

# TIBCO Spotfire S+® 8.2 for Solaris®/Linux® User's Guide

November 2010

TIBCO Software Inc.

#### IMPORTANT INFORMATION

SOME TIBCO SOFTWARE EMBEDS OR BUNDLES OTHER TIBCO SOFTWARE. USE OF SUCH EMBEDDED OR BUNDLED TIBCO SOFTWARE IS SOLELY TO ENABLE THE FUNCTIONALITY (OR PROVIDE LIMITED ADD-ON FUNCTIONALITY) OF THE LICENSED TIBCO SOFTWARE. THE EMBEDDED OR BUNDLED SOFTWARE IS NOT LICENSED TO BE USED OR ACCESSED BY ANY OTHER TIBCO SOFTWARE OR FOR ANY OTHER PURPOSE.

USE OF TIBCO SOFTWARE AND THIS DOCUMENT IS SUBJECT TO THE TERMS AND CONDITIONS OF A LICENSE AGREEMENT FOUND INEITHER Α SEPARATELY EXECUTED SOFTWARE LICENSE AGREEMENT, OR, IF THERE IS NO SUCH SEPARATE AGREEMENT, THE CLICKWRAP END USER LICENSE AGREEMENT WHICH IS DISPLAYED DURING DOWNLOAD OR INSTALLATION OF THE SOFTWARE (AND WHICH IS DUPLICATED IN TIBCO SPOTFIRE S+® LICENSES). USE OF THIS DOCUMENT IS SUBJECT TO THOSE TERMS AND CONDITIONS, AND YOUR USE HEREOF SHALL CONSTITUTE ACCEPTANCE OF AND AN AGREEMENT TO BE BOUND BY THE SAME.

This document contains confidential information that is subject to U.S. and international copyright laws and treaties. No part of this document may be reproduced in any form without the written authorization of TIBCO Software Inc.

TIBCO Software Inc., TIBCO, Spotfire, TIBCO Spotfire S+, Insightful, the Insightful logo, the tagline "the Knowledge to Act," Miner, Insightful S+, S-PLUS, TIBCO Spotfire S+ArrayAnalyzer, S+EnvironmentalStats, S+FinMetrics, S+NuOpt, S+SegTrial, S+SpatialStats, S+Wavelets, S-PLUS Graphlet, Spotfire S+ FlexBayes, Spotfire S+ Resample, TIBCO Spotfire Miner, TIBCO Spotfire S+ Server, TIBCO Spotfire Statistics Services, and TIBCO Spotfire Clinical Graphics are either registered trademarks or trademarks of TIBCO Software Inc. and/or subsidiaries of TIBCO Software Inc. in the United States and/or other countries. All other product and company names and marks mentioned in this document are the property of their respective owners and are mentioned for identification purposes only. This

software may be available on multiple operating systems. However, not all operating system platforms for a specific software version are released at the same time. Please see the readme.txt file for the availability of this software version on a specific operating system platform.

THIS DOCUMENT IS PROVIDED "AS IS" WITHOUT WARRANTY OF ANY KIND, EITHER EXPRESS OR IMPLIED, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE, OR NON-INFRINGEMENT, THIS DOCUMENT COULD INCLUDE TECHNICAL INACCURACIES OR TYPOGRAPHICAL ERRORS. CHANGES ARE PERIODICALLY ADDED TO THE INFORMATION HEREIN; THESE CHANGES WILL BE INCORPORATED IN NEW EDITIONS OF THIS DOCUMENT. TIBCO SOFTWARE INC. MAY MAKE IMPROVEMENTS AND/OR CHANGES IN THE PRODUCT(S) AND/OR THE PROGRAM(S) DESCRIBED IN THIS DOCUMENT AT ANY TIME.

Copyright © 1996-2010 TIBCO Software Inc. ALL RIGHTS RESERVED. THE CONTENTS OF THIS DOCUMENT MAY BE MODIFIED AND/OR QUALIFIED, DIRECTLY OR INDIRECTLY, BY OTHER DOCUMENTATION WHICH ACCOMPANIES THIS SOFTWARE, INCLUDING BUT NOT LIMITED TO ANY RELEASE NOTES AND "READ ME" FILES.

TIBCO Software Inc. Confidential Information

#### Reference

The correct bibliographic reference for this document is as follows:

TIBCO Spotfire S+® 8.2 for Solaris®/UNIX® User's Guide TIBCO Software Inc.

## Technical Support

For technical support, please visit http://spotfire.tibco.com/support and register for a support account.

#### TIBCO SPOTFIRE S+ BOOKS

#### Note about Naming

Throughout the documentation, we have attempted to distinguish between the language (S-PLUS) and the product (Spotfire S+).

- "S-PLUS" refers to the engine, the language, and its constituents (that is objects, functions, expressions, and so forth).
- "Spotfire S+" refers to all and any parts of the product beyond the language, including the product user interfaces, libraries, and documentation, as well as general product and language behavior.

The TIBCO Spotfire S+® documentation includes books to address your focus and knowledge level. Review the following table to help you choose the Spotfire S+ book that meets your needs. These books are available in PDF format in the following locations:

- In your Spotfire S+ installation directory (**SHOME**\help on Windows, **SHOME**/doc on UNIX/Linux).
- In the Spotfire S+ Workbench, from the Help ➤ Spotfire S+ Manuals menu item.
- In Microsoft<sup>®</sup> Windows<sup>®</sup>, in the Spotfire S+ GUI, from the **Help ▶ Online Manuals** menu item.

Spotfire S+ documentation.

Information you need if you	See the
Must install or configure your current installation of Spotfire S+; review system requirements.	Installtion and Administration Guide
Want to review the third-party products included in Spotfire S+, along with their legal notices and licenses.	Licenses

Spotfire S+ documentation. (Continued)

Information you need if you	See the
Are new to the S language and the Spotfire S+GUI, and you want an introduction to importing data, producing simple graphs, applying statistical models, and viewing data in Microsoft Excel <sup>®</sup> .	Getting Started Guide
Are a new Spotfire S+ user and need how to use Spotfire S+, primarily through the GUI.	User's Guide
Are familiar with the S language and Spotfire S+, and you want to use the Spotfire S+ plug-in, or customization, of the Eclipse Integrated Development Environment (IDE).	Spotfire S+ Workbench User's Guide
Have used the S language and Spotfire S+, and you want to know how to write, debug, and program functions from the <b>Commands</b> window.	Programmer's Guide
Are familiar with the S language and Spotfire S+, and you want to extend its functionality in your own application or within Spotfire S+.	Application Developer's Guide
Are familiar with the S language and Spotfire S+, and you are looking for information about creating or editing graphics, either from a <b>Commands</b> window or the Windows GUI, or using Spotfire S+ supported graphics devices.	Guide to Graphics
Are familiar with the S language and Spotfire S+, and you want to use the Big Data library to import and manipulate very large data sets.	Big Data User's Guide
Want to download or create Spotfire S+ packages for submission to the Comprehensive S-PLUS Archive Network (CSAN) site, and need to know the steps.	Guide to Packages

Spotfire S+ documentation. (Continued)

Information you need if you	See the
Are looking for categorized information about individual S-PLUS functions.	Function Guide
If you are familiar with the S language and Spotfire S+, and you need a reference for the range of statistical modelling and analysis techniques in Spotfire S+. Volume 1 includes information on specifying models in Spotfire S+, on probability, on estimation and inference, on regression and smoothing, and on analysis of variance.	Guide to Statistics, Vol. 1
If you are familiar with the S language and Spotfire S+, and you need a reference for the range of statistical modelling and analysis techniques in Spotfire S+. Volume 2 includes information on multivariate techniques, time series analysis, survival analysis, resampling techniques, and mathematical computing in Spotfire S+.	Guide to Statistics, Vol. 2

## **CONTENTS**

Chapter 1 Introduction	1
Welcome to Spotfire S+!	2
Installation	3
Creating Spotfire S+ Launchers	7
Help, Support, and Learning Resources	13
Typographic Conventions	20
Chapter 2 Getting Started	21
Introduction	23
Running Spotfire S+	24
Command Line Editing	32
Getting Help in Spotfire S+	35
S-PLUS Language Basics	41
Importing and Editing Data	57
Graphics in Spotfire S+	66
Statistics	71
Chapter 3 Working with the Graphical User	
Interface	77
The User Interface	78
Using Menus, Dialog Boxes, and Toolbars	79
Spotfire S+ Windows	87

Chapter 4 Importing and Exporting Data	93
Introduction	94
Dialogs	95
Supported File Types for Importing and Exporting	108
Examples	113
Chapter 5 Menu Graphics	119
Introduction	121
Scatter Plots	127
Visualizing One-Dimensional Data	152
Visualizing Two-Dimensional Data	169
Visualizing Three-Dimensional Data	178
Visualizing Multidimensional Data	186
Time Series	195
References	205
Chapter 6 Statistics	207
Introduction	210
Summary Statistics	216
Compare Samples	223
Power and Sample Size	269
Experimental Design	274
Regression	281
Analysis of Variance	308
Mixed Effects	314
Generalized Least Squares	318
Survival	322
Tree	328
Compare Models	333

	Contents
Cluster Analysis	336
Multivariate	348
Quality Control Charts	355
Resample	360
Smoothing	364
Time Series	368
References	375
Chapter 7 Customizing Your Spotfire S+ Session	377
Introduction	378
Setting Spotfire S+ Options	379
Setting Environment Variables	381
Customizing Your Session at Start-up and Closing	383
Using Personal Function Libraries	387
Specifying Your Working Directory	389
Specifying a Pager	390
<b>Environment Variables and printgraph</b>	391
Setting Up Your Window System	393

#### Contents

**INTRODUCTION** 

Welcome to Spotfire S+!	
Installation	3
Supported Platforms	3
Installation Instructions	4
Running Spotfire S+	5
Creating Spotfire S+ Launchers	7
Help, Support, and Learning Resources	13
Online Help	13
Online Manuals	16
Spotfire S+ on the Web	17
Training Courses	17
Books Using Spotfire S+	18
Typographic Conventions	20

#### **WELCOME TO SPOTFIRE S+!**

This release of Spotfire S+ is based on the latest version of the powerful, object-oriented S language developed at Lucent Technologies. S is a rich environment designed for interactive data discovery and is the only language created specifically for data visualization and exploration, statistical modeling, and programming with data.

Spotfire S+ continues to be the premier solution for your data analysis and technical graphing needs. The user interface provided in the GUI version gives you point-and-click access to data manipulation, graphing, and statistics. With Spotfire S+, you can program interactively using the S-PLUS programming language.

#### Note

As of Spotfire S+ 8.1, the Spotfire S+ Java GUI is deprecated. If you want to use a GUI with Spotfire S+, use the Spotfire S+ Workbench.

In a typical Spotfire S+ session, you can:

- Import data from virtually any source.
- Create plots easily from the command line or with the click of a button (in the GUI-enabled version).
- Control every detail of your graphics and produce stunning, professional-looking output for export to your report document.
- Perform statistical analyses from convenient dialogs in the menu system.
- Run analysis functions one at a time at the command line or in batches.
- Create your own functions.
- Completely customize your user interface.

#### INSTALLATION

## Supported Platforms

The 32-bit version of TIBCO Spotfire S+ for Solaris \*\binom{Linux} is supported on the following platforms and operating systems. The minimum recommended disk space for installing and running Spotfire S+ is also included:

**Table 1.1:** Supported 32-bit platforms for Solaris/Linux systems.

Platform	Operating System	Disk Space
Sun SPARC	Solaris 2.8, 2.9, 2.10 on SPARC processors	475 MB
Intel/AMD x86	Red Hat Enterprise Linux WS 4.0 and 5.0	475 MB

The 64-bit version of Spotfire S+ for Linux is supported on the following platform (but will not be released for the beta):

**Table 1.2:** Supported 64-bit platform for Solaris/Linux systems.

Platform	Operating System	Disk Space
Intel/AMD x86	Red Hat Enterprise Linux WS 4.0 and 5.0	500 MB

Note that previous versions of the listed operating systems may function with Spotfire S+, but they are not supported.

You will need a minimum of 60 MB RAM to run Spotfire S+ from the command line, and the Java GUI requires an additional 100 MB to run. Note that these values are minima; if you work with moderate-sized data sets, these numbers may be insufficient for your needs.

#### Java Runtime Environment (JRE)

The Java runtime environment (JRE) version 1.6.21 is included in Spotfire S+. Your operating system must support JRE 1.6.21 to run the Java-enabled version of Spotfire S+. The JRE provided by Spotfire S+ is installed as part of the Spotfire S+ distribution, and under normal circumstances it is used only by Spotfire S+. If you have a different version of the JRE on your system, the JRE used by Spotfire S+ should not interfere with your other JRE applications, which will continue to use the version you've previously installed.

See the Spotfire S+ release notes for specific information regarding the JRE on your platform. In particular, Solaris operating environments require various patches from Sun to run Java 1.6.21. The release notes contain pointers to Web site where you can download these patches.

## Installation Instructions

To install the software, follow these steps:

- 1. Unpack and copy the files from the distribution CD to an appropriate file on your system.
- 2. Run the CONFIGURE script to customize your installation.
- 3. Run the INSTALL script to copy the customization from the previous step to your system.
- 4. Run Spotfire S+.

Do not install this release over any existing version of Spotfire S+. Instead, designate a clean installation directory for Spotfire S+ and proceed with the installation as described in **INSTALL.TXT** located at the top level of your CD.

## Running Spotfire S+

Before starting Spotfire S+, you must do the following:

- Set your **DISPLAY** environment variable to your local machine.
- 2. Create a Spotfire S+ chapter to hold your work.

Setting your **DISPLAY** environment variable is necessary for the Java features in Spotfire S+. To set your display from a C-like shell (**csh**, **tcsh**, etc.), use the **setenv** command from the UNIX prompt:

```
setenv DISPLAY <display_name>
```

where <display\_name> is the name of your local machine. From the Bourne- and Korn-like shells (including **sh**, **ksh**, **bash**, etc.), use the following commands:

```
DISPLAY=<display_name>;export DISPLAY
```

Creating a Spotfire S+ chapter is necessary for storing the data objects and external files you create in Spotfire S+. The following commands create a Spotfire S+ chapter named **mysplus** for you to work in (be sure you don't have a **mysplus** directory in your home directory before typing these commands).

```
cd
mkdir mysplus
cd mysplus
Splus CHAPTER
```

You are now ready to start Spotfire S+. You can launch Spotfire S+ in a variety of modes. The following lists each mode and the corresponding UNIX command-line expression for launching it. In all of the commands below, **Splus** refers to the script you use to launch Spotfire S+ on your system.

Spotfire S+ command line without Java:

```
Splus
```

Spotfire S+ graphical user interface:

```
Splus -g
or
Splus -g &
```

• Spotfire S+ command line supporting Java calls, Java graphics, and the Java help interface:

```
Splus -j
```

The **-e** flag may be added to the Java enabled version to enable command-line editing. The **Commands** window in the graphical user interface always allows basic editing.

• Spotfire S+ command line supporting the Big Data library:

```
Splus -bigdata
```

Note that the Big Data library is not loaded by default in the command line version.

 Spotfire S+ command line supporting the Eclipse Workbench:

```
Splus -w | -workbench
```

Spotfire S+ includes two additional flags, -jit and -helpoff:

- The -jit flag works with the -g, -j, and -userapp flags and allows you to turn on the Java just-in-time compiler. This makes the graphical user interface and help system run faster but introduces instabilities that often lead to crashes. In particular, the just-in-time compiler often crashes while repainting graphical user interface elements such as the JavaHelp window and the **Data** window.
- The **-helpoff** flag is useful only with the **-g** flag. It turns off the automatic invisible startup of the help system. The invisible startup improves initial responsiveness of the help system but adds a significant memory footprint to the current session. If you want to optimize your available memory, this flag may prove useful.

#### CREATING SPOTFIRE S+ LAUNCHERS

Using the GNOME on LINUX or Solaris 10, or KDE window managers on LINUX, you can create custom application launchers for Spotfire S+, complete with a Spotfire S+ icon. This makes it possible to start Spotfire S+ by clicking the appropriate icon in the GNOME or KDE panel.

You can create multiple Spotfire S+ launchers to launch Spotfire S+ with different options. For example, you can create separate launchers for running the Spotfire S+ Workbench, for running the Spotfire S+ GUI, or for running the command-line version in an xterm. In fact, you could create task launchers for each Spotfire S+ CHAPTER in which you wish to run.

The following two sections describe:

- Creating LINUX or Solaris 10 application managers for GNOME.
- Creating LINUX application managers for KDE.

These instructions begin assuming that the Spotfire S+ command is installed in /usr/local/bin, and that Spotfire S+ is installed in [SHOME]. If these are not your installation locations, substitute the actual locations for your installation. See Figure 1.1 for an example of specifying selections for the GNOME application launcher properties.

#### Note

Menu selections and dialog box titles might vary according to the version of LINUX you are running.

Creating a
Spotfire S+
Application
Launcher under
GNOME

- 1. Right-click the GNOME panel (by default located at the top of the screen), and from the pop-up context menu, select **Add to Panel**.
- 2. From the menu, select **Launcher**.
- 3. In the **Create Launcher** dialog, set options as follows:

#### To set command-line Spotfire S+ to start with Java and cled, but not the Big Data library.

Set the following options in the **Create Launcher** dialog:

- Name: Splus
- **Generic Name**: Spotfire S+ command line
- **Comment**: Spotfire S+ with Java and cled, without Big Data.
- Command: /usr/local/bin/Splus -ej
- Type: Application
- Run in terminal: selected

#### To set Spotfire S+ Workbench with the Big Data library.

Set the following options in the **Create Launcher** dialog:

- Name: Splus Workbench
- Generic Name: Spotfire S+ Workbench
- Comment: Spotfire S+ Workbench with Big Data.
- Command: /usr/local/bin/Splus -workbench -bigdata
- Type: Application
- Run in terminal: cleared

#### To set Spotfire S+ GUI to start without the Big Data library.

#### Note

As of Spotfire S+ 8.1, the Spotfire S+ Java GUI is deprecated. If you want to use a GUI with Spotfire S+, use the Spotfire S+ Workbench.

Set the following options in the **Create Launcher** dialog:

- Name: Splus GUI
- Generic Name: Spotfire S+ GUI
- Comment: Spotfire S+ GUI without Big Data.
- **Command**: /usr/local/bin/Splus -g
- Type: Application

• Run in terminal: cleared

Do not close the dialog.

 While the Launcher Properties dialog is still open, click Icon. You are presented with a Browse icons dialog. Browse to [SHOME]/splus/lib/icons and select an appropriate icon. Click OK.

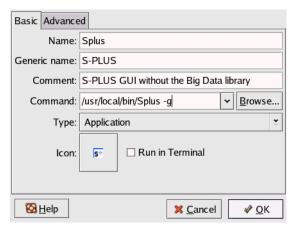


Figure 1.1: Create Launcher dialog with icon.

5. Close the **Launcher Properties** dialog. You should see the Spotfire S+ icon that you selected in the GNOME panel. Clicking it starts Spotfire S+ with the options you selected.



**Figure 1.2:** *GNOME panel with Spotfire S+ icon.* 

Creating a
Spotfire S+
Application
Launcher under
KDE:

 Right-click the KDE panel (by default located at the bottom of the screen) and select Add ➤ Special Button ➤ Non-KDE Application.

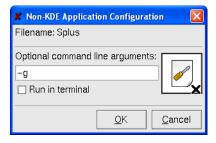


Figure 1.3: Non-KDE Application Configuration dialog.

2. Browse to the location of the Spotfire S+ executable.

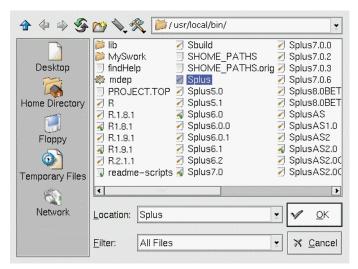
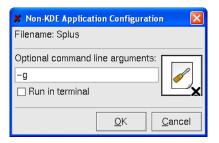


Figure 1.4: Select Executable dialog for KDE Panel.

3. Select Splus, and then click OK to display the **Non-KDE Application Configuration** dialog.



**Figure 1.5:** Non-KDE Application Configuration dialog set to run the Spotfire S+ GUI without the Big Data library.

4. In the **Non-KDE Application Configuration** dialog, set the options as follows:

#### To set command-line Spotfire S+ with cled.

Set the following options:

- Executable: /usr/local/bin/Splus
- Optional command line arguments: -e
- Run in terminal: selected

#### To set the Spotfire S+ Workbench to start with the Big Data library.

Set the following options:

- Executable: /usr/local/bin/Splus
- Optional command line arguments: -w -bigdata
- Run in terminal: cleared.

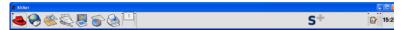
#### To set Spotfire S+ GUI to start without the Big Data library.

Set the following options:

- Executable: /usr/local/bin/Splus
- Optional command line arguments: -g
- Run in terminal: cleared

#### Chapter 1 Introduction

5. Do not close the dialog yet. To the right of the Executable box appears a generic icon. Select this icon to display the Select Icon - KDE Panel dialog. Select the Other icons option, and then browse to [SHOME]/splus/lib/icons and select the desired icon. Click Open, and then click OK. The Spotfire S+ icon you selected in the KDE panel appears. Clicking the icon starts Spotfire S+ with the selected options.



**Figure 1.6:** *Kicker panel with Spotfire S+ icon.* 

#### HELP, SUPPORT, AND LEARNING RESOURCES

There are a variety of ways to accelerate your progress with Spotfire S+. This section describes the learning and support resources available to Spotfire S+ users.

#### Online Help

Spotfire S+ offers an online JavaHelp system to make learning and using Spotfire S+ easier. Under the **Help** menu in the Spotfire S+ GUI, you will find detailed help on each function in the S-PLUS language. You can access the help system from the Spotfire S+ prompt or the **Commands** window in the GUI by typing help.start().

JavaHelp in Spotfire S+ uses Java to display the help files. To access JavaHelp, do one of the following:

- From the main menu in the Spotfire S+ GUI, choose Help ► Contents, Help ► Index, or Help ► Search to view the help system's table of contents, index, and search pages, respectively.
- From the Spotfire S+ prompt or the **Commands** window in the GUI, type help.start().

To turn the help system off, type help.off() at the Spotfire S+prompt.

As shown in Figure 1.7, the JavaHelp window has three main areas: the *toolbar*, the *navigation pane*, and the *topic pane*.

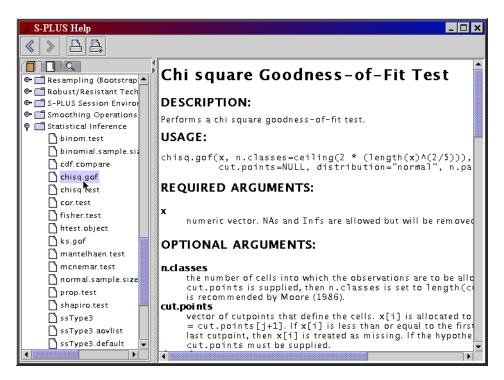


Figure 1.7: The Spotfire S+ JavaHelp window.

#### Using the toolbar

Table 1.3 lists the four buttons on the help window toolbar.

Table 1.3: Toolbar buttons in the JavaHelp window.

Button	Description
Previous	Returns to previously viewed help topic.
Next	Moves to next help topic in a previously-displayed sequence of topics.
Print 🖺	Prints the current help topic.

**Table 1.3:** Toolbar buttons in the JavaHelp window. (Continued)

Button	Description
Page Setup	Determines the orientation of the page for printing purposes.

#### Using the navigation pane

The navigation pane appears on the left side of the JavaHelp window. Like the help window itself, the left pane is divided into three parts:

the Table of Contents , Index , and Search pages:

- The **Table of Contents** page organizes help topics by category so related help files can be found easily. These categories appear as small folder icons, labeled with the name of the category. To open a category, double-click the icon or label. To select a topic within the category, double-click its page icon or the topic title.
- The **Index** page lists available help topics by keyword. Keywords are typically function names for S-PLUS language functions. Type a word in the text box and press ENTER to find the keywords that most closely match it.
- The Search tab provides a full-text search for the entire help system. Type the word or phrase you want to find in the text box and press ENTER. JavaHelp displays in the list box all help files containing that keyword. Double-click a title to display the desired help topic.

#### Using the topic pane

The topic pane appears on the right side of the help window and displays the help topics you choose. It usually appears with both vertical and horizontal scroll bars, but you can expand the JavaHelp window to increase the width of the right pane. Many help files are too long to be fully displayed in a single screen, so choose a convenient height for your JavaHelp window and then use the vertical scroll bars to scroll through the text.

#### Help at the **Command Line**

When working from the Spotfire S+ command line, you can obtain help for any S-PLUS function using the help or ? functions. For example, to open the help file for anova, simply type:

> help(anova)

or

> ?anova

Online Manuals For a description of the contents of available manuals, see the section TIBCO Spotfire S+ Books on page iv.

> To view a manual online, go to your SHOME/doc directory and select the desired title. These manuals are stored as pdf; they require the free Acrobat Reader to view them.

Table 1.4: Online manuals and associated pdf file names.

Manual	File Name
Application Developer's Guide	adg.pdf
Big Data User's Guide	bigdata.pdf
Function Guide	functionguide.pdf
Getting Started with Spotfire S+	getstart.pdf
Guide to Graphics	graphics.pdf
Guide to Packages	spluspackages.pdf
Guide to Statistics, Volume 1	statman1.pdf
Guide to Statistics, Volume 2	statman2.pdf

**Table 1.4:** Online manuals and associated pdf file names.

Manual	File Name
Programmer's Guide	pg.pdf
User's Guide	uguide.pdf
Workbench User's Guide	workbench.pdf

## Spotfire S+ on the Web

You can find Spotfire S+ on the TIBCO Web site at **www.tibco.com**. In these pages, you will find a variety of information, including:

- FAQ pages.
- · The most recent service packs.
- Training course information.
- Product information.
- Information on classroom use and related educational materials.

## Training Courses

TIBCO Spotfire Educational Services offers a number of courses designed to quickly make you efficient and effective at analyzing data with Spotfire S+. The courses are taught by professional statisticians and leaders in statistical fields. Courses feature a hands-on approach to learning, dividing class time between lecture and online exercises. All participants receive the educational materials used in the course, including lecture notes, supplementary materials, and exercise data on diskette.

#### Technical Support

For technical support, please visit http://spotfire.tibco.com/support and register for a support account.

## Books Using S-PLUS

#### General

Becker, R.A., Chambers, J.M., and Wilks, A.R. (1988). *The New S Language*. Wadsworth & Brooks/Cole, Pacific Grove, CA.

Burns, Patrick (1998). *S Poetry*. Download for free from http://www.seanet.com/~pburns/Spoetry.

Chambers, John (1998). *Programming with Data*. Springer-Verlag.

Krause, A. and Olson, M. (1997). *The Basics of S and S-PLUS*. Springer-Verlag, New York.

Lam, Longhow (1999). *An Introduction to S-PLUS. for Windows*. CANdiensten, Amsterdam.

Spector, P. (1994). An Introduction to S and S-PLUS. Duxbury Press, Belmont, CA.

#### **Data analysis**

Bowman, Adrian and Azzalini, Adelchi (1997). *Smoothing Methods*. Oxford University Press.

Bruce, A. and Gao, H.-Y. (1996). *Applied Wavelet Analysis with S-PLUS*. Springer-Verlag, New York.

Chambers, J.M. and Hastie, T.J. (1992). *Statistical Models in S.* Wadsworth & Brooks/Cole, Pacific Grove, CA.

Efron, Bradley and Tibshirani, Robert J. (1994). An Introduction to the Bootstrap. Chapman & Hall.

Everitt, B. (1994). A Handbook of Statistical Analyses Using S-PLUS. Chapman & Hall, London.

Härdle, W. (1991). Smoothing Techniques with Implementation in S. Springer-Verlag, New York.

Hastie, T. and Tibshirani, R. (1990). *Generalized Additive Models*. Chapman & Hall.

Huet, Sylvie, et al. (1997). Statistical Tools for Nonlinear Regression: with S-PLUS. Springer-Verlag.

Kaluzny, S.P., Vega, S.C., Cardoso, T.P., and Shelly, A.A. (1997). *S+SpatialStats User's Manual.* Springer-Verlag, New York.

Marazzi, A. (1992). Algorithms, Routines and S Functions for Robust Statistics. Wadsworth & Brooks/Cole, Pacific Grove, CA.

Millard, Steven (1998). *User's Manual for Environmental Statistics*. Companion book to the S+Environmental Stats module. (The S+Environmental Stats module is available through Dr. Millard.)

Selvin, S. (1998). *Modern Applied Biostatistical Methods: Using S-PLUS*. Oxford University Press.

Venables, W.N. and Ripley, B.D. (1999). *Modern Applied Statistics with S-PLUS*, Third Edition. Springer-Verlag, New York.

#### **Graphical techniques**

Chambers, J.M., Cleveland, W.S., Kleiner, B., and Tukey, P.A. (1983). *Graphical Techniques for Data Analysis*. Duxbury Press, Belmont, CA.

Cleveland, W.S. (1993). Visualizing Data. Hobart Press, Summit, NJ.

Cleveland, W.S. (1994). *The Elements of Graphing Data*, revised edition. Hobart Press, Summit, NJ.

#### TYPOGRAPHIC CONVENTIONS

Throughout this *User's Guide*, the following typographic conventions are used:

- This font is used for S-PLUS expressions and code samples.
- **This font** is used for elements of the Spotfire S+ user interface, for operating system files and commands, and for user input in dialog fields.
- *This font* is used for emphasis and book titles.
- CAP/SMALLCAP letters are used for key names. For example, the Shift key appears as SHIFT.
- When more than one key must be pressed simultaneously, the two key names appear with a hyphen (-) between them. For example, the key combination of SHIFT and F1 appears as SHIFT-F1.
- Menu selections are shown in an abbreviated form using the arrow symbol (►) to indicate a selection within a menu, as in File ► New.

## **GETTING STARTED**

Introduction	23
Running Spotfire S+	24
Creating a Working Directory	24
Starting Spotfire S+	24
Loading Libraries	27
Entering Expressions	28
Quitting Spotfire S+	29
Basic Syntax and Conventions	29
Command Line Editing	32
Getting Help in Spotfire S+	35
Starting and Stopping the Help System	35
Using the Help Window	35
Getting Help at the Spotfire S+ Prompt	37
Displaying Help in a Separate Window	39
Printing Help Files	40
Documen-tation Objects	40
S-PLUS Language Basics	41
Data Objects	41
Managing Data Objects	47
Functions	49
Operators	50
Expressions	52
Precedence Hierarchy	53
Optional Arguments to Functions	55
Access to Solaris and Linux	56
Importing and Editing Data	57
Reading a Data File	57
Editing Data	59
Built-in Data Sets	59
Quick Hard Copy	60

#### Chapter 2 Getting Started

Adding Row And Column Names	60
Extracting Subsets of Data	62
Graphics in Spotfire S+	66
Making Plots	66
Quick Hard Copy	69
Using the Graphics Window	69
Multiple Plot Layout	69
Statistics	71
Summary Statistics	71
Hypothesis Testing	72
Statistical Models	73

#### **INTRODUCTION**

This chapter provides basic information that everyone needs to use Spotfire S+ effectively. It describes the following tasks:

- Starting and quitting Spotfire S+
- · Getting help
- Using fundamental elements of the S-PLUS language
- Creating and manipulating basic data objects
- Opening graphics windows and creating basic graphics

#### **RUNNING Spotfire S+**

This section covers the basics of starting Spotfire S+, opening windows for graphics and help, and constructing S-PLUS expressions.

## Creating a Working Directory

Before running Spotfire S+ the first time, you should create a *working directory* specifically for Spotfire S+. This directory will contain any files you want to read into or export from Spotfire S+, as well as a .Data directory to hold your S-PLUS data objects, metadata objects, and help files. These working directories are called *chapters*, and are created with the S-PLUS CHAPTER utility. The first time you run Spotfire S+, it creates a chapter called MySwork which can function as a default working directory; however, it will also store more general user information. It is recommended that you create at least one chapter separate from MySwork, and using that for your day-to-day Spotfire S+ work.

To create a working directory named **myproj** in your home directory, type the following sequence of commands at the shell prompt and press RETURN after each command:

```
cd
mkdir myproj
cd myproj
Splus CHAPTER
```

The CHAPTER utility creates a .Data directory, which in turn contains three other directories at start-up: \_\_Meta, \_\_Shelp, and \_\_Hhelp. The .Data directory contains your normal data sets and functions, the \_\_Meta directory contains Spotfire S+ metadata such as method definitions, and the two \_\_\*help directories contain SGML and HTML versions of help files you create for your functions. All of these databases are initially empty, except for some possible marker files.

## Starting Spotfire S+

There are five basic ways to launch a Spotfire S+ session:

- 1. As a simple terminal-based application.
- 2. As a Java-controlled terminal-based application.

- 3. As a terminal-based application with command-line editing.
- 4. As a Java-based application with a graphical user interface.
- 5. As a batch operation.

#### Spotfire S+ as a Simple Terminal-Based Application

To start Spotfire S+, type the following at the shell prompt and press the RETURN key:

#### Splus

Note that only the "S" is capitalized.

When you press RETURN, a copyright message appears in your Spotfire S+ window. The first time you that you start Spotfire S+, you may also receive a message about initializing a new Spotfire S+ working directory. These messages are followed by the Spotfire S+ prompt.

#### Spotfire S+ as a Java-Controlled Terminal-Based Application

To start Spotfire S+ as a terminal-based Java application, type the following at the shell prompt and press the RETURN key:

#### Splus -j

Note that only the "S" is capitalized.

When you press RETURN, a copyright message appears in your Spotfire S+ window. The first time you that you start Spotfire S+, you may also receive a message about initializing a new Spotfire S+ working directory. These messages are followed by the Spotfire S+ prompt.

#### Spotfire S+ as a Terminal-Based Application with Command-Line Editing

To start Spotfire S+ with command-line editing, add the -e flag to your normal start-up command. Thus, for the standard terminal-based Spotfire S+, start the command-line editor as follows:

#### Splus -e

Note that only the "S" is capitalized.

For the Java-controlled terminal, start the command-line editor as follows:

#### Splus -j -e

When you press RETURN, a copyright message appears in your Spotfire S+ window. The first time you that you start Spotfire S+, you may also receive a message about initializing a new Spotfire S+ working directory. These messages are followed by the Spotfire S+ prompt.

For information on editing with the command-line editor, see the section Command Line Editing on page 32.

#### Spotfire S+ with a Graphical User Interface

To start Spotfire S+ with a graphical user interface, type the following at the shell prompt and press the RETURN key:

Note that only the "S" is capitalized. The & indicates to the shell that the graphical user interface will run in the background; this simply allows the interface to start as a separate X window while returning the prompt to your shell window.

#### Note

In TIBCO Spotfire S+ 8.1, the graphical user interface is deprecated. Users should consider using the Spotfire S+ Workbench instead.

When you press RETURN, you will see the Spotfire S+ splash screen. Shortly thereafter, the graphical user interface appears, with menus, a toolbar, and a **Commands** window.

A copyright message appears in the **Commands** window. The first time you that you start Spotfire S+, you may also receive a message about your specific environment and initializing a new Spotfire S+ working directory. These messages are followed by the Spotfire S+ prompt.

You can begin typing expressions in the **Commands** window, or you can use the menus and dialogs to perform Spotfire S+ tasks. Entering expressions is described in the section Spotfire S+ as a Batch Process; using the menus and dialogs is introduced in the chapter Working with the Graphical User Interface.

# Spotfire S+ as a Batch Process

Once you've created a function and verified that it works, you may want to use it with a large data set. Complicated analyses on large data sets can take some time, however, and your session is locked while Spotfire S+ performs its calculations. *Batch mode* provides one method for working around this. To run a set of commands in batch mode, simply create a file containing the S-PLUS expressions you want evaluated, and then type the following at the Solaris/Linux prompt:

```
Splus SBATCH -help
```

The -help option displays all the possible arguments, including input, output, log file name, working directory, etc. See the chapter on Verbose Logging in the *Application Developer's Guide* for information on running batch mode for Solaris/Linux processes.

When you run a Spotfire S+ process in batch mode, it begins immediately but is at a lower priority than interactive tasks. You can also run batch jobs from within a Spotfire S+ session by using the ! shell escape:

> !Splus SBATCH

#### Warning

When you run batch processes from within Spotfire S+, the results are invisible to your current session; your working database is not updated with the results of the batch job. To see the results of a batch process in your current session, you must *synchronize* the databases. See the chapter on Verbose Logging in the *Application Developer's Guide* for more details.

### Loading Libraries

All data sets in Spotfire S+ are stored in libraries. When we speak of "Spotfire S+," however, we usually mean the executable program and the objects in the libraries that are attached automatically at startup. The Spotfire S+ distribution contains additional libraries. To see a list and a description of each, at the command prompt, type

library()

Your default text editor opens and displays the information.

You can attach a library by using the library() function.

#### Note

In addition to loading libraries, you can find and download packages. See the *Guide to Packages* for more information about using packages.

# Entering Expressions

You can use Spotfire S+ by typing expressions after the prompt and pressing the RETURN key. You type an expression at the Spotfire S+ command prompt, and Spotfire S+ responds.

Among the simplest S-PLUS expressions are arithmetic expressions such as the following:

```
> 3+7
[1] 10
> 3*21
[1] 63
```

The symbols "+" and "\*" represent S-PLUS operators for addition and multiplication, respectively. In addition to the usual arithmetic and logical operators, S-PLUS has operators for special purposes. For example, the colon operator ":" is used to obtain sequences:

```
> 1:7
[1] 1 2 3 4 5 6 7
```

The [1] in each of the output lines is the *index* of the first Spotfire S+ response on the line of Spotfire S+ output. If Spotfire S+ is responding with a long vector of results, each line is preceded by the index of the first response of that line.

The most common S-PLUS expression is the *function call*. An example of a *function* in S-PLUS is c, which is used for "combining" comma-separated lists of items into a single object. Function calls are always followed by a pair of parentheses, with or without any *arguments* in the parentheses:

```
> c(3,4,1,6)
[1] 3 4 1 6
```

In all of our examples to this point, Spotfire S+ has simply returned a value. To reuse the value of a S-PLUS expression, you must *assign* it with the <- operator. For example, to assign the above expression to a S-PLUS object named newvec, type the following:

```
> newvec <- c(3, 4, 1, 6)
```

S-PLUS creates the object newvec and returns a Spotfire S+ prompt. To view the contents of the newly created object, just type its name:

```
> newvec [1] 3 4 1 6
```

# Quitting Spotfire S+

To quit Spotfire S+ and get back to your shell prompt, use the q function:

```
> q()
```

The () are required with the q command to quit Spotfire S+ because q is a S-PLUS function, and parentheses are required with all S-PLUS functions. In the Spotfire S+ graphical user interface, you can also select **File** ▶ **Exit** to exit Spotfire S+.

# Basic Syntax and Conventions

This section introduces basic typing syntax and conventions in Spotfire S+.

#### **Spaces**

S-PLUS ignores most spaces. For example:

```
> 3+ 7
[1] 10
```

However, do not put spaces in the middle of numbers or names, or an error will result. For example, if you wish to add 321 and 1, the expression 32 1+1 causes an error. Also, you should always put spaces around the two-character assignment operator <-; otherwise, you may perform a comparison instead of an assignment.

# Upper And Lower Case

S-PLUS is *case sensitive*, just like Solaris and Linux. All S-PLUS objects, arguments, and names are case sensitive. Hence, "QWERT" is different from "qwert". In the following example, the object SeX is defined as "M". You get an error message if you do not type "SeX" with the capitalization.

```
> SeX
[1] "M"
> sex
Problem: Object "sex" not found
```

#### **Continuation**

When you press the RETURN key and it is clear to Spotfire S+ that an expression is incomplete (for example, the last character is an operator, or there is a missing parenthesis), Spotfire S+ provides a *continuation* prompt to remind you to complete the expression. The default continuation prompt is "+".

Here are two examples of incomplete expressions that cause Spotfire S+ to respond with a continuation prompt:

```
> 3*
+ 21
[1] 63
> c(3,4,1,6
+)
[1] 3 4 1 6
```

In the first command, Spotfire S+ determined that the expression was not complete because the multiplication operator \* must be followed by a data object. In the second example, Spotfire S+ determined that c(3,4,1,6 was not complete because a right parenthesis is needed. In each of these cases, the user completed the expression after the continuation prompt (+), and then Spotfire S+ responded with the result of the complete evaluation.

#### Interrupting Evaluation Of An Expression

Sometimes you may want to stop the evaluation of a S-PLUS expression. For example, you may suddenly realize you want to use a different command, or the output display of data on the screen is extremely long and you don't want to look at all of it.

To interrupt Spotfire S+ from a terminal-based window, use the Solaris/Linux interrupt command, which consists of either CTRL-C (pressing the C key while holding down the CONTROL key) or the DELETE key on most systems. If neither CTRL-C nor DELETE stop the scrolling, consult your Solaris or Linux manual for use of the **stty** command to see what key performs the interrupt function, or consult your local system administrator.

To interrupt Spotfire S+ from the graphical user interface, press the ESC key on your keyboard.

#### **Error Messages**

Do not be afraid of making mistakes when using Spotfire S+. You will not break anything by making a mistake. Usually you get some sort of error message, after which you can try again.

Here are two examples of mistakes made by typing "improper" expressions:

```
> 32 1+1
Problem: Syntax error: illegal literal ("1") on input line
1
> .5(2,4)
Problem: Invalid object supplied as function
```

In the second command, we typed something that Spotfire S+ tried to interpret as a function because of the parentheses. However, there is no function named ".5".

### COMMAND LINE EDITING

Included with Spotfire S+ is a command line editor that can help improve your productivity. The Spotfire S+ command line editor enables you to recall and edit previously issued S-PLUS commands. The editor can do either **emacs**- or **vi**-style editing, and uses the first *valid* value in the following list of environment variables:

```
S_CLEDITOR
VISUAL
EDITOR
```

To be valid, the value for the environment variable must end in "vi" or "emacs." If none of the listed variables has a valid value, the command line editor defaults to **vi** style.

For example, issue the following command from the C shell to set your **S\_CLEDITOR** to **emacs**:

```
setenv S_CLEDITOR emacs
```

To use the command line editor within Spotfire S+, start Spotfire S+ with a -e option:

```
Splus -e
```

Table 2.1 summarizes the most useful editing commands for both **emacs**- and **vi**-style editing. With **vi**, the Spotfire S+ command line editor puts you in insert mode automatically. Thus, any editing commands must be preceded by an ESC.

**Table 2.1:** Command line editing in Spotfire S+.

Action	emacs keystrokes	vi keystrokes*
backward character	CTRL-B	Н
forward character	CTRL-F	L
previous line	CTRL-P	К
next line	CTRL-N	J

<b>Table 2.1:</b>	Command	line	editing	in L	Spotfire	S+.
-------------------	---------	------	---------	------	----------	-----

Action	emacs keystrokes	vi keystrokes*		
beginning of line	CTRL-A	SHIFT-6		
end of line	CTRL-E	SHIFT-4		
forward word	ESC,F	W		
backward word	ESC,B	В		
kill char	CTRL-D	X		
kill line	CTRL-K	SHIFT-D		
delete word	ESC,D	D,W		
search backward	CTRL-R	/		
yank	CTRL-Y	SHIFT-Y		
transpose chars	CTRL-T	X,P		
*In command mode. You must press ESC to enter command mode.				

As an example of using the command line editor, suppose you've started Spotfire S+ with the emacs option for the EDITOR environment variable. Attempt to create a plot by typing the following:

```
> plto(x,y)
Problem: Couldn't find a function definition for "plto"
```

Type CTRL-P to recall the previous line, then use CTRL-B to return to the "t" in "plto." Finally, type CTRL-T to transpose the "t" and the "o." Press RETURN to issue the edited command.

#### Chapter 2 Getting Started

To recall earlier commands, use backward search (CTRL-R in **emacs** mode, / in **vi** mode) followed by the command or first portion of command. For example, suppose you've recently issued the following command:

```
> plot(xdata, ydata, xlab="Predictor", ylab="Response")
```

To recall this command, type CTRL-R plot. The complete command is restored to your command line. You can then use other editing commands to edit it if desired, or you can press RETURN to issue the command again.

### **GETTING HELP IN SPOTFIRE S+**

If you need help at any time during a Spotfire S+ session, you can obtain it easily with the menu-driven help system, which uses Sun Microsystems' JavaHelp $^{TM}$ . The Spotfire S+ window-driven help system lets you select from broad categories of help topics. Within each category you can choose from a list of S-PLUS functions pertaining to that category.

### Starting and Stopping the Help System

The easiest way to access the help system is through the help window. To call up the help system, type help.start() at the > prompt. The help.start function no longer supports the gui argument, so don't type help.start(gui="motif") as you might have done in S-PLUS 3.4. A JavaHelp window appears, with a **Table of Contents** in the left pane. You will also see additional tabs for the **Index** and the **Search** capabilities.

To turn off the help system, type help.off() at the > prompt, and the JavaHelp window closes. To hide the help system temporarily, simply minimize or close the window (depending on your window manager).

In the Spotfire S+ graphical user interface, you can also select **Help** ► **Contents**, **Help** ► **Index**, or **Help** ► **Search** to view the help system's **Table of Contents**, **Index**, and **Search** lists, respectively. To close the GUI help window, click the **Close** button in the upper right corner of the interface. To turn the help system off, type help.off() in the **Commands** window.

# Using the Help Window

The Spotfire S+ help window contains two panes. At start-up, the left-hand pane contains the **Table of Contents** while the right-hand pane is empty. The right pane is used to display help text. The left pane is tabbed, and contains pages for the help system's **Table of Contents**, **Index**, and **Search** lists. You can replace the **Table of Contents** with an **Index**, which is a listing of all the topics currently available, or with the **Search** pane, which allows you to perform a full-text search on the current help set.

Use the following steps to get help on a topic with the **Table of Contents**:

- 1. Scan the **Table of Contents** on the left side of the help window until you find the desired category. Use the scroll bars and the mouse buttons to scroll through the list.
- 2. To select the category, double-click on the category name, or single-click on the lever next to the folder icon for the category. Once you select a category, a list of S-PLUS functions and data sets pertaining to that category appears below the category name.
- 3. Scroll through the list of objects under the category name until you find the desired function.
- 4. To select the function, click on the function name. After you select a function, Spotfire S+ formats the help file for that function and brings it up in the text pane.
- 5. Scroll through the help file using the scroll bars and the mouse buttons.
- 6. To print the formatted file, click the **Print** button on the JavaHelp toolbar.

Use the following steps to get help on a topic with the **Index**:

- 1. To select the help **Index**, click the middle tab in the left pane of the help window.
- 2. Move the pointer inside the **Find** text field.
- 3. Type the function name you wish to search for.
- 4. Press the RETURN key. In the text pane of the help window, Spotfire S+ displays the first help file in the **Index** list that matches the name of your function. To see help files for the remaining matches, continue to press the RETURN key.

Alternatively, you can scroll through the **Index** list until you find the function name that you want.

Use the following steps to get help on a topic with the full-text **Search**:

- 1. To select the help **Search**, click the right-most tab in the left pane of the help window.
- 2. Move the pointer inside the **Find** text field.
- 3. Type the word you wish to search for.
- 4. Press the RETURN key. A list of help topics matching your search criterion is displayed in the left pane. The topics are sorted in order of importance: the help files that contain your search criterion most often are displayed at the top of the list, along with the number of occurrences.
- 5. To select a function, double-click on the topic in the left pane of the help window. Once you select a topic, Spotfire S+ formats the help file for that function, brings it up in the text pane, and highlights your search criterion.

# Getting Help at the Spotfire S+ Prompt

You can access help easily at the Spotfire S+ prompt with the ? and help functions. The ? function has simpler syntax and requires no parentheses in most instances:

#### **REQUIRED ARGUMENTS:**

#### formula

a formula object, with the response on the left of a `~' operator and the terms, separated by + operators, on the right. The response may be a single numeric variable or a matrix.

#### OPTIONAL ARGUMENTS:

#### data

data frame in which to interpret the variables named in the formula, subset, and weights arguments. This may also be a single number to handle some special cases -- see below for details. If data is missing, the variables in the model formula should be in the search path.

. . .

If the JavaHelp system is running in your session, all requests for help files are sent to the help window. Otherwise, the help file is displayed in an available Help application such as 'lynx', 'links', 'less', or 'more'. You can specify a different help pager by using, for example, options(help.pager="vi"). Because vi is just a text editor, it displays the HTML formatting codes if you use vi to view your help files. To try another text-based HTML browser, set options(help.pager="yourBrowser") where yourBrowser specifies your particular HTML browser (such as the slynx program).

#### Note

The slynx program is not distributed with Spotfire S+; however, if you want to use it as a Help browser, you can download it it separately as part of the 'pkgutils' package (using the install.pkgutils() function), and then help() will use it.

The text in the Spotfire S+ help files is formatted for display using HTML. You can use the arrow keys to page through a help file; use the "q" key to exit a help file and return to the Spotfire S+ prompt.

The ? command is particularly useful for obtaining information on classes of objects. If you use the syntax class ? with the name of a class, Spotfire S+ offers documentation on the class. For example,

## 

You can call help with the name of a S-PLUS function, operator, or data set as argument. For instance, the following command displays the help file for the c function:

```
> help("c")
```

The quotation marks are optional for most functions, but are required for functions and operators containing special characters, such as <-. Quotation marks are also required for S-PLUS reserved words, such as for, in, and TRUE.

### Displaying Help in a Separate Window

The help function has an argument, window=T, that you can use to display your help files in a separate window from your Spotfire S+ session window. This allows you to view a help file while continuing to do work in your Spotfire S+ session. By default, the help window is a terminal window displaying the **slynx** browser, as determined by the setting of options()\$help.pager. If you want to change your browser settings, save the old options with the syntax oldopts <-options(help.pager="whatever"). To restore the **slynx** browser, call options(oldopts).

#### Chapter 2 Getting Started

The window=T argument applies only to terminal-based sessions of Spotfire S+. In the graphical user interface, the ? and help functions always display help files in a window that is separate from the **Commands** window. By default, the help window displays the **slynx** browser, as determined by the setting of options()\$help.pager.

### Printing Help Files

To print a help file, use the **Print** button in the JavaHelp window. For a more plainly formatted printed version, use the help function with the argument offline=T.

### Documentation Objects

Spotfire S+ does not support *creating* documentation objects, although you can still dump existing documentation objects and create help files used by the new Spotfire S+ help system. The sourceDoc function is defunct.

### **S-PLUS LANGUAGE BASICS**

This section introduces the most basic concepts you need to use the S-PLUS language: expressions, operators, assignments, data objects, and function calls.

### **Data Objects**

When you use Spotfire S+, you should think of your data sets as *data objects* belonging to a certain *class*. Each class has a particular *representation*, often defined as a named list of *slots*. Each slot, in turn, contains an object of some other class. Among the most common classes are "numeric", "character", "factor", "list", and "data.frame". This chapter introduces the most fundamental data objects; see the chapter Data Objects in the *Programmer's Guide* for a more detailed treatment.

The simplest type of data object is a one-way array of values, all of which are numbers, logical values, or character strings, but not a combination of those. For example, you can have an array of numbers: -2.0 3.1 5.7 7.3. Or you can have an array of logical values: T T F T F T F, where T stands for TRUE and F stands for FALSE. Or you can have an ordered set of character strings: "sharp claws", "COLD PAWS". These simple one-way arrays are called vectors when stored in S-PLUS. The class "vector" is a virtual class encompassing all basic classes whose objects can be characterized as one-way arrays. In a vector, any individual value can be extracted and replaced by referring to its *index*, or position in the array. The *length* of a vector is the number of values in the array; valid indices for a vector object x are in the range 1:length(x). Most vectors belong to one of the following classes: numeric, integer, logical, or character. For example, the vectors described above have length 4, 8, and 2 and class numeric, logical, and character, respectively.

S-PLUS assigns the class of a vector containing different kinds of values in a way that preserves the maximum amount of information: character strings contain the most information, numbers contain somewhat less, and logical values contain still less. S-PLUS coerces less informative values to equivalent values of the more informative type:

```
> c(17, TRUE, FALSE) [1] 17 1 0
```

```
> c(17, TRUE, "hello")
[1] "17" "TRUE" "hello"
```

#### Data Object Names

Object names must begin with a letter and may include any combinations of upper and lower case letters, numbers, and periods. For example, the following are all valid object names:

```
mydata
data.ozone
RandomNumbers
lottery.ohio.1.28.90
```

#### Warning

If you create S-PLUS data objects on a file system with more restrictive naming conventions than those your version of Spotfire S+ was compiled for, you may lose data if you violate the restrictive naming conventions. For example, if you are running Spotfire S+ on a machine allowing 255 character names and create S-PLUS objects on a machine restricting file names to 14 characters, object names greater than 14 characters will be truncated to the 14 character limit. If two objects share the same initial 14 characters, the latest object overwrites the earlier object. Spotfire S+ warns you whenever you attach a directory with more restrictive naming conventions than it is expecting.

#### Hint

You will not lose data if, when creating data objects on a file system with more restrictive naming conventions than your version of Spotfire S+ was compiled for, you restrict yourself to names that are unique under the more restrictive conventions. However, your file system may truncate or otherwise modify the object name. To recall the object, you must refer to it by its modified name. For example, if you create the object aov.devel.small on a file system with a 14 character limit, you should look for it in subsequent Spotfire S+ sessions with the 14 character name aov.devel.smal.

The use of periods often enhances the readability of similar data set names, as in the following:

```
data.1
data.2
data.3
```

Objects and methods created with S-PLUS 5.0 and later often follow a naming scheme that omits periods, but adds capital letters to enhance readability:

```
setMethod
signalSeries
```

#### Warning

You should not choose names that coincide with the names of S-PLUS functions. If you store a function with the same name as a built-in S-PLUS function, access to the S-PLUS function is temporarily prevented until you remove or rename the object you created. Spotfire S+ warns you when you have masked access to a function with a newly created function. To obtain a list of objects that mask other objects, use the masked function.

# Vector Data Objects

By now you are familiar with the most basic object in S-PLUS, the vector, which is a set of numbers, character values, logical values, etc. *Vectors must be of a single mode*: you cannot have a vector consisting of the values T, -2.3. If you try to create such a vector, S-PLUS coerces the elements to a common mode. For example:

```
> c(T,-2.3)
[1] 1.0 -2.3
```

Vectors are characterized by their *length* and *mode*. Length can be displayed with the length function, and mode can be displayed with the mode function.

#### Matrix Data Objects

An important data object type in S-PLUS is the *two-way array*, or *matrix* object. For example:

```
-3.0 2.1 7.6
2.5 -.5 -2.6
7.0 10.0 16.1
5.3 -21.0 -6.5
```

Matrices and their higher-dimensional analogues, *arrays*, are related to vectors, but have an extra structure imposed on them. S-PLUS treats these objects similarly by having the matrix and array classes inherit from another virtual class, the structure class.

To create a matrix, use the matrix function. The matrix function takes as arguments a vector and two numbers which specify the number of rows and columns. For example:

In this example, the first argument to matrix is a vector of integers from 1 through 12. The second and third arguments are the number of rows and columns, respectively. Each row and column is labeled: the row labels are [1,], [2,], [3,] and the column labels are [,1], [,2], [,3], [,4]. This notation for row and column numbers is derived from mathematical matrix notation.

In the above example, the vector 1:12 fills the first column first, then the second column, and so on. This is called filling the matrix "by columns." If you want to fill the matrix "by rows", use the optional argument byrow=T to matrix.

For a vector of given length used to fill the matrix, the number of rows determines the number of columns and vice versa. Thus, you need not provide both the number of rows and the number of columns as arguments to matrix; it is sufficient that you provide only one or the other. The following command produces the same matrix as above:

```
> matrix(1:12, 3)
```

You can also create this matrix by specifying the number of columns only. To do this, type:

```
> matrix(1:12, ncol=4)
```

You have to provide the optional argument ncol=4 in *name=value* form because, by default, the second argument is taken to be the number of rows. When you use the "by name" form ncol=4 as the second

argument, you override the default. See the section Optional Arguments to Functions on page 55 for further information on using optional arguments in function calls.

The array classes generally have three slots: a .Data slot to hold the actual values, a .Dim slot to hold the dimensions vector, and an optional .Dimnames slot to hold the row and column names. The most important slot for a matrix data object is the dimension slot .Dim. You can use the dim function to display the dimensions of an object:

```
> my.mat <- matrix(1:8,4,2)
> dim(my.mat)
[1] 4 2
```

This shows that the dimension of the matrix my.mat is 4 rows by 2 columns. Matrix objects also have length and mode, which correspond to the length and mode of the vector in the .Data slot. You can use the length and mode functions to view these characteristics of a matrix. Like vectors, a matrix object has a single mode. This means that you cannot create, for example, a two column matrix with one column of numeric data and one column of character data. For that, you must use a data frame.

#### Data Frame Objects

S-PLUS contains an object called a *data frame* which is very similar to a matrix object. A data frame object consists of rows and columns of data, just like a matrix object, except that the columns can be of different modes. The following object, baseball.df, is a data frame consisting of some baseball data from the 1988 season. The first two columns are factor objects (codes for names of players), the next two columns are numeric, and the last column is logical.

#### > baseball.df

```
bat.ID pitch.ID event.typ outs.play err.play
                              2
r1 pettg001 clemr001
                             14
                                         0
r2 whit1001 clemr001
r3 evand001 clemr001
                              3
                              2
r4 trama001 clemr001
                              3
                                         1
r5 andeb001 morrj001
                              2
                                         1
r6 barrm001 morrj001
                                                   F
                                         0
r7 boggw001 morrj001
                             21
r8 ricej001 morrj001
                              3
```

See the chapter Data Objects in the *Programmer's Manual* for further information on data frames. The chapter Chapter 4, Importing and Exporting Data discusses how to read in data frame objects from ASCII files.

#### **List Objects**

The *list* object is the most general and most flexible object for holding data in S-PLUS. A list is an ordered collection of *components*. Each list component can be any data object, and different components can be of different modes. For example, a list might have three components consisting of a vector of character strings, a matrix of numbers, and another list. Hence, lists are more general than vectors or matrices because they can have components of different types or modes, and they are more general than data frames because they are not restricted to having a rectangular (row by column) nature.

You can create lists with the list function. To create a list with two components, one a vector of mode "numeric" and one a vector of character strings, type the following:

```
> list(101:119,c("char string 1","char string 2"))
[[1]]:
   [1] 101 102 103 104 105 106 107 108 109 110 111 112 113
[14] 114 115 116 117 118 119
[[2]]:
[1] "char string 1" "char string 2"
```

The components of the list are labeled by double square-bracketed numbers, here [[1]] and [[2]]. This notation distinguishes the numbering of list components from vector and matrix numbering. After each component label, Spotfire S+ displays the contents of that component.

For greater ease in referring to list components, it is often useful to name the components. You do this by giving each argument in the list function its own name. For instance, you can create the same list as above, but name the components "a" and "b" and save the list data object with the name xyz:

```
> xyz <- list(a = 101:119,
+ b = c("char string 1", "char string 2"))
```

To take advantage of the component names from the list command, use the name of the list, followed by a \$ sign, followed by the name of the component. For example, the following two commands display components a and b, respectively, of the list xyz.

```
> xyz$a
  [1] 101 102 103 104 105 106 107 108 109 110 111 112 113
[14] 114 115 116 117 118 119
> xyz$b
[1] "char string 1" "char string 2"
```

# Managing Data Objects

In Spotfire S+, any object you create at the command line is permanently stored on disk until you remove it. This section describes how to name, store, list, and remove your data objects.

# Assigning Data Objects

To name and store data in Spotfire S+, use one of the *assignment* operators <- or =. For example, to create a vector consisting of the numbers 4, 3, 2, and 1 and store it with the name x, use the c function as follows:

```
> x < -c(4,3,2,1)
```

You type <- by with two keys on your keyboard: the "less than" key (<) followed by the minus (-) character, with no intervening space.

To store the vector containing the integers 1 through 10 in y, type:

```
> y <- 1:10
```

The following assignment expressions use the operator =, are identical to the two assignments above:

```
x = c(4,3,2,1)
y=1:10
```

The <- form of the assignment operator is highly suggestive and readable, so the examples in this manual use the arrow. The = is easier to type and matches the assignment operator in C, so many users prefer it. However, the S language also uses the = operator inside function calls for argument matching; if you want assign the value of an argument inside a function call, you must use the <- operator.

# Storing Data Objects

Data objects in your working directory are permanent. They remain even if you quit Spotfire S+ and start a new session later.

You can change the location where S-PLUS objects are stored by using the attach function. See the attach help file for further information. You can also change where your S-PLUS objects are located by explicitly specifying a new working directory. To do this, define the environment variable **S\_WORK**, which can specify one directory or a colon-separated list of directories. The first valid directory in the list is used as your working directory. For more information on working directories, see the section Creating a Working Directory on page 24.

# Listing Data Objects

To display a list of the data objects in your working directory, use the objects function as follows:

```
> objects()
```

If you created the vectors x and y in the section Assigning Data Objects on page 47, you see these listed in your working directory.

The S-PLUS function objects also searches for objects whose names match a character string given to it as an argument. The pattern search may include wildcard characters. For instance, the following expression displays all objects that start with the letter d:

```
> objects("d*")
```

For information on wildcards and how they work, see the help file for grep.

# Removing Data Objects

Because S-PLUS objects are permanent, you should remove objects you no longer need from time to time. You can use the rm function to remove objects. The rm function takes any number of objects as its arguments, and removes each one from your working database. For instance, to remove two objects named a and b, use the following expression:

```
> rm(a,b)
```

# Displaying Data Objects

To look at the contents of a stored data object, just type its name:

```
> x [1] 4 3 2 1
```

```
> y
[1] 1 2 3 4 5 6 7 8 9 10
```

#### **Functions**

A function is a S-PLUS expression that returns a value, usually after performing some operation on one or more arguments. For example, the c function returns a vector formed by combining its arguments. You *call* a function by typing an expression consisting of the name of the function followed by a pair of parentheses, which may enclose some arguments separated by commas. For example, runif is a function which produces random numbers uniformly distributed between 0 and 1. To have Spotfire S+ compute 10 such numbers, type runif(10):

```
> runif(10)
[1] 0.6033770 0.4216952 0.7445955 0.9896273 0.6072029
[6] 0.1293078 0.2624331 0.3428861 0.2866012 0.6368730
```

Spotfire S+ displays the results computed by the function, followed by a new prompt. In this case, the result is a vector object consisting of 10 random numbers generated by a uniform random number generator. The square-bracketed numbers, here [1] and [6], help you keep track of how many numbers are displayed on each line of the output, and help you locate particular numbers.

One of the functions in S-PLUS that you will use frequently is the function c which allows you to combine data values into a vector. For example:

```
> c(3, 7, 100, 103)
[1] 3 7 100 103
> c(T, F, F, T, T)
[1] T F F F T T
> c("sharp teeth", "COLD PAWS")
[1] "sharp teeth" "COLD PAWS"
> c("sharp teeth", 'COLD PAWS')
[1] "sharp teeth" "COLD PAWS"
```

The last example illustrates that either double quotes (") or single quotes (') can be used to delimit character strings.

Usually, you want to assign the result of a function to an object with another name that is permanently saved (until you choose to remove it). For example:

```
> weather <- c("hot day","COLD NIGHT")
> weather
[1] "hot day" "COLD NIGHT"
```

Some functions in S-PLUS are commonly used with no arguments. For example, recall that you quit Spotfire S+ by typing q(). The parentheses are still required so that Spotfire S+ can recognize that the expression is a function.

When you leave the parentheses out of a function call, the function text is displayed on the screen. Typing any object's name causes Spotfire S+ to print that object; a function object is simply the definition of the function. To call the function, simply retype the function name with parentheses. For instance, if you accidentally type q instead of q() when you try to quit Spotfire S+, the body of the function q is displayed. In this case the body of the function is only two lines long:

```
> q
function(...)
.Internal(q(...), "S_dummy", T, 33)
>
```

No harm has been done. All you need to do now is correctly type q(), and Spotfire S+ returns to your system prompt.

```
> q()
%
```

#### **Operators**

An *operator* is a function that has at most two arguments, and can be represented by one or more special symbols which appear between the two arguments. For example, the usual arithmetic operations of addition, subtraction, multiplication and division are represented by the operators +, -, \*, and /, respectively. Some simple calculations using the arithmetic operators are given in the examples below.

```
> 3+71
[1] 74
> 3*121
[1] 363
> (6.5 - 4)/5
[1] .5
```

The exponentiation operator is ^, which can be used as follows:

```
> 2 ^ 3 [1] 8
```

Some operators work with only one argument, and hence are called *unary* operators. For example, the subtraction operator - can act as a unary operator:

```
> -3 [1] -3
```

The colon (:) is an important operator for generating sequences of integers:

```
> 1:10
[1] 1 2 3 4 5 6 7 8 9 10
```

Table 2.2 lists the S-PLUS operators for comparison and logic. Comparisons are among the most common sources for logical data:

```
> (1:10) > 5
[1] F F F F F T T T T T
```

Comparisons and logical operations are frequently convenient for extracting subsets of data, and conditionals using logical comparisons play an important role in flow of control in functions.

<b>Table 2.2:</b>	Logical	and	comparison	operators.
-------------------	---------	-----	------------	------------

Operator	Explanation	Operator	Explanation
==	equal to	!=	not equal to
>	greater than	<	less than
>=	greater than or equal to	<=	less than or equal to
&	vectorized And	I	vectorized Or
&&	control And	П	control Or
!	not		

### **Expressions**

An *expression* is any combination of functions, operators, and data objects. Thus x < - c(4,3,2,1) is an expression that involves an operator (the assignment operator) and a function (the c function). Here are a few examples to give you an indication of the variety of expressions you can use in S-PLUS:

```
> 3 * runif(10)
 [1] 1.6006757 2.2312820 0.8554818 2.4478138 2.3561580
 [6] 1.1359854 2.4615688 1.0220507 2.8043721 2.5683608
> 3*c(2,11)-1
[1] 5 32
> c(2*runif(5),10,20)
[1] 0.6010921 0.3322045 1.0886723 0.3510106
[5] 0.9838003 10.0000000 20.0000000
> 3*c(2*x,5)-1
[1] 41 14
```

The last two examples illustrate a general feature of S-PLUS functions: arguments to functions can themselves be S-PLUS expressions.

Here are three examples of expressions which are important because they show how arithmetic works in Spotfire S+ when you use expressions involving both vectors and numbers. If x consists of the numbers 4, 3, 2, and 1, then the following operations work on each element of x:

```
> x-1
[1] 3 2 1 0
> 2*(x-1)
[1] 6 4 2 0
> x ^ 2
[1] 16 9 4 1
```

Any time you use an operator with a vector as one argument and a number as the other argument, the operation is performed on each component of the vector.

#### Hint

If you are familiar with the APL programming language, this treatment of vectors will be familiar to you.

### Precedence Hierarchy

The evaluation of S-PLUS expressions has a *precedence hierarchy*, shown in Table 2.3. Operators appearing higher in the table have higher precedence than those appearing lower; operators on the same line have equal precedence.

Among operators of equal precedence, evaluation proceeds from left to right within an expression. Whenever you are uncertain about the precedence hierarchy for evaluation of an expression, you should use parentheses to make the hierarchy explicit. S-PLUS shares a common feature of many computer languages that the innermost parentheses are evaluated first, and so on until the outermost parentheses are evaluated. In the following example, we assign the value 5 to a vector (of length 1) called x. We then use the *sequence* operator: and show the difference between how the expression is evaluated with and without parentheses.

 Table 2.3: Precedence of operators.

Operator	Use
\$	component selection
[ [[	subscripts, elements
۸	exponentiation
-	unary minus
:	sequence operator
%% %/% %*%	modulus, integer divide, matrix multiply
* /	multiply, divide
+ -	add, subtract
<> <= >= !=	comparison
!	not
&   &&	and, or
~	formulas
<<> <	assignments

#### Note

When using the  $\,^{\wedge}$  operator, the exponent must be an integer if the base is a negative number.

For example, in the expression 1: (x-1), (x-1) is evaluated first, and Spotfire S+ displays the integers from 1 to 4 as a result:

```
> x <- 5
> 1:(x-1)
[1] 1 2 3 4
```

However, when the parentheses are left off, the : operator has greater precedence than the - operator. The expression 1:x-1 is interpreted by Spotfire S+ to mean "take the integers from 1 to 5, and then subtract one from each integer". Hence, the output is of length 5 instead of length 4, and starts at 0 instead of 1:

```
> 1:x-1
[1] 0 1 2 3 4
```

When you use Spotfire S+, keep in mind the effect of parentheses and the default operator hierarchy.

# Optional Arguments to Functions

One powerful feature of S-PLUS functions is considerable flexibility through the use of *optional* arguments. At the same time, simplicity is maintained because sensible *defaults* for optional arguments have been built in, and the number of *required* arguments is kept to a minimum. You can determine which arguments are required and which are optional by looking in the help file under the REQUIRED ARGUMENTS and OPTIONAL ARGUMENTS sections.

For example, to produce 50 normal random numbers with mean 0 and standard deviation 1, use the following command:

```
> rnorm(50)
```

If you want to produce 50 normal random numbers with mean 3 and standard deviation 5, you can use any of the following:

```
> rnorm(50, 3, 5)
> rnorm(50, sd=5, mean=3)
> rnorm(50, m=3, s=5)
> rnorm(m=3, s=5, 50)
```

In the first expression, you supply the optional arguments by value. When supplying optional arguments by value, you must supply the arguments in the order they are given in the help file USAGE statement. In the second through fourth expressions, you supply the optional arguments by name. When supplying arguments by name, order is not important. However, we recommend that you supply optional arguments after required arguments for consistency of style. The third and fourth expressions above illustrate that you may abbreviate the formal names of optional arguments for convenience, so long as the abbreviations uniquely correspond to their respective argument names.

You will find that supplying arguments by name is convenient because you can supply them in any order. Of course, you do not need to specify *all* of the optional arguments. For instance, the following are two equivalent ways to produce 50 random normal numbers with mean 0 (the default), and standard deviation of 5:

```
> rnorm(50, m=0, s=5)
> rnorm(50, s=5)
```

### Access to Solaris and Linux

One important feature of Spotfire S+ is easy access to and use of Solaris and Linux tools. Spotfire S+ provides a simple shell escape character for issuing a single command from within Spotfire S+:

```
> !date
Mon Apr 15 17:46:25 PDT 1991
```

Here, date is a command which passes its result to Spotfire S+ for display as shown. You can use any command in place of date. Of course, if you have separate Solaris or Linux windows open on your workstation screen, you can simply move into another window to issue a command.

In addition to the escape function !, Spotfire S+ provides a unix function that is a more powerful way to execute commands. The unix function allows you to capture and manipulate output produced by Solaris or Linux within a Spotfire S+ session.

### IMPORTING AND EDITING DATA

There are many kinds and sizes of data sets that you may want to work on in Spotfire S+. The first step is to get your data into Spotfire S+ in appropriate data object form. In this section, we show you how to import data sets that exist as files and how to enter small data sets from your keyboard. For details on the **Import Data** dialog, see the chapter Importing and Exporting Data.

# Reading a Data File

The data you are interested in may have been created in Spotfire S+, but more likely it came to you in some other form. Perhaps your data is an ASCII file or is from someone else's work in another software package, such as SAS. You can read data from a variety of sources using the S-PLUS function importData.

For example, suppose you have a SAS file named **Exervirn.ssd01**. To import that file using the importData function, you must supply the file's name as the file argument:

```
> Exenvirn <- importData(file = "Exenvirn.ssd01")</pre>
```

After Spotfire S+ reads the data file, it assigns the data to the Exenvirn data frame.

### Entering Data From Your Keyboard

To get a small data set into Spotfire S+, create a S-PLUS data object using the scan() function as follows:

```
> mydata <- scan()</pre>
```

where *mydata* is any legal data object name. Spotfire S+ prompts you for input, as described in the following example. We enter 14 data values and assign them to the object diff.hs. At the Spotfire S+ prompt, type in the name diff.hs and assign to it the results of the scan command. Spotfire S+ responds with the prompt 1:, which means that you should enter the first value.

You can enter as many values per line as you like, separated by spaces. When you press RETURN, Spotfire S+ prompts with the index of the next value it is waiting for. In our example, Spotfire S+ responds with 6: because you entered 5 values on the first line. When you finish entering data, press RETURN in response to the: prompt, and Spotfire S+ returns to the Spotfire S+ command prompt (>).

The complete example appears on your screen as follows:

```
> diff.hs <- scan()
1: .06 .13 .14 -.07 -.05
6: -.31 .12 .23 -.05 -.03
11: .62 .29 -.32 -.71
15:
>
```

# Reading An ASCII File

Entering data from the keyboard is a relatively uncommon task in Spotfire S+. More typically, you have a data set stored as an ASCII file that you want to read into Spotfire S+. An ASCII file usually consists of numbers separated by spaces, tabs, newlines, or other delimiters.

Suppose you have a text file called **vec.data** in the same directory from which you started Spotfire S+, and suppose **vec.data** contains the following data:

```
62 60 63 59
63 67 71 64 65 66
88 66 71 67 68 68
56 62 60 61 63 64 63 59
```

You read the **vec.data** file into Spotfire S+ by using the scan command with "vec.data" as an argument:

```
> x <- scan("vec.data")</pre>
```

The quotation marks around the vec.data argument to scan are required. You can now type x to display the data object you have read into Spotfire S+.

If the file you want to read is not in the same directory from which you started Spotfire S+, you must use the entire path name. If the text file **vec.data** is in a subdirectory with path name **/usr/mabel/test/vec.data**, then type:

```
> x <- scan ("/usr/mabel/test/vec.data")</pre>
```

### **Editing Data**

After you have created a S-PLUS data object, you may want to change some of the data you have entered. The easiest way to modify simple vectors and S-PLUS functions is to use the fix function, which uses the editor specified in your Spotfire S+ session options. By default, the editor used is **vi**.

With fix, you create a copy of the original data object, edit it, then reassign the result under its original name. If you have a favorite editor, you can use it by specifying it with the options function. For example, if you prefer to use the **emacs** editor, you can set this up easily as follows:

```
> options(editor="emacs")
```

To create a *new* data object by modifying an existing object, use the vi function, assigning the result to a new name. For example, if you want to create your own version of a system function such as lm, you can use vi as follows:

```
> my.lm <- vi(lm)
```

#### Warning

If you do not assign the output from the vi function, the changes you make are simply scrolled across the screen, and are not incorporated into any function definition. The value is also stored in the object .Last.value until a new value is returned by Spotfire S+. You can therefore recover the changes by *immediately* typing the following:

```
> myfunction <- .Last.value
```

### Built-in Data Sets

Spotfire S+ comes with a large number of *built-in* data sets. These data sets provide examples for illustrating the capabilities of Spotfire S+ without requiring you to enter your own data. When Spotfire S+ is used as a teaching aid, the built-in data sets provide a foundation for problem assignments in data analysis.

To have Spotfire S+ display any of the built-in data sets, just type its name at the > prompt. The built-in data sets include data objects of various types, and are stored in a **data** directory of your search path. To see the databases that are attached to your search path by default, type search() at the Spotfire S+ command prompt:

Your working directory is attached in the first position of your search path, and the **data** directory is attached in the fourth position. To see a listing of the built-in objects in the **data** directory, use the objects function as follows:

```
> objects("data")
[1] "\001"
                    "..min.script.id"
                                          ".Copyright"
[4] ".Original"
                    ".PostScript.Options" ".Program"
                         "CHAR"
[7] ".Random.seed"
                                          "Defunct.funs"
                                          "LGL"
[10] "Deprecated.funs"
                        "INT"
                         "Puromycin"
[13] "Lubricant"
                                          "REAL"
[16] . . .
```

### Quick Hard Copy

To obtain a quick hard copy of your S-PLUS objects, use the 1pr function. For example, to print the object diff.hs, use the following command:

```
> lpr(diff.hs)
```

A copy of your data will be sent to your standard printer.

### Adding Row And Column Names

Names can be added to a number of different types of S-PLUS objects. In this section we discuss adding labels to vectors and matrices.

#### Adding Names To Vectors

To add names to a vector of data, use the names function. You assign a character vector of length equal to the length of the data vector as the names attribute for the vector. For example, the following commands assign the integers 1 through 5 to a vector x, and assign the spelled out words for those integers to the names attribute of the vector:

```
> x <- 1:5
> names(x) <- c("one", "two", "three", "four", "five")
> x
  one two three four five
    1    2    3    4    5
```

You also use names to display the names associated with a vector:

```
> names(x)
one two three four five
```

You should note that the class of simple data objects such as vectors may be changed when names are added. If a vector does not include names, Spotfire S+ recognizes it as a simple "numeric" object. When names are added, however, the class of the object changes to "named":

```
> data.class(x)
[1] "named"
```

## Adding Names To Matrices

In a matrix, both the rows and columns can be named. Often the columns have meaningful alphabetic word names because the columns represent different *variables*, while the row names are either integer values indicating the observation number or character strings identifying "case" labels. Lists are useful for adding row names and column names to a matrix, as we now illustrate.

The dimnames argument to the matrix function is used to name the rows and columns of the matrix. The dimnames argument must be a list with exactly 2 components. The first component gives the labels for the matrix rows, and the second component gives the names for the matrix columns. The length of the first component in the dimnames list is equal to the number of rows, and the length of the second component is equal to the number of columns.

For example, if we add a dimnames argument to the matrix command, the resulting matrix will have the row and column labels specified:

You can assign row and column names to existing matrices using the dimnames function, which works much like the names function for vectors:

# Extracting Subsets of Data

Another powerful feature of the S-PLUS language is the ability to extract subsets of data for viewing or further manipulation. The examples in this section illustrate subset extraction for vectors and matrices only. However, similar techniques can be used to extract subsets of data from other S-PLUS data objects.

# Subsetting From Vectors

Suppose you create a vector of length 5, consisting of the integers 5, 14, 8, 9, 5:

```
> x <- c(5, 14, 8, 9, 5)
> x
[1] 5 14 8 9 5
```

To display a single element of this vector, just type the vector's name followed by the element's index within square brackets. For example, type x[1] to display the first element and x[4] to display the fourth element:

```
> x[1]
[1] 5
> x[4]
[1] 9
```

To display more than one element at a time, use the c function within the square brackets. The following command displays the second and fifth elements of x:

```
> x[c(2,5)]
[1] 14 5
```

Use negation to display all elements *except* a a specified element or list of elements. For instance, x[-4] displays all elements except the fourth:

```
> x[-4]
[1] 5 14 8 5
```

Similarly, x[-c(1,3)] displays all elements except the first and third:

```
x[-c(1,3)] [1] 14 9 5
```

A more advanced use of subsetting uses a logical expression within the [] characters. Logical expressions divide a vector into two subsets: one for which a given condition is true, and one for which the condition is false. When used as a subscript, the expression returns the subset for which the condition is true.

For instance, the following expression selects all elements with values greater than 8:

```
> x[x>8]
[1] 14 9
```

In this case, the second and fourth elements of x, with values 14 and 9, meet the requirements of the logical expression x > 8, and are therefore displayed. As usual in Spotfire S+, you can assign the result of the subsetting operation to another object. For example, you could assign the subset in the above expression to an object named y, and then display y or use it in subsequent calculations:

```
> y <- x[x>8]
> y
[1] 14 9
```

In the next section you will see that the same subsetting principles apply to matrix data objects, although the syntax is a little more complicated to account for both dimensions in a matrix.

#### Subsetting From Matrix Data Objects

A single element of a matrix can be selected by typing its coordinates inside the square brackets as an ordered pair, separated by commas. We use the built-in data set state.x77 to illustrate. The first number inside the [] operator is the row index, and the second number is the column index. The following command displays the value in the third row, eighth column of state.x77:

```
> state.x77[3,8]
[1] 113417
```

You can also display an element, using row and column dimnames, if such labels have been defined. To display the above value, which happens to be in the row named "Arizona" and the column named "Area", use the following command:

```
> state.x77["Arizona", "Area"]
[1] 113417
```

To select sequential rows and/or columns from a matrix object, use the : operator. The following expression selects the first 4 rows and columns 3 through 5 and assigns the result to the object x:

```
> x <- state.x77[1:4, 3:5]
> x
         Illiteracy Life Exp Murder
 Alabama
                2.1
                        69.05
                                15.1
                1.5
                        69.31
                                11.3
  Alaska
 Arizona
                1.8
                        70.55
                                7.8
                1.9
                        70.66
                                10.1
Arkansas
```

The c function can be used to select non-sequential rows and/or columns of matrices, just as it was used for vectors. For instance, the following expression chooses rows 5, 22, and 44, and columns 1, 4, and 7 of state.x77:

As before, if row or column names have been defined, they can be used in place of the index numbers:

Selecting All Rows or All Columns From a Matrix Object

To select all of the rows in a matrix, leave the expression before the comma (in the square brackets) blank. To select all columns in a matrix, leave the expression after the comma blank. The following command chooses all columns in state.x77 for the rows corresponding to California, Michigan, and Utah. In the expression, the closing bracket appears immediately after the comma; this means that all columns are selected.

```
> state.x77[c("California","Michigan","Utah"), ]
           Population Income Illiteracy Life Exp Murder
California
                21198
                        5114
                                     1.1
                                            71.71
                                                    10.3
  Michigan
                 9111
                        4751
                                     0.9
                                            70.63
                                                    11.1
                 1203
                        4022
                                     0.6
                                            72.90
                                                    4.5
      Utah
           HS Grad Frost
                           Area
California
              62.6
                      20 156361
              52.8
                     125
                          56817
  Michigan
              67.3 137
                          82096
      Utah
```

#### **GRAPHICS IN SPOTFIRE S+**

Graphics are central to the Spotfire S+ philosophy of looking at your data visually as a first and last step in any data analysis. With its broad range of built-in graphics functions and its programmability, Spotfire S+ lets you look at your data from many angles. This section describes how to use Spotfire S+ to create simple command-line plots. To put Spotfire S+ to work creating the many other types of plots, see the chapters Traditional Graphics and Traditional Trellis Graphics in the Spotfire S+ documentation.

This section is geared specifically to graphics that are created by S-PLUS functions and displayed in motif windows. For information on manipulating **Graph** windows in the GUI, see the chapter Working with the Graphical User Interface. For information on creating plots from the **Graph** menu options in the GUI, see the chapter Menu Graphics.

#### **Making Plots**

Plotting engineering, scientific, financial or marketing data, including the preparation of camera-ready copy on a laser printer, is one of the most powerful and frequently used features of Spotfire S+. S-PLUS has a wide variety of plotting and graphics functions for you to use.

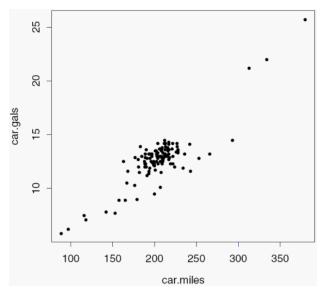
The most frequently used S-PLUS plotting function is plot. When you call a plotting function, a Spotfire S+ graphics window displays the requested plot:

```
> plot(car.miles)
```

The argument car.miles is a S-PLUS built-in vector data object. Since there is no other argument to plot, the data are plotted against their natural index or observation numbers, 1 through 120. Since you may be interested in gas mileage, you can plot car.miles against car.gals. This is also easy to do with plot:

```
> plot(car.gals, car.miles)
```

The result is shown in Figure 2.1.



**Figure 2.1:** A Spotfire S+ plot.

You can use many S-PLUS functions besides plot to display graphical results in the Spotfire S+ graphics window. Many of these functions are listed in Table 2.4 and Table 2.5, which display, respectively, high-level and low-level plotting functions. High-level plotting functions create new plots and axes, while low-level plotting functions typically add to an existing plot.

**Table 2.4:** Common high-level plotting functions.

barplot, hist	Bar graph, histogram
boxplot	Boxplot
brush	Brush pair-wise scatter plots; spin 3D axes
contour, image, persp, symbols	3D plots
coplot	Conditioning plot
dotchart	Dot chart
faces, stars	Display multivariate data

 Table 2.4: Common high-level plotting functions. (Continued)

map	Plot all or part of the U.S. (this function is part of the maps library)
pairs	Plot all pair-wise scatter plots
pie	Pie chart
plot	Generic plotting
qqnorm, qqplot	Normal and general QQ-plots
scatter.smooth	Scatter plot with a smooth curve
tsplot	Plot a time series
usa	Plot the boundary of the U.S.

 Table 2.5:
 Common low-level plotting functions.

abline	Add line in intercept-slope form
axis	Add axis
box	Add a box around plot
contour, image, persp, symbols	Add 3D information to plot
identify	Use mouse to identify points on a graph
legend	Add a legend to the plot
lines, points	Add lines or points to a plot
mtext, text	Add text in the margin or in the plot
stamp	Add date and time information to the plot
title	Add title, x-axis labels, y-axis labels, and/or subtitle to plot

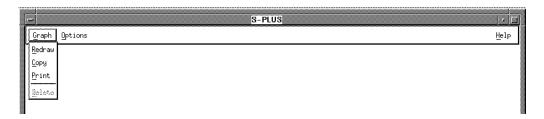
#### Quick Hard Copy

Each graphics window offers a simple, straightforward way to obtain a hard copy of the picture you have composed on the screen: the **Print** option under the **Graph** pull-down menu. You can exercise more control over your instant hard copy, by specifying whether the copy is in landscape or portrait orientation, which printer the hard copy is sent to, and for HP-Laserjet systems, the dpi (dots per inch) resolution of the printout.

# Using the Graphics Window

You can use a mouse to perform basic functions in a graphics window, such as redrawing or copying a graph. The standard graphics window, also known as the motif device (Figure 2.2) has a set of pull-down menus providing a mouse-based point and click capability for copying, redrawing and printing hard copy on a printer.

In general, you select actions by pulling down the appropriate menu, and clicking the left mouse button.



**Figure 2.2:** *The* motif *window*.

#### Copying A Graph

Each graphics window provides a mechanism to copy a graph on the screen. This option allows you to "freeze" a picture in one state, but continue to modify the original. The motif device has a **Copy** choice under the **Graph** pull-down menu.

## Redrawing A Graph

Each graphics window provides a mechanism for "redrawing" a graph. This option can be used to refresh the picture if your screen has become cluttered. The motif device offers the **Redraw** option as a selection from the **Graph** pull-down menu.

#### Multiple Plot Layout

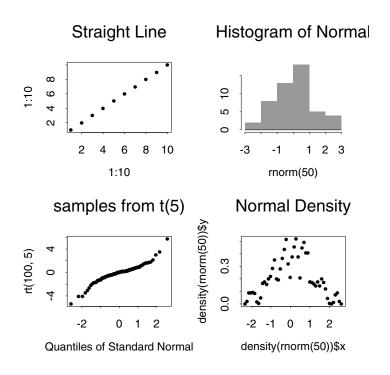
It is often desirable to display more than one plot in a window or on a single page of hard copy. To do so, you use the S-PLUS function par to control the layout of the plots. The following example shows how

to use par for this purpose. The par command is used to control and customize many aspects of Spotfire S+ plots. See the chapter Traditional Graphics for further information on the par command.

In this example, we use par to set up a a window or a page that has four plots in two rows of two each. Following the par command, we issue four plotting commands. Each command creates a simple plot with a main title.

```
> par(mfrow=c(2,2))
> plot(1:10,1:10,main="Straight Line")
> hist(rnorm(50),main="Histogram of Normal")
> qqnorm(rt(100,5),main="Samples from t(5)")
> plot(density(rnorm(50)),main="Normal Density")
```

The result is shown in Figure 2.3.



**Figure 2.3:** A multiple plot layout.

#### **STATISTICS**

S-PLUS includes functions for doing all kinds of statistical analysis, including hypothesis testing, linear regression, analysis of variance, contingency tables, factor analysis, survival analysis, and time series analysis. Estimation techniques for all these branches of statistics are described in detail in the manual *Guide to Statistics*.

This section gives overviews of the functions that produce summary statistics, perform hypothesis tests, and fit statistical models. This section is geared specifically to statistical analyses that are generated by S-PLUS command-line functions. For information on the options available under the **Statistics** menu in the GUI, see the Statistics chapter.

#### Summary Statistics

S-PLUS includes functions for calculating all of the standard summary statistics for a data set, together with a variety of robust and/or resistant estimators of location and scale. Table 2.6 lists of the most common functions for summary statistics.

The summary function is a generic function that provides appropriate summaries for different types of data. For example, an object of class 1m created by fitting a linear model has a summary that includes the table of estimated coefficients, their standard errors, and t-values, along with other information. The summary for a standard vector is a six-number table of the minimum, maximum, mean, median, and first and third quartiles:

**Table 2.6:** Common functions for summary statistics.

cor	Correlation coefficient
cummax, cummin, cumprod, cumsum	Cumulative maximum, minimum, product, and sum
diff	Create sequential differences
max, min	Maximum and minimum

-un-10 -100 dominion functions for cumumary countries ( dominional)		
pmax, pmin	Maxima and minima of several vectors	
mean	Arithmetic mean	
median	50th percentile	
prod	Product of elements of a vector	
quantile	Compute empirical quantiles	
range	Returns minimum and maximum of a vector	
sample	Random sample or permutation of a vector	
sum	Sum elements of a vector	
summary	Summarize an object	
var	Variance and covariance	

 Table 2.6:
 Common functions for summary statistics. (Continued)

#### Hypothesis Testing

S-PLUS contains a number of functions for doing classical hypothesis testing, as shown in Table 2.7. The following example illustrates how to use t.test to perform a two-sample t-test to detect a difference in means. This example uses two random samples generated from N(0,1) and N(1,1) distributions. We set the random number seed with the function set.seed so this example is reproducible:

```
> set.seed(19)
> x <- rnorm(10)
> y <- rnorm(5, mean=1)
> t.test(x,y)
   Standard Two-Sample t-Test

data: x and y
t = -1.4312, df = 13, p-value = 0.176
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
   -1.7254080   0.3502894
sample estimates:
   mean of x mean of y
   -0.4269014   0.2606579
```

**Table 2.7:** S-PLUS functions for hypothesis testing.

Test	Description
t.test	Student's one- or two-sample t-test
wilcox.test	Wilcoxon rank sum and signed-rank sum tests
chisq.test	Pearson's chi square test for 2D contingency table
var.test	F test to compare two variances
kruskal.test	Kruskal-Wallis rank sum test
fisher.test	Fisher's exact test for 2D contingency table
binom.test	Exact binomial test
friedman.test	Friedman rank sum test
mcnemar.test	McNemar's chi square test
prop.test	Proportions test
cor.test	Test for zero correlation
mantelhaen.test	Mantel-Haenszel chi square test

#### Statistical Models

Most of the statistical modeling functions in S-PLUS follow a unified modeling paradigm in which the input data are represented as a data frame and the model to be fit is represented as a formula. Formulas can be saved as separate S-PLUS objects and supplied as arguments to the modeling functions. A partial listing of S-PLUS modeling functions is given in Table 2.8.

In a formula, you specify the response variable first, followed by a tilde ( $\sim$ ) and the terms to be included in the model. Variables in formulas can be any expression that evaluates to a numeric vector, a factor or ordered factor, or a matrix. Table 2.9 gives a summary of the formula syntax.

 Table 2.8:
 S-PLUS modeling functions.

Function	Description
aov, manova	Analysis of variance models
1 m	Linear model (regression)
glm	Generalized linear model (including logistic and Poisson regression)
gam	Generalized additive model
loess	Local regression model
tree	Classification and regression tree models
nls, ms	Nonlinear models
lme, nlme	Mixed-effects models
factanal	Factor analysis
princomp	Principal components analysis
pam, fanny, diana, agnes, daisy, clara	Cluster analysis

 Table 2.9: Summary of the S-PLUS formula S-PLUS syntax.

Expression	Meaning
A ~ B	A is modeled as B
B + C	Include both B and C in the model
B - C	Include all of B except what is in C in the model
B:C	The interaction between B and C
B*C	Include B, C, and their interaction in the model
C %in% B	C is nested within B
B/C	Include B and C %in% B in the model

The following sample Spotfire S+ session illustrates some steps to fit a regression model to the fuel.frame data containing five variables for 60 cars. We do not show the output; type these commands at your Spotfire S+ prompt and you'll get a good feel for doing data analysis with the S-PLUS language.

```
> names(fuel.frame)
> par(mfrow=c(3,2))
> plot(fuel.frame)
> pairs(fuel.frame)
> attach(fuel.frame)
> par(mfrow=c(2,1))
> scatter.smooth(Mileage ~ Weight)
> scatter.smooth(Fuel ~ Weight)
> lm.fit1 <- lm(Fuel ~ Weight)</pre>
> lm.fit1
> names(lm.fit1)
> summary(lm.fit1)
> qqnorm(residuals(lm.fit1))
> plot(lm.influence(lm.fit1)$hat, type="h",
     xlab = "Case Number", ylab = "Hat Matrix Diagonal")
> o.type <- ordered(Type, c("Small", "Sporty", "Compact",</pre>
     "Medium", "Large", "Van"))
> par(mfrow=c(1,1))
> coplot(Fuel ~ Weight | o.type,
     given.values=sort(unique(o.type)))
> lm.fit2 <- update(lm.fit1, . ~ . + Type)</pre>
> lm.fit3 <- update(lm.fit2, . ~ . + Weight:Type)</pre>
> anova(lm.fit1, lm.fit2, lm.fit3)
> summary(lm.fit3)
```

#### Chapter 2 Getting Started

# WORKING WITH THE GRAPHICAL USER INTERFACE

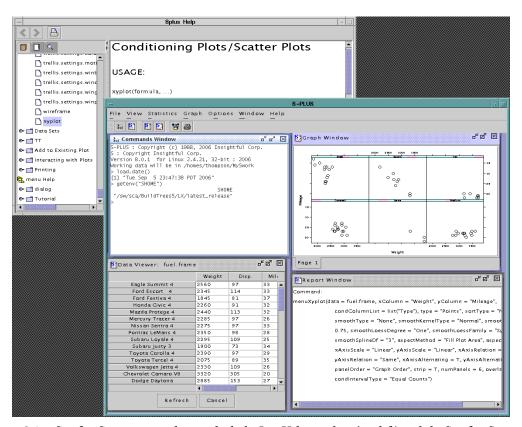
The User Interface	78
Using Menus, Dialog Boxes, and Toolbars	79
Using the Mouse	79
Using the Keyboard	80
Using Windows	80
Using Main Menus	84
Specifying Options in Dialogs	84
Using Toolbar Buttons	86
Spotfire S+ Windows	87
Objects Summary	87
Data Viewer	87
Graph Window	88
Commands Window	89
Report Window	89
Spotfire S+ Menus	90
Spotfire S+ Dialogs	01

#### THE USER INTERFACE

Spotfire S+ is a full-featured statistics and graphics application designed for easy, intuitive analysis and visualization of data. The Java-based graphical user interface makes this work even easier. This chapter gives an overview of its menus, windows, and toolbars.

#### Note

As of Spotfire S+ 8.1, the Spotfire S+ Java GUI is deprecated. If you want to use a GUI with Spotfire S+, use the Spotfire S+ Workbench.



**Figure 3.1:** Spotfire S+ in action; showing both the JavaHelp window (top left) and the Spotfire S+ graphical user interface (below right). Within the Spotfire S+ window, note the **Graph** window (top right), the **Data Viewer** (below left), and **Report** window (below right).

#### USING MENUS, DIALOG BOXES, AND TOOLBARS

Spotfire S+ menus, dialogs and toolbars contain all the options you need to view data, create graphs, and perform statistical analyses. You can use your mouse or your keyboard to access Spotfire S+ menus. Dialogs can be accessed by selecting menu options. Mouse, keyboard and window terms used throughout this document are defined below.

## Using the Mouse

Throughout this document, the following conventions are used to describe mouse operations.

- **Pointing**: moving the mouse to position the pointer over an object.
- **Clicking**: pointing at an object and quickly pressing and releasing the left mouse button. Some tasks in Spotfire S+ require a *double-click*, which is achieved by quickly pressing and releasing the left mouse button twice.
- **Right-Clicking**: pointing at a selected object and quickly pressing and releasing the right mouse button.
- **Dragging**: pointing at the object, then holding down the left mouse button while moving the mouse. Releasing the left mouse button "drops" the object in the new location.

The mouse pointer changes shape to indicate what action is taking place. The following table shows the different mouse pointer shapes and the significance of each.

**Table 3.1:** Different shapes of the mouse pointer.

Pointer	Mouse Action
1/3	Selection mouse pointer.
I	Text indicator, slanted pointer indicates italic text.
₹ <u></u>	Displayed when Move or Size is selected from the Control menu; allows the window to be moved or resized.
⇔ ĴĴ	Change the size of the window vertically or horizontally when positioned on a window border.
<b>2</b>	Change the size of two sides of the window when positioned on the corner of a window border.
	Indicates that a command is being processed; you should wait for a different mouse pointer before going on to other tasks.

#### Using the **Keyboard**

Throughout this document, the following conventions are used to reference keys.

- Key names appear in SMALLCAPS letters. For example, the Shift key appears as SHIFT.
- When more than one key must be pressed simultaneously, the two key names appear with a plus (+) between them. For example, the key combination of SHIFT and F1 appears as SHIFT+F1.
- The up, down, left, and right direction keys (represented on the keyboard by arrows) are useful for moving objects around the page. They are referred to as the UP direction key, the DOWN direction key, the LEFT direction key, and the RIGHT direction key.

**Using Windows** In Spotfire S+ you can operate on multiple windows, making it easy to view different data sets and display multiple graphs. The graphical user interface is contained within a single main window, and has multiple subwindows.

The Control-menu box is always in the upper-left corner of the main Spotfire S+ window. Click once on the Control-menu box for a list of commands that control the size, shape, and attributes of the window. Click twice on the Control-menu box to quit Spotfire S+.

The title bar displays the name of the window. If more than one window is open, the title bar of the current (or active) window is a different color or intensity than other title bars.

The Minimize button is represented in the main Spotfire S+ window by a small box, and in the subwindows by a small box with an arrow pointing into it. When this button is clicked, the window is reduced to an icon.

The Maximize button is represented in the main Spotfire S+ window by a large box, and in the subwindows by a large box with an arrow pointing out of it. When this button is clicked, the main Spotfire S+ window enlarges to fill the entire desktop, or the subwindow enlarges to fill the entire Spotfire S+ window.

The Restore button replaces the Maximize button when the window is maximized. The Restore button contains a large square with an arrow pointing into it, and it returns the window to its previous size.

**The Close button** is available only in the subwindows, and is not included as part of the main Spotfire S+ window. The Close button is represented by a square with an "X" in it, and it is used to close the **Commands** window, the **Report** window, **Graph** windows, etc.

The menu bar is a list of the available menus. Each menu contains a list of commands or actions.

The scroll bars let you scroll up and down through a window.

The window border surrounds the entire window. You can lengthen or shorten any side of the border by dragging it with the mouse.

The window corner can be used to drag any two sides of the window.

The mouse pointer is displayed if you have a mouse installed. The mouse is usually in the form of an arrow, an I, or a crosshair (+). For more information, see the section Using the Mouse on page 79.

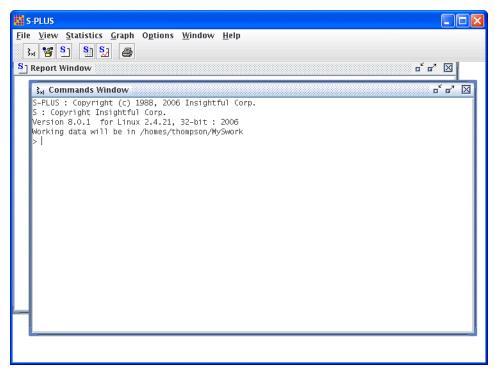


Figure 3.2: The opening main window of Spotfire S+ includes a Commands window. Notice that the main window has a Control-menu and Minimize and Maximize buttons, while the contained window has Minimize, Maximize and Close buttons (top right). Subwindows can be sized and moved, but only within the confines of the main Spotfire S+ window.

### Switching to a Different Window

At any time you can have many windows open simultaneously in Spotfire S+. The number of windows is limited only by your system's memory resources. To switch from one window to another window, click on any portion of the preferred window that is visible. Alternatively, you can select the preferred window from the list at the bottom of the **Window** menu.

## Moving and Sizing Windows

A maximized window cannot be moved or resized. A smaller window can be moved or resized within the confines of the application window. Note that not all windows can be resized.

#### To move a window or dialog

- 1. Click in the window or dialog to make it active.
- 2. Click and drag the title bar until the window or dialog is in the desired location.

#### To resize a window

- Click in the window to make it active.
- 2. Position the mouse over one of the four window borders.
- 3. The mouse changes to a double-headed arrow when it is over the border.
- 4. Click and drag the border to the desired size.

#### To expand a window to maximum size

- 1. Click in the window to make it active.
- 2. Click the **Maximize** button on the title bar, or double-click the title bar. Note that the **Maximize** button changes to the **Restore** button.

### Viewing Multiple Windows

In Spotfire S+, each type of object, such as a graph or data set, is displayed in a separate window. You can also have multiple windows of the same graph or data set open at the same time. You have several options for viewing multiple windows.

#### To view the windows tiled

• From the **Window** menu, choose **Tile**.

#### To view the windows layered, with only the title bars visible

• From the **Window** menu, choose **Cascade**.

#### Closing Windows To close a window

• Click the **Close** button on the title bar of the window.

#### To close all open windows

 Double-click the Control-menu box, or choose Exit from the File menu. This closes all open windows and quits Spotfire S+.

#### Using Main Menus

When you choose one of the main menu options, a list of additional options drops down. You can choose any of the options in the list. Menu options with a ▶ symbol at the end of the line display a submenu when selected. Menu commands with an ellipsis (...) after the command display a dialog box when selected.

#### To choose a menu option

Point to the desired menu option and click the left mouse button

or

Press the ALT key to access the menu bar, and then press the underlined key in the desired menu option.

To cancel a menu, click outside the menu or press ESC.

# Specifying Options in Dialogs

Choosing a menu option often displays a dialog. You can use dialogs to specify information about a particular action. Spotfire S+ has two types of dialogs: action dialogs and property dialogs. Action dialogs carry out commands such as creating a graph. Property dialogs display and allow you to modify the properties and characteristics in your Spotfire S+ session.

Dialogs can contain multiple, tabbed pages of options. To see the options on a different page of the dialog, click the page name. When you choose **OK** or **Apply** (or press CTRL+ENTER), any changes made on any of the tabbed pages are applied to the selected object.

Most of Spotfire S+ dialogs are modeless. They can be moved around on the screen and they remain open until you choose to close them. This means you can make changes in a dialog and see the effect without closing the dialog. This is useful when you are experimenting with changes to an object and want to see the effect of each change. The **Apply** button can be used to apply changes without closing the dialog. When you are ready to close the dialog, you can either choose **Cancel** or click the **Close** box on the dialog.

#### Note

Choosing OK closes the dialog and executes the command specified by it. If you do not wish the command to execute after the dialog closes, perhaps because you have already clicked on Apply, choose Cancel instead of OK.

## The OK, Cancel, and Apply Buttons

When you are finished setting options in a dialog box, you can click on the **OK**, **Cancel** or **Apply** buttons.

- **OK**: choose the **OK** button or press CTRL+ENTER to close the dialog box and carry out the action.
- Cancel: choose the Cancel button to close the dialog box and discard any of the changes you have made in the dialog. Sometimes changes cannot be canceled (for example, when changes have made with Apply, or when changes have been made outside of the dialog with the mouse).
- Apply: choose the Apply button to carry out the action without closing the dialog. Most of the Spotfire S+ dialogs have an Apply button, which acts much like an OK button except it does not close the dialog box. You can specify changes in the dialog box and then choose the Apply button to see your changes, keeping the dialog open so that you can make more changes without having to re-select the dialog.

## Typing and Editing in Dialog Boxes

Table 3.2 lists special keys for navigating through and performing tasks in dialog boxes. In addition, many dialogs contain text edit boxes, which allow you to type in information such as file names and graph titles.

 Action
 Special Keys

 Move to the next option in the dialog
 TAB

 Move to a specific option and select it
 ALT+underlined letter in the option name. Press again to move to additional options with the same underlined letter.

 Display a drop-down list
 DOWN direction key

 Select an item from a list
 UP or DOWN direction keys to move,

**Table 3.2:** Shortcut keys in dialog boxes.

#### To replace text in a dialog

1. Select the existing text with the mouse, or press ALT+underlined letter in the option name.

ENTER key to close the list

2. Type the new text. Any highlighted text is immediately overwritten when you begin typing the new text.

#### To edit text in a text box

- 1. Position the insertion point in the text box. If text is highlighted, it will be replaced when you begin typing.
- 2. Edit the text.

#### Using Toolbar Buttons

Toolbars contain buttons that are shortcuts to menu selections. You can use toolbar buttons to perform file operations such as opening a new **Graph** window or printing a window. To select a toolbar button, position the mouse pointer over the desired button and click. For example, you can print your current **Graph** window by clicking on the **Print** button.

#### SPOTFIRE S+ WINDOWS

The Spotfire S+ user interface contains five types of windows: the **Objects Summary**, **Data Viewer**, **Graph** window, **Commands** window, and **Report** window. These windows allow you to easily organize your work session, work with data and graphs simultaneously, and automate repetitive tasks.

#### Objects Summary

The **Objects Summary** window, shown in Figure 3.3, gives a brief overview of the objects in your working database. To open an **Objects Summary** window in your Spotfire S+ session, select **View Dobjects Summary**.

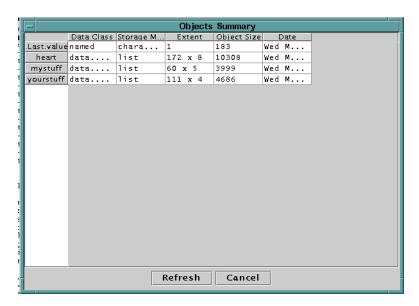


Figure 3.3: An Objects Summary window: several can be open simultaneously.

#### **Data Viewer**

The **Data Viewer**, shown in Figure 3.4, displays data sets in a non-editable tabular format. To view a data set, select **View** ▶ **New Data Viewer** from the main menu. A dialog appears that prompts you for the name of a S-PLUS data set. If the data set is in your working database, you can select its name from the pull-down list; otherwise, type the name directly in the **Data Set** field and click **OK**.

Data Viewer: fuel.frame 🗗 🗗 🗵			
	Weight	Disp.	N.
Eagle Summit 4	2560	97	33
Ford Escort 4	2345	114	33
Ford Festiva 4	1845	81	37
Honda Civic 4	2260	91	32
Mazda Protege 4	2440	113	32
Mercury Tracer 4	2285	97	26
Nissan Sentra 4	2275	97	33
Pontiac LeMans 4	2350	98	28
Subaru Loyale 4	2295	109	25
Subaru Justy 3	1900	73	34
Toyota Corolla 4	2390	97	29
Toyota Tercel 4	2075	89	35
Volkswagen Jetta 4	2330	109	26
Chevrolet Camaro V8	3320	305	20
Dodge Daytona	2885	153	27
Ford Mustang V8	3310	302	19
Ford Probe	2695	133	30
Honda Civic CRX Si 4	2170	97	33
Honda Prelude Si 4WS 4	2710	125	27
Nissan 240SX 4	2775	146	24 🕶
	4 38888888888	#	<b>)</b>
Refresh	Cancel		

Figure 3.4: The Data Viewer.

It is important to note that only objects of class "data.frame" are recognized by the dialogs in the Spotfire S+ graphical user interface. This means that the **Data Viewer** cannot find or display matrices, vectors, or time series objects; to display objects of these types, you must first convert them to class "data.frame".

#### **Graph Window**

By default, Spotfire S+ displays graphics in a Java graphics window, as shown in Figure 3.5. Each **Graph** window can contain one or more graphs, and you can work with multiple graph windows in your Spotfire S+ session.

There are four different ways to create a graphics window:

- 1. Generate plots from the dialogs in the **Graph** menu.
- 2. Generate plots from functions called in the **Commands** window.
- 3. Select View ▶ New Graph Window, or click on the New Graph Window toolbar button. This opens a blank graphics window.
- 4. Explicitly call the java.graph() device in the **Commands** window, which also opens a blank graphics window.

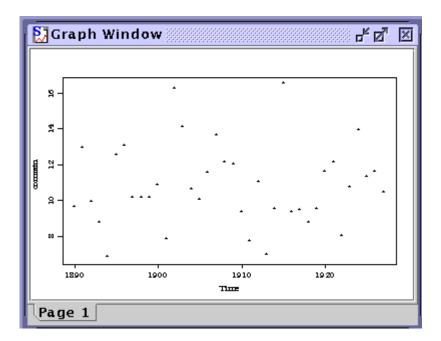


Figure 3.5: A Graph window displaying a Trellis graph.

## Commands Window

The **Commands** window allows you to access the powerful S-PLUS programming language. You can modify existing functions or create new ones tailored to your specific analysis needs by using the **Commands** window. By default, the **Commands** window is open when you start Spotfire S+. See the chapter Getting Started for examples of typing expressions and working from the **Commands** window.

## Report Window

When a dialog is launched, output is directed to the **Report** window, shown in Figure 3.6. Text in the **Report** window can be formatted before cutting and pasting it into another application. The **Report** window is a place-holder for the text output resulting from any operation in Spotfire S+. For example, error messages and warnings are sometimes placed in a **Report** window.

**Figure 3.6:** A **Report** window is an option for holding textual output.

#### Spotfire S+ Menus

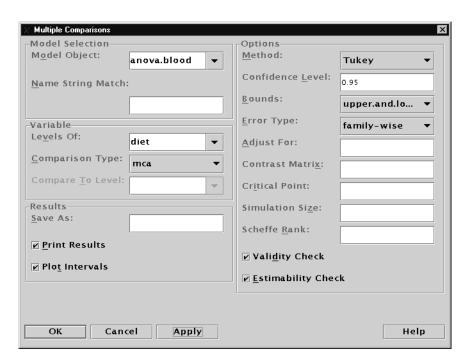
When you choose one of the main menu options, a list of additional options drops down. You can choose from any of the active options in the list. Menu options with a ▶ symbol at the end of the line display submenus when selected. Menu items with an ellipsis (...) after the command display a dialog when selected. Table 3.3 gives brief descriptions of each of the main Spotfire S+ menus.

**Table 3.3:** The main Spotfire S+ menus.

Main menu	Notes
File	Importing, exporting, saving, and printing files.
View	Standard options such as whether the Commands and Report windows are open.
Statistics	See the Statistics chapter.
Graph	See the Menu Graphics chapter.
Options	General settings for options, styles, and color schemes.
Window	Standard windows controls such as Cascade and Tile.
Help	Gives on-line access to the Spotfire S+ help system.

#### Spotfire S+ Dialogs

Dialogs can contain multiple tabbed pages of options, as shown in Figure 3.7. To see the options on a different page of the dialog, check the page name. When you choose **OK** or **Apply**, any changes made on any of the tabbed pages are applied to the selected objects.



**Figure 3.7:** A Spotfire S+ dialog for performing multiple comparisons.

Chapter 3 Working with the Graphical User Interface

# IMPORTING AND EXPORTING DATA

Introduction	94
Dialogs	95
The Import Data Dialog	95
Filtering Rows	101
Format Strings	103
The Export Data Dialog	104
Supported File Types for Importing and Exporting	108
Examples	113
Importing and Exporting Subsets of Data	113
Importing and Exporting Character Data	116

#### INTRODUCTION

Spotfire S+ can read a wide variety of data formats, which makes importing data straightforward. Spotfire S+ also allows you to export data sets for use in other applications. The primary tools for importing and exporting data are command-line functions named importData and exportData, respectively. In the graphical user interface, these functions are implemented in the **Import Data** and **Export Data** dialogs. We discuss the dialogs and their options in this chapter; for detailed discussions on the functions themselves, see the online help files or the *Programmer's Guide*.

#### **DIALOGS**

## The Import Data Dialog

To import data from the graphical user interface, select **File** ► **Import Data**. The **Import Data** dialog appears, as shown in Figure 4.1.

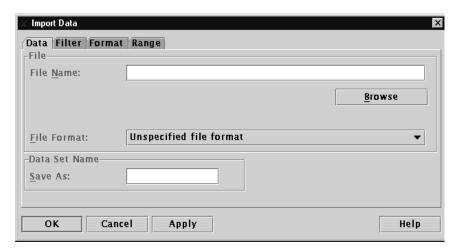


Figure 4.1: The Data page of the Import Data dialog.

#### Note

As of Spotfire S+ 8.1, the Spotfire S+ Java GUI is deprecated. If you want to use a GUI with Spotfire S+, use the Spotfire S+ Workbench.

#### The Data page

The **Data** page, shown in Figure 4.1, allows you to navigate to a particular directory, choose the file to be imported, specify a particular file format, and name the S-PLUS object in which the data should be stored. Descriptions of the individual fields are:

- **File Name**: Select or type the name of the file to import. To navigate to the directory that contains your data file, click on the **Browse** button.
- File Format: Select the format of the file to import. See the section Supported File Types for Importing and Exporting for details on the selections in this list.

• Save As: Enter a valid name for the S-PLUS object in which the data should be stored. If an object with this name already exists, its contents are overwritten. A valid name is any combination of alphanumeric characters (including the period character ".") that does not start with a number. Names are case-sensitive, so X and x refer to different objects.

#### Note

By default, the **Import Data** dialog looks for files in your current working directory, which is one level up from your **.Data** directory. If the file you wish to import is located in another directory, either click on the **Browse** button to search for it, or explicitly type the path to the file in the **File Name** field.

#### The Filter page

The **Filter** page, shown in Figure 4.2, allows you to subset the data to be imported. By specifying a query, or *filter* expression, you gain additional functionality; it is possible to import random samples of your data using a filter, for example. By default, the import filter is blank and thus imports all of the data. Descriptions of the individual fields are given below.

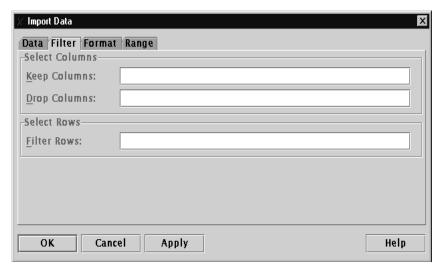


Figure 4.2: The Filter page of the Import Data dialog.

- Keep Columns: Specify a character vector of column names or numeric vector of column numbers that should be imported from the data file. Only one of Keep Columns and Drop Columns can be specified.
- Drop Columns: Specify a character vector of column names or numeric vector of column numbers that should *not* be imported from the data file. Only one of **Keep Columns** and **Drop Columns** can be specified.
- Filter Rows: Specify a logical expression for selecting the rows that should be imported from the data file. See the section Filtering Rows for a description of the syntax accepted by this field.

#### The Format page

The **Format** page, shown in Figure 4.3, contains options specific to ASCII, SAS, and SPSS data files. In addition, the **Format** page allows you to specify the data types of imported character expressions. Descriptions of the individual fields are given below.

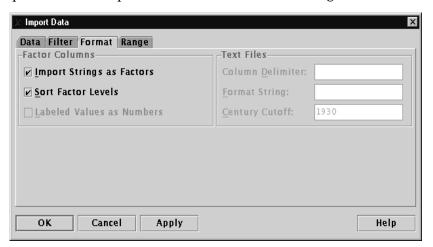


Figure 4.3: The Format page of the Import Data dialog.

• **Import Strings as Factors**: If this option is selected, then all character strings are converted to factor variables when the data file is imported. Otherwise, they are imported with the data class "character".

- **Sort Factor Levels**: If this option is selected, then Spotfire S+ (alphabetically) sorts the levels for all factor variables that are created from character strings. Otherwise, the levels are defined in the order they are read in from the data file.
- **Labeled Values as Numbers**: If this option is selected, then SAS and SPSS variables that have labels are imported as numbers. Otherwise, the value labels are imported.
- Column Delimiter: When importing an ASCII text file, this field specifies the character delimiters to use. The expressions \n and \t are the only multi-character delimiters allowed, and denote a newline and a tab, respectively. Double quotes are reserved characters, and therefore cannot be used as standard delimiters. If a delimiter is not supplied, Spotfire S+ searches the file automatically for the following, in the order given: tabs, commas, semicolons, and vertical bars. If none of these are detected, blank spaces are treated as delimiters.
- **Format String**: This field is required when importing a formatted ASCII text file (FASCII). A *format string* specifies the data types and formats of the imported columns. For more details on the syntax accepted by this field, see the section Format Strings.
- **Century Cutoff**: When importing an ASCII text file, this field specifies the origin for two-digit dates. Dates with two-digit years are assigned to the 100-year span that starts with this numeric value. The default value of 1930 thus reads the date 6/15/30 as June 15, 1930, while the date 12/29/29 is interpreted as December 29, 2029.

### The Range page

The **Range** page, shown in Figure 4.4, contains options that allow you to filter rows and columns when importing data from a spreadsheet (Excel and Lotus files, etc.). Descriptions of the individual fields are given below.

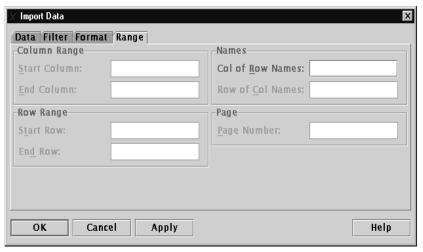


Figure 4.4: The Range page of the Import Data dialog.

- **Start Column**: Specify an integer that corresponds to the first column to be imported from the spreadsheet. For example, a value of 5 causes Spotfire S+ to begin reading data from the file at column 5. By default, the first column in the spreadsheet is used.
- **End Column**: Specify an integer that corresponds to the final column to be imported from the spreadsheet. By default, the final column in the spreadsheet is used, and Spotfire S+ imports everything that follows the **Start Column**.
- **Start Row**: Specify an integer that corresponds to the first row to be imported from the spreadsheet. For example, a value of 10 causes Spotfire S+ to begin reading data from the file at row 10. By default, the first row in the spreadsheet is used.
- End Row: Specify an integer that corresponds to the final row to be imported from the spreadsheet. By default, the final row in the spreadsheet is used, and Spotfire S+ imports everything that follows the Start Row.

### Chapter 4 Importing and Exporting Data

- Col of Row Names: Specify an integer denoting the column
  of the data file that should be used for row names. The chosen
  column is not included in the S-PLUS data set that gets
  created. You can use this option with ASCII text files as well
  as with spreadsheets.
- Row of Col Names: Specify an integer denoting the row of the data file that should be used for column names. The chosen row is not included in the S-PLUS data set that gets created. By default, Spotfire S+ attempts to formulate sensible column names from the first imported row.
- **Page Number**: Specify the page number of the spreadsheet that should be imported.

### Note

Because the underscore "\_" is a reserved character in S-PLUS, the **Import Data** dialog converts all column names that have underscores in them so that they contain periods "." instead.

### **Filtering Rows**

The **Filter Rows** field in the **Import Data** dialog accepts logical expressions that specify the rows to be imported from the data file. The filter must be written in terms of the original column names in the file, and not in terms of the variable names specified by the **Row of Col Names** field. Note that the filter is *not* evaluated by S-PLUS. This means that expressions containing built-in S-PLUS functions (such as mean) are not allowed. One special exception to this rule deals with missing values: you can use NA to denote missing values in the logical expressions, though you cannot use NA-specific functions such as is.na and na.exclude.

Table 4.1 lists the logical operators that are accepted by the **Filter Rows** field. Thus, to select all rows that do not have missing values in the id column, type id != NA. To import all rows corresponding to 10-year-old children who weigh less than 150 pounds, type Age==10 & Weight<150. In the filter expression, the variable name should be on the left side of the logical operator; i.e., type Age > 12 instead of 12 < Age.

**Table 4.1:** Logical operators accepted by the *Filter Rows* field.

Operator	Description
=	equal to
!=	not equal to
<	less than
>	greater than
<=	less than or equal to
>=	greater than or equal to
&	logical and
1	logical or
!	negation

The wildcard characters? (for single characters) and \* (for strings of arbitrary length) can be used to select subgroups of character variables. For example, the logical expression account == ?????22 selects all rows for which the account variable is six characters long and ends in 22. The expression id == 3\* selects all rows for which id starts with 3, regardless of the length of the string.

You can use the built-in variable @rownum to import specific row numbers. For example, the expression @rownum < 200 imports the first 199 rows of the data file.

### **Sampling functions**

Three functions that permit random sampling of your data are available to use in a **Filter Rows** expression:

- samp.rand: accepts a single numeric argument prop, where 0 ≤ prop ≤ 1. Rows are selected randomly from the data file with a probability of prop.
- samp.fixed: accepts two numeric arguments, sample.size and total.observations. The first row is drawn from the data file with a probability of sample.size/total.observations. The ith row is drawn with a probability of (sample.size i)/(total.observations i), where i = 1, 2, ..., sample.size.
- samp.syst: accepts a single numeric argument n. Every *n*th row is selected systematically from the data file after a random start.

Expressions are evaluated from left to right, so you can sample a subset of the rows in your data file by first subsetting, and then sampling. For example, to import a random sample of half the rows corresponding to high school graduates, use the expression schooling>=12 & samp.rand(0.5).

The sampling functions use the Spotfire S+ random number generator to create random samples. You can therefore use the set.seed function in the **Commands** window to produce the same data sample repeatedly. For more details, see the help files for set.seed and .Random.seed.

### Format Strings

Format strings are used when importing data from, or exporting data to, fixed-format text files (FASCII). With a format string, you specify how each character in the imported file should be treated. You must use a format string, together with the FASCII file type, if the columns in your data file are not separated by delimiters.

### The Import Data dialog

In the **Import Data** dialog, a valid format string includes a percent % sign followed by the data type, for each column in the data file. Available data types are: s, which denotes a character string; f, which denotes a numeric value; and the asterisk \*, which denotes a skipped column. One of the characters specified in the **Column Delimiters** field must separate each specification in the string. For example, the format string

imports the first column of the data file as type "character", the second and fourth columns as "numeric", and skips the third column altogether.

If a variable is designated as "numeric" and the value of a cell cannot be interpreted as a number, the cell is filled in with a missing value. Incomplete rows are also filled in with missing values.

### Note

Some dates in text files may be imported automatically as numbers. After importing data that contain dates, you should check the class of each column in Spotfire S+, and change them to the appropriate data types if necessary.

Note that format strings and field width specifications are irrelevant for regular ASCII files, and are therefore ignored. For fixed-format ASCII text files, however, you can specify an integer that defines the width of each field. For example, the format string

imports the first four entries in each row as a numeric column. The next six entries in each row are read as characters, the next three are skipped, and then six more entries are imported as another character column.

### The Export Data dialog

When exporting to a fixed-format ASCII text file, the syntax accepted by the **Format String** field is similar to the **Import Data** option. In addition to the data type, however, the precision of numeric values can also be specified. For example, the format string

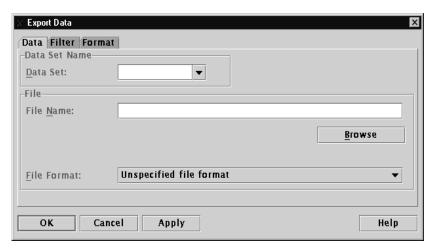
```
%3, %7.2, %4, %5.2
```

exports the first and third columns as whole numbers with 3 and 4 digits, respectively. The second and fourth columns each have two decimal digits of precision. The precision value is ignored if it is given for a character column; if the precision is not specified, is assumed to be zero. If you export row names for your data set, the first entry in the format string is reserved for the row names.

Specifying a format string can potentially speed up the export of data sets that have many character columns. If a format string is not specified, Spotfire S+ must check the width of every entry in a character or factor column, and determine a width large enough for all values in the column. Since many of the supported file types use fixed widths, considerable space can be saved by specifying a narrow width for character columns that have many short values and only a few long values; with this approach, the few long values are truncated.

## The Export Data Dialog

To export data from the graphical user interface, select **File** ► **Export Data**. The **Export Data** dialog appears, as shown in Figure 4.5.



**Figure 4.5:** The **Data** page of the **Export Data** dialog.

### The Data page

The **Data** page, shown in Figure 4.5, allows you to name the S-PLUS object to be exported, navigate to the directory in which the file should be stored, and specify a particular file format. Descriptions of the individual fields are given below.

- **Data Set**: Enter the name of the S-PLUS object to be exported. Names are case-sensitive, so X and x refer to different objects.
- **File Name**: Select or type the name of the file that should contain the contents of the data set. Spotfire S+ notifies you if the file already exists, and then gives you the opportunity to either overwrite the file's contents or cancel the export. To navigate to a particular directory, click on the **Browse** button.
- **File Format**: Select the format of the exported data file. See the section Supported File Types for Importing and Exporting for details on the selections in this list.

#### Note

By default, the **Export Data** dialog saves files in your current working directory, which is one level up from your **.Data** directory. If you wish to export a file to another directory, either click on the **Browse** button to search for it, or explicitly type the path to the file in the **File Name** field.

### The Filter page

The **Filter** page, shown in Figure 4.6, allows you to subset the data to be exported. By specifying a filter expression, you gain additional functionality; it is possible to export random samples of your data using a filter, for example. By default, the export filter is blank and thus exports all of the data. Descriptions of the individual fields are given below.

- Keep Columns: Specify a character vector of column names or numeric vector of column numbers that should be exported from the data set. Only one of Keep Columns and Drop Columns can be specified.
- **Drop Columns**: Specify a character vector of column names or numeric vector of column numbers that should *not* be exported from the data set. Only one of **Keep Columns** and **Drop Columns** can be specified.

• **Filter Rows**: Specify a logical expression for selecting the rows that should be exported from the data set. See the section Filtering Rows for a description of the syntax accepted by this field. Although the discussion in that section is specific to the **Import Data** dialog, the descriptions are analogous for the **Export Data** dialog.

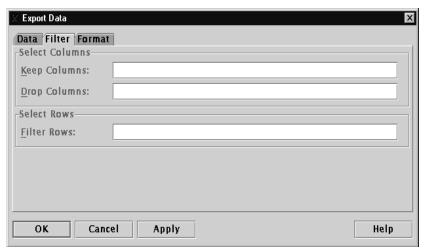


Figure 4.6: The Filter page of the Export Data dialog.

### The Format page

The **Format** page, shown in Figure 4.7, contains options specific to ASCII text files and factor variables. In addition, the **Format** page allows you to specify whether row names and column names should be exported from your data set. Descriptions of the individual fields are given below.

- **Export Column Names:** If this option is selected, then Spotfire S+ includes the column names of the data set as the first row in the file.
- **Export Row Names**: If this option is selected, then Spotfire S+ includes the row names of the data set as the first column in the file.
- Quote Character Strings: If this option is selected, then all
  factors and character variables in the data set are exported
  with quotation marks, so that they are recognized as strings.

- **Column Delimiter**: When exporting to an ASCII text file, this field specifies the character delimiters to use. The expressions \n and \t are the only multi-character delimiters allowed, and denote a newline and a tab, respectively. Double quotes are reserved characters, and therefore cannot be used as standard delimiters. By default, S-PLUS uses commas as delimiters.
- **Format String**: When exporting to an ASCII text file, this field specifies the data types and formats of the exported columns. For more details on the syntax accepted by this field, see the section Format Strings.

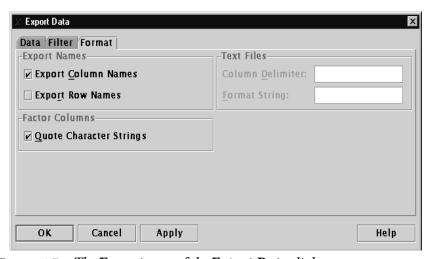


Figure 4.7: The Format page of the Export Data dialog.

# SUPPORTED FILE TYPES FOR IMPORTING AND EXPORTING

Table 4.2 lists all the supported file formats for importing and exporting data. Note that Spotfire S+ both imports from and exports to all the listed types with two exceptions: SigmaPlot (.jnb) files are import only and HTML  $(.htm^*)$  tables are export only.

### Note

As of Spotfire S+ version 8.2, native database drivers are deprecated. In lieu of these drivers, you should use JDBC drivers for all supported database vendors.

**Table 4.2:** Supported file types for importing and exporting data.

Format	Туре	Default Extension	Notes
ASCII File	"ASCII"	.csv .asc, .csv, .txt, .prn .asc, .dat, .txt, .prn	Comma delimited.  Delimited.  Whitespace delimited; space delimited; tab delimited; user-defined delimiter.
dBASE File	"DBASE"	.dbf	II, II+, III, IV files.
DIRECT-DB2	"DIRECT-DB2"		DB2 database connection. No file argument should be specified.
DIRECT-ORACLE	"DIRECT- ORACLE"	.ora	Oracle database connection. No file argument should be specified.
DIRECT-SQL	"DIRECT-SQL"		Microsoft SQL Server database connection. No file argument should be specified. This option is available only in Spotfire S+ for Windows.

 Table 4.2: Supported file types for importing and exporting data. (Continued)

Format	Туре	Default Extension	Notes
DIRECT-SYBASE	"DIRECT- SYBASE"		Sybase database connection. No file argument should be specified.
Epi Info File	"EPI"	.rec	
Fixed Format ASCII File	"FASCII"	.fix, .fsc	
FoxPro File	"FOXPRO"	.dbf	
Gauss Data File	"GAUSS", "GAUSS96"	.dat	Automatically reads the related <b>DHT</b> file, if any, as GAUSS 89. If no <b>DHT</b> file is found, reads the <b>.DAT</b> file as GAUSS96. GAUSS96 is available in Solaris/Linux only.
HTML Table	"HTML"	.htm*	Export only.
Lotus 1-2-3 Worksheet	"LOTUS"	.wk*, .wr*	
MATLAB Matrix	"MATLAB"  "MATLAB7" (export only)	.mat	File must contain a single matrix. Spotfire S+ recognizes the file's platform of origin on import. On export, specify type="MATLAB" to create a pre-MATLAB 7 version file; otherwise, specify type="MATLAB7" to export the MATLAB 7 file format.
Minitab Workbook	"MINITAB"	.mtw	Versions 8 through 12.
Microsoft Access File	"ACCESS"	.mdb	Microsoft Access file. This file type is available only in Spotfire S+ for Windows.

### Chapter 4 Importing and Exporting Data

 Table 4.2: Supported file types for importing and exporting data. (Continued)

Format	Туре	Default Extension	Notes
Microsoft Excel Worksheet	"EXCEL" "EXCELX"	.xl? .xlsx	Versions 2.1 through 2007. Note that "EXCELX" and the new file extension, ".xlsx" are for files imported from or exported to Excel 2007.
ODBC	"ODBC"	Not applicable	For Informix (.ifx), Oracle (.ora), and Sybase (.syb) databases. This file type is available only in Spotfire S+ for Windows.
Oracle	"Oracle"	.ora	Same as "DIRECT-ORACLE". Oracle database connection. No file argument should be specified.
Paradox Data File	"PARADOX"	.db	
QuattroPro Worksheet	"QUATTRO"	.wq?, .wb?	
S-PLUS File	"SPLUS"	.sdd	Windows, DEC Solaris/Linux. Uses data.restore() to import file.
STATA	"STATA"  "STATASE" (export only)	.dta	Portable across platforms (UNIX, Windows, and Mac). Can import STATA files and export STATA or STATASE.  When exporting a STATA dataset, you are limited to 2,047 characters. For larger STATA datasets (up to 32,767 variables), specify type="STATASE".

 Table 4.2: Supported file types for importing and exporting data. (Continued)

Format	Туре	Default Extension	Notes
SAS File	"SAS", "SASV6"	.sd2	SAS version 6 files, Windows.
	"SAS1", "SAS6UX32"	.ssd01	SAS version 6 files, HP, IBM, Sun Solaris.
	"SAS4", "SAS6UX64"	.ssd04	SAS version 6 files, Digital UNIX.
	"SAS7"	.sas7bdat, .sd7	SAS version 7 or 8 files, current platform.
	"SAS7WIN"	.sas7bdat, .sd7	SAS version 7 or later data files, Windows.
	"SAS7UX32"	.sas7bdat, .sd7	SAS version 7 or later data files, Solaris (SPARC), HP-UX, IBM AIX.
	"SAS7UX64"	.sas7bdat, .sd7	SAS version 7 or later data files, Digital/Compaq UNIX.
SAS Transport File	"SAS_TPT"	.xpt, .tpt	Version 6.x. Some special export options may need to be specified in your SAS program. We suggest using the SAS Xport engine (not PROC CPORT) to read and write these files.
	"SAS_CPORT"	.stc, .cpt	CPORT files created by SAS versions 7.01 through 9.01 can be imported.
SigmaPlot File	"SIGMAPLOT"	.jnb	Import only.

### Chapter 4 Importing and Exporting Data

 Table 4.2: Supported file types for importing and exporting data. (Continued)

Format	Туре	Default Extension	Notes
SPSS Data File	"SPSS"	.sav	OS/2; Windows; HP, IBM, Sun, DEC UNIX.
SPSS Portable File	"SPSSP"	.por	
Stata Data File	"STATA"	.dta	Versions 2.0 and higher.
Sybase	"SYBASE"	Same as "DIRECT-SYBASE". Same as "DIRECT-SYBAS	
SYSTAT File	"SYSTAT"	.syd, .sys	Double- or single-precision <b>.sys</b> files.

### **EXAMPLES**

# Importing and Exporting Subsets of Data

In the following examples, we import and export subsets of the built-in data set car.test.frame, using the options in the **Filter** page of the **Import Data** and **Export Data** dialogs. The car.test.frame data is taken from the April 1990 issue of *Consumer Reports*, and contains 60 observations (rows) and 8 variables (columns). Observations of price, manufacturing country, reliability, mileage, type, weight, engine displacement, and horsepower were taken for each of sixty cars. This data set is shown in Figure 4.8.

	Price	Country	Reliability	Mileage	Type	Weight	Disp.	НР
Eagle Summit 4	8895	USA	4	33	Small	2560	97	113
Ford Escort 4	7402	USA	2	33	Small	2345	114	90
Ford Festiva 4	6319	Korea	4	37	Small	1845	81	63
Honda Civic 4	6635	Japan/USA	5	32	Small	2260	91	92
Mazda Protege 4	6599	Japan	5	32	Small	2440	113	103
Mercury Tracer 4	8672	Mexico	4	26	Small	2285	97	82
Nissan Sentra 4	7399	Japan/USA	5	33	Small	2275	97	90
Pontiac LeMans 4	7254	Korea	1	28	Small	2350	98	74
Subaru Loyale 4	9599	Japan	5	25	Small	2295	109	90
Subaru Justy 3	5866	Japan	NA.	34	Small	1900	73	73
Toyota Corolla 4	8748	Japan/USA	5	29	Small	2390	97	102
Toyota Tercel 4			<u> </u>					-
Volkswagen Jetta 4	6488	Japan	5	35	Small	2075	89	78
Chevrolet Camaro V8	9995	Germany	3	26	Small	2330	109	100
Dodge Daytona	11545	USA	1	20	Sporty	3320	305	170
Refresh Cancel								

Figure 4.8: The car.test.frame data in a Data Viewer.

### Using the Keep Columns and Drop Columns options

- 1. Open the **Export Data** dialog.
- Type car.test.frame in the Data Set field. Type car.keep.txt in the File Name field, and choose ASCII file tab delimited from the File Format list.
- 3. Click on the **Filter** tab and type **2,3,5** in the **Keep Columns** field.
- 4. Click on the **Format** tab and check the **Export Row Names** box.
- Click OK.

Spotfire S+ creates a tab-delimited text file named **car.keep.txt** in your working directory. The file contains the row names in car.test.frame in addition to the three specified columns: Price, Country, and Mileage. Because we checked the **Export Row Names** box, the row names are considered the first column in the exported data set. This is why a **Keep Columns** value of **2,3,5** actually exports the first, second, and fourth variables in the data set.

The syntax for the **Drop Columns** field is similar, as the following example shows.

- 1. Open the **Import Data** dialog.
- Type car.keep.txt in the File Name field, and choose ASCII file tab delimited from the File Format list. Type car.drop in the Save As field.
- 3. Click on the **Filter** tab and type **Country, Mileage** in the **Drop Columns** field. This imports all columns from the text file except those named Country and Mileage.
- 4. Click on the **Range** tab and type **1** in the **Col of Row Names** field. This forces Spotfire S+ to use the first column in the text file as the row names in the data frame.
- 5. Click **OK**.

The car.drop data set, shown in Figure 4.9, contains only the pricing data from car.test.frame. Whether used in the **Import Data** or **Export Data** dialog, the **Keep Columns** and **Drop Columns** fields can be specified as either a list of column numbers or a list of variable names.

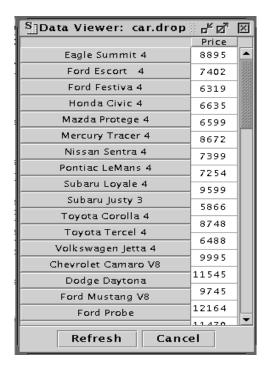


Figure 4.9: The car. drop data set in a Data Viewer.

### Using the Filter Rows option

- 1. Open the **Export Data** dialog.
- 2. Type car.test.frame in the **Data Set** field. Type car.filter.xls in the **File Name** field, and choose **Excel Worksheet** from the **File Format** list.
- 3. Click on the **Filter** tab and type **Price** < 10000 & **Mileage** > 27 in the **Filter Rows** field.
- 4. Click on the **Format** tab and check the **Export Row Names** box.
- Click **OK**.

Spotfire S+ creates an Excel file named **car.filter.xls** in your working directory. The file contains the 11 observations from car.test.frame for which the Price variable is less than \$10,000 and the Mileage variable is greater than 27 miles per gallon.

### Importing and Exporting Character Data

To illustrate the options relating to character data in the **Import Data** and **Export Data** dialogs, we create a simple data set named animal. The following S-PLUS command generates a data frame that has five entries: dog, cat, bird, hyena, and goat:

We can export the text file with the following steps:

- 1. Open the **Export Data** dialog.
- Type animal in the Data Set field and animal.txt in the File Name field. Select ASCII file - space delimited from the File Format list.
- 3. Click on the **Format** tab and deselect the **Export Column Names** option.
- 4. Click **OK**.

Spotfire S+ creates a text file named **animal.txt** in your working directory that contains the five entries from animal, each with a set of surrounding quotes. The following steps import the data into Spotfire S+ as character strings:

- 1. Open the **Import Data** dialog.
- Type animal.txt in the File Name field, and select ASCII file space delimited from the File Format list. Type animal.char in the Data Set field.
- 3. Click on the **Format** tab, and deselect the **Import Strings as Factors** and **Sort Factor Levels** options.
- 4. Click **Apply**.

Spotfire S+ recognizes animal.char as having data class "AsIs":

```
> animal.char
   Coll
1   dog
2   cat
3   bird
4   hyena
5   goat
> data.class(animal.char$Coll)
[1] "AsIs"
```

To formally convert the animal.char column, we can use the character or as.character functions.

The steps below import the **animal.txt** data as a factor variable:

- 1. Click on the **Data** tab in the open **Import Data** dialog, and type animal.fac in the **Data Set** field.
- 2. Click on the **Format** tab. Select the **Import Strings as Factors** option, but leave **Sort Factor Levels** box unchecked.
- 3. Click **Apply**.

The animal.fac object is identical to animal.char, but Spotfire S+ now interprets the data as a factor variable:

Note that the levels of the factor appear in the same order as they do in the text file. The steps given below sort the levels alphabetically instead.

### Chapter 4 Importing and Exporting Data

- 1. Click on the **Data** tab in the open **Import Data** dialog, and type animal.fac2 in the **Data Set** field.
- 2. Click on the **Format** tab and select the **Sort Factor Levels** option.
- 3. Click **OK**.

The levels of the factor variable are now sorted alphabetically:

```
> data.class(animal.fac2$Col1)
[1] "factor"
> levels(animal.fac2$Col1)
[1] "bird" "cat" "dog" "goat" "hyena"
```

### **MENU GRAPHICS**

Introduction	121
Overview	122
General Procedure	124
Dialogs	125
Dialog Fields	125
Graph Options	126
Scatter Plots	127
A Basic Example	128
Line Plots	131
Grouping Variables	133
Line Fits	134
Nonparametric Curve Fits	138
Multipanel Conditioning	147
Visualizing One-Dimensional Data	152
Density Plots	153
Histograms	157
QQ Math Plots	159
Bar Charts	161
Dot Plots	164
Pie Charts	166
Visualizing Two-Dimensional Data	169
Box Plots	169
Strip Plots	173
QQ Plots	175
Visualizing Three-Dimensional Data	178
Contour Plots	178
Level Plots	180
Surface Plots	182
Cloud Plots	184

### Chapter 5 Menu Graphics

Visualizing Multidimensional Data	186
Scatterplot Matrices	186
Parallel Plots	189
Multipanel Trellis Graphics	191
Time Series	195
Line Plots	195
High-Low Plots	199
Stacked Bar Plots	202
References	205

### INTRODUCTION

The power of Spotfire S+ comes from the integration of its graphics capabilities with its statistical analysis routines. In the Statistics chapter, we show how statistical procedures are performed in Spotfire S+. In this chapter, we introduce the Spotfire S+ graphics that are built into the menu options. It is not necessary to read this entire chapter before you begin generating graphics. Once you've acquired a basic understanding of the way the **Graph** dialogs are organized, you can refer directly to a section of interest.

The dialogs under the **Graph** menu give you access to nearly all of the Trellis functions in S-PLUS: xyplot, densityplot, histogram, qqmath, barchart, dotplot, piechart, bwplot, stripplot, qq, contourplot, levelplot, wireframe, splom, and parallel. Due to the complicated syntax that these functions require, Trellis graphics usually have the steepest learning curve among users. With the graphical user interface, however, you can create highly involved Trellis graphics as easily as you create scatter plots and histograms.

We begin this chapter by presenting general information about the graphics dialogs, and devote the remaining sections to descriptions and examples for each of them. The presentation of the **Scatter Plot** dialog contains the most detail of all the graphics in this chapter. If you are interested in the basic options under the **Titles**, **Axes**, and **Multipanel Conditioning** tabs of the graphics dialogs, see the section Scatter Plots. For all other graphs, we focus on the dialog options specific to particular plot types.

The Spotfire S+ graphical user interface is designed to create complicated graphs easily and quickly for exploratory data analysis. Not all of the Spotfire S+ functionality has been built into the menu options, however, and it is therefore necessary to use command line functions in some sections throughout this chapter. For completely customized graphics, you will likely need to resort to the command line functions as well.

### **Overview**

Figure 5.1 displays many elements of the Spotfire S+ interface.

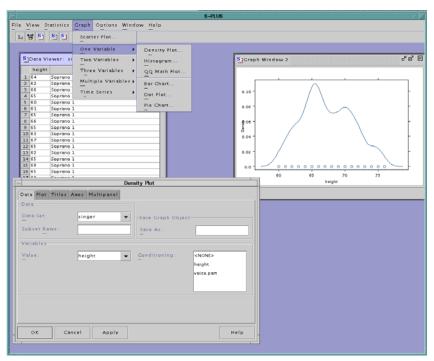


Figure 5.1: Graphics-related menus and windows.

### Note

As of Spotfire S+ 8.1, the Spotfire S+ Java GUI is deprecated. If you want to use a GUI with Spotfire S+, use the Spotfire S+ Workbench.

- **Graph menu**: The **Graph** menu gives you access to nearly all of the Trellis functions available in Spotfire S+. The procedures are logically grouped, with submenus that allow you to precisely specify the procedure you want to use. For example, Figure 5.1 displays the menu tree for density plots. It is selected by choosing **Graph** ▶ **One Variable** ▶ **Density Plot**.
- Graph dialogs: The open dialog in Figure 5.1 is entitled Density Plot and is used to display a density estimate for a data set.

• Data Viewer: The open window on the left in Figure 5.1 is a Data viewer, which you can use to see a data set in its entirety. The Data viewer is not a data editor, however, and you cannot use it to modify or create a new data set.

- **Graph Window**: A **Graph** window displays the graphics you create. Figure 5.1 shows the density estimate for a variable in a data set.
- Commands Window (not shown): The Commands window contains the Spotfire S+ command line prompt, which you can use to call S-PLUS functions that are not yet implemented in the menu options.
- Report Window (not shown): Any error, warning, or informational message generated by a graphics dialog is printed in the Report window.

### General Procedure

The basic procedure for creating graphs is the same regardless of the type of graph chosen.

- 1. Choose the graph you want to create from the **Graph** menu. The dialog corresponding to that procedure opens.
- 2. Select the data set, variables, and options for the procedure you have chosen. (These are slightly different for each dialog.) Click the **OK** or **Apply** button to generate the graph. If you click **OK**, the dialog closes when the graph is generated; if you click **Apply**, the dialog remains open. We use the **Apply** button extensively in the examples throughout this chapter, as it allows us to experiment with dialog options and build graphs incrementally.
- 3. Check for messages. If a message is generated, it appears in the **Report** window.
- 4. Check the result. If everything went well, your graph is displayed in a **Graph** window.

If you want, you can change the variables, parameters, or options in the dialog and click **Apply** to generate new results. Spotfire S+ makes it easy to experiment with options and to try variations on your analysis.

### **Dialogs**

Much of the graphics functionality in Spotfire S+ can be accessed through the **Graph** menu. The **Graph** menu includes dialogs for creating one-, two-, and three-dimensional plots, as well as Trellis graphics and time series plots. Many of the dialogs consist of tabbed pages that allow for some formatting, so that you can include legends, titles, and axis labels in your plots. Each dialog has a corresponding function that is executed using dialog inputs as values for function arguments. Usually, it is only necessary to fill in a few fields on the first page of a tabbed dialog to launch the function call.

### **Dialog Fields**

Many dialogs include a **Data Set** field. To specify a data set, you can either type its name directly in the **Data Set** field, or make a selection from the dropdown list. Note that the **Data Set** field recognizes objects of class "data.frame" only, and does not accept matrices, vectors, or time series. For this reason, we periodically drop to the **Commands** window in this chapter to create objects that are accepted by the menu options.

Most dialogs that fit statistical models include a **Subset Rows** field that you can use to specify only a portion of a data set. To use a subset of your data in an analysis, enter a S-PLUS expression in the **Subset Rows** field that identifies the rows to use. The expression can evaluate to a vector of logical values: true values indicate which rows to include in the analysis, and false values indicate which rows to drop. Alternatively, the expression can specify a vector of row indices. For example:

- The expression Species=="bear" includes only rows for which the Species column contains bear.
- The expression Age>=13 & Age<20 includes only rows that correspond to teenage values of the Age variable.
- The expression 1:20 includes the first 20 rows of the data.

To use all rows in a data set, leave the **Subset Rows** field blank.

Note that the **Data Set** field recognizes objects of class "data.frame" only, and does not accept matrices or vectors. One exception to this is the **Time Series** graphics dialogs, which recognize objects of class "timeSeries" only. For this reason, we periodically drop to the **Commands** window in this chapter to create objects that are accepted by the menu options.

### **Graph Options**

The **Options** menu contains a few options that affect the graphics you create from the interface. In particular:

- The Options ➤ Dialog Options window includes a Create New Graph Window check box. If this box is selected, as it is by default, then a new Graph window is created each time you click OK or Apply.
- The **Options** ► **Set Graph Colors** window allows you to select a color scheme for your graphics.
- The **Options** ► **Graph Options** window governs whether tabbed pages in **Graph** windows are deleted, preserved, or written over when a new plot is generated.

### **SCATTER PLOTS**

The scatter plot is the fundamental visual technique for viewing and exploring relationships in two-dimensional data. In this section, we discuss many of the options available in the **Scatter Plot** dialog, including grouping variables, smoothing, and conditioning. In addition, we also show how you can use the **Scatter Plot** dialog to create one-dimensional line plots of each of your variables. For details on creating line plots specifically for time series data, see the section Time Series.

### Creating a scatter plot

From the main menu, choose **Graph** ▶ **Scatter Plot**. The **Scatter Plot** dialog opens, as shown in Figure 5.2.

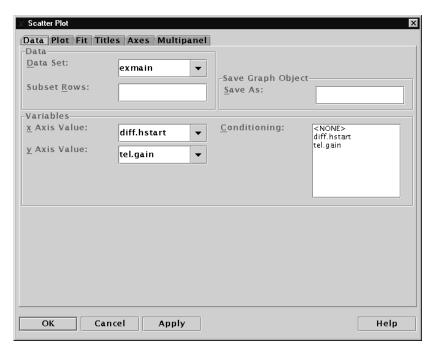


Figure 5.2: The Scatter Plot dialog.

### A Basic Example

The "main gain" data in Table 5.1 present the relationship between the number of housing starts and the number of new main telephone extensions. The observations were recorded once per year on the first of January, for a total of fourteen years beginning in 1971. The first column, "New Housing Starts," is the change in new housing starts from one year to the next in a geographic area around New York City; the units are "sanitized" for confidentiality. The second column, "Gain in Main Residential Telephone Extensions," is the increase in main residential telephone extensions for the same geographic area, again in sanitized units. In this example, we explore the relationship between these two variables using scatter plots.

**Table 5.1:** *Main gain data.* 

New Housing Starts	Gain in Main Residential Telephone Extensions
0.06	1.135
0.13	1.075
0.14	1.496
-0.07	1.611
-0.05	1.654
-0.31	1.573
0.12	1.689
0.23	1.850
-0.05	1.587
-0.03	1.493
0.62	2.049
0.29	1.942
-0.32	1.482
-0.71	1.382

### Setting up the data

The data in Table 5.1 are best represented as a data set with two variables. To create this data set, type the following in the **Commands** window:

```
> exmain <- data.frame(</pre>
+ diff.hstart = c(0.06, 0.13, 0.14, -0.07, -0.05, -0.31,
+ 0.12, 0.23, -0.05, -0.03, 0.62, 0.29, -0.32, -0.71),
+ tel.gain = c(1.135, 1.075, 1.496, 1.611, 1.654, 1.573,
+ 1.689, 1.850, 1.587, 1.493, 2.049, 1.942, 1.482, 1.382))
> exmain
   diff.hstart tel.gain
 1
          0.06
                   1.135
 2
          0.13
                   1.075
 3
          0.14
                   1.496
 4
         -0.07
                   1.611
 5
         -0.05
                   1.654
 6
         -0.31
                   1.573
 7
          0.12
                   1.689
 8
          0.23
                   1.850
 9
         -0.05
                   1.587
10
         -0.03
                   1.493
11
          0.62
                   2.049
12
          0.29
                   1.942
13
         -0.32
                   1.482
14
         -0.71
                   1.382
```

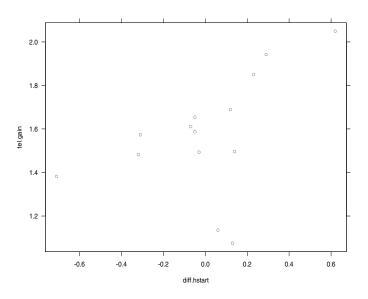
### **Exploratory data analysis**

If you are responsible for planning the number of new residence extensions that should be installed, you might be interested in whether there is a strong relationship between diff.hstart and tel.gain. If there is, you can use diff.hstart to predict tel.gain. As a first step in assessing whether there appears to be a strong relationship between the two variables, make a scatter plot:

- 1. Open the **Scatter Plot** dialog.
- 2. Type exmain in the **Data Set** field.
- 3. Select diff.hstart as the **x Axis Value** and tel.gain as the **y Axis Value**.

- 4. Click on the **Axes** tab and select **Horizontal** for the **Tick Marks Label Orientation**. This option places horizontal tick labels on both the *x* and *y* axes. By default, labels are parallel to the axes, so that *x* axis tick labels are horizontal and *y* axis labels are vertical.
- 5. Click **Apply** to leave the dialog open.

The plot is shown in Figure 5.3.



**Figure 5.3:** Scatter plot of tel.gain versus diff.hstart.

The plot immediately reveals two important features in the data. With the exception of two of the data points, there is a positive and roughly linear relationship between new housing starts and the increase in residential telephone extensions. The two exceptional data points are well detached from the remainder of the data; such data points are called *outliers*. In the exmain data, the two outliers correspond to the first two observations.

### Formatting the graph

You can format a graph with the options in the **Plot**, **Titles**, and **Axes** tabs of the **Scatter Plot** dialog. In the **Plot** tab, you can change the color, style, or size of the plotting symbols and lines. In the **Titles** tab, you can modify axes labels and place a main title on the graph. In the **Axes** tab, you can change the aspect ratio, scale, relation, limits, and tick-label orientation of your axes. For example:

- 1. Click on the **Plot** tab in the open **Scatter Plot** dialog. Select **Diamond, Solid** as the **Plotting Style**.
- Click on the Titles tab. Type The Main Gain Data for the Main Title, New Housing Starts for the x Axis Label, and Gain in Residential Telephone Extensions for the y Axis Label.
- 3. Click on the **Axes** tab. Type **-0.9**, **0.7** in the **X Limits** field and **0.9**, **2.1** in the **Y Limits** field.
- 4. Click **OK** to close the dialog.

A new **Graph** window appears displaying the changes you made.

### **Line Plots**

Scatter plots are useful tools for visualizing the relationship between any two variables, regardless of whether there is any particular ordering of the *x* axis variable. On the other hand, one of the two variables you want to visualize may be ordered, so that the order in which the observations were taken is as important to the analysis as the values themselves. A line plot, or *index plot*, is a helpful tool for displaying one-dimensional ordered data. In a line plot, the ordered data are plotted along the *y* axis and their corresponding indices are plotted on the *x* axis. This kind of plot arises often in time series data; for details on the line plots available under the **Time Series** graphics menu, see the section Time Series.

### Example

In the section A Basic Example on page 128, we created a scatter plot of the variables in the exmain data set. In this example, we create a line plot of the tel.gain variable.

- 1. If you have not done so already, create the exmain data set with the instructions given on page 129.
- 2. Open the **Scatter Plot** dialog.
- 3. Type exmain in the **Data Set** field.
- 4. Select tel.gain as the y Axis Value. This plots the values in tel.gain against a vector of indices that is the same length as tel.gain.
- 5. Click on the **Plot** tab and select **Both Points & Lines** from the **Type** list.
- Click on the **Titles** tab. Type **index** for the **x Axis Label** and **Gain in Residential Telephone Extensions** for the **y Axis Label**.
- 7. Click on the **Axes** tab and select **Horizontal** for the **Tick Marks Label Orientation**. This option places horizontal tick labels on both the *x* and *y* axes. By default, labels are parallel to the axes, so that *x* axis tick labels are horizontal and *y* axis labels are vertical.
- 8. Click **OK**.

The result is shown in Figure 5.4. The fourteen values in tel.gain, representing observations made in the years 1971-1984, are plotted sequentially using both points and lines. The observation from 1971 corresponds to the point with the smallest x coordinate, and the observation from 1984 corresponds to the point with the largest x coordinate. From the plot, we can easily see that gains in new residential telephone extensions were at their lowest during the first two years of the study, rose rapidly in the third year, and then oscillated up and down starting in year 6 of the study.

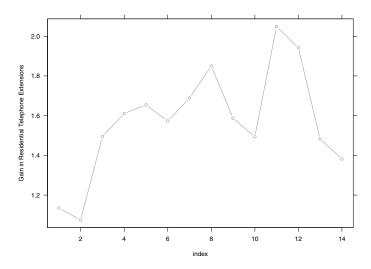


Figure 5.4: Line plot of tel.gain.

### Grouping Variables

It is often useful to plot multiple two-dimensional scatter plots on the same set of axes according to the value of a third factor (categorical) variable. In the **Scatter Plot** dialog, you can choose to vary such scatter plots by symbol color, style, or size. In addition, legends can be included, and are placed on the right side of the graphics area.

### **Example**

The data set Puromycin has 23 rows representing the measurement of initial velocity (vel) of a biochemical reaction for 6 different concentrations of substrate (conc) and two different cell treatments (state). In this example, we plot velocity versus concentration with different symbols for the two treatment groups, treated and untreated.

- Open the Scatter Plot dialog.
- 2. Type Puromycin in the **Data Set** field.
- 3. Select conc as the x Axis Value and vel as the y Axis Value.

- 4. Click on the **Plot** tab and select state as the **Group** Variable. Check the boxes for Vary Symbol Style and Include Legend.
- 5. Click on the **Axes** tab and select **Horizontal** for the **Tick Marks Label Orientation**. This option places horizontal tick labels on both the *x* and *y* axes. By default, labels are parallel to the axes, so that *x* axis tick labels are horizontal and *y* axis labels are vertical.
- 6. Click **OK**.

The result is displayed in Figure 5.5.

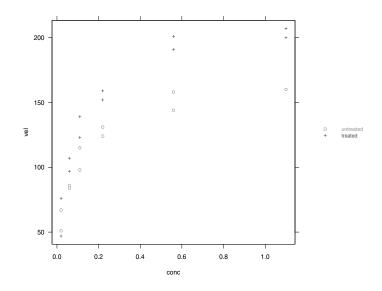


Figure 5.5: Scatter plot of the Puromycin data.

### **Line Fits**

You can fit a straight line to your scatter plot data and superpose the fit with the data. Such a fit helps you visually assess how well the data conforms to a linear relationship between two variables. When the linear fit seems adequate, the fitted straight line plot provides a good visual indication of both the slope of bivariate data, and the variation of the data about the straight line fit. The **Scatter Plot** dialog includes two kinds of line fits in the **Fit** tab, as described below.

- **Linear Least Squares**: computes a line fit via a least squares algorithm.
- **Robust MM**: computes a line fit via a robust fitting criterion. Robust line fits are useful for fitting linear relationships when the random variation in the data is not Gaussian (normal), or when the data contain significant outliers.

# Linear Least Squares

The method of *least squares* fits a line to data so that the sum of the squared residuals is minimized. Suppose a set of n observations of the response variable  $y_i$  correspond to a set of values of the predictor  $x_i$  according to the model  $\hat{y} = f(\hat{x})$ , where  $\hat{y} = (y_1, y_2, ..., y_n)$  and  $\hat{x} = (x_1, x_2, ..., x_n)$ . The *i*th *residual*  $r_i$  is defined as the difference between the *i*th observation  $y_i$  and the *i*th fitted value  $\hat{y}_i = \hat{f}(x_i)$ : that is,  $r_i = y_i - \hat{y}_i$ . The method of least squares finds a set of fitted

values that minimizes the sum  $\sum_{i=1}^{n} r_i^2$ .

#### **Example**

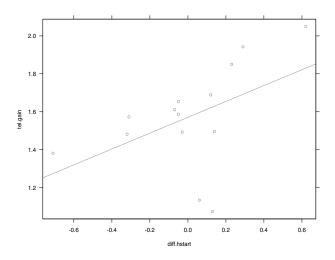
In the section A Basic Example on page 128, we created a scatter plot of the exmain data. You can fit a straight line to the data by the method of least squares and display the result superposed on a scatter plot of the data. The following steps illustrate how to do this.

- 1. If you have not done so already, create the exmain data set with the instructions given on page 129.
- 2. Open the **Scatter Plot** dialog.
- 3. Type exmain in the **Data Set** field.
- 4. Select diff.hstart as the x Axis Value and tel.gain as the y Axis Value.
- 5. Click on the **Fit** tab and select **Least Squares** as the **Regression Type**.

6. Click on the **Axes** tab and select **Horizontal** for the **Tick Marks Label Orientation**. This option places horizontal tick labels on both the *x* and *y* axes. By default, labels are parallel to the axes, so that *x* axis tick labels are horizontal and *y* axis labels are vertical.

#### 7. Click **OK**.

The result is shown in Figure 5.6.



**Figure 5.6:** Scatter plot of tel.gain versus diff.hstart with a least squares line fit.

Notice that the two outliers in the data appear to influence the least squares fit by pulling the line downward. This reduces the slope of the line relative to the remainder of the data.

#### **Robust MM**

The least squares fit of a straight line is not *robust*, and outliers can have a large influence on the location of the line. A robust method is one that is not significantly influenced by outliers, no matter how large. Robust fitting methods are useful when the random variation in the data is not normal (Gaussian), or when the data contain significant outliers. In such situations, standard least squares may return inaccurate fits. *Robust MM* is one robust fitting method used to guard against outlying observations. The MM method is the robust procedure currently recommended by TIBCO Software Inc.

In this example, we fit a robust line to the exmain data.

- 1. If you have not done so already, create the exmain data set with the instructions given on page 129.
- 2. Open the **Scatter Plot** dialog.
- 3. Type exmain in the **Data Set** field.
- 4. Select diff.hstart as the **x Axis Value** and tel.gain as the **y Axis Value**.
- 5. Click on the **Fit** tab and select **Robust** as the **Regression Type**.
- 6. Click on the **Axes** tab and select **Horizontal** for the **Tick Marks Label Orientation**. This option places horizontal tick labels on both the *x* and *y* axes. By default, labels are parallel to the axes, so that *x* axis tick labels are horizontal and *y* axis labels are vertical.
- 7. Click **OK**.

The result is shown in Figure 5.7.

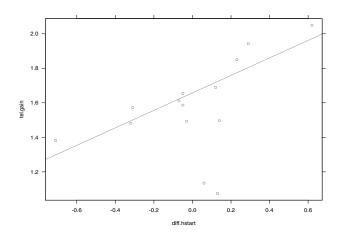


Figure 5.7: Scatter plot of tel. gain versus diff. hstart with robust MM line.

Compare Figure 5.6 to Figure 5.7 and note how much the two outliers influence the least squares line.

# **Curve Fits**

Nonparametric In the previous section, we fit linear parametric functions to scatter plot data. Frequently, you do not have enough prior information to determine what kind of parametric function to use. In such cases, you can fit a *nonparametric curve*, which does not assume a particular type of relationship.

> Nonparametric curve fits are also called *smoothers* since they attempt to create a smooth curve showing the general trend in the data. The simplest smoothers use a running average, where the fit at a particular x value is calculated as a weighted average of the y values for nearby points. The weight given to each point decreases as the distance between its x value and the x value of interest increases. In the simplest kind of running average smoother, all points within a certain distance (or window) from the point of interest are weighted equally in the average for that point. The window width is called the bandwidth of the smoother, and is usually given as a percentage of the total number of data points. Increasing the bandwidth results in a smoother curve fit but may miss rapidly changing features. Decreasing the bandwidth allows the smoother to track rapidly changing features more accurately, but results in a rougher curve fit.

> More sophisticated smoothers add variations to the running average approach. For example, smoothly decreasing weights or local linear fits may be used. However, all smoothers have some type of smoothness parameter (bandwidth) controlling the smoothness of the curve. The issue of good bandwidth selection is complicated and has been treated in many statistical research papers. You can, however, gain a good feeling for the practical consequences of varying the bandwidth by experimenting with smoothers on real data.

This section describes how to use four different types of smoothers.

- **Kernel Smoother**: a generalization of running averages in which different weight functions, or *kernels*, may be used. The weight functions provide transitions between points that are smoother than those in the simple running average approach.
- **Loess Smoother**: a noise-reduction approach that is based on local linear or quadratic fits to the data.

- **Spline Smoother**: a technique in which a sequence of polynomials is pieced together to obtain a smooth curve.
- **Supersmoother**: a highly automated variable span smoother. It obtains fitted values by taking weighted combinations of smoothers with varying bandwidths.

In particular, we illustrate how a smoother's bandwidth can be used to control the degree of smoothness in a curve fit.

Kernel Smoothers A kernel smoother is a generalization of running averages in which different weight functions, or kernels, may be used. The weight functions provide transitions between points that are smoother than those in the simple running average approach. The default kernel is the normal or Gaussian kernel, in which the weights decrease with a Gaussian distribution away from the point of interest. Other choices include a triangle, a box, and the Parzen kernel. In a triangle kernel, the weights decrease linearly as the distance from the point of interest increases, so that the points on the edge of the smoothing window have a weight near zero. A box or boxcar smoother weighs each point within the smoothing window equally, and a *Parzen kernel* is a box convolved with a triangle.

#### Example

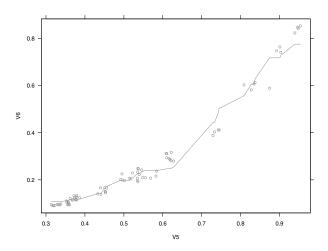
The sensors data set contains the responses of eight different semiconductor element sensors to varying levels of nitrous oxide (NOx) in a container of air. The engineers who designed these sensors study the relationship between the responses of these eight sensors to determine whether using two sensors, instead of one, allows a more precise measurement of the concentration of NOx. Prior investigation has revealed that there may be a nonlinear relationship between the responses of the two sensors, but not much is known about the details of the relationship. In the examples below, we use kernel smoothers to graphically explore the relationship between the fifth and sixth sensors.

First, create a scatter plot of sensor 5 versus sensor 6 with a box kernel:

- Open the **Scatter Plot** dialog.
- Type sensors in the **Data Set** field.
- Select V5 as the **x Axis Value** and V6 as the **y Axis Value**.

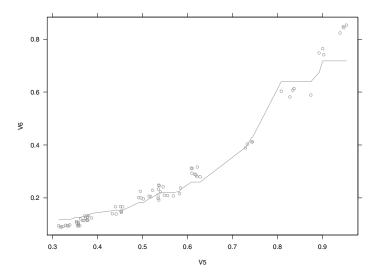
- 4. Click on the **Fit** tab. Select **Kernel** as the **Smoothing Type** and **Box** as the **Kernel**.
- 5. Click on the **Axes** tab and select **Horizontal** for the **Tick Marks Label Orientation**. This option places horizontal tick labels on both the *x* and *y* axes. By default, labels are parallel to the axes, so that *x* axis tick labels are horizontal and *y* axis labels are vertical.
- 6. Click **Apply** to leave the dialog open.

This results are shown in Figure 5.8.



**Figure 5.8:** Sensor 5 versus sensor 6 with a box kernel smoother line.

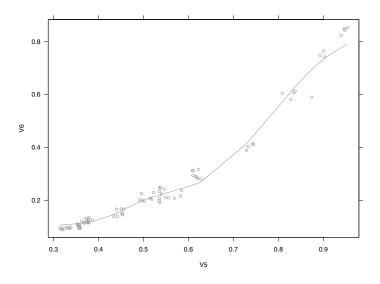
You can experiment with the smoothing parameter by varying the value in the **Bandwidth** field. For example, click on the **Fit** tab in the open **Scatter Plot** dialog. By default, no bandwidth value is specified. Instead, the standard deviation of the x variable is used to compute a good estimate for the bandwidth; this allows the default bandwidth to scale with the magnitude of the data. Type various values between 0.1 and 0.6 in the **Bandwidth** field, clicking **Apply** each time you choose a new value. Each time you click **Apply**, a new **Graph** window appears that displays the updated curve. Note how the smoothness of the fit is affected. Which bandwidth produces the best "eyeball" curve fit? The box kernel smoother with a bandwidth choice of 0.3 is shown in Figure 5.9.



**Figure 5.9:** Sensor 5 versus sensor 6 with a box kernel smoother line using a bandwidth of 0.3.

To obtain a smoother curve, we can experiment with the remaining three kernels. For example, click on the **Fit** tab in the open **Scatter Plot** dialog, choose **Parzen** as the **Kernel**, and click **Apply**. Again, you can also vary the bandwidth choice to see how the smoothness of the fit is affected. Type various values in the **Bandwidth** field, clicking **Apply** each time you choose a new value. Each time you click **Apply**, a new **Graph** window appears that displays the updated curve. The Parzen kernel smoother with a bandwidth choice of 0.15 is shown in Figure 5.10.

When you are finished experimenting, click **OK** to close the dialog.



**Figure 5.10:** Sensor 5 versus sensor 6 with a Parzen kernel smoother line using a bandwidth of 0.15.

#### **Loess Smoothers**

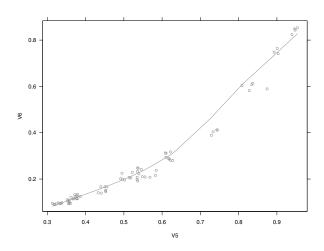
The *loess smoother*, developed by W.S. Cleveland and others at Bell Laboratories (1979), is a clever approach to smoothing that is essentially a noise-reduction algorithm. It is based on local linear or quadratic fits to the data: at each point, a line or parabola is fit to the points within the smoothing window, and the predicted value is taken as the *y* value for the point of interest. Weighted least squares is used to compute the line or parabola in each window. Connecting the computed *y* values results in a smooth curve.

For loess smoothers, the bandwidth is referred to as the *span* of the smoother. The span is a number between 0 and 1, representing the percentage of points that should be included in the fit for a particular smoothing window. Smaller values result in less smoothing, and very small values close to 0 are not recommended. If the span is not specified, an appropriate value is computed using cross-validation. For small samples (n < 50), or if there are substantial serial correlations between observations close in x value, a prespecified fixed span smoother should be used.

In this example, we use loess smoothers to graphically explore the relationship between the fifth and sixth sensors in the sensors data set.

- 1. Open the **Scatter Plot** dialog.
- 2. Type sensors in the **Data Set** field.
- 3. Select V5 as the **x Axis Value** and V6 as the **y Axis Value**.
- 4. Click on the **Fit** tab and select **Loess** as the **Smoothing Type**.
- 5. Click on the **Axes** tab and select **Horizontal** for the **Tick Marks Label Orientation**. This option places horizontal tick labels on both the *x* and *y* axes. By default, labels are parallel to the axes, so that *x* axis tick labels are horizontal and *y* axis labels are vertical.
- 6. Click **Apply** to leave the dialog open.

The result is shown in Figure 5.11.



**Figure 5.11:** Sensor 5 versus sensor 6 with a loess smoother line.

You can experiment with the smoothing parameter by varying the value in the **Span** field. For example, click on the **Fit** tab in the open **Scatter Plot** dialog. The bandwidth used to create Figure 5.11 is the default value of 0.75. Since the sensors data set has eighty

observations, this means that  $0.75 \times 80 = 60$  values are included in the calculation at each point. Type various values between 0.1 and 1 in the **Span** field, clicking **Apply** each time you choose a new value. Each time you click **Apply**, a new **Graph** window appears that displays the updated curve. Note how the smoothness of the fit is affected.

You can also experiment with the degree of the polynomial that is used in the local fit at each point. If you select **Two** as the **Degree** in the **Fit** tab, local quadratic fits are used instead of local linear fits. The **Family** field in the **Fit** tab governs the assumed distribution of the errors in the smoothed curve. The default family is **Symmetric**, which combines local fitting with a robustness feature that guards against distortion by outliers. The **Gaussian** option employs strictly local fitting methods, and can be affected by large outliers. When you are finished experimenting, click **OK** to close the dialog.

#### Spline Smoothers

Spline smoothers are computed by piecing together a sequence of polynomials. Cubic splines are the most widely used in this class of smoothers, and involve locally cubic polynomials. The local polynomials are computed by minimizing a penalized residual sum of squares. Smoothness is assured by having the value, slope, and curvature of neighboring polynomials match at the points where they meet. Connecting the polynomials results in a smooth fit to the data. The more accurately a smoothing spline fits the data values, the rougher the curve, and vice versa.

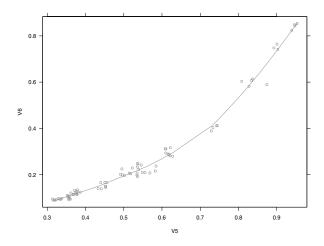
The smoothing parameter for splines is called the *degrees of freedom*. The degrees of freedom controls the amount of curvature in the fit, and corresponds to the degree of the local polynomials. The lower the degrees of freedom, the smoother the curve. The degrees of freedom automatically determines the smoothing window, by governing the trade-off between smoothness of the fit and fidelity to the data values. For n data points, the degrees of freedom should be between 1 and n-1. Specifying n-1 degrees of freedom results in a curve that passes through each of the data points exactly.

In this example, we use spline smoothers to graphically explore the relationship between the fifth and sixth sensors in the sensor data set.

- Open the **Scatter Plot** dialog.
- 2. Type sensors in the **Data Set** field.
- 3. Select V5 as the **x Axis Value** and V6 as the **y Axis Value**.
- 4. Click on the **Fit** tab and select **Smoothing Spline** as the **Smoothing Type**.
- 5. Click on the **Axes** tab and select **Horizontal** for the **Tick Marks Label Orientation**. This option places horizontal tick labels on both the *x* and *y* axes. By default, labels are parallel to the axes, so that *x* axis tick labels are horizontal and *y* axis labels are vertical.
- 6. Click **Apply** to leave the dialog open.

You can experiment with the smoothing parameter by varying the value in the **Degrees of Freedom** field. For example, click on the **Fit** tab in the open **Scatter Plot** dialog. The degrees of freedom is set to 3 by default, which corresponds to cubic splines. The sensors data set has eighty observations, so type various integer values between 1 and 79 in the **Degrees of Freedom** field (or select values from the dropdown list). If **Crossvalidate** is selected as the **Degrees of Freedom**, the smoothing parameter is computed internally by cross-validation. Click **Apply** each time you choose a new value, and a new **Graph** window appears that displays the updated curve. Note how the smoothness of the fit is affected. When you are finished experimenting, click **OK** to close the dialog.

The spline smoother with 6 degrees of freedom is shown in Figure 5.12.



**Figure 5.12:** Sensor 5 versus sensor 6 with a spline smoother line using 6 degrees of freedom.

# Friedman's Supersmoother

The *supersmoother* is a highly automated variable span smoother. It obtains fitted values by taking a weighted combination of smoothers with varying bandwidths. Like loess smoothers, the main parameter for supersmoothers is called the *span*. The span is a number between 0 and 1, representing the percentage of points that should be included in the fit for a particular smoothing window. Smaller values result in less smoothing, and very small values close to 0 are not recommended. If the span is not specified, an appropriate value is computed using cross-validation. For small samples (n < 50), or if there are substantial serial correlations between observations close in x value, a prespecified fixed span smoother should be used.

In this example, we use a supersmoother to graphically explore the relationship between the fifth and sixth sensors in the sensors data set.

- Open the **Scatter Plot** dialog.
- 2. Type sensors in the **Data Set** field.
- 3. Select V5 as the **x Axis Value** and V6 as the **y Axis Value**.
- 4. Click on the **Fit** tab and select **Supersmoother** as the **Smoothing Type**.
- 5. Click **Apply** to leave the dialog open.

A **Graph** window is created containing a plot. As in the previous examples, you can experiment with the smoothing parameter by varying the value in the **Span** field. For example, click on the **Fit** tab in the open **Scatter Plot** dialog. By default, no span value is specified, so it is computed internally by cross-validation. Type various values between 0.1 and 1 in the **Span** field, clicking **Apply** each time you choose a new value. Each time you click **Apply**, a new **Graph** window appears that displays the updated curve. Note how the smoothness of the fit is affected. When you are finished experimenting, click **OK** to close the dialog.

# Multipanel Conditioning

In the section Grouping Variables, we plotted multiple twodimensional scatter plots on the same set of axes according to the value of a third factor (categorical) variable. It is also possible to place multiple scatter plots on separate axes, conditioned on the value of a third variable. When a conditioning variable is categorical, Spotfire S+ generates plots for each level. When a conditioning variable is numeric, conditioning is automatically carried out on the sorted unique values; each plot represents either an equal number of observations or an equal range of values.

The **Scatter Plot** dialog, as well as many other dialogs in the **Graph** menu, includes options for specifying conditioning variables, arranging the plots, and labeling the panels. For additional detailed examples on conditioning in the **Graph** dialogs, see the section Visualizing Multidimensional Data.

#### Example I

The ethanol data set records 88 measurements from an experiment in which ethanol was burned in a single cylinder automobile test engine. The three variables in the experiment are the concentration of nitric oxide and nitrogen dioxide in the engine's exhaust (NOX), the compression ratio of the engine (C), and the equivalence ratio at which the engine was run (E). In this example, we examine the relationship between NOX and E for various values of C.

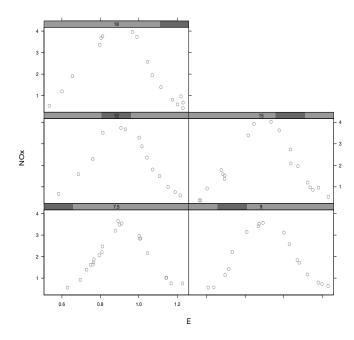
The conditioning variable C is numeric and has 6 unique values: 7.5, 9.0, 12.0, 15.0, and 18.0. We create scatter plots of NOx versus E for each value of these values. Spotfire S+ displays the conditioned plots, or *panels*, in the same order that the levels function returns the values of the conditioning variable. The effect is the same if we declare the conditioning variable to be a factor directly:

```
> ethanol.fac <- factor(ethanol$C)
> levels(ethanol.fac)
[1] "7.5" "9" "12" "15" "18"
```

In the multipanel graph, the individual scatter plots are therefore placed in order from C=7.5 to C=18.

By default, Spotfire S+ displays the individual scatter plots in succession from the bottom left corner of the **Graph** window to the top right corner. Figure 5.13 displays the plots generated by the steps below. The scatter plot for C=7.5 is in the lower left corner of the window, the plot for C=9.0 is to the right of it, etc.

- 1. Open the **Scatter Plot** dialog.
- 2. Type ethanol in the **Data Set** field.
- 3. Select E as the **x Axis Value** and NOx as the **y Axis Value**. Highlight C in the **Conditioning** box.
- 4. Click on the **Axes** tab. Set the **Aspect Ratio** to be a **Specified Value** and type 0.5 for the **Ratio Value**.
- 5. Select **Horizontal** for the **Tick Marks Label Orientation**. This option places horizontal tick labels on both the *x* and *y* axes. By default, labels are parallel to the axes, so that *x* axis tick labels are horizontal and *y* axis labels are vertical.
- 6. Click on the **Multipanel** tab. Select **Unique Values** as the **Interval Type**, and click **Apply** to leave the dialog open.



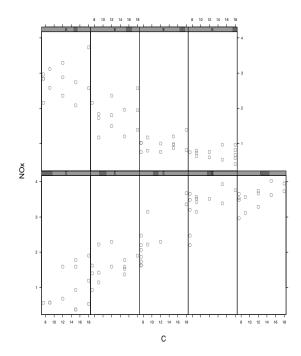
**Figure 5.13:** Scatter plots of NOx versus E for various values of C.

You can change the layout of the plots in the **Graph** window with the options in the **Multipanel** tab of the open **Scatter Plot** dialog. For example, to start the individual plots in the upper left corner of the window instead of the lower left corner, select **Table Order** from the **Panel Order** list. This places the plot for C=7.5 in the upper left corner, the plot for C=9.0 to the right of it, and so on. You can also specify the number of rows and columns in the layout, and the number of pages is computed accordingly. Conversely, you can specify the number of pages, and the panels are placed in appropriate rows and columns. When you are finished experimenting, click **OK** to close the dialog.

In this example, we examine the relationship between NOx and C for various values of E. However, E varies in a nearly continuous way: there are 83 unique values out of 88 observations. Since E is a continuous variable, each panel represents either an equal number of observations or an equal range of values.

- 1. Open the **Scatter Plot** dialog.
- 2. Type ethanol in the **Data Set** field.
- 3. Select C as the **x Axis Value** and NOx as the **y Axis Value**. Highlight E in the **Conditioning** box.
- 4. Click on the **Axes** tab. Set the **Aspect Ratio** to be **Bank to** 45 **Degree**.
- 5. Select **Horizontal** for the **Tick Marks Label Orientation**. This option places horizontal tick labels on both the *x* and *y* axes. By default, labels are parallel to the axes, so that *x* axis tick labels are horizontal and *y* axis labels are vertical.
- 6. Suppose we want to generate a  $2 \times 5$  grid containing 9 scatter plots, with an equal number of observations in each panel. Click on the **Multipanel** tab. Type 5 for the # **of Columns** and 2 for the # **of Rows**. Type 9 in the # **of Panels** field and 0.25 as the **Overlap Fraction**.
- 7. Click **Apply** to leave the dialog open.

The result is displayed in Figure 5.14. Since the **Panel Order** is set to **Graph Order** by default, the minimum values of E are in the lower left panel and the maximum values are in the upper right panel. To place the plot with the minimum values in the upper left corner of the window instead, click on the **Multipanel** tab in the open **Scatter Plot** dialog and select **Table Order** as the **Panel Order**. To generate plots according to equal-length intervals of the values in E, select **Equal Ranges** as the **Interval Type**.



**Figure 5.14:** Scatter plots of NOx versus C for various values of E.

The **Overlap Fraction** in the **Multipanel Conditioning** tab governs the amount of points that are shared by successive intervals of the conditioning variable. The endpoints of the intervals are chosen to make either the number of points (if **Equal Counts** is chosen) or the length of the intervals (if **Equal Ranges** is chosen) as nearly equal as possible. At the same time, the amount of points shared by successive intervals is kept as close to the **Overlap Fraction** as possible. If the **Overlap Fraction** is between 0 and 1, it is the fraction of points shared between adjacent intervals. If the **Overlap Fraction** is greater than or equal to 1, it is the number of points shared between adjacent intervals.

When you are finished experimenting, click **OK** to close the dialog.

# VISUALIZING ONE-DIMENSIONAL DATA

A *one-dimensional data object* is sometimes referred to as a (single) *data sample*, a set of *univariate observations*, or simply a batch of data. In this section, we examine a number of basic plot types useful for exploring a one-dimensional data object.

- **Density Plot**: an estimate of the underlying probability density function for a data set.
- Histogram: a display of the number of data points that fall in each of a specified number of intervals. A histogram gives an indication of the relative density of the data points along the horizontal axis.
- **QQ Math Plot**: an extremely powerful tool for determining a good approximation to a data set's distribution. The most common is the *normal probability plot*, or *normal qqplot*, which is used to test whether the distribution of a data set is nearly Gaussian.
- **Bar Chart**: a display of the relative magnitudes of observations in a data set. A bar is plotted for each data point, where the height of a bar is determined by the value of the data point. The **Bar Chart** dialog can also tabulate counts for a factor variable in a data set.
- **Dot Plot**: a tool that displays the same information as a bar chart or pie chart, but in a form that is often easier to grasp.
- **Pie Chart**: a graph that shows the share of individual values in a variable, relative to the sum total of all the values.

These visualization plots are simple but powerful exploratory data analysis tools that can help you quickly grasp the nature of your data. Such an understanding can help you avoid the misuse of statistical inference methods, such as using a method appropriate only for a normal (Gaussian) distribution when the distribution is strongly nonnormal.

# **Density Plots**

As a first step in analyzing one-dimensional data, it is often useful to study the shape of its distribution. A *density plot* displays an estimate of the underlying probability density function for a data set, and allows you to approximate the probability that your data fall in any interval.

In Spotfire S+, density plots are essentially kernel smoothers. The algorithm used to compute the plots is therefore similar to those presented in the section Nonparametric Curve Fits. A smoothing window is centered on each *x* value, and the predicted *y* value in the density plot is calculated as a weighted average of the *y* values for nearby points. The size of the smoothing window is called the *bandwidth* of the smoother. Increasing the bandwidth results in a smoother curve but may miss rapidly changing features. Decreasing the bandwidth allows the smoother to track rapidly changing features more accurately, but results in a rougher curve fit. The **Density Plot** dialog includes various methods for estimating good bandwidth values.

The weight given to each point in a smoothing window decreases as the distance between its *x* value and the *x* value of interest increases. *Kernel functions* specify the way in which the weights decrease: kernel choices for density plots include a cosine curve, a normal (Gaussian) kernel, a rectangle, and a triangle. The default kernel is Gaussian, where the weights decrease with a normal (Gaussian) distribution away from the point of interest. A rectangular kernel weights each point within the smoothing window equally, and a triangular kernel has linearly decreasing weights. In a cosine kernel, weights decrease with a cosine curve away from the point of interest.

### Creating a density plot

From the main menu, choose **Graph** ▶ **One Variable** ▶ **Density Plot**. The **Density Plot** dialog opens, as shown in Figure 5.15.

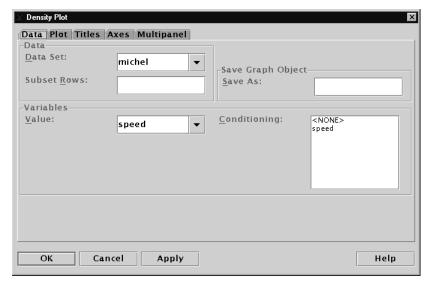


Figure 5.15: The **Density Plot** dialog.

In 1876, the French physicist Cornu reported a value of 299,990 km/sec for c, the speed of light. In 1879, the American physicist A.A. Michelson carried out several experiments to verify and improve Cornu's value. Michelson obtained the following 20 measurements of the speed of light:

```
850 740 900 1070 930 850 950 980 980 880
1000 980 930 650 760 810 1000 1000 960 960
```

To obtain Michelson's actual measurements, add 299,000 km/sec to each of the above values.

The 20 observations can be thought of as observed values of 20 random variables with a common but unknown mean-value location  $\mu$ . If the experimental setup for measuring the speed of light is free of bias, then it is reasonable to assume that  $\mu$  is the true speed of light. In evaluating these data, we seek answers to at least four questions, listed below.

- 1. What is the speed of light  $\mu$ ?
- 2. Has the speed of light changed relative to our best previous value  $\mu_0 = 299,990$  km/sec?
- 3. What is the uncertainty associated with our answers to (1) and (2)?
- 4. What is the shape of the distribution of the data?

The first three questions were probably in Michelson's mind when he gathered his data. The last two must be answered to determine which techniques can obtain valid statistical inferences from the data. In this example, we use density plots to graphically analyze the distribution of the Michelson data. In the Statistics chapter, we revisit these data and perform various statistical tests to answer questions (2) and (3).

#### Setting up the data

We begin analyzing the Michelson data by first creating a S-PLUS data frame that contains it. To do this, type the following in the **Commands** window:

```
> michel <- data.frame(speed = c(850, 740, 900,
+ 1070, 930, 850, 950, 980, 980, 880, 1000, 980,
+ 930, 650, 760, 810, 1000, 1000, 960, 960))
```

### **Exploratory data analysis**

To obtain a useful exploratory view of the Michelson data, create a density plot as follows:

- 1. Open the **Density Plot** dialog.
- 2. Type michel in the **Data Set** field.
- 3. Select speed as the **Value**.
- 4. Click **Apply** to leave the dialog open.

The result is shown in Figure 5.16. The rug at the bottom of the density plot shows the unique x values in the data set.

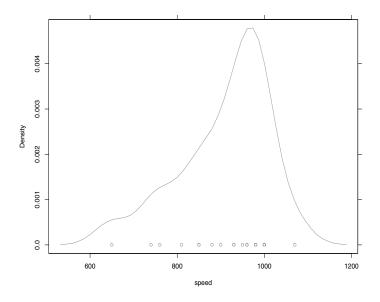


Figure 5.16: Density estimate of the Michelson data.

To experiment with the smoothing kernel, click on the **Plot** tab in the open **Density Plot** dialog and choose a new function from the **Window Type** list. The **Number of Points** field specifies the number of equally spaced points at which to estimate the density; the **From** and **To** fields define the range of the equally spaced points. The **Width Method** field specifies the algorithm for computing the width of the smoothing window. Available methods are the histogram bin (**Hist Bin**), normal reference density (**Normal Ref**), biased crossvalidation (**Biased CV**), unbiased cross-validation (**Unbiased CV**), and Sheather & Jones pilot estimation of derivatives (**Est Deriv**). You can also define your own window by selecting **Specified Value** from the **Width Method** list, and then typing a number for the **Width Value**. For more information on the methods used to compute the width of a smoothing window, see Venables and Ripley (1999).

When you are finished experimenting, click **OK** to close the dialog.

# **Histograms**

*Histograms* display the number of data points that fall in each of a specified number of intervals. A histogram gives an indication of the relative density of the data points along the horizontal axis. For this reason, density plots are often superposed with (scaled) histograms.

By default, the **Histogram** dialog displays vertical bars. For details on horizontal bar plots, see the section Bar Charts.

#### Creating a histogram

From the main menu, choose **Graph** ▶ **One Variable** ▶ **Histogram**. The **Histogram** dialog opens, as shown in Figure 5.17.

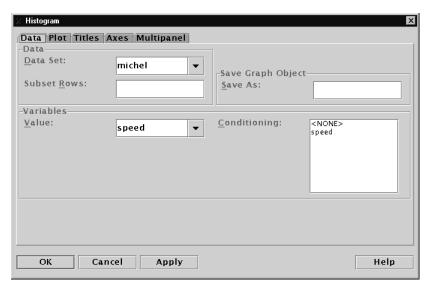


Figure 5.17: The Histogram dialog.

#### **Example**

In the section Density Plots on page 153, we created a probability density estimate for the michel data. In this example, we plot a histogram of the data.

- 1. If you have not done so already, create the michel data set with the instructions given on page 155.
- 2. Open the **Histogram** dialog.
- 3. Type michel in the **Data Set** field and select speed as the **Value**.

- 4. Click on the **Axes** tab and select **Horizontal** for the **Tick Marks Label Orientation**. This option places horizontal tick labels on both the *x* and *y* axes. By default, labels are parallel to the axes, so that *x* axis tick labels are horizontal and *y* axis labels are vertical.
- 5. Click **Apply** to leave the dialog open.

The result is shown in Figure 5.18.

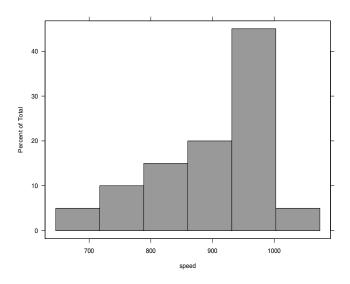


Figure 5.18: Histogram of the Michelson data.

By default, Spotfire S+ displays histograms scaled as probability densities. To display the raw counts in each histogram bin instead, click on the **Plot** tab in the open **Histogram** dialog and select **Count** as the **Bar Height Type**.

Spotfire S+ computes the number of intervals in a histogram automatically to balance the trade-off between obtaining smoothness and preserving detail. To experiment with the algorithm used to compute the intervals, click on the **Plot** tab in the open **Histogram** dialog. There are three algorithms available in the **Binning Method** list: **Freedman-Diaconi**, **Scott**, and **Sturges**. You can also define your own number of intervals by selecting **Specified Value** from the

**Binning Method** list, and then typing a number for the **Number of Bins**. For more information on the methods used to compute the number of bins, see Venables and Ripley (1999).

When you are finished experimenting, click **OK** to close the dialog.

### **QQ Math Plots**

The quantile-quantile plot, or *qqplot*, is an extremely powerful tool for determining a good approximation to a data set's distribution. In a qqplot, the ordered data are graphed against quantiles of a known theoretical distribution. If the data points are drawn from the theoretical distribution, the resulting plot is close to a straight line in shape. The most common in this class of one-dimensional plots is the *normal probability plot*, or *normal qqplot*, which is used to test whether the distribution of a data set is nearly normal (Gaussian).

#### Creating a QQ math plot

From the main menu, choose **Graph** ▶ **One Variable** ▶ **QQ Math Plot**. The **QQ Math Plot** dialog opens, as shown in Figure 5.19.

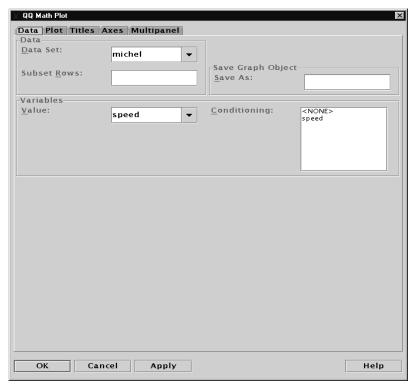


Figure 5.19: The QQ Math Plot dialog.

In the section Density Plots on page 153, we created a probability density estimate for the michel data. In this example, we compare the data to a normal (Gaussian) distribution.

- 1. If you have not done so already, create the michel data set with the instructions given on page 155.
- 2. Open the **QQ Math Plot** dialog.
- 3. Type michel in the **Data Set** field and select speed as the **Value**.
- 4. Click **Apply** to leave the dialog open.

The result is shown in Figure 5.20.

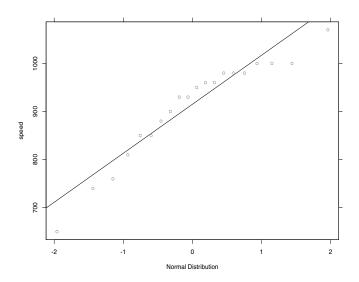


Figure 5.20: Normal QQ plot for the Michelson data.

By default, Spotfire S+ includes a reference line in qqplots. To omit the line from a graph, deselect the **Include Reference Line** option in the **Plot** page of the dialog.

The points in Figure 5.20 do not fall particularly close to a straight line, which suggests that the data may not be normally distributed. You can experiment with the chosen theoretical distribution by varying the selection in the **Distribution** list. For example, click on

the **Plot** tab in the open **QQ Math Plot** dialog. By default, the **Distribution** is **normal** with a **Mean** of 0 and a **Std. Deviation** of 1. Select **t** as the **Distribution**, type 5 in the **Deg of Freedom** 1 box, and click **Apply**. Does the *t* distribution with 5 degrees of freedom produce a more linear qqplot? When you are finished experimenting, click **OK** to close the dialog.

#### **Bar Charts**

A *bar chart* displays a bar for each point in a set of observations, where the height of a bar is determined by the value of the data point. The **Bar Chart** dialog also contains an option for tabulating the values in your data set according to the levels of a categorical variable. This allows you to view a count of the observations that are associated with each level of a factor variable.

By default, Spotfire S+ generates horizontal bar charts from the menu options. If you require vertical bar charts, you should use the command line function barplot.

#### Creating a bar chart

From the main menu, choose **Graph** ▶ **One Variable** ▶ **Bar Chart**. The **Bar Chart** dialog opens, as shown in Figure 5.21.

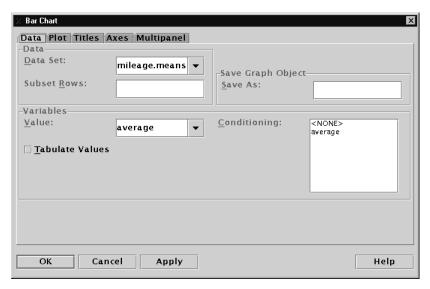


Figure 5.21: The Bar Chart dialog.

#### Example I

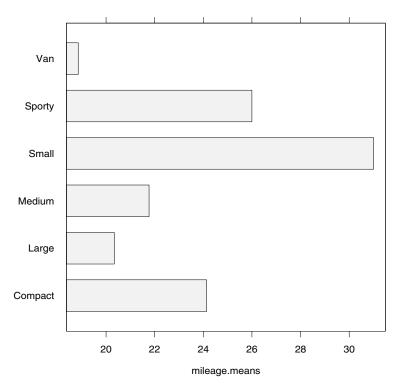
The data set fuel.frame is taken from the April 1990 issue of *Consumer Reports*. It contains 60 observations (rows) and 5 variables (columns). Observations of weight, engine displacement, mileage, type, and fuel were taken for each of sixty cars. In this example, we graphically analyze the average mileage for each of the six types of cars.

To create a mileage.means data set containing the average Mileage for each Type of car, type the following in the **Commands** window:

Create a bar chart of the mileage.means data as follows:

- 1. Open the **Bar Chart** dialog.
- 2. Type mileage.means in the **Data Set** field.
- 3. Select average as the **Value**. Deselect the **Tabulate Values** option.
- 4. Click on the **Titles** tab and type mileage.means for the **X Axis Label**.
- 5. Click **OK**.

The horizontal bar chart is shown in Figure 5.22. Note that the bars in the chart are placed according to the order in the data set: Compact, the first element in mileage.means, appears with the smallest y value in the chart, and Van, the last element in mileage.means, appears with the largest y value.



**Figure 5.22:** A bar chart of average mileage in the fuel. frame data set.

In this example, we tabulate the number of cars in the fuel.frame data set for each level of the Type factor variable.

- 1. Open the **Bar Chart** dialog.
- 2. Type fuel.frame in the **Data Set** field.
- 3. Select Type as the **Value**.
- 4. Verify that the **Tabulate Values** option is checked.
- 5. Click **OK**.

A **Graph** window appears that displays a bar chart of the tabulated values in fuel.frame. Note that the bars in the chart are placed according to the levels in the Type variable: Compact, the first level Type, appears with the smallest y value in the chart, and Van, the last

level in Type, appears with the largest *y* value. You can view the order of the levels in a factor variable by using the levels function in the **Commands** window:

```
> levels(fuel.frame$Type)
[1] "Compact" "Large" "Medium" "Small" "Sporty" "Van"
```

#### **Dot Plots**

The dot plot was first described by Cleveland in 1985 as an alternative to bar charts and pie charts. The dot plot displays the same information as a bar chart or pie chart, but in a form that is often easier to grasp. Instead of bars or pie wedges, dots and gridlines are used to mark the data values in dot plots. In particular, the dot plot reduces most data comparisons to straightforward length comparisons on a common scale.

#### Creating a dot plot

From the main menu, choose **Graph** ▶ **One Variable** ▶ **Dot Plot**. The **Dot Plot** dialog opens, as shown in Figure 5.23.

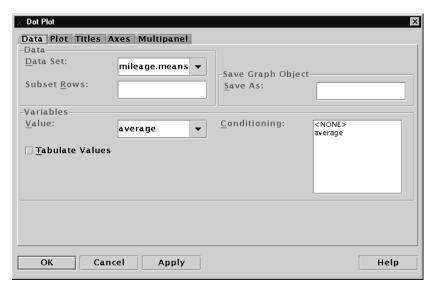


Figure 5.23: The Dot Plot dialog.

#### Example I

In the section Bar Charts on page 161, we used bar charts to graphically display the mileage.means data set. In this example, we create a dot plot of these data.

- 1. If you have not done so already, create the mileage.means data set with the instructions given on page 162.
- 2. Open the **Dot Plot** dialog.
- 3. Type mileage.means in the **Data Set** field.
- 4. Select average as the **Value**. Deselect the **Tabulate Values** option.
- Click on the **Titles** tab and type mileage.means for the **X**Axis Label.
- 6. Click **OK**.

The result is shown in Figure 5.24. Note that the plot labels are placed according to the order in the data set: Compact, the first element in mileage.means, appears with the smallest y value in the plot, and Van, the last element in mileage.means, appears with the largest y value.

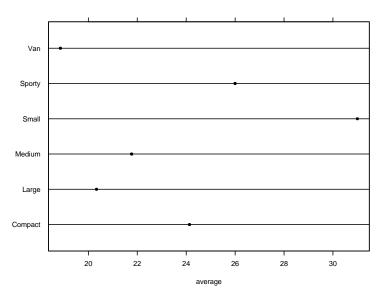


Figure 5.24: Dot plot of average mileage in the fuel. frame data set.

In this example, we tabulate the number of cars in the fuel.frame data set for each level of the Type factor variable.

- 1. Open the **Dot Plot** dialog.
- 2. Type fuel.frame in the **Data Set** field.
- 3. Select Type as the **Value**.
- 4. Verify that the **Tabulate Values** option is checked.
- Click OK.

A **Graph** window appears that displays a dot plot of the tabulated values in fuel.frame. Note that the plot labels are placed according to the levels in the Type variable: Compact, the first level Type, appears with the smallest y value in the chart, and Van, the last level in Type, appears with the largest y value. You can view the order of the levels in a factor variable by using the levels function in the **Commands** window:

```
> levels(fuel.frame$Type)
[1] "Compact" "Large" "Medium" "Small" "Sporty" "Van"
```

### **Pie Charts**

A *pie chart* shows the share of individual values in a variable, relative to the sum total of all the values. Pie charts display the same information as bar charts and dot plots, but can be more difficult to interpret. This is because the size of a pie wedge is relative to a sum, and does not directly reflect the magnitude of the data value. Because of this, pie charts are most useful when the emphasis is on an individual item's relation to the whole; in these cases, the sizes of the pie wedges are naturally interpreted as percentages. When such an emphasis is not the primary point of the graphic, a bar chart or a dot plot is preferred.

### Creating a pie chart

From the main menu, choose **Graph** ▶ **One Variable** ▶ **Pie Chart**. The **Pie Chart** dialog opens, as shown in Figure 5.25.

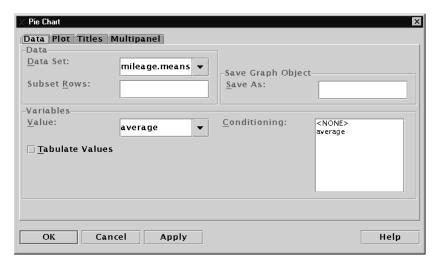


Figure 5.25: The Pie Chart dialog.

#### Example I

In the section Bar Charts on page 161, we used bar charts to graphically display the mileage.means data set. In this example, we create a pie chart of these data.

- 1. If you have not done so already, create the mileage.means data set with the instructions given on page 162.
- 2. Open the **Pie Chart** dialog.
- 3. Type mileage.means in the **Data Set** field.
- 4. Select average as the **Value**.
- 5. Deselect the **Tabulate Values** option.
- 6. Click **Apply** to leave the dialog open.

By default, Spotfire S+ includes a legend to match the pie wedges with their labels. If you would like to include labels on the slices instead, click on the **Plot** tab in the open **Pie Chart** dialog. Deselect the **Include Legend** option and check the boxes for **Include Slice Labels** and **Rotate Labels**. Click **OK**, and a new **Graph** window appears displaying the changes you made. The result is similar to Figure 5.26.

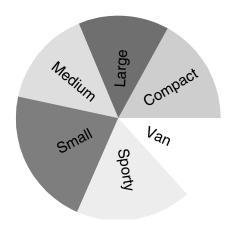


Figure 5.26: Pie chart of the mileage. means data.

Because the average mileage of each type of car cannot be easily interpreted as a fraction of the total mileage, Figure 5.26 does not convey the information in mileage.means very well. We can see that small cars get slightly better mileage on average, since the corresponding pie wedge is the largest in the chart. Other than that, the size of the pie wedges simply imply that the mileage of the cars are relatively close in value when compared to the sum total. To refine these conclusions, we would need to view a bar chart or a dot plot of the data.

### Example 2

In this example, we tabulate the number of cars in the fuel.frame data set for each level of the Type factor variable.

- 1. Open the **Pie Chart** dialog.
- 2. Type fuel.frame in the **Data Set** field. Select Type as the **Value**.
- 3. Verify that the **Tabulate Values** option is checked and click **OK**.

A **Graph** window appears that displays a pie chart of the tabulated values in the fuel.frame data set. A pie chart makes more visual sense in this example than it did in the previous example, because each level of Type can be viewed as a fraction of the total number of observations in fuel.frame.

# VISUALIZING TWO-DIMENSIONAL DATA

Two-dimensional data are often called *bivariate* data, and the individual, one-dimensional components of the data are referred to as *variables*. Two-dimensional plots help you quickly grasp the nature of the relationship between the two variables that constitute bivariate data. For example, you might want to know whether the relationship is linear or nonlinear, if the variables are highly correlated, if there any outliers or distinct clusters, etc. In this section, we examine a number of basic plot types useful for exploring a two-dimensional data object.

- **Box Plot**: a graphical representation showing the center and spread of a distribution, as well as any outlying data points.
- **Strip Plot**: a one-dimensional scatter plot.
- **QQ Plot**: a powerful tool for comparing the distributions of two sets of data.

When you couple two-dimensional plots of bivariate data with onedimensional visualizations of each variable's distribution, you gain a thorough understanding of your data.

#### **Box Plots**

A box plot, or box and whisker plot, is a clever graphical representation showing the center and spread of a distribution. A box is drawn that represents the bulk of the data, and a line or a symbol is placed in the box at the median value. The width of the box is equal to the interquartile range, or IQR, which is the difference between the third and first quartiles of the data. The IQR indicates the spread of the distribution for the data. Whiskers extend from the edges of the box to either the extreme values of the data, or to a distance of  $1.5 \times IQR$  from the median, whichever is less. Data points that fall outside of the whiskers may be outliers, and are therefore indicated by additional lines or symbols.

By default, Spotfire S+ generates horizontal box plots from the menu options. If you require vertical box plots, you should use the command line function boxplot.

#### Creating a box plot

From the main menu, choose **Graph** ▶ **Two Variables** ▶ **Box Plot**. The **Box Plot** dialog opens, as shown in Figure 5.27.

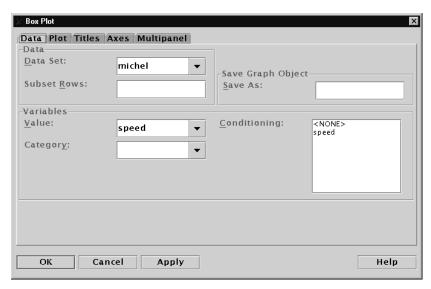


Figure 5.27: The Box Plot dialog.

#### Example I

In the section Density Plots on page 153, we created a probability density estimate for the michel data. In this example, we view a box plot of the data.

- 1. If you have not done so already, create the michel data set with the instructions given on page 155.
- 2. Open the **Box Plot** dialog.
- 3. Type michel in the **Data Set** field.
- 4. Select speed as the **Value** and leave the **Category** field blank.
- 5. Click **Apply** to leave the dialog open.

The result is shown in Figure 5.28.

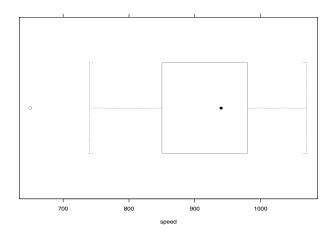


Figure 5.28: Box plot of the Michelson data.

The symbol used to indicate the median in each of the boxes is a solid circle by default. To change the symbol, click on the **Plot** tab in the open **Box Plot** dialog. Choose a new symbol from the **Select Symbol** list, and click **Apply** to see the changes. When you are finished experimenting, click **OK** to close the dialog.

#### Example 2

The lottery.payoff, lottery2.payoff, and lottery3.payoff vectors contain the payoffs for the winning 3-digit numbers in the New Jersey State Pick-It lottery. The lottery.payoff object contains 254 values, corresponding to the drawings from May 22, 1975 to March 16, 1976. The lottery2.payoff object contains 254 values corresponding to drawings from the 1976-1977 lottery, and lottery3.payoff contains 252 values corresponding to the 1980-1981 lottery. In this example, we examine the distributions of these data using box plots.

To create a data frame of the lottery payoff vectors that is suitable for the **Box Plot** dialog, we can use the make.groups function:

```
> lottery.payoffs <- make.groups(
+ "1975" = lottery.payoff,
+ "1977" = lottery2.payoff,
+ "1981" = lottery3.payoff)</pre>
```

#### > lottery.payoffs

```
data which
1 190.0 1975
2 120.5 1975
3 285.5 1975
4 184.0 1975
5 384.5 1975
6 324.5 1975
7 114.0 1975
8 506.5 1975
9 290.0 1975
10 869.5 1975
11 668.5 1975
12 83.0 1975
13 . . .
```

The data column is a numeric variable containing the payoff values from each of the three vectors. The which column is a factor variable with three levels, corresponding to the chosen names "1975", "1977", and "1981". Thus, lottery.payoff appears at the beginning of the data frame, lottery2.payoff is in the middle, and lottery3.payoff is at the end of the data set.

Once you have generated the lottery.payoffs data, create a box plot as follows:

- 1. Open the **Box Plot** dialog.
- 2. Type lottery.payoffs in the **Data Set** field.
- 3. Select data as the **Value**.
- 4. Select which as the **Category**.
- 5. Click **OK**.

The result is displayed in Figure 5.29.

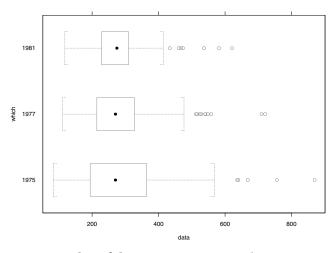


Figure 5.29: Box plots of the lottery.payoffs data.

# **Strip Plots**

A *strip plot* can be thought of as a one-dimensional scatter plot. Strip plots are similar to box plots in overall layout, but they display all of the individual data points instead of the box plot summary.

# Creating a strip plot

From the main menu, choose **Graph** ► **Two Variables** ► **Strip Plot**. The **Strip Plot** dialog opens, as shown in Figure 5.30.

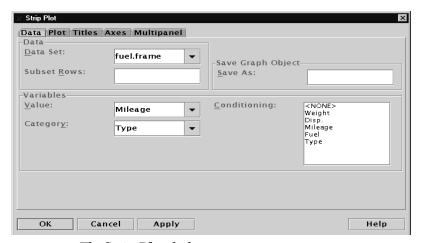


Figure 5.30: The Strip Plot dialog.

In this example, we graphically analyze the mileage for each of the six types of cars in the fuel.frame data.

- Open the Strip Plot dialog.
- 2. Type fuel.frame in the **Data Set** field.
- 3. Select Mileage as the **Value** and Type as the **Category**.
- 4. Click on the **Titles** tab and select **NONE** for the **Y Axis Label**.
- 5. Click **Apply** to leave the dialog open.

At first glance, there appears to be very few points in the strip plot. This is because points with the same x coordinate overlap each other in the horizontal strips. You can distinguish points very near to each other by adding random vertical noise to the points' coordinates. This alleviates some of the overlap in a strip plot's symbols. To do this, click on the **Plot** tab in the open **Strip Plot** dialog and check the **Jitter Symbols Vertically** option. Click **OK** to close the dialog and see the updated graph. The result is shown in Figure 5.31.

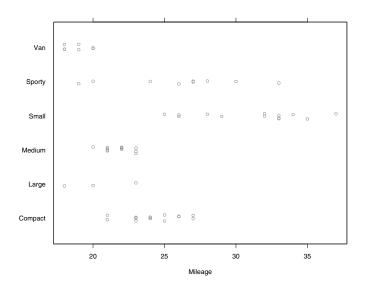


Figure 5.31: Strip plot of mileage in the fuel. frame data set.

# **QQ Plots**

In the section Visualizing One-Dimensional Data, we introduced the quantile-quantile plot, or *qqplot*, as an extremely powerful tool for determining a good approximation to a data set's distribution. In a one-dimensional qqplot, the ordered data are graphed against quantiles of a known theoretical distribution. If the data points are drawn from the theoretical distribution, the resulting plot is close to a straight line in shape.

We can also use qqplots with two-dimensional data to compare the distributions of the variables. In this case, the ordered values of the variables are plotted against each other. If the variables have the same distribution shape, the points in the qqplot cluster along a straight line. The **QQ Plot** dialog creates a qqplot for the two groups in a binary variable. It expects a numeric variable and a factor variable with exactly two levels; the values of the numeric variable corresponding to each level are then plotted against each other.

#### Creating a QQ plot

From the main menu, choose **Graph** ► **Two Variables** ► **QQ Plot**. The **QQ Plot** dialog opens, as shown in Figure 5.32.

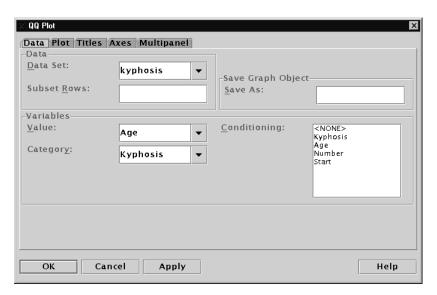


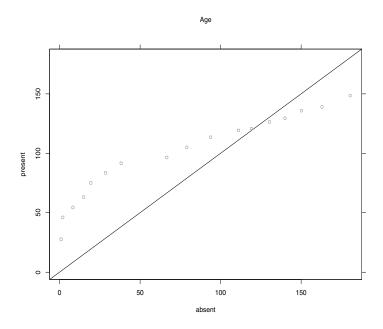
Figure 5.32: The QQ Plot dialog.

The kyphosis data set has 81 rows representing data on 81 children who have had corrective spinal surgery. The outcome Kyphosis is a binary variable, and the other three columns Age, Number, and Start, are numeric. Kyphosis is a post-operative deformity which is present in some children receiving spinal surgery. We are interested in examining whether the child's age, the number of vertebrae operated on, or the starting vertebra influence the likelihood of the child having a deformity. As an exploratory tool, we test whether the distributions of Age, Number, and Start are the same for the children with and without kyphosis. To do this, we create applots for each of the variables.

- 1. Open the **QQ Plot** dialog.
- 2. Type kyphosis in the **Data Set** field.
- 3. Select Kyphosis as the **Category**.
- 4. Select Age as the **Value**. Click on the **Titles** tab and type Age for the **Main Title**. Click **Apply**.
- 5. Click on the **Data** tab and select Number as the **Value**. Change the **Main Title** to Number and click **Apply**.
- 6. Click on the **Data** tab and select Start as the **Value**. Change the **Main Title** to Start and click **OK**.

By default, Spotfire S+ includes a reference line in qqplots. To omit the line from a graph, deselect the **Include Reference Line** option in the **Plot** page of the dialog.

The three qqplots appear in separate **Graph** windows. The only variable that clusters near the straight line drawn in the qqplots is Age, as shown in Figure 5.33. This suggests that the Age values corresponding to the two levels in Kyphosis come from roughly the same distribution. In other words, the children with and without kyphosis do not differ significantly in the distribution of their ages. On the other hand, the children do differ significantly in the distributions of how many vertebrae were involved in the operation, as well as which vertebra was the starting vertebra.



**Figure 5.33:** Normal applot of Age, for the two groups in the binary Kyphosis variable.

# VISUALIZING THREE-DIMENSIONAL DATA

Three-dimensional data have three columns, or *variables*, of univariate data, and the relationships between variables form a surface in 3D space. Because the depth cues in three-dimensional plots are sometimes insufficient to convey all of the information, special considerations must be made when visualizing three-dimensional data. Instead of viewing the surface alone, we can analyze projections, slices, or rotations of the surface. In this section, we examine a number of basic plot types useful for exploring a three-dimensional data object.

- **Contour Plot**: uses contour lines to represent heights of three-dimensional data in a flat, two-dimensional plane.
- Level Plot: uses colors to represent heights of threedimensional data in a flat, two-dimensional plane. Level plots and contour plots are essentially identical, but they have defaults that allow you to view a particular surface differently.
- **Surface Plot**: approximates the shape of a data set in three dimensions.
- Cloud Plot: displays a three-dimensional scatter plot of points.

# **Contour Plots**

A *contour plot* is a representation of three-dimensional data in a flat, two-dimensional plane. Each contour line represents a height in the *z* direction from the corresponding three-dimensional surface. Contour plots are often used to display data collected on a regularly-spaced grid; if gridded data is not available, interpolation is used to fit and plot contours.

# Creating a contour plot

From the main menu, choose **Graph** ► **Three Variables** ► **Contour Plot**. The **Contour Plot** dialog opens, as shown in Figure 5.34.

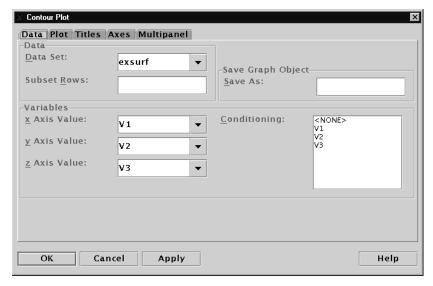


Figure 5.34: The Contour Plot dialog.

The exsurf data set has 1271 rows and 3 columns: V1, V2, and V3. It is an example data set that is useful for demonstrating the functionality of three-dimensional plots over a regular grid. In this example, we use contour plots to explore the shape of the exsurf data.

- 1. Open the **Contour Plot** dialog.
- 2. Type exsurf in the **Data Set** field.
- 3. Select V1 as the x Axis Value, V2 as the y Axis Value, and V3 as the z Axis Value.
- 4. Click **Apply** to leave the dialog open.

The result is shown in Figure 5.35.

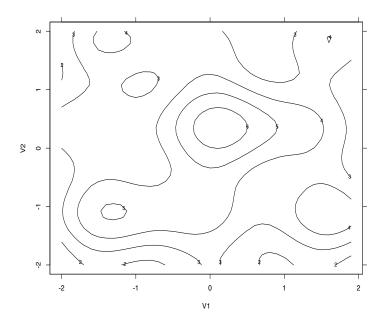


Figure 5.35: Contour plot of the exsurf data.

By default, Spotfire S+ uses 7 slices through the three-dimensional surface to produce the lines in a contour plot. If you want to increase or decrease the number of contour lines, click on **Plot** tab in the open **Contour Plot** dialog and enter a new value for the **Number of Cuts**. The **Use Pretty Contour Levels** option determines whether the contour lines are chosen at rounded *z* values, which allows them to be labelled clearly. When you are finished experimenting, click **OK** to close the dialog.

# **Level Plots**

A *level plot* is essentially identical to a contour plot, but it has default options that allow you to view a particular surface differently. Like contour plots, level plots are representations of three-dimensional data in flat, two-dimensional planes. Instead of using contour lines to indicate heights in the *z* direction, however, level plots use colors. Specifically, level plots include color fills and legends by default, and they do not include contour lines or labels.

#### Creating a level plot

From the main menu, choose **Graph** ▶ **Three Variables** ▶ **Level Plot**. The **Level Plot** dialog opens, as shown in Figure 5.36.

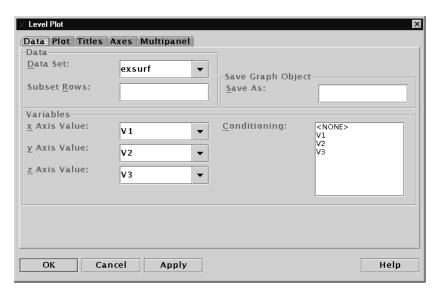


Figure 5.36: The Level Plot dialog.

#### **Example**

In this example, we use level plots to explore the shape of the exsurf data set.

- 1. Open the **Level Plot** dialog.
- 2. Type exsurf in the **Data Set** field.
- 3. Select V1 as the x Axis Value, V2 as the y Axis Value, and V3 as the z Axis Value.
- 4. Click **OK**.

A **Graph** window appears that displays the level plot and its corresponding legend.

#### **Surface Plots**

A *surface plot* is an approximation to the shape of a three-dimensional data set. Surface plots are used to display data collected on a regularly-spaced grid; if gridded data is not available, interpolation is used to fit and plot the surface.

#### Creating a surface plot

From the main menu, choose **Graph** ▶ **Three Variables** ▶ **Surface Plot**. The **Surface Plot** dialog opens, as shown in Figure 5.37.

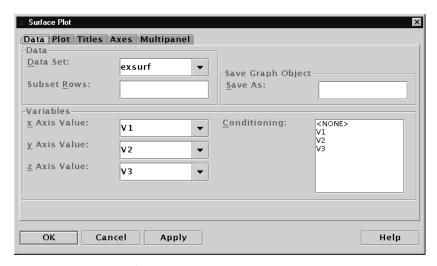


Figure 5.37: The Surface Plot dialog.

### Example

In this example, we create a surface plot of the exsurf data set.

- 1. Open the **Surface Plot** dialog.
- 2. Type exsurf in the **Data Set** field.
- 3. Select V1 as the x Axis Value, V2 as the y Axis Value, and V3 as the z Axis Value.
- 4. Click **Apply** to leave the dialog open.

The result is shown in Figure 5.38.

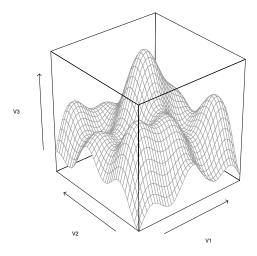


Figure 5.38: Surface plot of the exsurf data.

The arrows along the axes in Figure 5.38 indicate the direction of increasing values for each of the variables. To include tick marks instead of arrows, click on the **Axes** tab in the open **Surface Plot** dialog and check the **Include Tick Marks and Labels** box.

By default, Spotfire S+ rotates a surface plot 40 degrees about the z axis and -60 degrees about the x axis before displaying it. To change this setting, enter new values in the **Rotation** fields; rotating each axis 0 degrees results in a view from the top of the surface, looking down in the x-y plane. The **Distance Factor** controls the distance from the surface to the viewer. A distance factor of 0 implies the viewer is right at the object, and a factor of 1 implies the viewer is infinitely far away. The **Zoom Factor** controls the overall scaling for the drawn surface. Zoom values larger than 1 enlarge the object, and values less than 1 compress the object.

If you would like to create a surface plot with colors, click on the **Plot** tab in the open **Surface Plot** dialog and check the **Include Fills** box. Click **OK** to close the dialog, and a new **Graph** window appears that displays the changes you made.

#### **Cloud Plots**

A *cloud plot* is a three-dimensional scatter plot of points. Typically, a static 3D scatter plot is not effective because the depth cues of single points are insufficient to give a strong 3D effect. On some occasions, however, cloud plots can be useful for discovering simple characteristics about the three variables.

#### Creating a cloud plot

From the main menu, choose **Graph** ▶ **Three Variables** ▶ **Cloud Plot**. The **Cloud Plot** dialog opens, as shown in Figure 5.39.

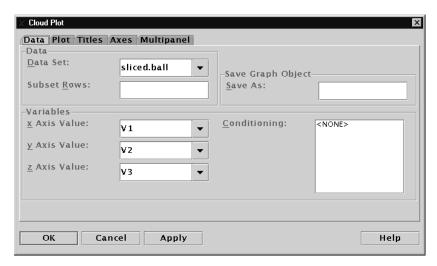


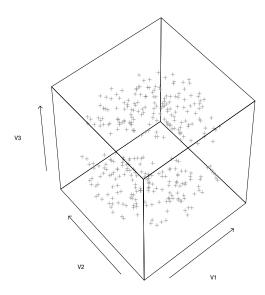
Figure 5.39: The Cloud Plot dialog.

#### **Example**

The sliced.ball data set contains three variables that comprise a set of points uniformly distributed in a three-dimensional sphere, except that a central slice of the points has been removed. The removed slice is oriented so that all two-dimensional projections of the data appear to be uniformly distributed over a disk. In addition, the slice is not visible in the initial three-dimensional view. In this example, we discover the location of the slice by rotating a cloud plot.

- 1. Open the **Cloud Plot** dialog.
- 2. Type sliced.ball in the **Data Set** field.
- 3. Select V1 as the **x Axis Value**, V2 as the **y Axis Value**, and V3 as the **z Axis Value**. Click **Apply** to leave the dialog open.

Note that the removed slice of data points is not visible in the initial graph. To rotate the scatter plot, click on the **Axes** tab in the open **Cloud Plot** dialog. The options in the **Axes** tab are identical to those in the **Surface Plot** dialog. Experiment with different **Rotation** values, clicking **Apply** each time you enter a new set of numbers. Each time you click **Apply**, a new **Graph** window appears displaying the rotated view of the surface. In particular, the values of -42, 0, and 40 clearly show the missing slice of data points, as displayed in Figure 5.40. When you are finished experimenting, click **OK** to close the dialog.



**Figure 5.40:** Cloud plot of the sliced.ball data set, showing the missing slice of data points.

# **VISUALIZING MULTIDIMENSIONAL DATA**

In the previous sections, we discussed visual tools for simple one-, two-, and three-dimensional data sets. With lower-dimensional data, all of the basic information in the data may be easily viewed in a single set of plots. Different plots provide different types of information, but deciding which plots to use is fairly straightforward.

With multidimensional data, however, visualization is more involved. In addition to univariate and bivariate relationships, variables may have interactions such that the relationship between any two variables changes depending on the remaining variables. Standard one- and two-variable plots do not allow us to look at interactions between multiple variables, and must therefore be complemented with techniques specifically designed for multidimensional data. In this section, we discuss both standard and novel visualization tools for multidimensional data.

- Scatterplot Matrix: displays an array of pairwise scatter plots illustrating the relationship between any pair of variables.
- **Parallel Plot**: displays the variables in a data set as horizontal panels, and connects the values for a particular observation with a set of line segments.

Two additional techniques for visualizing multidimensional data are grouping variables and multipanel conditioning. We briefly discussed both of these tools in the section Scatter Plots, and we intersperse more detailed examples below. The conditioning options that we discuss are not specific to scatter plots, but are available in most dialogs under the **Graph** menu. You can therefore use the options to create multiple histograms, box plots, etc., conditioned on the value of a particular variable in your data set.

# Scatterplot Matrices

A *scatterplot matrix* is a powerful graphical tool that enables you to quickly visualize multidimensional data. It is an array of pairwise scatter plots illustrating the relationship between any pair of variables in a multivariate data set. Often, when faced with the task of analyzing data, the first step is to become familiar with the data. Generating a scatterplot matrix greatly facilitates this process.

#### Creating a scatterplot matrix

From the main menu, choose **Graph** ▶ **Multiple Variables** ▶ **Scatterplot Matrix**. The **Scatterplot Matrix** dialog opens, as shown in Figure 5.41.

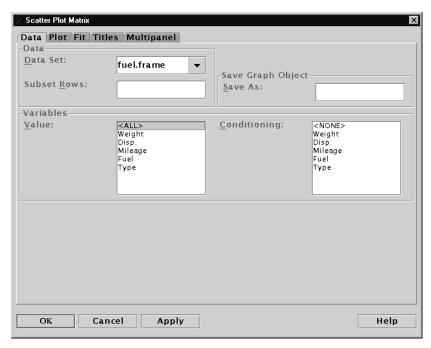


Figure 5.41: The Scatterplot Matrix dialog.

#### Example

In this example, we create a scatterplot matrix of the fuel.frame data.

- 1. Open the **Scatterplot Matrix** dialog.
- 2. Type fuel.frame in the **Data Set** field.
- 3. Select  $\langle ALL \rangle$  in the **Variables** box to create a  $5 \times 5$  scatterplot matrix that includes all variables.
- 4. Click **Apply** to leave the dialog open.

The result is shown in Figure 5.42.

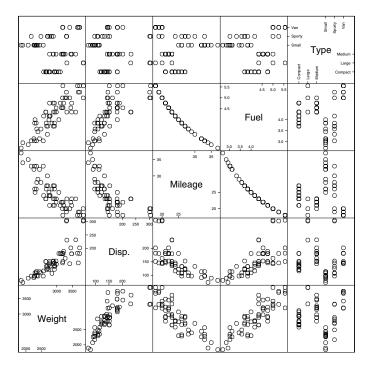


Figure 5.42: Scatterplot matrix of the fuel. frame data. A number of strong relationships appears.

From the figure, you can immediately see a number of strong linear relationships. For example, the weight of a car and its fuel consumption have a positive linear relationship: as Weight increases, so does Fuel. Note that the factor variable Type has been converted to a numeric variable and plotted. The six levels of Type (Compact, Large, Medium, Small, Sporty, and Van) simply take the values 1 through 6 in this conversion.

The **Scatterplot Matrix** dialog contains the same options as the **Scatter Plot** dialog for grouping variables, fitting lines, and smoothing. Thus, you can add curve fits or distinguish the levels of a grouping variable in each of the panels of a scatterplot matrix. For example, to add least squares line fits to each of the plots in Figure 5.42, click on the **Fit** tab in the open **Scatterplot Matrix** dialog. Select **Least Squares** as the **Regression Type** and click **OK**. As an

additional example, the following steps create a matrix of the four numeric variables in fuel.frame, distinguishing the different levels of Type in each scatter plot:

- 1. Open the **Scatterplot Matrix** dialog.
- 2. Type fuel.frame in the **Data Set** field.
- 3. CTRL-click to highlight Weight, Disp., Mileage, and Fuel in the **Variables** box.
- Click on the Plot tab. Select Type in the Group Variable list, and check the boxes for Vary Symbol Style and Include Legend.
- 5. Click **OK**.

A new **Graph** window appears displaying the scatterplot matrix.

#### **Parallel Plots**

A *parallel coordinates plot* displays the variables in a data set as horizontal panels, and connects the values for a particular observation with a set of line segments. These kinds of plots show the relative positions of observation values as coordinates on parallel horizontal panels.

#### Creating a parallel plot

From the main menu, choose **Graph** ▶ **Multiple Variables** ▶ **Parallel Plot**. The **Parallel Plot** dialog opens, as shown in Figure 5.43.

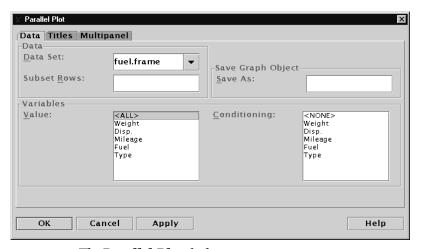


Figure 5.43: The Parallel Plot dialog.

In this example, we create a parallel coordinates plot of the fuel.frame data.

- 1. Open the **Parallel Plot** dialog.
- 2. Type fuel.frame in the **Data Set** field.
- 3. Select **<ALL>** in the **Variables** box to create a 5-panel plot that includes all variables.
- 4. Click **OK**.

The result is shown in Figure 5.44.

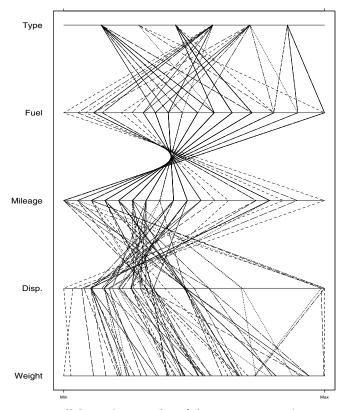


Figure 5.44: Parallel coordinates plot of the fuel. frame data set.

# Multipanel Trellis Graphics

Trellis graphics allow you to view relationships between different variables in your data set through conditioning. Suppose you have a data set based on multiple variables, and you want to see how plots of two variables change in relation to a third "conditioning" variable. With Trellis graphics, you can view your data in a series of panels, where each panel contains a subset of the original data divided into intervals of the conditioning variable. When a conditioning variable is categorical, Spotfire S+ generates plots for each level. When a conditioning variable is numeric, conditioning is automatically carried out on the sorted unique values; each plot represents either an equal number of observations or an equal range of values.

A wide variety of graphs can be conditioned using Trellis graphics, and many of the dialogs under the **Graph** menu include Trellis display options. In the section Scatter Plots, we illustrate how conditioning can be used with scatter plots to reveal relationships in multivariate data. In this section, we present another detailed example that shows the functionality of Trellis graphics.

#### Example

The barley data set contains observations from a 1930s agricultural field trial that studied barley crops. At six sites in Minnesota, ten varieties of barley were grown for each of two years, 1931 and 1932. The data are the yields for all combinations of site, variety, and year, so there are a total of  $6 \times 10 \times 2 = 120$  observations. The data first appeared in a 1934 report published by the experimenters, and has been analyzed and re-analyzed ever since. R.A. Fisher presented the data for five of the sites in his classic book, *The Design of Experiments* (1971). Publication in the book made the data famous; many other statisticians subsequently analyzed the data, usually to illustrate a new statistical method.

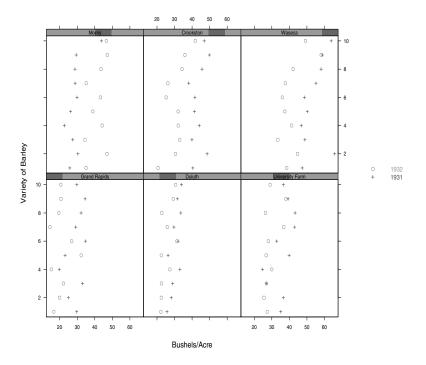
In the early 1990s, Bill Cleveland of AT&T (now Lucent Technologies) analyzed the barley data using Trellis graphics. The results were quite surprising, and the basis of Cleveland's analysis is repeated here for illustrative purposes. For historical details about the barley experiment, see the Cleveland (1993) reference.

#### **Exploratory data analysis**

We are interested in exploring how barley yield varies based on combinations of the variety, year, and site variables. Trellis graphics are particularly useful for displaying effects and interactions between variables. We create a scatter plot of yield and variety conditioned on site, and vary the plotting symbol by year. Because site is a factor variable with six levels, our Trellis graph will have six panels labeled with the names of the sites. In addition, year is a factor variable with two levels, so each panel in our Trellis graph will include two different plotting symbols.

- Select Graph ► Scatter Plot to open the Scatter Plot dialog.
- 2. Type barley in the **Data Set** field. Select yield as the **x Axis Value** and variety as the **y Axis Value**. Highlight site in the **Conditioning** box.
- Click on the Plot tab and select year as the Group Variable.
   Check the boxes for Vary Symbol Style and Include Legend.
- 4. Click on the **Titles** tab. Type **Bushels/Acre** for the **X Axis Label** and **Variety of Barley** for the **Y Axis Label**.
- 5. Click on the **Axes** tab and select **Horizontal** for the **Tick Marks Label Orientation**. This option places horizontal tick labels on both the *x* and *y* axes. By default, labels are parallel to the axes, so that *x* axis tick labels are horizontal and *y* axis labels are vertical.
- 6. Click **Apply** to leave the dialog open.

The resulting graph is shown in Figure 5.45.



**Figure 5.45:** Unformatted Trellis plot of barley yields for 1931 and 1932.

To simplify the comparison of barley yields across sites, we make two changes to the layout of the panels in Figure 5.45:

- First, we stack the six panels in one column. To do this, click on the Multipanel Conditioning tab in the open Scatter Plot dialog. Type 1 for the # of Columns and 6 for the # of Rows.
- 2. Next, we set the aspect ratio of each panel to 0.5. To do this, click on the **Axes** tab in the open **Scatter Plot** dialog. Set the **Aspect Ratio** to be a **Specified Value** and type 0.5 as the **Ratio Value**.

Click **OK** to close the dialog, and a new **Graph** window appears that displays the updated set of plots. The final Trellis graphic looks similar to the one shown in Figure 5.46.

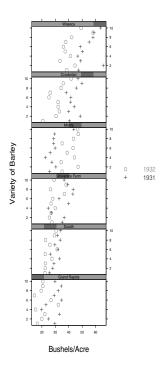


Figure 5.46: Formatted Trellis plot of barley yields for 1931 and 1932.

Examine Figure 5.46 to find a discrepancy in the barley data. It appears in the Morris panel: for all other sites, 1931 has significantly higher overall yields than 1932, but the reverse is true at the Morris site. More importantly, the amount by which the 1932 yield exceeds the 1931 yield at Morris is similar to the amounts by which 1931 exceeds 1932 at the other five sites. Either an extraordinary natural event (such as disease or a local weather anomaly) produced a strange coincidence, or the years for the Morris data were inadvertently reversed. More Trellis graphics, statistical modeling of the data, and some background checks on the experiment led to the conclusion that the data are in error. But it was a Trellis graphic like the one in Figure 5.46 that originally led Cleveland to this conclusion.

# TIME SERIES

Time series are multivariate data sets that are associated with a set of ordered positions, where the positions are an important feature of the values and their analysis. These data can arise in many contexts. For example, in the financial marketplace, trading tickers record the price and quantity of each trade at particular times throughout the day. Such data can be analyzed to assist in making market predictions. This section discusses three plots that are helpful in visualizing time series data.

- Line Plots: successive values of the data are connected by straight lines.
- High-Low Plots: vertical lines are used to indicate the daily, monthly, or yearly extreme values in a time series, and hatch marks are drawn on the lines to represent the opening and closing values. This type of plot is most often used to display financial data.
- **Stacked Bar Plots**: multiple *y* values determine segment heights in a bar chart.

Note that the dialogs for these time series plots recognize objects of class "timeSeries" only, and do not accept data frames, matrices, or vectors. For this reason, we periodically drop to the **Commands** window in this section to create objects that are accepted by the menu options.

# **Line Plots**

With time series data, it is often useful to view a *line plot*, where the successive values of the data are connected by straight lines. By using straight line segments to connect the points, you can see more clearly the overall trend or shape in the ordered data values.

# Creating a line plot

From the main menu, choose **Graph** ▶ **Time Series** ▶ **Line Plot**. The **Time Series Line Plot** dialog opens, as shown in Figure 5.47.

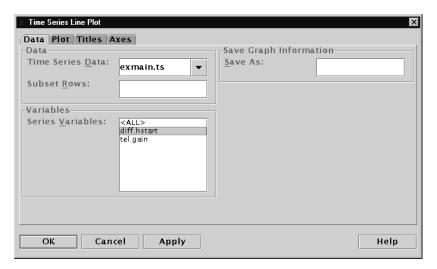


Figure 5.47: The Time Series Line Plot dialog.

In the section Scatter Plots on page 127, we created the exmain data set. The variables in exmain are both time series: tel.gain and diff.hstart contain values recorded once per year on the first of January for the 14 years beginning in 1971. In this example, we use the **Time Series Line Plot** dialog to analyze these variables.

If you have not done so already, create the exmain data set with the instructions given on page 129. The exmain data is stored in an object of class "data.frame". We must therefore convert it to class "timeSeries" before it can be recognized by the dialogs under the **Time Series** menu. To do this, type the following in the **Commands** window:

```
> exmain.ts <- timeSeries(exmain,
+ from = timeCalendar(d=1, m=1, y=1971), by = "years")</pre>
```

The from and by arguments in the call to timeSeries define the appropriate units for the time series data.

#### **Exploratory data analysis**

To begin our analysis, we create a line plot of diff.hstart:

- 1. Open the **Time Series Line Plot** dialog.
- 2. Type exmain.ts in the **Time Series Data** field.
- 3. Highlight diff. hstart in the **Series Variables** box.
- 4. Click on the **Titles** tab and type **New Housing Starts** for the **Y Axis Label**.
- 5. Click **Apply** to leave the dialog open.

The result is shown in Figure 5.48. The fourteen values in diff.hstart, representing observations made in the years 1971-1984, are plotted sequentially.

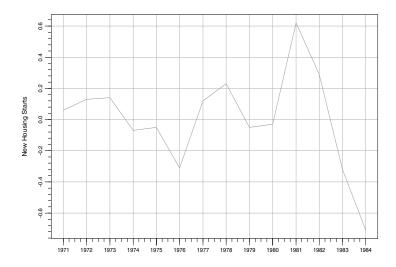


Figure 5.48: A time series line plot of diff. hstart.

By default, Spotfire S+ includes a reference grid in time series line plots. To leave the grid out of your graphics, click on the **Axes** tab in the open **Time Series Line Plot** dialog and deselect the **Include Reference Grid** option. To include both points and lines in the graph, click on the **Plot** tab and select **Both Points & Lines** from the **Type** list. When you are finished experimenting, click **OK** to close the dialog.

Now that you have seen the time series behavior of diff.hstart, you may be interested in seeing that of tel.gain as well. The steps below place line plots of both variables on the same set of axes:

- 1. Open the **Time Series Line Plot** dialog.
- 2. Type exmain.ts in the **Time Series Data** field.
- 3. CTRL-click to highlight diff.hstart and tel.gain in the **Series Variables** box.
- 4. Click on the **Plot** tab and select **Both Points & Lines** from the **Type** list. Check the boxes for **Vary Line Style** and **Include Legend**.
- Click on the **Titles** tab and type **The Main Gain Data** as the **Main Title**.
- 6. Click **OK**.

The result is shown in Figure 5.49.

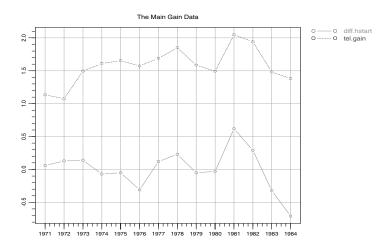


Figure 5.49: Time series line plots of tel.gain and diff.hstart.

Viewing line plots of tel.gain and diff.hstart is a simple yet powerful complement to viewing scatter plots of these variables alone. Using both plot types gives you a more complete understanding of the data. Earlier in this chapter, we determined that the first two observations in exmain were outliers. The time series line plots reveal that the tel.gain values during the first two years

were the smallest during the 14-year study. At the same time, the diff. hstart values during the first two years were near their overall average for the 14-year time period. Furthermore, notice that except for the first four years, there is a striking correlation pattern between the two variables: whenever one increases, so does the other. In comparison to the final years of the study, it appears that the relative behavior of the two variables is different during the 1971-1974 time period.

**High-Low Plots** A high-low plot typically displays lines indicating the daily, monthly, or yearly extreme values in a time series. These kinds of plots can also include average, opening, and closing values, and are referred to as high-low-open-close plots in these cases. Meaningful high-low plots can thus display from three to five columns of data, and illustrate simultaneously a number of important characteristics about time series data. Because of this, they are most often used to display financial data.

> In typical high-low plots, vertical lines are drawn to indicate the range of values in a particular time unit (i.e., day, month, or year). If opening and closing values are included in the plot, they are represented by small horizontal hatch marks on the lines: leftpointing hatch marks indicate opening values and right-pointing marks indicate closing values. One variation on the high-low plot is the *candlestick plot*. Where typical high-low plots display the opening and closing values of a financial series with lines, candlestick plots use filled rectangles. The color of the rectangle indicates whether the difference is positive or negative. In Spotfire S+, white rectangles represent positive differences, when closing values are larger than opening values. Blue rectangles indicate negative differences, when opening values are larger than closing values.

# Creating a high-low plot

From the main menu, choose **Graph** ▶ **Time Series** ▶ **High-Low Plot**. The **Time Series High-Low Plot** dialog opens, as shown in Figure 5.50.

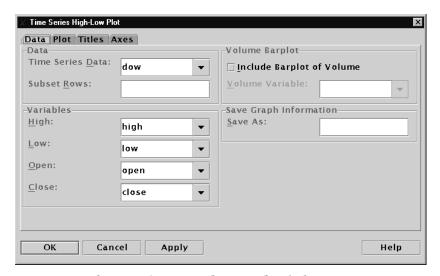


Figure 5.50: The Time Series High-Low Plot dialog.

The djia data set is a multivariate time series taken from the Ohio State University web site. It contains the high, low, opening, and closing prices, as well as the daily trading volume, for the Dow Jones Industrial Average. The data set has the closing price only from 1915 through September 1928, and it contains the high, low, and closing prices from October 1928 through March 9, 1984. The high, low, opening, and closing prices from March 12, 1984 through December 1986 are included. The high, low, opening, and closing prices, as well as the trading volume, are included for January 1987 through February 1990. In this example, we create high-low plots for a portion of the djia data set.

# Setting up the data

Suppose we want to analyze financial data for a period of time surrounding the stock market crash of 1987. The command below uses the positions function to extract a subset of the djia time series that corresponds to the period between September 1, 1987 and November 1, 1987.

```
> dow <- djia[positions(djia) >= timeDate("09/01/87") &
+ positions(djia) <= timeDate("11/01/87"), ]
> dow
                       high
  Positions
               open
                                low
                                      close volume
09/01/1987 2666.77 2695.47 2594.07 2610.97 193450
 09/02/1987 2606.98 2631.06 2567.76 2602.04 199940
 09/03/1987 2621.81 2642.22 2560.11 2599.49 165200
 09/04/1987 2604.11 2617.19 2556.28 2561.38 129070
 09/07/1987 2561.38 2561.38 2561.38 2561.38
 09/08/1987 2551.18 2571.43 2493.78 2545.12 242880
 09/09/1987 2544.48 2570.63 2522.80 2549.27 164910
 09/10/1987 2578.13 2595.50 2549.43 2576.05 179790
 09/11/1987 2586.26 2625.96 2575.41 2608.74 178020
 09/14/1987 2624.36 2634.57 2587.85 2613.04 154380
```

#### **Exploratory data analysis**

Create a high-low plot of the dow time series as follows:

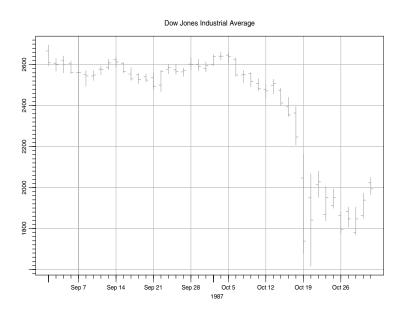
- 1. Open the **Time Series High-Low Plot** dialog.
- 2. Type dow in the **Time Series Data** field.
- 3. Select high in the **High** list and low in the **Low** list.
- 4. Click **Apply** to leave the dialog open.

To place lines on the graph for the opening and closing prices in the dow time series, click on the **Data** tab in the open **Time Series High-Low Plot** dialog. Select open in the **Open** list and close in the **Close** list, and then click **Apply**. The plot is shown in Figure 5.51.

To include a panel with a barplot of the trading volume, check the **Include Barplot of Volume** box and select volume as the **Volume Variable**. If you prefer candlestick-style indicators instead of lines in high-low-open-close plots, click on the **Plot** tab and select **Candlestick** from the **Type** list.

It is also possible to superpose a moving average line on a high-low plot or candlestick plot. To do this, click on the **Plot** tab in the open **Time Series High-Low Plot** dialog, highlight **Specified Number** in the **Days in Average** box, and type 5 for the **Specified Number**. In our example, this computes a 5-business-day moving average of the closing stock prices in the dow time series. By default, the moving averages are calculated for the closing prices only; if closing values are not included in the data, moving averages are not plotted.

When you are finished experimenting, click **OK** to close the dialog.



**Figure 5.51:** High-low-open-close plot for a portion of the djia time series corresponding to the 1987 stock market crash.

# Stacked Bar Plots

A *stacked bar plot* is a chart in which multiple *y* values can represent segment heights for the bar at a single *x* value.

# Creating a stacked bar plot

From the main menu, choose **Graph** ▶ **Time Series** ▶ **Stacked Bar Plot**. The **Time Series Stacked Bar Plot** dialog opens, as shown in Figure 5.52.

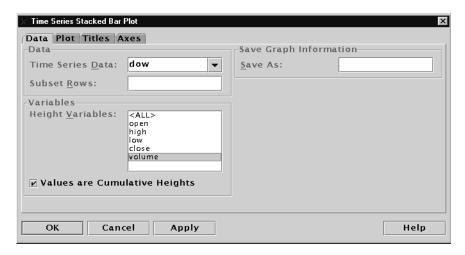


Figure 5.52: The Time Series Stacked Bar Plot dialog.

In this example, we create a bar plot of the trading volume data from the dow time series. If you have not done so already, create the dow time series with the instructions given on page 200. The following steps generate the bar plot displayed in Figure 5.53.

- 1. Open the **Time Series Stacked Bar Plot** dialog.
- 2. Type dow in the **Time Series Data** field.
- 3. Select volume in the **Height Variables** list.
- 4. Click **OK**.

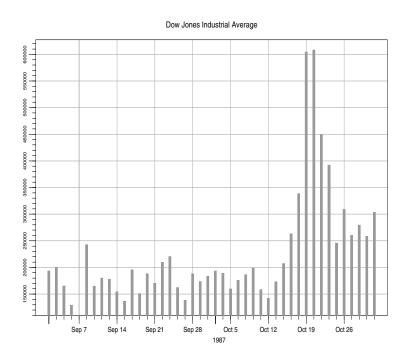


Figure 5.53: Bar plot of the trading volume data in the dow time series.

# REFERENCES

Chambers, J.M., Cleveland, W.S., Kleiner, B. & Tukey, P.A. (1983). *Graphical Methods for Data Analysis*. Belmont, California: Wadsworth.

Cleveland, W.S. (1979). Robust locally weighted regression and smoothing scatterplots. *Journal of the American Statistical Association*, 74: 829-836.

Cleveland, W.S. (1985). *The Elements of Graphing Data*. Monterrey, California: Wadsworth.

Cleveland, W.S. (1993). *Visualizing Data*. Murray Hill, New Jersey: AT&T Bell Laboratories.

Fisher, R.A. (1971). The Design of Experiments (9th ed.). New York: Hafner.

Friedman, J.H. (1984). *A Variable Span Smoother*. Technical Report No. 5, Laboratory for Computational Statistics. Department of Statistics, Stanford University, California.

Venables, W.N. & Ripley B.D. (1999). *Modern Applied Statistics with S-PLUS* (3rd ed.). New York: Springer.

# Chapter 5 Menu Graphics

# **STATISTICS**

	7
	1
l	

Introduction	210
Overview	211
Basic Procedure	213
Dialogs	213
Dialog Fields	214
Plotting From the Statistics Dialogs	215
Statistics Options	215
Saving Results From an Analysis	215
Summary Statistics	216
Summary Statistics	216
Crosstabulations	218
Correlations	221
Compare Samples	223
One-Sample Tests	223
Two-Sample Tests	234
K-Sample Tests	245
Counts and Proportions	255
Power and Sample Size	269
Normal Mean	269
Binomial Proportion	271
Experimental Design	274
Factorial	274
Orthogonal Array	275
Design Plot	276
Factor Plot	277
Interaction Plot	279
Regression	281
Linear Regression	282
Robust MM Regression	288
Robust LTS Regression	290

# Chapter 6 Statistics

Stepwise Linear Regression	291
Generalized Additive Models	294
Local (Loess) Regression	295
Nonlinear Regression	296
Generalized Linear Models	301
Log-Linear (Poisson) Regression	302
Logistic Regression	303
Probit Regression	306
Analysis of Variance	308
Fixed Effects ANOVA	308
Random Effects ANOVA	309
Multiple Comparisons	311
Mixed Effects	314
Linear	314
Nonlinear	315
Generalized Least Squares	318
Linear	318
Nonlinear	319
Survival	322
Nonparametric Survival	322
Cox Proportional Hazards	323
Parametric Survival	325
Life Testing	326
Tree	328
Tree Models	328
Tree Tools	329
Compare Models	333
Cluster Analysis	336
Compute Dissimilarities	336
K-Means Clustering	337
Partitioning Around Medoids	339
Fuzzy Partitioning	340
Agglomerative Hierarchical Clustering	342
Divisive Hierarchical Clustering	344
Monothetic Clustering	346
Multivariate	348
Discriminant Analysis	348
Factor Analysis	349

Principal Components MANOVA	351 353
Quality Control Charts	355
Continuous Grouped	355
Continuous Ungrouped	356
Counts and Proportions	358
Resample	360
Bootstrap Inference	360
Jackknife Inference	362
Smoothing	364
Kernel Smoother	365
Local Regression (Loess)	365
Spline Smoother	366
Supersmoother	366
Examples	367
Time Series	368
Autocorrelations	368
ARIMA	371
Lag Plot	373
Spectrum Plot	374
References	375

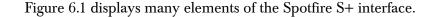
# INTRODUCTION

The power of Spotfire S+ comes from the integration of its graphics capabilities with its statistical analysis routines. In other chapters throughout this manual, we introduce Spotfire S+ graphics. In this chapter, we show how statistical procedures are performed in Spotfire S+.

It is not necessary to read this entire chapter before you perform a statistical analysis. Once you've acquired a basic understanding of the way statistics are performed, you can refer directly to a section of interest.

We begin this chapter by presenting general information on using the statistics dialogs, and devote the remaining sections to descriptions and examples for each of these dialogs. Wherever possible, we complement statistical examples with plots generated by the graphics dialogs. However, not all of the Spotfire S+ functionality has been built into the menu options, and it is therefore necessary to use command line functions in some sections.

#### **Overview**



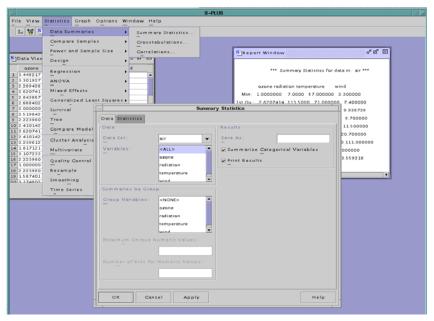


Figure 6.1: Statistics-related menus and windows.

- Statistics menu: The Statistics menu gives you access to nearly all of the statistical procedures available in Spotfire S+. The procedures are logically grouped, with submenus that allow you to precisely specify the procedure you want to use. For example, in Figure 6.1 the menu tree for summary statistics is shown. It is selected by choosing Statistics ▶ Data Summaries ▶ Summary Statistics.
- Statistics dialogs: The open dialog in Figure 6.1 is entitled Summary Statistics, and is used to specify which data summaries to calculate.
- **Data Viewer**: The open window on the left in Figure 6.1 is a **Data** viewer, which you can use to see a data set in its entirety. The **Data** viewer is not a data editor, however, and you cannot use it to modify or create a new data set.

- **Report Window**: The **Report** window displays the results of statistical analyses. In Figure 6.1, a **Report** window shows the results of the chosen summary statistics. In addition, any error, warning, or informational message generated by a statistics dialog is printed in the **Report** window.
- Commands Window (not shown): The Commands window contains the Spotfire S+ command line prompt, which you can use to call S-PLUS functions that are not yet implemented in the menu options.
- **Graph Window** (not shown): A **Graph** window displays the graphics created from the statistics menus.

# Basic Procedure

The basic procedure for analyzing data is the same regardless of the type of analysis.

- Choose the statistical procedure (summary statistics, linear regression, ANOVA, etc.) you want to perform from the Statistics menu. The dialog corresponding to that procedure opens.
- 2. Select the data set, variables, and options for the procedure you have chosen. (These are slightly different for each dialog.) Click the **OK** or **Apply** button to conduct the analysis. If you click **OK**, the dialog closes when the graph is generated; if you click **Apply**, the dialog remains open.
- 3. Check for messages. If a message is generated, it appears in the **Report** window.
- 4. Check the result. If everything went well, the results of your analysis are displayed in the **Report** window. Some statistics procedures also generate plots.

If you want, you can change the variables, parameters, or options in the dialog and click **Apply** to generate new results. Spotfire S+ makes it easy to experiment with options and to try variations on your analysis.

# **Dialogs**

Most of the statistical functionality of Spotfire S+ can be accessed through the **Statistics** menus. The **Statistics** menu includes dialogs for creating data summaries and fitting statistical models. Many of the dialogs consist of tabbed pages that allow for a complete analysis, including model fitting, plotting, and prediction. Each dialog has a corresponding function that is executed using dialog inputs as values for function arguments. Usually, it is only necessary to fill in a few fields on the first page of a tabbed dialog to launch the function call.

# **Dialog Fields**

Many dialogs include a **Data Set** field. To specify a data set, you can either type its name directly in the **Data Set** field, or make a selection from the dropdown list. Note that the **Data Set** field recognizes objects of class "data.frame" only, and does not accept matrices, vectors, or time series. For this reason, we periodically drop to the **Commands** window in this chapter to create objects that are accepted by the menu options.

Most dialogs that fit statistical models include a **Subset Rows** field that you can use to specify only a portion of a data set. To use a subset of your data in an analysis, enter a S-PLUS expression in the **Subset Rows** field that identifies the rows to use. The expression can evaluate to a vector of logical values: true values indicate which rows to include in the analysis, and false values indicate which rows to drop. Alternatively, the expression can specify a vector of row indices. For example:

- The expression Species=="bear" includes only rows for which the Species column contains bear.
- The expression Age>=13 & Age<20 includes only rows that correspond to teenage values of the Age variable.
- The expression 1:20 includes the first 20 rows of the data.

To use all rows in a data set, leave the **Subset Rows** field blank.

Some dialogs require a **Formula**. To specify a formula, you can type one directly in the **Formula** field, or click the **Create Formula** button to bring up a dialog that builds a formula for you. Some dialogs, such as the **Generalized Additive Models** dialog, require special formulas; in these cases, the special terms available are listed in the **Formula Builder**.

Most dialogs have a **Save As** field that corresponds to the name of the object in which the results of the analysis are saved. Many of the modeling dialogs also have one or more **Save In** fields. The **Save In** field corresponds to the name of a data set in which new columns are saved. Examples of new columns include fitted values, residuals, predictions, and standard errors.

# Plotting From the Statistics Dialogs

Most of the statistics dialogs produce default plots that are appropriate for the analysis. Many have several plot options, usually on a separate **Plot** tab.

The **Options** menu contains a few options that affect the graphics you create from the statistics menus. In particular:

- The Options ➤ Dialog Options window includes a Create New Graph Window check box. If this box is selected, as it is by default, then a new Graph window is created each time you generate a statistics plot.
- The **Options** ▶ **Set Graph Colors** window allows you to select a color scheme for your graphics.
- The Options ➤ Graph Options window governs whether tabbed pages in Graph windows are deleted, preserved, or written over when a new plot is generated.

# Statistics Options

The **Options** ▶ **Dialog Options** window includes an **Echo Dialog Command** check box. If this box is selected, the command associated with a dialog action is printed before its output in the **Report** window. This allows you to copy and paste the commands used for your analyses into your own S-PLUS functions.

# Saving Results From an Analysis

A statistical model object may be created by specifying a name for the object in the **Save As** field of a dialog. Once the execution of a dialog function completes, the object shows up in your working database. You can then access the object from the **Commands** window. This allows you to do plotting and prediction for a model without relaunching an entire dialog.

# SUMMARY STATISTICS

One of the first steps in analyzing data is to create summaries. This can be done numerically through the **Summary Statistics**, **Crosstabulations**, and **Correlations and Covariances** dialogs.

- **Summary Statistics:** calculates summary statistics, such as the mean, median, variance, total sum, quartiles, etc.
- **Crosstabulations:** tabulates the number of cases for each combination of factors between your variables, and generates statistics for the table.
- **Correlations:** calculates correlations or covariances between variables.

These three procedures can be found under the **Statistics** ▶ **Data Summaries** menu.

# Summary Statistics

The **Summary Statistics** dialog provides basic univariate summaries for continuous variables, and it provides counts for categorical variables. Summaries may be calculated within groups based on one or more grouping variables.

# **Computing summary statistics**

From the main menu, choose **Statistics** ▶ **Data Summaries** ▶ **Summary Statistics**. The **Summary Statistics** dialog opens, as shown in Figure 6.2.

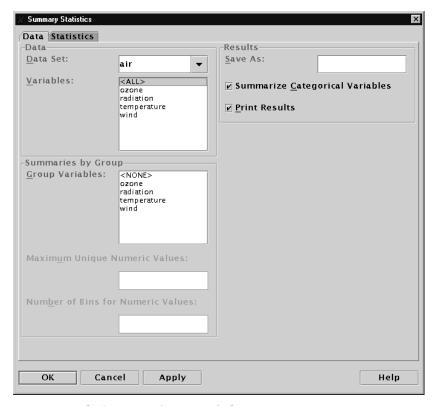


Figure 6.2: The Summary Statistics dialog.

We use the data set air. This data set measures the ozone concentration, wind speed, temperature, and radiation of 111 consecutive days in New York. In this example, we calculate summary statistics for these data.

- 1. Open the **Summary Statistics** dialog.
- 2. Type air in the **Data Set** field.
- 3. Select the variables you want summary statistics for in the **Variables** field. For this example, we choose **<ALL>** (the default).

- 4. Click on the **Statistics** tab to see the statistics available. For this example, select the **Variance** and **Total Sum** check boxes.
- 5. Make sure the **Print Results** check box is selected to ensure that the results are printed in the **Report** window.
- 6. Click **OK**. A **Report** window containing the following output is created, if one does not already exist:

***	Summary	Statistics	for data in:	air ***
	ozone	radiation	temperature	wind
Min:	1.00	7.00	57.00	2.30
1st Qu.:	2.62	113.50	71.00	7.40
Mean:	3.25	184.80	77.79	9.94
Median:	3.14	207.00	79.00	9.70
3rd Qu.:	3.96	255.50	84.50	11.50
Max:	5.52	334.00	97.00	20.70
Total N:	111.00	111.00	111.00	111.00
NA's :	0.00	0.00	0.00	0.00
Variance:	0.79	8308.74	90.82	12.67
Std Dev.:	0.89	91.15	9.53	3.56
Sum:	360.50	20513.00	8635.00	1103.20

7. If the above output is not displayed, check the **Report** window for error messages.

We are done. As you can see, calculating summary statistics is straightforward. Other statistical procedures use the same basic steps that we did in this example.

# Crosstabulations

The **Crosstabulations** dialog produces a table of counts for all combinations of specified categorical (factor) variables. In addition, it calculates cell percentages and performs a chi-square test for independence. The **Crosstabulations** dialog returns results in an ASCII formatted table.

The chi-square test for independence is useful when the data consist of the number of occurrences of an outcome for various combinations of categorical covariates. It is used to determine whether the number of occurrences is due to the marginal values of the covariates, or whether it is influenced by an interaction between covariates.

#### **Computing crosstabulations**

From the main menu, choose **Statistics Data Summaries Crosstabulations**. The **Crosstabulations** dialog opens, as shown in Figure 6.3.

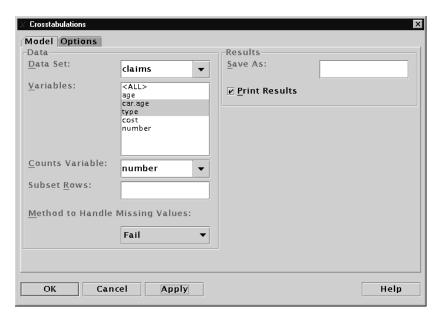


Figure 6.3: The Crosstabulations dialog.

#### Example

Consider the data set claims, which has the components age, car.age, type, cost, and number. The original data were taken from 8,942 insurance claims. The 128 rows of the claims data set represent all possible combinations of the three predictor variables (columns) age, car.age, and type. An additional variable, number, gives the number of claims in each cell. The outcome variable, cost, is the average cost of the claims.

We can use a contingency table to examine the distribution of the number of claims by car age and type. The corresponding test for independence tells us whether the effect of age upon the likelihood of a claim occurring varies by car type, or whether the effects of car age and type are independent.

To construct a contingency table for the claims data:

- 1. Open the **Crosstabulations** dialog.
- 2. Type claims in the **Data Set** field.
- 3. In the **Variables** field, click on car.age and then CTRL-click type. This selects both variables for the analysis.
- 4. In the **Counts Variable** field, scroll through the list of variables and select number.
- Click OK.

The table below appears in the **Report** window. Each cell in the table contains the number of claims for that car age and type combination, along with the row percentage, column percentage, and total percentage of observations falling in that cell. The results of the test for independence indicate that the percentage of observations in each cell is significantly different from the product of the total row percentage and total column percentage. Thus, there is an interaction between the car age and type, which influences the number of claims. That is, the effect of car age on the number of claims varies by car type.

4 - 7	538	1746	941	324	3549
	0.1516	0.4920	0.2651	0.0913	0.397
	0.4240	0.4491	0.3472	0.3014	
	0.0602	0.1953	0.1052	0.0362	
8-9	187	400	191	+   44	822
	0.2275	0.4866	0.2324	0.0535	0.092
	0.1474	0.1029	0.0705	0.0409	
	0.0209	0.0447	0.0214	0.0049	
10+	153	204	61	19	437
	0.3501	0.4668	0.1396	0.0435	0.049
	0.1206	0.0525	0.0225	0.0177	
	0.0171	0.0228	0.0068	0.0021	
ColTotl	+  1269	+  3888	+  2710	+  1075	++  8942
	•	0.43	•	•	į į
Test for independence of all factors Chi^2 = 588.2952 d.f.= 9 (p=0) Yates' correction not used					

# **Correlations**

The **Correlations and Covariances** dialog produces the basic bivariate summaries of correlations and covariances.

# **Computing correlations and covariances**

From the main menu, choose **Statistics** ▶ **Data Summaries** ▶ **Correlations**. The **Correlations** and **Covariances** dialog opens, as shown in Figure 6.4.

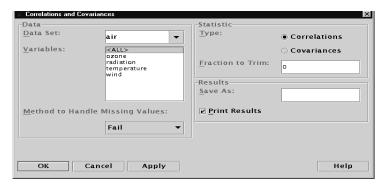


Figure 6.4: The Correlations and Covariances dialog.

In the section Summary Statistics on page 216, we looked at univariate summaries of the data set air. We now generate the correlations between all four variables of the data set. Here are the basic steps:

- 1. Open the **Correlations and Covariances** dialog.
- 2. Type air in the **Data Set** field.
- 3. Choose **<ALL>** in the **Variables** field.
- 4. Click **OK**.

The **Report** window displays the correlations between the four variables:

```
*** Correlation for data in: air ***

ozone radiation temperature wind
ozone 1.0000000 0.4220130 0.7531038 -0.5989278
radiation 0.4220130 1.0000000 0.2940876 -0.1273656
temperature 0.7531038 0.2940876 1.0000000 -0.4971459
wind -0.5989278 -0.1273656 -0.4971459 1.0000000
```

Note the strong correlation of 0.75 between ozone and temperature: as temperature increases, so do the ozone readings. The negative correlation of -0.60 between ozone and wind indicates that ozone readings decrease as the wind speed increases. Finally, the correlation of -0.50 between wind and temperature indicates that the temperature decreases as the wind increases (or that the temperature increases as the wind decreases).

# **COMPARE SAMPLES**

# One-Sample Tests

Spotfire S+ supports a variety of statistical tests for testing a hypothesis about a single population. Most of these tests involve testing a parameter against a hypothesized value. That is, the null hypothesis has the form  $H_0$ :  $\Theta = \Theta_0$ , where  $\Theta$  is the parameter of interest and  $\Theta_0$  is the hypothesized value of our parameter.

- One-sample t-test: a test for the population mean  $\mu$ . We test if the population mean is a certain value. For small data sets, we require that the population have a normal distribution.
- One-sample Wilcoxon signed-rank test: a nonparametric test for the population mean  $\mu$ . As with the t-test, we test if the population mean is a certain value, but we make no distributional assumptions.
- One-sample Kolmogorov-Smirnov goodness-of-fit test: a test to determine if the data come from a hypothesized distribution. This is the preferred goodness-of-fit test for a continuous variable.
- One-sample chi-square goodness-of-fit test: a test to see if the data come from a hypothesized distribution. This is the preferred goodness-of-fit test for a discrete variable.

# One-Sample t-Test

A *one-sample t-test* is used to test whether the mean for a variable has a particular value. The main assumption in a t-test is that the data come from a Gaussian (normal) distribution. If this is not the case, then a nonparametric test, such as the Wilcoxon signed-rank test, may be a more appropriate test of location.

### Performing a one-sample t-test

From the main menu, choose **Statistics** ▶ **Compare Samples** ▶ **One Sample** ▶ **t Test**. The **One-sample t Test** dialog opens, as shown in Figure 6.5.

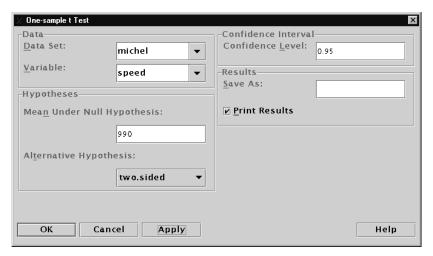


Figure 6.5: The One-sample t Test dialog.

In 1876, the French physicist Cornu reported a value of 299,990 km/sec for c, the speed of light. In 1879, the American physicist A.A. Michelson carried out several experiments to verify and improve Cornu's value. Michelson obtained the following 20 measurements of the speed of light:

```
850
      740
           900
                1070
                       930
                                  950
                                       980
                            850
                                             980
                                                  880
                 650
                       760
                            810 1000 1000
1000
                                             960
                                                  960
```

To obtain Michelson's actual measurements, add 299,000 km/sec to each of the above values.

In the chapter Menu Graphics, we created a michel data set containing the Michelson data. For convenience, we repeat the S-PLUS command here:

```
> michel <- data.frame(speed = c(850, 740, 900,
+ 1070, 930, 850, 950, 980, 980, 880, 1000, 980,
+ 930, 650, 760, 810, 1000, 1000, 960, 960))
```

#### **Exploratory data analysis**

To obtain a useful exploratory view of the Michelson data, create the following plots: a boxplot, a histogram, a density plot, and a QQ normal plot. You can create these plots from the **Graph** menu or the **Commands** window. The function below packages the four exploratory data analysis (EDA) plots into one S-PLUS call:

```
> eda.shape <- function(x) {</pre>
     par(mfrow = c(2, 2))
     hist(x)
+
+
     boxplot(x)
     iqd < summary(x)[5] - summary(x)[2]
+
     plot(density(x, width = 2 * iqd),
          xlab = "x", ylab = "", type = "l")
+
+
     qqnorm(x)
+
     qqline(x)
     invisible()
+
+ }
```

#### > eda.shape(michel\$speed)

The plots that eda.shape generates for the Michelson data are shown in Figure 6.6. We want to evaluate the shape of the distribution to see if our data are normally distributed. These plots reveal a distinctly skewed distribution toward the left (that is, toward smaller values). The distribution is thus not normal and probably not even "nearly" normal. We should therefore not use Student's t-test for our statistical inference, since it requires normality for small samples.

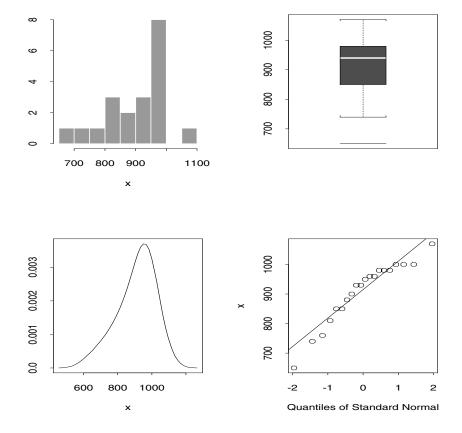


Figure 6.6: Exploratory data analysis plots for the Michelson data.

The solid horizontal line in the box plot is located at the *median* of the data, and the upper and lower ends of the box are located at the *upper* and *lower quartiles* of the data, respectively. To obtain precise values for the median and quartiles, use the **Summary Statistics** dialog.

- 1. Open the **Summary Statistics** dialog.
- 2. Enter michel as the **Data Set**.

- 3. Click on the Statistics tab, and deselect all options except Mean, Minimum, First Quartile, Median, Third Quartile, and Maximum.
- 4. Click **OK**. The output appears in the **Report** window.

```
*** Summary Statistics for data in: michel ***

Min: 650.000

1st Qu.: 850.000

Mean: 909.000

Median: 940.000

3rd Qu.: 980.000

Max: 1070.000
```

The summary shows, from top to bottom, the smallest observation, the first quartile, the mean, the median, the third quartile, and the largest observation. From this summary, you can compute the *interquartile range*, IQR = 3Q - 1Q. The interquartile range provides a useful criterion for identifying outliers: any observation that is more than 1.5 3 IQR above the third quartile or below the first quartile is a suspected outlier.

#### Statistical inference

Because the Michelson data are probably not normal, you should use the Wilcoxon signed-rank test for statistical inference, rather than the Student's t-test. For illustrative purposes, we use both.

To compute Student's t confidence intervals for the population mean-value location parameter  $\mu$ , we use the **One-sample t Test** dialog. This dialog also computes Student's t significance test p-values for the parameter  $\mu_0 = 299,990$ .

- 1. Open the **One-sample t Test** dialog.
- 2. Type michel in the **Data Set** field.
- 3. Select speed as the **Variable**.

- 4. Suppose you want to test the null hypothesis value  $\mu_0 = 990$  (plus 299,000) against a two-sided alternative, and you want to construct 95% confidence intervals. Enter 990 as the **Mean Under Null Hypothesis**.
- Click **OK**.

The results of the one-sample t-test appear in the **Report** window.

The computed mean of the Michelson data is 909, and the p-value is 0.0027, which is highly significant. Clearly, Michelson's average value of 299,909 km/sec for the speed of light is significantly different from Cornu's value of 299,990 km/sec.

Spotfire S+ returns other useful information besides the p-value, including the t-statistic value, the degrees of freedom, the sample mean, and the confidence interval.

# One-Sample Wilcoxon Signed-Rank Test

The *Wilcoxon signed-rank test* is used to test whether the median for a variable has a particular value. Unlike the one-sample t-test, it does not assume that the observations come from a Gaussian (normal) distribution.

### Performing a one-sample Wilcoxon signed-rank test

From the main menu, choose **Statistics** ► **Compare Samples** ► **One Sample** ► **Wilcoxon Signed-Rank Test**. The **One-sample Wilcoxon Test** dialog opens, as shown in Figure 6.7.

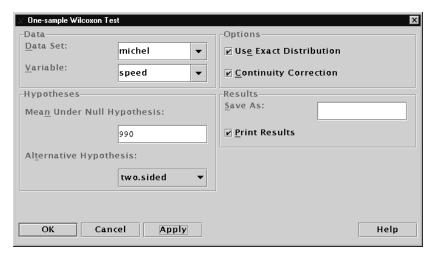


Figure 6.7: The One-sample Wilcoxon Test dialog.

In the section One-Sample t-Test on page 223, we performed a t-test on the Michelson data. The test concludes that Michelson's average value for the speed of light (299,909 km/sec) is significantly different from Cornu's value of 299,990 km/sec. However, we have noted that the data may not be normal, so the results of the t-test are suspect. We now conduct a Wilcoxon signed-rank test to see if the two values for the speed of light differ significantly from each other.

- 1. If you have not done so already, create the michel data set with the instructions given on page 155 in the Menu Graphics chapter.
- 2. Open the **One-sample Wilcoxon Test** dialog.
- 3. Type michel in the **Data Set** field.
- 4. Select speed as the Variable.
- 5. Enter 990 as the **Mean Under Null Hypothesis**.
- Click **OK**.

#### The **Report** window shows:

```
Wilcoxon signed-rank test

data: speed in michel
signed-rank normal statistic with correction Z = -3.0715,
p-value = 0.0021
alternative hypothesis: true mu is not equal to 990
```

You may also receive a warning message that there are duplicate values in the variable speed. You can ignore this message. The p-value of 0.0021 is close to the t-test p-value of 0.0027 for testing the same null hypothesis with a two-sided alternative. Thus, the Wilcoxon signed-rank test confirms that Michelson's average value for the speed of light of 299,909 km/sec is significantly different from Cornu's value of 299,990 km/sec.

### Kolmogorov-Smirnov Goodness-of-Fit

The *Kolmogorov-Smirnov goodness-of-fit test* is used to test whether the empirical distribution of a set of observations is consistent with a random sample drawn from a specific theoretical distribution. It is generally more powerful than the chi-square goodness-of-fit test for continuous variables. For discrete variables, the chi-square test is generally preferable.

If parameter values for the theoretical distribution are not available, they may be estimated from the observations automatically as part of the test for normal (Gaussian) or exponential distributions. For other distributions, the chi-square test must be used if parameters are to be estimated. In this case, the parameters are estimated from the data separately from the test, and then entered into the dialog.

### Performing a one-sample Kolmogorov-Smirnov goodness-of-fit test

From the main menu, choose **Statistics** ► **Compare Samples** ► **One Sample** ► **Kolmogorov-Smirnov GOF**. The **One-sample Kolmogorov-Smirnov Goodness-of-Fit Test** dialog opens, as shown in Figure 6.8.

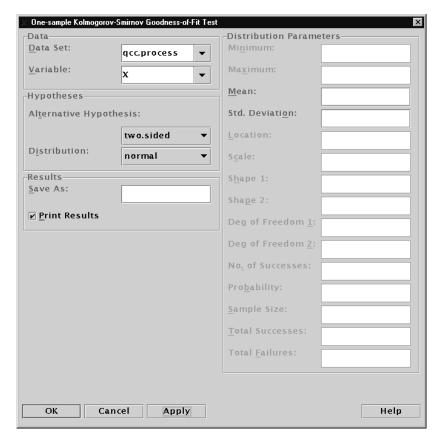


Figure 6.8: The One-sample Kolmogorov-Smirnov Goodness-of-Fit Test dialog.

We create a data set called qcc.process that contains a simulated process with 200 measurements. Ten measurements per day were taken for a total of twenty days. We use the rnorm function to generate the data set from a Gaussian distribution.

```
# Use set.seed for reproducibility.
> set.seed(21)
> qcc.process <- data.frame(X = rnorm(200, mean=10),
+ Day = unlist(lapply(1:20,
+ FUN=function(x) rep(x, times=10))))</pre>
```

#### > qcc.process

```
X Day
   9.755851
  8.959829
3 10.223913
4 10.362865
  9.477088
6 10.236104
  8.009497
8 10.213798
  9.929919
10 9.656944
11 9.304599
               2
               2
12 10.749046
13 . . .
```

We can use the Kolmogorov-Smirnov goodness-of-fit test to confirm that qcc.process is Gaussian:

- Open the One-sample Kolmogorov-Smirnov Goodnessof-Fit Test dialog. The Distribution is normal by default.
- 2. Select qcc.process as the **Data Set**.
- 3. Select X as the **Variable**.
- 4. Click **OK**.

A summary of the goodness-of-fit test appears in the **Report** window. The p-value of 0.5 indicates that we do not reject the hypothesis that the data are normally distributed. The summary also contains estimates of the mean and standard deviation for the distribution.

The **Report** window contains a warning indicating that the Dallal-Wilkinson approximation used in this test is most accurate for extreme p-values (p-values  $\leq 0.1$ ). Our actual calculated p-value is 0.776, which is set to 0.5 in the summary to indicate that the null hypothesis is not rejected, but our estimate of the p-value is not highly accurate.

### Chi-Square Goodness-of-Fit

The *chi-square goodness-of-fit test* uses Pearson's chi-square statistic to test whether the empirical distribution of a set of observations is consistent with a random sample drawn from a specific theoretical distribution.

Chi-square tests apply to any type of variable: continuous, discrete, or a combination of these. If the hypothesized distribution is discrete and the sample size is large (n > 50), the chi-square is the only valid test. In addition, the chi-square test easily adapts to the situation in which parameters of a distribution are estimated. However, for continuous variables, information is lost by grouping the data.

When the hypothesized distribution is continuous, the Kolmogorov-Smirnov test is more likely than the chi-square test to reject the null hypothesis when it should be rejected. The Kolmogorov-Smirnov test is more powerful than the chi-square test, and hence is preferred for continuous distributions.

#### Performing Pearson's chi-square test

From the main menu, choose Statistics ▶ Compare Samples ▶ One Sample ▶ Chi-square GOF. The One-sample Chi-Square Goodness-of-Fit Test dialog opens, as shown in Figure 6.9.

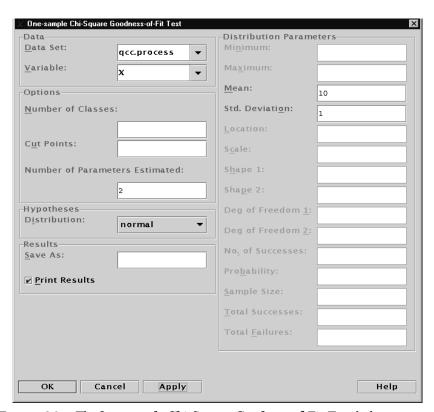


Figure 6.9: The One-sample Chi-Square Goodness-of-Fit Test dialog.

In the previous section, we created a data set called qcc.process that contains a simulated process with 200 measurements. Ten measurements per day were taken for a total of twenty days. We can use the chi-square goodness-of-fit test to confirm that qcc.process is Gaussian:

- 1. If you have not done so already, create the qcc.process data set with the instructions given on page 231.
- 2. Open the **One-sample Chi-Square Goodness-of-Fit Test** dialog. The **Distribution** is **normal** by default.
- 3. Select qcc.process as the **Data Set**.
- 4. Select X as the **Variable**.
- 5. For the chi-square test, we must specify parameter estimates for the mean and standard deviation of the distribution. Enter 10 as the **Mean** and 1 as the **Std. Deviation**. If you do not know good parameter estimates for your data, you can use the **Summary Statistics** dialog to compute them.
- 6. Since we are estimating the mean and standard deviation of our data, we should adjust for these parameter estimates when performing the goodness-of-fit test. Enter 2 as the **Number of Parameters Estimated**.
- 7. Click **OK**.

A summary of the goodness-of-fit test appears in the **Report** window.

# Two-Sample Tests

Spotfire S+ supports a variety of statistical tests for comparing two population parameters. That is, we test the null hypothesis that  $H_0\colon \Theta_1=\Theta_2$ , where  $\Theta_1$  and  $\Theta_2$  are the two population parameters.

• Two-sample t-test: a test to compare two population means  $\mu_1$  and  $\mu_2$ . For small data sets, we require that both populations have a normal distribution. Variations of the two-sample t-test, such as the paired t-test and the two-sample t-test with unequal variances, are also supported.

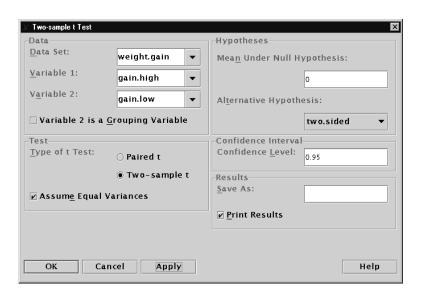
- Two-sample Wilcoxon test: a nonparametric test to compare two population means  $\mu_1$  and  $\mu_2$ . As with the t-test, we test if  $\mu_1 = \mu_2$ , but we make no distributional assumptions about our populations. Two forms of the Wilcoxon test are supported: the signed rank test and the rank sum test.
- Kolmogorov-Smirnov goodness-of-fit test: a test to determine whether two samples come from the same distribution.

# Two-Sample t-Test

The *two-sample t-test* is used to test whether two samples come from distributions with the same means. This test handles both paired and independent samples. The samples are assumed to come from Gaussian (normal) distributions. If this is not the case, then a nonparametric test, such as the Wilcoxon rank sum test, may be a more appropriate test of location.

#### Performing a two-sample t-test

From the main menu, choose Statistics ▶ Compare Samples ▶ Two Samples ▶ t Test. The Two-sample t Test dialog opens, as shown in Figure 6.10.



**Figure 6.10:** The **Two-sample t Test** dialog.

Suppose you are a nutritionist interested in the relative merits of two diets, one featuring high protein and the other featuring low protein. Do the two diets lead to differences in mean weight gain? Consider the data in Table 6.1, which shows the weight gains (in grams) for two lots of female rats under the two diets. The first lot, consisting of 12 rats, was given the high-protein diet, and the second lot, consisting of 7 rats, was given the low-protein diet. These data appear in section 6.9 of Snedecor and Cochran (1980).

**Table 6.1:** Weight gain data.

High Protein	Low Protein
134	70
146	118
104	101
119	85
124	107
161	132
107	94
83	
113	
129	
97	
123	

The high-protein and low-protein samples are presumed to have mean-value location parameters  $\mu_H$  and  $\mu_L$ , and standard deviation scale parameters  $\sigma_H$  and  $\sigma_L$ , respectively. While you are primarily interested in whether there is any difference in the mean values, you may also be interested in whether the two diets result in different variabilities, as measured by the standard deviations. This example shows you how to use Spotfire S+ to answer such questions.

#### Setting up the data

The data consist of two sets of observations, so they are appropriately described in Spotfire S+ as a data frame with two variables. Because Spotfire S+ requires data frame columns to be of equal length, we must pad the column representing the low-protein samples with NAs. To create such a data frame, type the following in the **Commands** window:

```
\rightarrow weight.gain \leftarrow data.frame(gain.high=c(134, 146, 104, 119,
+ 124, 161, 107, 83, 113, 129, 97, 123), gain.low=c(70, 118,
+ 101, 85, 107, 132, 94, NA, NA, NA, NA, NA))
> weight.gain
 gain.high gain.low
        134
                   70
        146
                  118
        104
                  101
        119
                   85
        124
                  107
        161
                  132
        107
                   94
         83
                   NA
        113
                   NA
        129
                   NA
         97
                   NA
        123
                   NA
```

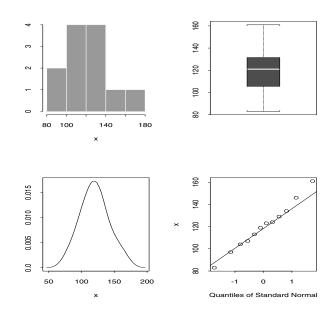
# **Exploratory data analysis**

To begin, we want to evaluate the shape of the distribution to see if both our variables are normally distributed. To do this, create the following plots for each of the variables: a boxplot, a histogram, a density plot, and a QQ normal plot. You can create these plots from

the **Graph** menu or from the **Commands** window. We use the function eda.shape defined in the section One-Sample t-Test on page 223:

#### > eda.shape(weight.gain\$gain.high)

The plots that eda.shape generates for the high-protein group are shown in Figure 6.11. They indicate that the data come from a nearly normal distribution, and there is no indication of outliers. The plots for the low-protein group, which we do not show, support the same conclusions.



**Figure 6.11:** Exploratory data analysis plots for the high-protein diet.

#### Statistical inference

Is the mean weight gain the same for the two groups of rats? Specifically, does the high-protein group show a higher average weight gain? From our exploratory data analysis, we have good reason to believe that Student's t-test provides a valid test of our hypotheses. As in the one-sample case, you can obtain confidence intervals and hypothesis test p-values for the difference  $\mu_1 - \mu_2$ 

between the two mean-value location parameters  $\mu_1$  and  $\mu_2$ . To do this, we use the **Two-sample t Test** and **Two-sample Wilcoxon Test** dialogs.

Each two-sample test is specified by a hypothesis to be tested, the confidence level, and a hypothesized  $\mu_0$  that refers to the *difference* of the two sample means. However, because of the possibility that the two samples may be from different distributions, you may also specify whether the two samples have equal variances. To determine the correct setting for the option **Assume Equal Variances**, you can either use informal inspection of the variances and box plots, or conduct a formal F-test to check for equality of variance. If the heights of the boxes in the two box plots are approximately the same, then so are the variances of the two samples. In the weight.gain example, the box plots indicate that the equal variance assumption probably holds. To check this assumption, we calculate the variances exactly:

- 1. Open the **Summary Statistics** dialog.
- 2. Enter weight.gain as the **Data Set**.
- 3. Click on the **Statistics** tab, and select the **Variance** check box.
- 4. Click **OK**.

The following output appears in the **Report** window:

```
*** Summary Statistics for data in: weight.gain ***

gain.high gain.low
Min: 83.00000 70.00000

1st Qu.: 106.25000 89.50000
Mean: 120.00000 101.00000
Median: 121.00000 101.00000
3rd Qu.: 130.25000 112.50000
Max: 161.00000 132.00000
Total N: 12.00000 12.00000
NA's: 0.00000 5.00000
Variance: 457.45455 425.33333
Std Dev.: 21.38819 20.62361
```

The actual variances of our two samples are 457.4 and 425.3, respectively. These values support our assertion of equal variances.

We are interested in two alternative hypotheses: the two-sided alternative that  $\mu_H - \mu_L = 0$  and the one-sided alternative that  $\mu_H - \mu_L > 0$ . To test these, we run the standard two-sample t-test twice, once with the default two-sided alternative and a second time with the one-sided alternative hypothesis greater.

- 1. Open the **Two-sample t Test** dialog.
- 2. Type weight.gain in the **Data Set** field.
- Select gain.high as Variable 1 and gain.low as Variable 2. By default, the Variable 2 is a Grouping Variable check box should not be selected, and the Assume Equal Variances check box should be selected.
- 4. Click **Apply**.

The result appears in the **Report** window:

The p-value is 0.0757, so the null hypothesis is rejected at the 0.10 level but not at the 0.05 level. The confidence interval is (-2.2,40.2). In other words, we conclude at the 0.05 level that there is no significant difference in the weight gain between the two diets.

To test the one-sided alternative that  $\mu_H - \mu_L > 0$ , we change the **Alternative Hypothesis** field to greater in the **Two-sample t Test** dialog. Click **OK** to perform the test and see the output shown below.

#### Standard Two-Sample t-Test

In this case, the p-value is just half of the p-value for the two-sided alternative. This relationship between the p-values holds in general. You also see that when you use the greater alternative hypothesis, you get a lower confidence bound. This is the natural one-sided confidence interval corresponding to the "greater than" alternative.

# Two-Sample Wilcoxon Test

The *Wilcoxon rank sum test* is used to test whether two sets of observations come from the same distribution. The alternative hypothesis is that the observations come from distributions with identical shape but different locations. Unlike the two-sample t-test, this test does not assume that the observations come from normal (Gaussian) distributions. The Wilcoxon rank sum test is equivalent to the Mann-Whitney test.

For paired data, specify "signed rank" as the type of Wilcoxon rank test.

### Performing a two-sample Wilcoxon rank test

From the main menu, choose **Statistics** ► **Compare Samples** ► **Two Samples** ► **Wilcoxon Rank Test**. The **Two-sample Wilcoxon Test** dialog opens, as shown in Figure 6.12.

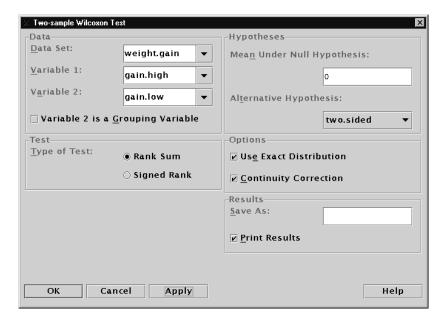


Figure 6.12: The Two-sample Wilcoxon Test dialog.

In the section Two-Sample t-Test on page 235, we conducted a test to see if the mean weight gain from a high-protein diet differs from that of a low-protein diet. The two-sample t-test was significant at the 0.10 level but not at the 0.05 level. Since normality holds, a two-sample t-test is probably most appropriate for these data. However, for illustrative purposes we conduct a two-sample Wilcoxon test to see if the two diets differ in mean weight gain. We conduct a two-sided test, where the null hypothesis is that the difference in diets is 0; that is, we test if the mean weight gain is the same for each diet.

- 1. If you have not done so already, create the weight.gain data set with the instructions given on page 237.
- 2. Open the **Two-sample Wilcoxon Test** dialog.

- 3. Specify weight.gain as the **Data Set**.
- 4. Select gain.high as Variable 1 and gain.low as Variable 2. By default, the Variable 2 is a Grouping Variable check box should not be selected, and the Type of Rank Test should be set to Rank Sum. Click OK.

The **Report** window shows the following output:

```
Wilcoxon rank-sum test

data: x: gain.high in weight.gain , and y: gain.low in
  weight.gain

rank-sum normal statistic with correction Z = 1.6911,
  p-value = 0.0908

alternative hypothesis: true mu is not equal to 0
```

You may also see a warning in the **Report** window because the value 107 appears twice in the data set. The warning can be ignored for now. The p-value of 0.0908 is based on the normal approximation, which is used because of ties in the data. It is close to the t-statistic p-value of 0.0757. It therefore supports our conclusion that the mean weight gain is not significantly different at level 0.05 in the high- and low-protein diets.

## Kolmogorov-Smirnov Goodness-of-Fit

The two-sample Kolmogorov-Smirnov goodness-of-fit test is used to test whether two sets of observations could reasonably have come from the same distribution. This test assumes that the two samples are random and mutually independent, and that the data are measured on at least an ordinal scale. In addition, the test gives exact results only if the underlying distributions are continuous.

## Perform a two-sample Kolmogorov-Smirnov goodness-of-fit test

From the main menu, choose **Statistics** ► **Compare Samples** ► **Two Samples** ► **Kolmogorov-Smirnov GOF**. The **Two-sample Kolmogorov-Smirnov Goodness-of-Fit Test** dialog opens, as shown in Figure 6.13.

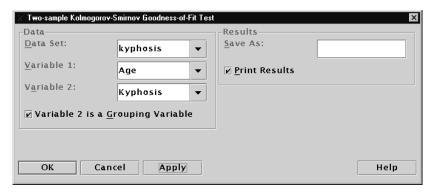


Figure 6.13: The Two-sample Kolmogorov-Smirnov Goodness-of-Fit Test dialog.

The kyphosis data set has 81 rows representing data on 81 children who have had corrective spinal surgery. The outcome Kyphosis is a binary variable, and the other three columns Age, Number, and Start, are numeric. Kyphosis is a post-operative deformity which is present in some children receiving spinal surgery. We are interested in examining whether the child's age, the number of vertebrae operated on, or the starting vertebra influence the likelihood of the child having a deformity. As an exploratory tool, we test whether the distributions of Age, Number, and Start are the same for the children with and without kyphosis.

- 1. Open the **Two-sample Kolmogorov-Smirnov Goodness-of-Fit Test** dialog.
- 2. Type kyphosis in the **Data Set** field.
- 3. We perform separate tests for each of the three covariates, in each case grouping by Kyphosis. Select Kyphosis as **Variable 2**. Select the **Variable 2** is a **Grouping Variable** check box.
- 4. Select Age as **Variable 1**. Click **Apply**.
- 5. Select Number as **Variable 1**. Click **Apply**.
- 6. Select Start as **Variable 1**. Click **OK**.

A **Report** window appears with three goodness-of-fit summaries. The p-values for Age, Number, and Start are 0.076, 0.028, and 0.0002, respectively. This suggests that the children with and without kyphosis do not differ significantly in the distribution of their ages, but do differ significantly in the distributions of how many vertebrae were involved in the operation, as well as which vertebra was the starting vertebra. This is consistent with the logistic regression model fit to these data later, in the section Logistic Regression on page 303.

**K-Sample Tests** Spotfire S+ supports a variety of techniques to analyze group mean differences in designed experiments.

- One-way analysis of variance: a simple one-factor analysis of variance. No interactions are assumed among the main effects. That is, the k samples are considered independent, and the data must be normally distributed.
- Kruskal-Wallis rank sum test: a nonparametric alternative to a one-way analysis of variance. No distributional assumptions are made.
- **Friedman rank sum test**: a nonparametric analysis of means of a one-factor designed experiment with an unreplicated blocking variable.

The **ANOVA** dialog provides analysis of variance models involving more than one factor; see the section Analysis of Variance on page 308.

## One-Way Analysis of Variance

The One-Way Analysis of Variance dialog generates a simple analysis of variance (ANOVA) table when there is a grouping variable available that defines separate samples of the data. No interactions are assumed among the main effects; that is, the samples are considered to be independent. The ANOVA tables include F-statistics, which test whether the mean values for all of the groups are equal. These statistics assume that the observations are normally (Gaussian) distributed.

For more complex models or ANOVA with multiple predictors, use the **Analysis of Variance** dialog.

### Perform a one-way ANOVA

From the main menu, choose Statistics ▶ Compare Samples ▶ k Samples ▶ One-way ANOVA. The One-way Analysis of Variance dialog opens, as shown in Figure 6.14.

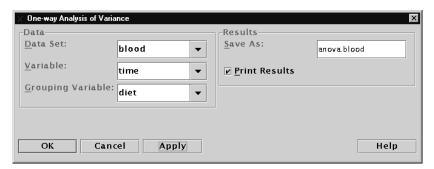


Figure 6.14: The One-way Analysis of Variance dialog.

#### **Example**

The simplest kind of experiments are those in which a single continuous *response* variable is measured a number of times for each of several *levels* of some experimental *factor*. For example, consider the data in Table 6.2 (from Box, Hunter, and Hunter (1978)). The data consist of numerical values of blood coagulation times for each of four diets. Coagulation time is the continuous response variable, and diet is a *qualitative* variable, or *factor*, having four levels: A, B, C, and D. The diets corresponding to the levels A, B, C, and D were determined by the experimenter.

Your main interest is to see whether or not the factor "diet" has any effect on the mean value of blood coagulation time. Experimental factors such as "diet" are often called the *treatments*.

Formal statistical testing for whether the factor levels affect the mean coagulation time is carried out using analysis of variance (ANOVA). This method needs to be complemented by exploratory graphics to provide confirmation that the model assumptions are sufficiently correct to validate the formal ANOVA conclusion. Spotfire S+provides tools for you to do both the data exploration and the formal ANOVA.

	Di	et	
A	В	С	D
62	63	68	56
60	67	66	62
63	71	71	60
59	64	67	61
	65	68	63
	66	68	64
			63
			59

**Table 6.2:** Blood coagulation times for four diets.

## Setting up the data

We have one factor variable diet and one response variable time. The data are appropriately described in Spotfire S+ as a data set with two columns. The data presented in Table 6.2 can be generated by typing the following in the **Commands** window:

```
> diet <- factor(c(rep("A",4), rep("B",6), rep("C",6),
+ rep("D",8)))
> Time <- scan()
1: 62 60 63 59
5: 63 67 71 64 65 66
11: 68 66 71 67 68 68
17: 56 62 60 61 63 64 63 59
25:</pre>
```

```
> blood <- data.frame(diet=diet, time=Time)</pre>
> blood
   diet time
 1
            62
 2
       Α
            60
 3
       Α
            63
 4
       Α
            59
 5
       В
            63
       В
            67
       В
            71
 8
       В
            64
 9
       В
            65
10
       В
            66
11
            68
12
       C
            66
13
       C
            71
14
       C
            67
15
            68
16
       С
            68
17
       D
            56
18
       D
            62
19
       D
            60
20
       D
            61
21
       D
            63
22
       D
            64
23
       D
            63
24
       D
            59
```

## **Exploratory data analysis**

Box plots are a quick and easy way to get a first look at the data:

```
> boxplot(split(blood$time, blood$diet),
+ xlab="diet", ylab="time")
```

The resulting box plots are similar to those in Figure 6.15. This plot indicates that the responses for diets A and D are quite similar, while the median responses for diets B and C are considerably larger relative to the variability reflected by the heights of the boxes. Thus, you suspect that diet has an effect on blood coagulation time.

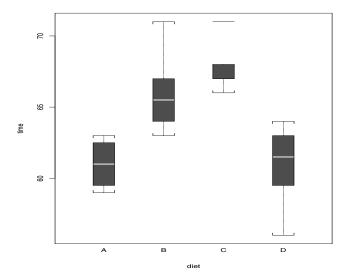


Figure 6.15: Box plots for each of the four diets in the blood data set.

### The one-way layout model and analysis of variance

The classical model for experiments with a single factor is

$$y_{ij} = \mu_i + \varepsilon_{ij}$$
  $j = 1, ..., J_i$   
 $i = 1, ..., I$ 

where  $\mu_i$  is the mean value of the response for the *i*th level of the experimental factor. There are I levels of the experimental factor, and  $J_i$  measurements  $y_{i1}, y_{i2}, ..., y_{iJ_i}$  are taken on the response variable for level i of the experimental factor. Using the treatment terminology, there are I treatments and  $\mu_i$  is called the *i*th treatment mean. The is often called the *one-way layout* model. For the blood coagulation experiment, there are I = 4 diets, and the means  $\mu_1$ ,

 $\mu_2$ ,  $\mu_3$ , and  $\mu_4$  correspond to diets A, B, C, and D, respectively. The numbers of observations are  $J_A=4$ ,  $J_B=6$ ,  $J_C=6$ , and  $J_D=8$ .

You may carry out the analysis of variance using the **One-way Analysis of Variance** dialog.

- 1. Open the **One-way Analysis of Variance** dialog.
- 2. Type blood in the **Data Set** field.
- 3. Select time as the **Variable** and diet as the **Grouping Variable**.
- 4. To generate multiple comparisons in a later section, we save the results by typing anova.blood in the **Save As** field.
- 5. Click **OK** to perform the ANOVA.

The results are displayed in the **Report** window:

```
*** One-Way ANOVA for data in time by diet ***
Call:
   aov(formula = time ~ diet, data = blood)
                diet Residuals
Sum of Squares 228
                           112
Deg. of Freedom
                3
                            20
Residual standard error: 2.366432
Estimated effects may be unbalanced
          Df Sum of Sq Mean Sq F Value
                                                Pr(F)
     diet 3
                   228
                          76.0 13.57143 0.00004658471
Residuals 20
                  112
                          5.6
```

The p-value is equal to 0.000047, which is highly significant; we therefore conclude that diet does affect blood coagulation times.

## Kruskal-Wallis Rank Sum Test

The *Kruskal-Wallis rank test* is a nonparametric alternative to a one-way analysis of variance. The null hypothesis is that the true location parameter for *y* is the same in each of the groups. The alternative hypothesis is that *y* is different in at least one of the groups. Unlike one-way ANOVA, this test does not require normality.

#### Performing a Kruskal-Wallis rank sum test

From the main menu, choose Statistics ▶ Compare Samples ▶ k Samples ▶ Kruskal-Wallis Rank Test. The Kruskal-Wallis Rank Sum Test dialog opens, as shown in Figure 6.16.

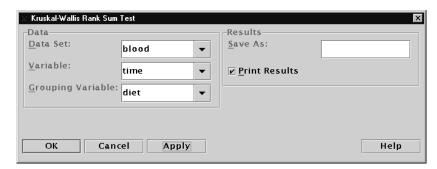


Figure 6.16: The Kruskal-Wallis Rank Sum Test dialog.

#### **Example**

In the section One-Way Analysis of Variance on page 245, we concluded that diet affects blood coagulation times. The one-way ANOVA requires the data to be normally distributed. The nonparametric Kruskal-Wallis rank sum test does not make any distributional assumptions and can be applied to a wider variety of data. We now conduct the Kruskal-Wallis rank sum test on the blood data set.

- 1. If you have not done so already, create the blood data set with the instructions given on page 247.
- 2. Open the Kruskal-Wallis Rank Sum Test dialog.
- 3. Type blood in the **Data Set** field.
- 4. Select time as the **Variable** and diet as the **Grouping Variable**, and click **OK**.

The **Report** window displays the result:

```
Kruskal-Wallis rank sum test
data: time and diet from data set blood
Kruskal-Wallis chi-square = 17.0154, df = 3,
p-value = 0.0007
alternative hypothesis: two.sided
```

The p-value is 0.0007, which is highly significant. The Kruskal-Wallis rank sum test confirms the results of our one-way ANOVA.

## Friedman Rank Test

The *Friedman rank test* is appropriate for data arising from an unreplicated complete block design. In these kinds of designs, exactly one observation is collected from each experimental unit, or *block*, under each treatment. The elements of *y* are assumed to consist of a groups effect, plus a blocks effect, plus independent and identically distributed residual errors. The interaction between groups and blocks is assumed to be zero.

In the context of a two-way layout with factors groups and blocks, a typical null hypothesis is that the true location parameter for y, net of the blocks effect, is the same in each of the groups. The alternative hypothesis is that it is different in at least one of the groups.

#### Performing a Friedman rank test

From the main menu, choose Statistics ➤ Compare Samples ➤ k Samples ➤ Friedman Rank Test. The Friedman Rank Sum Test dialog opens, as shown in Figure 6.17.

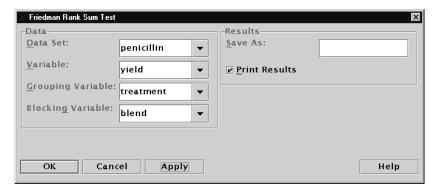


Figure 6.17: The Friedman Rank Sum Test dialog.

#### Example

The data set shown in Table 6.3 was first used by Box, Hunter, and Hunter in 1978. The data was collected to determine the effect of treatments A, B, C, and D on the yield of penicillin in a penicillin manufacturing process. The response variable is yield, and the

treatment variable is treatment. There is a second factor, blend, since a separate blend of the corn-steep liquor had to be made for each application of the treatments.

Our main interest is in determining whether the treatment factor affects yield. The blend factor is of only secondary interest; it is a blocking variable introduced to increase the sensitivity of the inference for treatments. The order of the treatments within blocks was chosen at random. Hence, this is a randomized block experiment.

**Table 6.3:** The effect of four treatments on the yield of penicillin.

blend	treatment	yield
1	A	89
2	A	84
3	A	81
4	A	87
5	A	79
1	В	88
2	В	77
3	В	87
4	В	92
5	В	81
1	С	97
2	С	92
3	С	87
4	С	89
5	С	80
1	D	94
2	D	79
3	D	85
4	D	84
5	D	88

#### Setting up the data

To create a penicillin data set containing the information in Table 6.3, type the following in the **Commands** window:

```
> blend <- factor(rep(c("Blend 1", "Blend 2", "Blend 3",
+ "Blend 4", "Blend 5"), times=4))
> treatment <- factor(c(rep("A",5), rep("B",5), rep("C",5),</pre>
rep("D",5)))
> yield <- scan()</pre>
1: 89 84 81 87 79
6: 88 77 87 92 81
11: 97 92 87 89 80
16: 94 79 85 84 88
21:
> penicillin <- data.frame(blend, treatment, yield)</pre>
> penicillin
     blend treatment yield
1 Blend 1
                        89
2 Blend 2
                        84
3 Blend 3
                        81
4 Blend 4
                   Α
                        87
5 Blend 5
                       79
6 Blend 1
                       88
7 Blend 2
                  В
                       77
8 . . .
```

#### Statistical inference

We use the Friedman rank test to test the null hypothesis that there is no treatment effect.

- 1. Open the **Friedman Rank Sum Test** dialog.
- 2. Type penicillin in the **Data Set** field.
- 3. Select yield as the **Variable**, treatment as the **Grouping Variable**, and blend as the **Blocking Variable**.
- 4. Click **OK**.

A summary for the Friedman test appears in the **Report** window. The p-value is 0.322, which is not significant. This p-value is computed using an asymptotic chi-squared approximation.

# Counts and Proportions

Spotfire S+ supports a variety of techniques to analyze counts and proportions.

- **Binomial Test:** an exact test used with binomial data to assess whether the data come from a distribution with a specified proportion parameter.
- Proportions Parameters: a chi-square test to assess whether a binomial sample has a specified proportion parameter, or whether two binomial samples have the same proportion parameter.
- **Fisher's Exact Test:** a test for independence between the rows and columns of a contingency table.
- **McNemar's Test:** a test for independence in a contingency table when matched variables are present.
- **Mantel-Haenszel Test:** a chi-square test of independence for a three-dimensional contingency table.
- **Chi-square Test:** a chi-square test for independence for a two-dimensional contingency table.

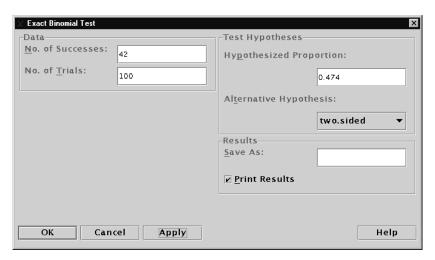
Binomial data are data representing a certain number k of successes out of n trials, where observations occur independently with probability p of a success. Contingency tables contain counts of the number of occurrences of each combination of two or more categorical (factor) variables.

#### **Binomial Test**

The *exact binomial test* is used with binomial data to assess whether the data are likely to have come from a distribution with a specified proportion parameter p. Binomial data are data representing a certain number k of successes out of n trials, where observations occur independently with probability p of a success. Examples include coin toss data.

#### Performing an exact binomial test

From the main menu, choose Statistics ▶ Compare Samples ▶ Counts and Proportions ▶ Binomial Test. The Exact Binomial Test dialog opens, as shown in Figure 6.18.



**Figure 6.18:** The **Exact Binomial Test** dialog.

## **Example**

When you play roulette and bet on red, you expect your probability of winning to be close to, but slightly less than 0.5. You expect this because, in the United States, a roulette wheel has 18 red slots, 18 black slots, and two additional slots labeled "0" and "00." This gives a total of 38 slots into which the ball can fall. Thus, for a fair or perfectly balanced wheel, you expect the probability of red to be  $p_0 = 18/38 = 0.474$ . You hope that the house is not cheating you by altering the roulette wheel so that the probability of red is less than 0.474.

For example, suppose you bet on red 100 times and red comes up 42 times. You wish to ascertain whether these results are reasonable with a fair roulette wheel.

- 1. Open the **Exact Binomial Test** dialog.
- 2. Enter 42 as the **No. of Successes**. Enter 100 as the **No. of Trials**.

- 3. Enter 0.474 as the **Hypothesized Proportion**.
- 4. Click **OK**.

A summary of the test appears in the **Report** window. The p-value of 0.3168 indicates that our sample is consistent with data drawn from a binomial distribution with a proportions parameter of 0.474. Hence, the roulette wheel seems to be fair.

## Proportions Parameters

The *proportions parameters test* uses a Pearson's chi-square statistic to assess whether a binomial sample has a specified proportion parameter p. In addition, it can assess whether two or more samples have the same proportion parameter. As the proportions parameters test uses a normal approximation to the binomial distribution, it is less powerful than the exact binomial test. Hence, the exact binomial test is usually preferred. The advantages of the proportions parameters test are that it provides a confidence interval for the proportions parameter, and that it may be used with multiple samples.

#### Performing a proportions parameters test

From the main menu, choose **Statistics** ► **Compare Samples** ► **Counts and Proportions** ► **Proportions Parameters**. The **Proportions Test** dialog opens, as shown in Figure 6.19.

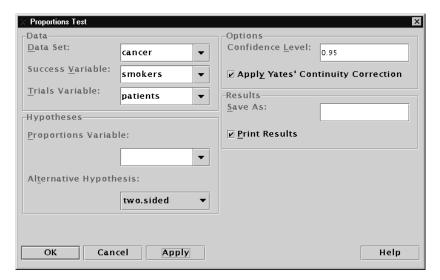


Figure 6.19: The Proportions Test dialog.

Sometimes you may have multiple samples of subjects, with each subject characterized by the presence or absence of some characteristic. An alternative, but equivalent, terminology is that you have three or more sets of trials, with each trial resulting in a success or failure. For example, the data set shown in Table 6.4 summarizes the results of four different studies of lung cancer patients, as presented by Fleiss (1981). Each study has a certain number of patients, and for each study a certain number of the patients were smokers.

smokers	patients
83	86
90	93
129	136
70	82

**Table 6.4:** Four different studies of lung cancer patients.

## Setting up the data

To create a cancer data set containing the information in Table 6.4, type the following in the **Commands** window:

```
> cancer <- data.frame(smokers = c(83, 90, 129, 70),
+ patients = c(86, 93, 136, 82))
> cancer
  smokers patients
1
       83
                 86
2
       90
                93
3
      129
               136
4
       70
                82
```

#### Statistical inference

For the cancer data, we are interested in whether the probability of a patient being a smoker is the same in each of the four studies. That is, we wish to test whether each of the studies involve patients from a homogeneous population.

- 1. Open the **Proportions Test** dialog.
- 2. Type cancer in the **Data Set** field.
- 3. Select smokers as the **Success Variable** and patients as the **Trial Variable**.
- 4. Click **OK**.

A summary of the test appears in the **Report** window. The p-value of 0.0056 indicates that we reject the null hypothesis of equal proportions parameters. Hence, we cannot conclude that all groups have the same probability that a patient is a smoker.

## Fisher's Exact Test

Fisher's exact test is a test for independence between the row and column variables of a contingency table. When the data consist of two categorical variables, a contingency table can be constructed reflecting the number of occurrences of each factor combination. Fisher's exact test assesses whether the value of one factor is independent of the value of the other. For example, this might be used to test whether political party affiliation is independent of gender. Certain types of homogeneity, for example, homogeneity of proportions in a  $k \times 2$  table, are equivalent to the independence hypothesis. Hence, this test may also be of interest in such cases.

As this is an exact test, the total number of counts in the crossclassification table cannot be greater than 200. In such cases, the chisquare test of independence is preferable.

## Performing Fisher's exact test

From the main menu, choose Statistics ► Compare Samples ► Counts and Proportions ► Fisher's Exact Test. The Fisher's Exact Test dialog opens, as shown in Figure 6.20.

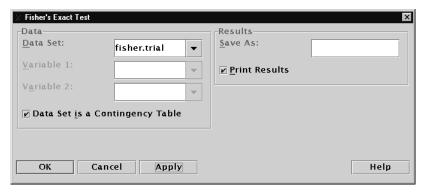


Figure 6.20: The Fisher's Exact Test dialog.

The data set shown in Table 6.5 contains a contingency table summarizing the results of a clinical trial. Patients were divided into a treatment group which received an experimental drug, and a control group which did not. These patients were then monitored for 28 days, with their survival status noted at the end of the study.

Table 6.5:	A contingency	table summarizin	ng the results o	of a clinical trial.
------------	---------------	------------------	------------------	----------------------

	Control	Treated
Died	17	7
Survived	29	38

## Setting up the data

To create a fisher.trial data set containing the information in Table 6.5, type the following in the **Commands** window:

```
> fisher.trial <- data.frame(c(17,29), c(7,38),
+ row.names=c("Died", "Survived"))
> names(fisher.trial) <- c("Control", "Treated")</pre>
```

#### > fisher.trial

```
Control Treated
Died 17 7
Survived 29 38
```

#### Statistical inference

We are interested in examining whether the treatment affected the probability of survival.

- 1. Open the **Fisher's Exact Test** dialog.
- 2. Type fisher.trial in the **Data Set** field.
- 3. Select the **Data Set is a Contingency Table** check box.
- 4. Click **OK**.

A summary of the test appears in the **Report** window. The p-value of 0.0314 indicates that we reject the null hypothesis of independence. Hence, we conclude that the treatment affects the probability of survival.

#### McNemar's Test

In some experiments with two categorical variables, one of the variables specifies two or more groups of individuals that receive different treatments. In such situations, matching of individuals is often carried out in order to increase the precision of statistical inference. However, when matching is carried out, the observations usually are not independent. In such cases, the inference obtained from the chi-square test, Fisher's exact test, and Mantel-Haenszel test is not valid because these tests all assume independent observations.

McNemar's test allows you to obtain a valid inference for experiments where matching is carried out. McNemar's statistic is used to test the null hypothesis of symmetry: namely, that the probability of an observation being classified into cell [i,j] is the same as the probability of being classified into cell [j,i]. The returned p-value should be interpreted carefully. Its validity depends on the assumption that the cell counts are at least moderately large. Even when cell counts are adequate, the chi-square is only a large-sample approximation to the true distribution of McNemar's statistic under the null hypothesis.

#### Performing McNemar's test

From the main menu, choose Statistics ► Compare Samples ► Counts and Proportions ► McNemar's Test. The McNemar's Chi-Square Test dialog opens, as shown in Figure 6.21.

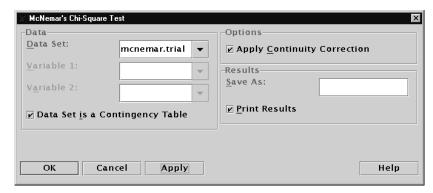


Figure 6.21: The McNemar's Chi-Square Test dialog.

#### **Example**

The data set shown in Table 6.6 contains a contingency table of matched pair data, in which each count is associated with a matched pair of individuals.

	B,Survive	B,Die
A,Survive	90	16
A,Die	5	510

**Table 6.6:** Contingency table of matched pair data.

In this table, each entry represents a pair of patients, one of whom was given treatment A while the other was given treatment B. For instance, the 5 in the lower left cell means that in five pairs, the person with treatment A died, while the individual the person was paired with survived. We are interested in the relative effectiveness of treatments A and B in treating a rare form of cancer.

A pair in the table for which one member of a matched pair survives while the other member dies is called a *discordant pair*. There are 16 discordant pairs in which the individual who received treatment A survived and the individual who received treatment B died. There are five discordant pairs with the reverse situation, in which the individual who received treatment A died and the individual who received treatment B survived. If both treatments are equally effective, then we expect these two types of discordant pairs to occur with nearly equal frequency. Put in terms of probabilities, the null hypothesis is that  $p_1 = p_2$ , where  $p_1$  is the probability that the first type of discordancy occurs and  $p_2$  is the probability that the second type of discordancy occurs.

#### Setting up the data

To create a mcnemar.trial data set containing the information in Table 6.6, type the following in the **Commands** window:

#### Statistical inference

We use McNemar's test to examine whether the treatments are equally effective.

- 1. Open the McNemar's Square Test dialog.
- 2. Type mcnemar.trial in the **Data Set** field.
- 3. Select the **Data Set is a Contingency Table** check box.
- 4. Click **OK**.

A summary of the test appears in the **Report** window. The p-value of 0.0291 indicates that we reject the null hypothesis of symmetry in the table. This suggests that the two treatments differ in their efficacy.

## Mantel-Haenszel Test

The *Mantel-Haenszel test* performs a chi-square test of independence on a three-dimensional contingency table. It is used for a contingency table constructed from three factors. As with McNemar's test, the returned p-value should be interpreted carefully. Its validity depends on the assumption that certain sums of expected cell counts are at least moderately large. Even when cell counts are adequate, the chi-square is only a large-sample approximation to the true distribution of the Mantel-Haenszel statistic under the null hypothesis.

#### Performing a Mantel-Haenszel test

From the main menu, choose Statistics ▶ Compare Samples ▶ Counts and Proportions ▶ Mantel-Haenszel Test. The Mantel-Haenszel's Chi-Square Test dialog opens, as shown in Figure 6.22.

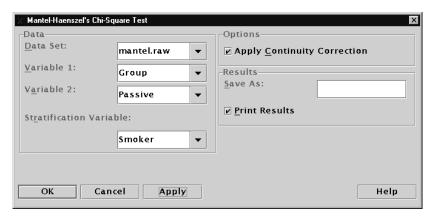


Figure 6.22: The Mantel-Haenszel's Chi-Square Test dialog.

### **Example**

The data set shown in Table 6.7 contains a three-way contingency table summarizing the results from a cancer study. The first column indicates whether an individual is a smoker. In the second column, "Case" refers to an individual who had cancer and "Control" refers to an individual who did not have cancer. The third column indicates whether an individual is a *passive smoker*. A passive smoker is a person who lives with a smoker, so it is therefore possible for a person to be considered both a smoker and a passive smoker. The fourth column indicates the number of individuals with each combination of Smoker, Group, and Passive values.

Smoker	Group	Passive	Number
Yes	Case	Yes	120
Yes	Case	No	111
Yes	Control	Yes	80
Yes	Control	No	155
No	Case	Yes	161
No	Case	No	117
No	No Control Yes		130
No	Control	No	124

**Table 6.7:** A three-way contingency table summarizing the results of a cancer study.

We are primarily interested in whether passive smoke influences the likelihood of getting cancer. However, smoking status could be a confounding variable because both smoking and passive smoking are related to the outcome, cancer status. We would like to use the information on smoking status to produce an overall test of independence between cancer status and passive smoking status. You can do so for two or more  $2 \times 2$  tables with the Mantel-Haenszel test.

## Setting up the data

To create a mantel.trial data set containing the information in Table 6.7, type the following in the **Commands** window:

```
> mantel.trial <- data.frame(
+ Smoker = factor(c(rep("Yes",4), rep("No",4))),
+ Group = factor(c("Case", "Case", "Control", "Control",
+ "Case", "Case", "Control", "Control")),
+ Passive = factor(c("Yes", "No", "Yes", "No", "Yes", "No",
+ "Yes", "No")),
+ Number = c(120, 111, 80, 155, 161, 117, 130, 124))</pre>
```

#### > mantel.trial

	Smoker	Group	Passive	Number
1	Yes	Case	Yes	120
2	Yes	Case	No	111
3	Yes	Control	Yes	80
4	Yes	Control	No	155
5	No	Case	Yes	161
6	No	Case	No	117
7	No	Control	Yes	130
8	No	Control	No	124

The mantel.trial data set has eight rows representing the eight possible combinations of three factors with two levels each. However, the **Mantel-Haenszel Chi-Square Test** dialog requires data to be in its raw form, and does not accept data in a contingency table. To recreate the raw data, type the following in the **Commands** window:

```
> mantel.raw <- mantel.trial[rep(1:8,mantel.trial$Number),]</pre>
```

This replicates each of the integers 1 to 8 as many times as indicated by the corresponding count in the Number column. We use the mantel.raw data frame in the example analysis below.

#### Statistical inference

We use the **Mantel-Haenszel Chi-Square Test** dialog to test the independence between cancer status and passive smoking status.

- 1. Open the **Mantel-Haenszel's Chi-Square Test** dialog.
- 2. Type mantel.raw in the **Data Set** field.
- 3. Select Group as **Variable 1**, Passive as **Variable 2**, and Smoker as the **Stratification Variable**.
- 4. Click **OK**.

A summary of the test appears in the **Report** window. The p-value of 0.0002 indicates that we reject the null hypothesis of independence between cancer status and passive smoking.

## **Chi-Square Test**

The chi-square test performs a Pearson's chi-square test on a twodimensional contingency table. This test is relevant to several types of null hypotheses: statistical independence of the rows and columns, homogeneity of groups, etc. The appropriateness of the test to a particular null hypothesis and the interpretation of the results depend on the nature of the data at hand. In particular, the sampling scheme is important in determining the appropriate of a chi-square test.

The p-value returned by a chi-square test should be interpreted carefully. Its validity depends heavily on the assumption that the expected cell counts are at least moderately large; a minimum size of five is often quoted as a rule of thumb. Even when cell counts are adequate, the chi-square is only a large-sample approximation to the true distribution of chi-square under the null hypothesis. If the data set is smaller than is appropriate for a chi-square test, then Fisher's exact test may be preferable.

#### Performing Pearson's chi-square test

From the main menu, choose Statistics ► Compare Samples ► Counts and Proportions ► Chi-square Test. The Pearson's Chi-Square Test dialog opens, as shown in Figure 6.23.

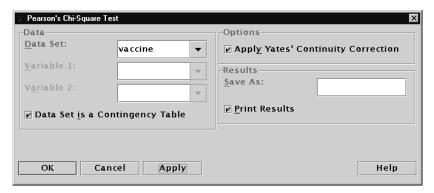


Figure 6.23: The Pearson's Chi-Square Test dialog.

#### Example

The data set shown in Table 6.8 contains a contingency table with results from Salk vaccine trials in the early 1950s. There are two categorical variables for the Salk trials: vaccination status, which has the two levels "vaccinated" and "placebo," and polio status, which has the three levels "no polio," "non-paralytic polio," and "paralytic polio." Of 200,745 individuals who were vaccinated, 24 contracted non-paralytic polio, 33 contracted paralytic polio, and the remaining 200,688 did not contract any kind of polio. Of 201,229 individuals

who received the placebo, 27 contracted non-paralytic polio, 115 contracted paralytic polio, and the remaining 201,087 did not contract any kind of polio.

<b>Table 6.8:</b>	A contingency	rtable summariz	zing the results	of th	e Salk vaccine	trials.
-------------------	---------------	-----------------	------------------	-------	----------------	---------

	None	Nonparalytic	Paralytic	
Vaccinated	200,688	24	33	
Placebo	201,087	27	115	

When working with contingency table data, the primary interest is most often determining whether there is any association in the form of statistical dependence between the two categorical variables whose counts are displayed in the table. The null hypothesis is that the two variables are statistically independent.

### Setting up the data

To create a vaccine data set containing the information in Table 6.8, type the following in the **Commands** window:

#### Statistical inference

We perform a chi-square test of independency for the vaccine data.

- 1. Open the **Pearson's Chi-Square Test** dialog.
- 2. Type vaccine in the **Data Set** field.
- 3. Select the **Data Set is a Contingency Table** check box, and click **OK**.

A summary of the test appears in the **Report** window. The p-value of 0 indicates that we reject the null hypothesis of independence. Vaccination and polio status are related.

## **POWER AND SAMPLE SIZE**

When designing a study, one of the first questions to arise is how large a sample size is necessary. The sample size depends upon the minimum detectable difference of interest, the acceptable probability of rejecting a true null hypothesis (alpha), the desired probability of correctly rejecting a false null hypothesis (power), and the variability within the population(s) under study.

Spotfire S+ provides power and sample size calculations for one and two sample tests of normal means or binomial proportions.

- Normal power and sample size: computes sample sizes for statistics that are asymptotically normally distributed, such as a sample mean. Alternatively, it may be used to calculate power or minimum detectable difference for a sample of a specified size.
- Binomial power and sample size: computes sample sizes
  for statistics that are asymptotically binomially distributed,
  such as a proportion. Alternatively, it may be used to calculate
  power or minimum detectable difference for a sample of a
  specified size.

## **Normal Mean**

The **Normal Power and Sample Size** dialog assists in computing sample sizes for statistics that are asymptotically normally distributed. Alternatively, it may be used to calculate power or minimum detectable difference for a sample of a specified size.

## Computing power and sample size for a mean

From the main menu, choose **Statistics** ▶ **Power and Sample Size** ▶ **Normal Mean**. The **Normal Power and Sample Size** dialog opens, as shown in Figure 6.24.

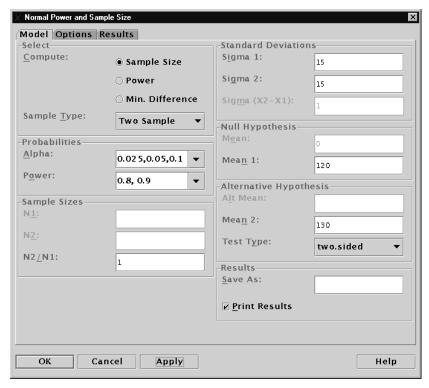


Figure 6.24: The Normal Power and Sample Size dialog.

A scientist is exploring the efficacy of a new treatment. The plan is to apply the treatment to half of a study group, and then compare the levels of a diagnostic enzyme in the treatment subjects with the untreated control subjects. The scientist needs to determine how many subjects are needed in order to determine whether the treatment significantly changes the concentration of the diagnostic enzyme.

Historical information indicates that the average enzyme level is 120, with a standard deviation of 15. A difference in average level of 10 or more between the treatment and control groups is considered to be of clinical importance. The scientist wants to determine what sample

sizes are necessary for various combinations of alpha (the probability of falsely claiming the groups differ when they do not) and power (the probability of correctly claiming the groups differ when they do).

The **Normal Power and Sample Size** dialog produces a table of sample sizes for various combinations of alpha and power.

- 1. Open the **Normal Power and Sample Size** dialog.
- 2. Select Two Sample as the **Sample Type**.
- 3. Enter 120 as **Mean1**, 130 as **Mean2**, and 15 for both **Sigma1** and **Sigma2**.
- 4. Enter 0.025, 0.05, 0.1 for **Alpha**, and enter 0.8, 0.9 for **Power**. We calculate equal sample sizes for all combinations of these alpha and power values.
- 5. Click **OK**.

A power table is displayed in the **Report** window. The table indicates what sample sizes n1 and n2 are needed for each group at various levels of alpha and power. For example, the scientist needs 36 subjects per group to determine a difference of 10 at an alpha of 0.05 and power of 0.8.

	***	Powe	r Tabl	e **	*				
	${\sf mean1}$	sd1	mean2	sd2	delta	alpha	power	n1	n2
1	120	15	130	15	10	0.025	0.8	43	43
2	120	15	130	15	10	0.050	0.8	36	36
3	120	15	130	15	10	0.100	0.8	28	28
4	120	15	130	15	10	0.025	0.9	56	56
5	120	15	130	15	10	0.050	0.9	48	48
6	120	15	130	15	10	0.100	0.9	39	39

## Binomial Proportion

The **Binomial Power and Sample Size** dialog assists in computing sample sizes for statistics that are asymptotically binomially distributed. Alternatively, it may be used to calculate power or minimum detectable difference for a sample of a specified size.

## Computing power and sample size for a proportion

From the main menu, choose **Statistics** ▶ **Power and Sample Size** ▶ **Binomial Proportion**. The **Binomial Power and Sample Size** dialog opens, as shown in Figure 6.25.

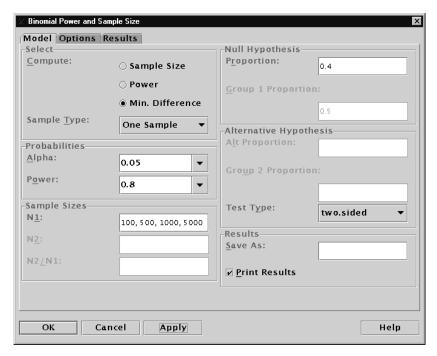


Figure 6.25: The Binomial Power and Sample Size dialog.

Historically, 40% of the voters in a certain congressional district vote for the Democratic congressional candidate. A pollster is interested in determining the proportion of Democratic voters in an upcoming election. The pollster wants to know how sizable a difference could be detected for various sample sizes. That is, how much would the proportion of Democratic voters in the sample have to differ from the historical proportion of 40% to claim that the proportion is significantly different from the historical norm?

- 1. Open the **Binomial Power and Sample Size** dialog.
- 2. Select **Min. Difference** as the value to **Compute**. Enter 0.4 as the **Proportion** and 100, 500, 1000, 5000 as the sample sizes **N1** to consider.
- 3. Click **OK**.

A power table is displayed in the **Report** window. The table indicates the detectable differences delta for each sample size. For example, with 1000 observations the pollster could determine whether the proportion varies from 40% by at least 4.34%.

```
*** Power Table ***
             p.alt
                       delta alpha power
                                           n1
1
    0.4 0.5372491 0.1372491
                              0.05
                                     0.8
                                          100
    0.4 0.4613797 0.0613797
                              0.05
                                     0.8
                                          500
    0.4 0.4434020 0.0434020 0.05
                                     0.8 1000
    0.4 0.4194100 0.0194100 0.05
                                     0.8 5000
```

## **EXPERIMENTAL DESIGN**

Typically, a researcher begins an experiment by generating a design, which is a data set indicating the combinations of experimental variables at which to take observations. The researcher then measures some outcome for the indicated combinations, and records this by adding a new column to the design data set. Once the outcome is recorded, exploratory plots may be used to examine the relationship between the outcome and the experimental variables. The data may then be analyzed using ANOVA or other techniques.

The Factorial Design and Orthogonal Array Design dialogs create experimental designs. The Design Plot, Factor Plot, and Interaction Plot dialogs produce exploratory plots for designs.

### **Factorial**

The **Factorial Design** dialog creates a *factorial* or *fractional factorial* design. The basic factorial design contains all possible combinations of the variable levels, possibly replicated and randomized. A fractional factorial design excludes some combinations based upon which model effects are of interest.

## Creating a factorial design

From the main menu, choose **Statistics** ▶ **Design** ▶ **Factorial**. The **Factorial Design** dialog opens, as shown in Figure 6.26.

imes Factorial Design	×
Design Structure	-Names
Levels: 3, 2	Fa <u>c</u> tor Names:
<u>N</u> umber of Replications:	Ro <u>w</u> Names:
1	-Randomization-
<u>F</u> raction:	□ <u>R</u> andomize Row Order
	Restricted Factors:
	-Results-
	Save <u>I</u> n: exfac.design
OK Cancel Apply	Help

**Figure 6.26:** The **Factorial Design** dialog.

We create a design with 3 levels of the first variable and two levels of the second.

- 1. Open the **Factorial Design** dialog.
- 2. Specify 3, 2 as the **Levels**.
- 3. Type exfac.design in the **Save In** field.
- 4. Click OK.

An exfac.design data set containing the design is created. You can view exfac.design with either the **Commands** window or the **Data** viewer.

## Orthogonal Array

The **Orthogonal Array Design** dialog creates an orthogonal array design. *Orthogonal array designs* are essentially very sparse fractional factorial designs, constructed such that inferences may be made regarding main (first-order) effects. Level combinations necessary for estimating second- and higher-order effects are excluded in the interest of requiring as few measurements as possible.

### Generating an orthogonal array design

From the main menu, choose **Statistics** ▶ **Design** ▶ **Orthogonal Array**. The **Orthogonal Array Design** dialog opens, as shown in Figure 6.27.

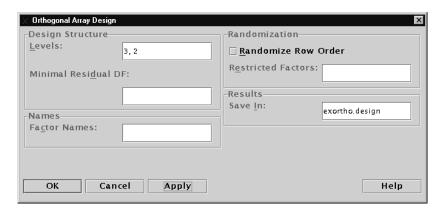


Figure 6.27: The Orthogonal Array Design dialog.

We create a design with 3 levels of the first variable and two levels of the second.

- 1. Open the **Orthogonal Array Design** dialog.
- 2. Specify 3, 2 as the **Levels**.
- 3. Type exortho.design in the **Save In** field.
- 4. Click **OK**.

An exortho.design data set containing the design is created. You can view exortho.design with either the **Commands** window or the **Data** viewer. In this simple example, the orthogonal array design is equivalent to the design created in the section Factorial on page 274.

## **Design Plot**

A *design plot* displays a function of a variable for each level of one or more corresponding factors. The default function is the mean.

### Creating a design plot

From the main menu, choose **Statistics** ▶ **Design** ▶ **Design Plot**. The **Design Plot** dialog opens, as shown in Figure 6.28.

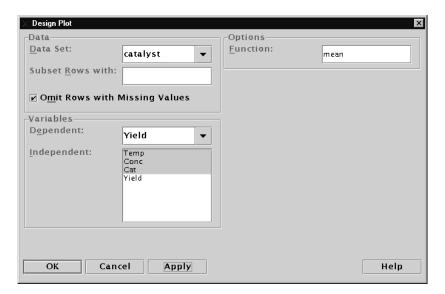


Figure 6.28: The Design Plot dialog.

The catalyst data set comes from a designed experiment. Its eight rows represent all possible combinations of two temperatures (Temp), two concentrations (Conc), and two catalysts (Cat). The fourth column represents the response variable Yield. We are interested in determining how temperature, concentration, and catalyst affect the Yield. Prior to fitting an ANOVA model, we can use various plots to examine the relationship between these variables. We start with a design plot.

- 1. Open the **Design Plot** dialog.
- 2. Type catalyst in the **Data Set** field.
- 3. Select Yield as the **Dependent** variable.
- 4. CTRL-click to select Temp, Conc, and Cat as the **Independent** variables.
- 5. Click **OK**.

A design plot appears in a **Graph** window. This plot has a vertical bar for each factor, and a horizontal bar indicating the mean of Yield for each factor level.

## **Factor Plot**

A *factor plot* consists of side by side plots comparing the values of a variable for different levels of a factor. By default, box plots are used. See the plot.factor help file for details.

## Creating a factor plot

From the main menu, choose **Statistics** ▶ **Design** ▶ **Factor Plot**. The **Factor Plot** dialog opens, as shown in Figure 6.29.

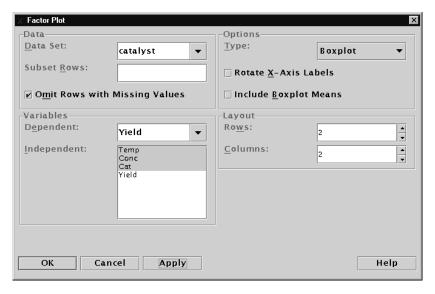


Figure 6.29: The Factor Plot dialog.

We create factor plots for the catalyst data set as follows:

- 1. Open the **Factor Plot** dialog.
- 2. Type catalyst in the **Data Set** field.
- 3. Select Yield as the **Dependent** variable.
- 4. CTRL-click to select Temp, Conc, and Cat as the **Independent** variables.
- 5. Change the number of **Rows** and number of **Columns** to **2**. This specifies a  $2 \times 2$  grid of plots.
- 6. Click **OK**.

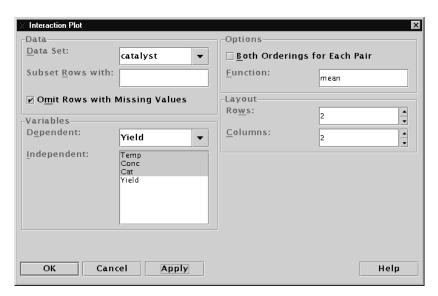
A factor plot appears in a **Graph** window. For each factor there is a set of box plots for Yield, with a separate box plot for each factor level.

# Interaction Plot

An *interaction plot* displays the levels of one factor along the x-axis, the response on the y-axis, and the points corresponding to a particular level of a second factor connected by lines. This type of plot is useful for exploring or discovering interactions.

### Creating an interaction plot

From the main menu, choose **Statistics** ▶ **Design** ▶ **Interaction Plot**. The **Interaction Plot** dialog opens, as shown in Figure 6.30.



**Figure 6.30:** The Interaction Plot dialog.

#### Example

We create interaction plots for the catalyst data set as follows:

- 1. Open the **Interaction Plot** dialog.
- 2. Type catalyst in the **Data Set** field.
- 3. Select Yield as the **Dependent** variable
- 4. CTRL-click to select Temp, Conc, and Cat as the **Independent** variables.
- 5. Change the number of **Rows** and number of **Columns** to **2**. This specifies a  $2 \times 2$  grid of plots.
- 6. Click **OK**.

# Chapter 6 Statistics

An interaction plot appears in a **Graph** window. For each pair of factors, a set of lines is created showing the mean of Yield for each level of the second factor at each level of the first factor. If the lines in a plot cross, it suggests that an interaction is present between the two factors.

## REGRESSION

Regression is the standard technique for assessing how various predictors relate to a response. This section discusses the regression techniques available from the **Statistics Regression** menu.

- Linear regression: predicting a continuous response as a linear function of predictors using a least-squares fitting criterion.
- **Robust MM regression**: predicting a continuous response using an MM based robust fitting criterion.
- **Robust LTS regression**: predicting a continuous response using a least-trimmed-squares fitting criterion.
- Stepwise linear regression: selecting which variables to employ in a linear regression model using a stepwise procedure.
- **Generalized additive models:** predicting a general response as a sum of nonparametric smooth univariate functions of the predictors.
- Local (loess) regression: predicting a continuous response as a nonparametric smooth function of the predictors using least-squares.
- **Nonlinear regression**: predicting a continuous response as a nonlinear function of the predictors using least-squares.
- Generalized linear models: predicting a general response as a linear combination of the predictors using maximum likelihood.
- Log-linear (Poisson) regression: predicting counts using Poisson maximum likelihood.

- **Logistic regression**: predicting a binary response using binomial maximum likelihood with a logistic link.
- **Probit regression:** predicting a binary response using binomial maximum likelihood with a probit link.

# Linear Regression

Linear regression is used to describe the effect of continuous or categorical variables upon a continuous response. It is by far the most common regression procedure. The linear regression model assumes that the response is obtained by taking a specific linear combination of the predictors and adding random variation (error). The error is assumed to have a Gaussian (normal) distribution with constant variance, and to be independent of the predictor values.

Linear regression uses the method of *least-squares*, in which a line is fit that minimizes the sum of the squared residuals. Suppose a set of n observations of the response variable  $y_i$  correspond to a set of values of the predictor  $x_i$  according to the model  $\hat{y} = f(\hat{x})$ , where  $\hat{y} = (y_1, y_2, ..., y_n)$  and  $\hat{x} = (x_1, x_2, ..., x_n)$ . The ith residual  $r_i$  is defined as the difference between the ith observation  $y_i$  and the ith fitted value  $\hat{y}_i = \hat{f}(x_i)$ : that is,  $r_i = y_i - \hat{y}_i$ . The method of least

squares finds a set of fitted values that minimizes the sum  $\sum_{i=1}^{n} r_i^2$ .

If the response of interest is not continuous, then logistic regression, probit regression, log-linear regression, or generalized linear regression may be appropriate. If the predictors affect the response in a nonlinear way, then nonlinear regression, local regression, or generalized additive regression may be appropriate. If the data contain outliers or the errors are not Gaussian, then robust regression may be appropriate. If the focus is on the effect of categorical variables, then ANOVA may be appropriate. If the observations are correlated or random effects are present, then the mixed effect or generalized least squares model may be appropriate.

Other dialogs related to linear regression are **Stepwise Linear Regression**, **Compare Models**, and **Multiple Comparisons**. The **Stepwise Linear Regression** dialog uses a stepwise procedure to suggest which variables to include in a model. **Compare Models** provides tests for determining which of several models is most appropriate. **Multiple Comparisons** calculates effects for categorical predictors in linear regression or ANOVA.

#### Fitting a linear regression model

From the main menu, choose **Statistics** ▶ **Regression** ▶ **Linear**. The **Linear Regression** dialog opens, as shown in Figure 6.31.

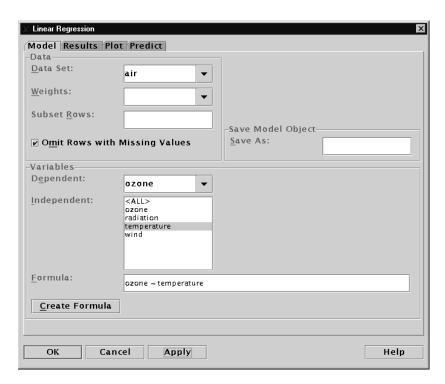
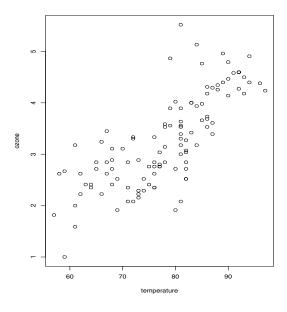


Figure 6.31: The Linear Regression dialog.

## **Example**

We examine the air pollution data in the example data set air. This is a data set with 111 observations (rows) and 4 variables (columns). It is taken from an environmental study that measured the four variables

ozone, solar radiation, temperature, and wind speed for 111 consecutive days. We first create a scatter plot of the temperature and ozone variables in air, as shown in Figure 6.32.



**Figure 6.32:** A scatter plot of ozone versus temperature.

From the scatter plot, we hypothesize a linear relationship between temperature and ozone concentration. We choose ozone as the response and temperature as the single predictor. The choice of response and predictor variables is driven by the subject matter in which the data arise, rather than by statistical considerations.

- 1. Open the **Linear Regression** dialog.
- 2. Type air in the **Data Set** field.
- 3. Type ozone ~ temperature in the Formula field. Alternatively, select ozone as the **Dependent** variable and temperature as the **Independent** variable. As a third way of generating a formula, click the **Create Formula** button and select ozone as the **Response** variable and temperature as a **Main Effect**. You can use the **Create Formula** button to

create complicated linear models and learn the notation for model specifications. The on-line help discusses formula creation in detail.

- 4. Go to the **Plot** page on the **Linear Regression** dialog and check the seven main diagnostic plots.
- 5. Click **OK** to do the linear regression.

Spotfire S+ generates a **Graph** window with seven diagnostic plots. You can access these plots by clicking the seven page tabs at the bottom of the **Graph** window. The plots appear similar to those shown in Figure 6.33. Spotfire S+ prints the results of the linear regression in the **Report** window:

```
*** Linear Model ***
Call: lm(formula = ozone ~ temperature, data = air,
  na.action = na.exclude)
Residuals:
  Min
      10 Median
                              Max
-1.49 -0.4258 0.02521 0.3636 2.044
Coefficients:
              Value Std. Error t value Pr(>|t|)
(Intercept) -2.2260 0.4614 -4.8243 0.0000
temperature 0.0704 0.0059 11.9511
                                       0.0000
Residual standard error: 0.5885 on 109 degrees of freedom
Multiple R-Squared: 0.5672
F-statistic: 142.8 on 1 and 109 degrees of freedom, the
  p-value is 0
```

The Value column under Coefficients gives the coefficients of the linear model, allowing us to read off the estimated regression line as follows:

```
ozone = -2.2260 + 0.0704 \times temperature
```

The column named Std. Error in the output gives the estimated standard error for each coefficient. The Multiple R-Squared term tells us that the model explains about 57% of the variation in ozone. The F-statistic is the ratio of the mean square of the regression to the estimated variance; if there is no relationship between

temperature and ozone, this ratio has an F distribution with 1 and 109 degrees of freedom. The ratio here is clearly significant, so the true slope of the regression line is probably not 0.

## Diagnostic plots for linear models

How good is the fitted linear regression model? Is temperature an adequate predictor of ozone concentration? Can we do better? Questions such as these are essential any time you try to explain data with a statistical model. It is not enough to fit a model; you must also assess how well the model fits the data, and be prepared to modify the model or abandon it altogether if it does not satisfactorily explain the data.

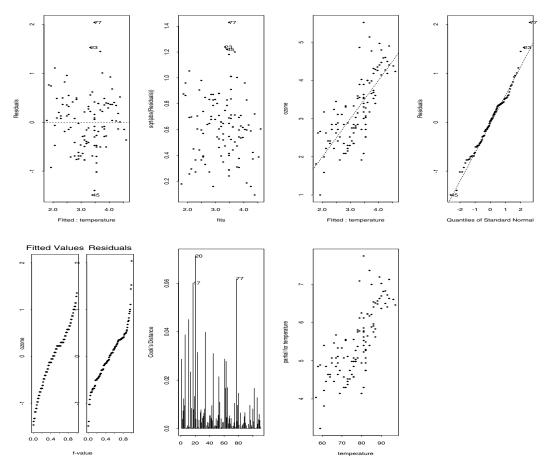


Figure 6.33: Seven diagnostic plots created by the Linear Regression dialog.

The simplest and most informative method for assessing the fit is to look at the model graphically, using an assortment of plots that, taken together, reveal the strengths and weaknesses of the model. For example, a plot of the response against the fitted values gives a good idea of how well the model has captured the broad outlines of the data. Examining a plot of the residuals against the fitted values often reveals unexplained structure left in the residuals, which should appear as nothing but noise in a strong model. The plotting options for the **Linear Regression** dialog provide these two plots, along with the following useful plots:

- Square root of absolute residuals against fitted values. This plot is
  useful in identifying outliers and visualizing structure in the
  residuals.
- Normal quantile plot of residuals. This plot provides a visual test of the assumption that the model's errors are normally distributed. If the ordered residuals cluster along the superimposed quantile-quantile line, you have strong evidence that the errors are indeed normal.
- Residual-fit spread plot, or r-f plot. This plot compares the spread of the fitted values with the spread of the residuals. Since the model is an attempt to explain the variation in the data, you hope that the spread in the fitted values is much greater than that in the residuals.
- Cook's distance plot. Cook's distance is a measure of the influence of individual observations on the regression coefficients.
- Partial residual plot. A partial residual plot is a plot of  $r_i = b_k x_{ik}$  versus  $x_{ik}$ , where  $r_i$  is the ordinary residual for the ith observation,  $x_{ik}$  is the ith observation of the kth predictor, and  $b_k$  is the regression coefficient estimate for the kth predictor. Partial residual plots are useful for detecting nonlinearities and identifying possible causes of unduly large residuals.

The line  $y = \hat{y}$  is shown as a dashed line in the third plot of the top row in Figure 6.33. In the case of simple regression, this line is visually equivalent to the regression line. The regression line appears

to model the trend of the data reasonably well. The residuals plots (left two plots in the top row of Figure 6.33) show no obvious pattern, although five observations appear to be outliers. By default, the three most extreme values are identified in each of the residuals plots and in the Cook's distance plot.

Another useful diagnostic plot is the normal plot of residuals (right plot in the top row of Figure 6.33). The normal plot gives no reason to doubt that the residuals are normally distributed. The r-f plot, on the other hand (left plot in the bottom row of Figure 6.33), shows a weakness in this model: the spread of the residuals is actually greater than the spread in the original data. However, if we ignore the five outlying residuals, the residuals are more tightly grouped than the original data.

The Cook's distance plot shows four or five heavily influential observations. Because the regression line fits the data reasonably well, the regression is significant, and the residuals appear normally distributed, we feel justified in using the regression line as a way to estimate the ozone concentration for a given temperature. One important issue remains, however: the regression line explains only 57% of the variation in the data. We may be able to do somewhat better by considering the effect of other variables on the ozone concentration.

# Robust MM Regression

Robust regression models are useful for fitting linear relationships when the random variation in the data is not Gaussian (normal), or when the data contain significant outliers. In such situations, standard linear regression may return inaccurate estimates.

The *robust MM regression* method returns a model that is almost identical in structure to a standard linear regression model. This allows the production of familiar plots and summaries with a robust model. The MM method is the robust regression procedure currently recommended by TIBCO Software Inc.

## Performing robust MM regression

From the main menu, choose **Statistics** ▶ **Regression** ▶ **Robust MM**. The **Robust MM** Linear **Regression** dialog opens, as shown in Figure 6.34.

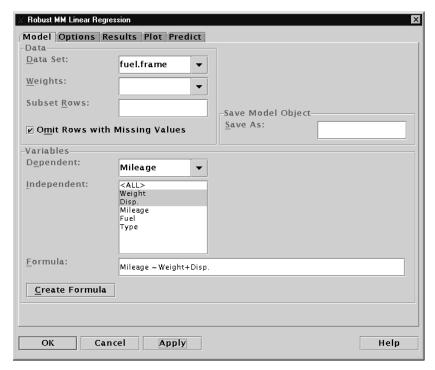


Figure 6.34: The Robust MM Linear Regression dialog.

The data set fuel.frame is taken from the April 1990 issue of *Consumer Reports*. It contains 60 observations (rows) and 5 variables (columns). Observations of weight, engine displacement, mileage, type, and fuel were taken for each of sixty cars. In the fuel.frame data, we predict Mileage by Weight and Disp. using robust MM regression.

- 1. Open the **Robust MM Linear Regression** dialog.
- 2. Type fuel.frame in the **Data Set** field.
- 3. Type Mileage~Weight+Disp. in the **Formula** field. Alternatively, select Mileage as the **Dependent** variable and CTRL-click to select Weight and Disp. as the **Independent** variables. As a third way of generating a formula, click the **Create Formula** button, select Mileage as the **Response**

variable, and CTRL-click to select Weight and Disp. as the **Main Effects**. You can use the **Create Formula** button to create complicated linear models and learn the notation for model specifications. The on-line help discusses formula creation in detail.

4. Click **OK** to fit the robust MM regression model.

A summary of the model appears in the **Report** window.

# Robust LTS Regression

The *robust LTS regression* method performs least-trimmed-squares regression. It has less detailed plots and summaries than standard linear regression and robust MM regression.

#### Performing robust LTS regression

From the main menu, choose **Statistics** ▶ **Regression** ▶ **Robust LTS**. The **Robust LTS Linear Regression** dialog opens, as shown in Figure 6.35.

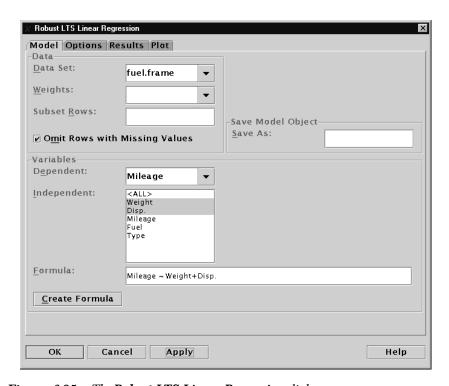


Figure 6.35: The Robust LTS Linear Regression dialog.

In the fuel.frame data, we predict Mileage by Weight and Disp. using robust LTS regression.

- 1. Open the **Robust LTS Linear Regression** dialog.
- 2. Type fuel. frame in the **Data Set** field.
- 3. Type Mileage~Weight+Disp. in the Formula field. Alternatively, select Mileage as the Dependent variable and CTRL-click to select Weight and Disp. as the Independent variables. As a third way of generating a formula, click the Create Formula button, select Mileage as the Response variable, and CTRL-click to select Weight and Disp. as the Main Effects. You can use the Create Formula button to create complicated linear models and learn the notation for model specifications. The on-line help discusses formula creation in detail.
- 4. Click **OK** to fit the robust LTS regression model.

A summary of the model appears in the **Report** window.

# Stepwise Linear Regression

One step in the modeling process is determining what variables to include in the regression model. *Stepwise linear regression* is an automated procedure for selecting which variables to include in a regression model. Forward stepwise regression adds terms to the model until additional terms no longer improve the goodness-of-fit. At each step the term is added that most improves the fit. Backward stepwise regression drops terms from the model so long as dropping terms does not significantly decrease the goodness-of-fit. At each step the term is dropped whose removal least degrades the fit. Stepwise regression also has the option of alternating between adding and dropping terms. This is the default method used.

## Performing stepwise linear regression

From the main menu, choose **Statistics** ▶ **Regression** ▶ **Stepwise**. The **Stepwise Linear Regression** dialog opens, as shown in Figure 6.36.

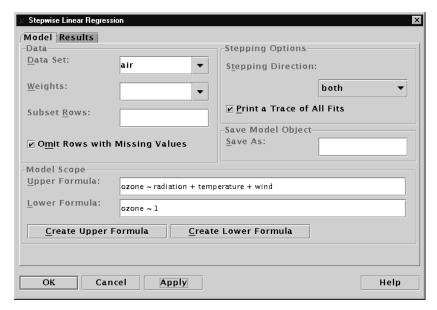


Figure 6.36: The Stepwise Linear Regression dialog.

We apply stepwise regression to the air data.

- 1. Open the **Stepwise Linear Regression** dialog.
- 2. Type air in the **Data Set** field.
- 3. We must supply a formula representing the most complex model to consider. Specify ozone ~ radiation + temperature + wind as the **Upper Formula**.
- 4. We must also supply a formula representing the simplest model to consider. Specify ozone ~ 1 as the **Lower Formula**. The 1 indicates inclusion of just an intercept term.
- Click **OK**.

Stepwise regression uses the Cp statistic as a measure of goodness-of-fit. This is a statistic which rewards accuracy while penalizing model complexity. In this example, dropping any term yields a model with a Cp statistic that is smaller than that for the full model. Hence, the full model is selected as the best model.

#### The summary of the steps appears in the **Report** window.

```
*** Stepwise Regression ***
  *** Stepwise Model Comparisons ***
Start: AIC= 29.9302
ozone ~ radiation + temperature + wind
Single term deletions
Model:
ozone ~ radiation + temperature + wind
scale: 0.2602624
           Df Sum of Sq RSS
    <none>
                       27.84808 29.93018
  radiation 1 4.05928 31.90736 33.46893
temperature 1 17.48174 45.32982 46.89140
      wind 1 6.05985 33.90793 35.46950
  *** Linear Model ***
Call: lm(formula = ozone ~ radiation + temperature + wind,
data = air, na.action = na.exclude)
Residuals:
   Min 10 Median 30 Max
-1.122 -0.3764 -0.02535 0.3361 1.495
Coefficients:
             Value Std. Error t value Pr(>|t|)
(Intercept) -0.2973  0.5552  -0.5355  0.5934
  radiation 0.0022 0.0006 3.9493 0.0001
temperature 0.0500 0.0061
                             8.1957 0.0000
      wind -0.0760 0.0158 -4.8253 0.0000
Residual standard error: 0.5102 on 107 degrees of freedom
Multiple R-Squared: 0.6807
F-statistic: 76.03 on 3 and 107 degrees of freedom, the
p-value is 0
```

# Generalized Additive Models

Generalized additive models extend linear models by flexibly modeling additive nonlinear relationships between the predictors and the response. Whereas linear models assume that the response is linear in each predictor, additive models assume only that the response is affected by each predictor in a smooth way. The response is modeled as a sum of smooth functions in the predictors, where the smooth functions are estimated automatically using smoothers. Additive models may be useful for obtaining a final fit, or for exploring what types of variable transformations might be appropriate for use in a standard linear model.

#### Fitting an additive model

From the main menu, choose **Statistics** ▶ **Regression** ▶ **Generalized Additive**. The **Generalized Additive Models** dialog opens, as shown in Figure 6.37.

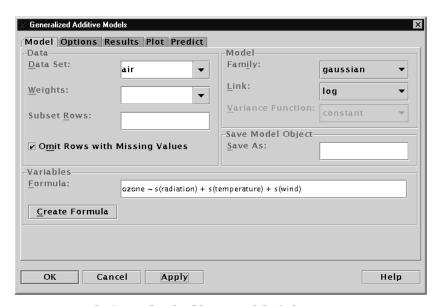


Figure 6.37: The Generalized Additive Models dialog.

## Example

We fit an additive model for the air data.

- 1. Open the **Generalized Additive Models** dialog.
- 2. Type air in the **Data Set** field.

- 3. Specify ozone ~ s(radiation) + s(temperature) + s(wind) as the **Formula**.
- 4. On the **Plot** page of the dialog, select the **Partial Residuals** and **Include Partial Fits** check boxes. This indicates that we want plots of the partial residuals and partial fits for each predictor.
- 5. Click **OK**.

A summary of the additive model appears in the **Report** window. A multipage **Graph** window appears with one partial residual plot on each page.

# Local (Loess) Regression

Local regression is a nonparametric generalization of multivariate polynomial regression. It is best thought of as a way to fit general smooth surfaces. A wide variety of options are available for specifying the form of the surface.

#### Fitting a local regression

From the main menu, choose **Statistics** ▶ **Regression** ▶ **Local** (**Loess**). The **Local** (**Loess**) **Regression** dialog opens, as shown in Figure 6.38.

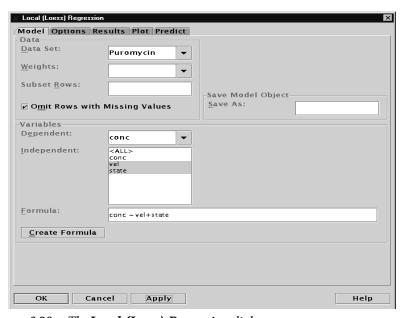


Figure 6.38: The Local (Loess) Regression dialog.

The data set Puromycin has 23 rows representing the measurement of initial velocity of a biochemical reaction for 6 different concentrations of substrate and two different cell treatments. The section Nonlinear Regression describes these data in detail and discusses a theoretical model for the data. Before fitting a theoretical model, we can use the **Local (Loess) Regression** dialog to fit nonparametric smooth curves to the data.

Our model consists of a separate curve for each treatment group. We predict the response conc by the variables vel and state. Since state is a factor, this fits a separate smooth curve in vel for each level of state.

- 1. Open the **Local** (**Loess**) **Regression** dialog.
- 2. Type Puromycin in the **Data Set** field.
- 3. Type conc~vel+state in the **Formula** field. Alternatively, select conc as the **Dependent** variable and CTRL-click to select vel and state as the **Independent** variables. As a third way of generating a formula, click the **Create Formula** button, select conc as the **Response** variable, and CTRL-click to select vel and state as the **Main Effects**. You can use the **Create Formula** button to create complicated linear models and learn the notation for model specifications. The on-line help discusses formula creation in detail.
- 4. On the **Plot** page of the dialog, select **Cond. Plots of Fitted vs Predictors**. This type of plot displays a separate plot in one variable for different subsets of another variable. In our case, it plots a separate curve for each level of state.
- Click **OK**.

A summary of the loess model is presented in the **Report** window, and a **Graph** window displays the conditional plot.

# Nonlinear Regression

Nonlinear regression uses a specific nonlinear relationship to predict a continuous variable from one or more predictor variables. The form of the nonlinear relationship is usually derived from an application-specific theoretical model.

The **Nonlinear Regression** dialog fits a nonlinear regression model. To use nonlinear regression, specify the form of the model in S-PLUS syntax and provide starting values for the parameter estimates.

### Fitting a nonlinear least squares regression

From the main menu, choose **Statistics** ▶ **Regression** ▶ **Nonlinear**. The **Nonlinear Regression** dialog opens, as shown in Figure 6.39.

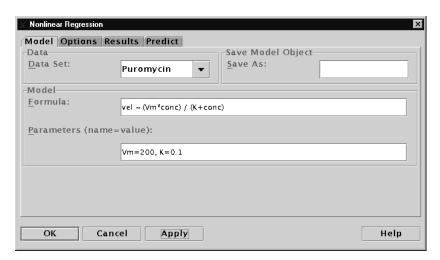


Figure 6.39: The Nonlinear Regression dialog.

#### Example

The data set Puromycin has 23 rows representing the measurement of initial velocity of a biochemical reaction for 6 different concentrations of substrate and two different cell treatments. Figure 6.40 plots velocity versus concentration with different symbols for the two treatment groups (treated and untreated).

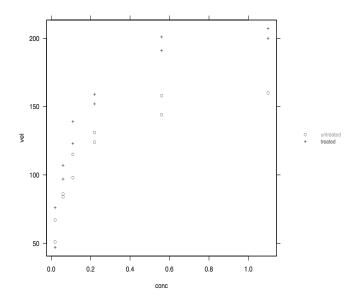


Figure 6.40: Scatter plot of the Puromycin data.

The relationship between velocity and concentration is known to follow a Michaelis-Menten relationship:

$$V = \frac{V_{max}c}{K+c} + \varepsilon$$

where V is the velocity, c is the enzyme concentration,  $V_{max}$  is a parameter representing the asymptotic velocity as  $c \to \infty$ , K is the Michaelis parameter, and  $\epsilon$  is experimental error. Assuming the treatment with the drug would change  $V_{max}$  but not K, the optimization function is:

$$S(V_{max}, K) = \sum \left(V_i - \frac{(V_{max} + \Delta V_{max} I_{\{treated\}}(state))c_i}{K + c_i}\right)^2$$

where  $I_{\{treated\}}$  is the function indicating whether the cell was treated with Puromycin.

We first fit the simpler model in which a single curve is fit for both groups. We then add a term reflecting the influence of treatment.

In order to fit a nonlinear regression model, we must specify the form of the nonlinear model, the name of the data set, and starting values for the parameter estimates. Examination of Figure 6.40 suggests starting values of V=200 and K=0.1, treating all observations as a single group. We fit a Michaelis-Menten relationship between velocity and concentration as follows:

- 1. Open the **Nonlinear Regression** dialog.
- 2. Type Puromycin in the **Data Set** field.
- 3. Type the Michaelis-Menten relationship vel~(Vm\*conc)/ (K+conc) into the **Formula** field.
- 4. Type the parameter starting values Vm=200, K=0.1 into the **Parameters** field.
- 5. Click **OK**.

The following results appear in the **Report** window.

The printed results provide parameter estimates, standard errors, and t-values, as well as the residual standard error and correlation of parameter estimates.

We now fit a model containing a treatment effect:

- 1. Open the **Nonlinear Regression** dialog.
- 2. Type Puromycin in the **Data Set** field.
- 3. Type the Michaelis-Menten relationship vel ~ ((Vm+delV \* (state == "treated")) \* conc)/(K + conc) into the **Formula** field.
- 4. Figure 6.40 suggests starting values of Vm=160 and delV=40, while the previous model suggests K=0.05. Type the starting values Vm=160, delV=40, K=0.05 into the **Parameters** field.
- 5. Click **OK**.

The following results appear in the **Report** window.

```
*** Nonlinear Regression Model ***

Formula: vel ~ ((Vm + delV * (state == "treated")) * conc)/(K + conc)

Parameters:

Value Std. Error t value
Vm 166.6010000 5.80726000 28.68840
delV 42.0245000 6.27201000 6.70032
K 0.0579659 0.00590968 9.80863

Residual standard error: 10.5851 on 20 degrees of freedom

Correlation of Parameter Estimates:

Vm delV
delV -0.5410
K 0.6110 0.0644
```

The printed results provide parameter estimates, standard errors, and t-values, as well as the residual standard error and correlation of parameter estimates. The magnitude of the t-statistic for delV confirms that the treatment affects the maximum velocity.

# Generalized Linear Models

Generalized linear models are generalizations of the familiar linear regression model to situations where the response is discrete or the model varies in other ways from the standard linear model. The most widely used generalized linear models are logistic regression models for binary data and log-linear (Poisson) models for count data.

#### Fitting a generalized linear model

From the main menu, choose **Statistics** ▶ **Regression** ▶ **Generalized Linear**. The **Generalized Linear Models** dialog opens, as shown in Figure 6.41.

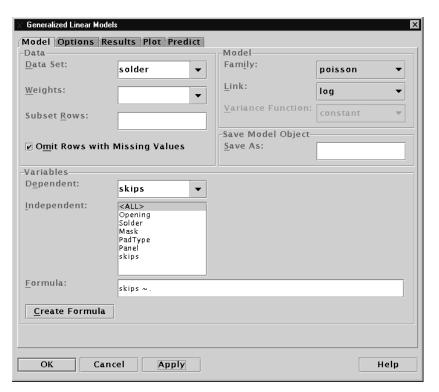


Figure 6.41: The Generalized Linear Models dialog.

## **Example**

The solder data set contains 900 observations (rows) that are the results of an experiment that varied five factors relevant to the wave-soldering procedure for mounting components on printed circuit boards. The response variable skips is a count of how many solder

skips appeared in a visual inspection. We can use the **Generalized Linear Models** dialog to assess which process variables affect the number of skips.

- 1. Open the **Generalized Linear Models** dialog.
- 2. Type solder in the **Data Set** field.
- 3. Select skips as the **Dependent** variable and **<ALL>** in the **Independent** variable list. This generates skips ~ . in the **Formula** field.
- 4. Select poisson as the **Family**. The **Link** changes to log, which is the canonical link for a Poisson model.
- Click OK.

A summary of the Poisson regression appears in the **Report** window.

# Log-Linear (Poisson) Regression

Count data are frequently modeled using *log-linear regression*. In log-linear regression, the response is assumed to be generated from a Poisson distribution, with a centrality parameter that depends upon the values of the covariates.

#### Fitting a log-linear (Poisson) regression

From the main menu, choose **Statistics** ▶ **Regression** ▶ **Log-linear** (**Poisson**). The **Log-linear** (**Poisson**) **Regression** dialog opens, as shown in Figure 6.42.

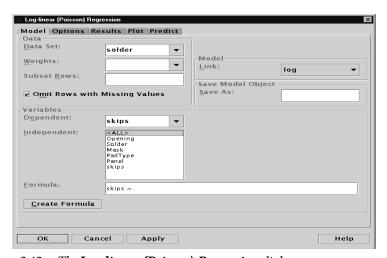


Figure 6.42: The Log-linear (Poisson) Regression dialog.

In this example, we fit a Poisson regression to the solder data.

- 1. Open the **Log-linear** (**Poisson**) **Regression** dialog.
- 2. Type solder in the **Data Set** field.
- 3. Select skips as the **Dependent** variable and **<ALL>** in the **Independent** variable list. This generates skips ~ . in the **Formula** field.
- Click OK.

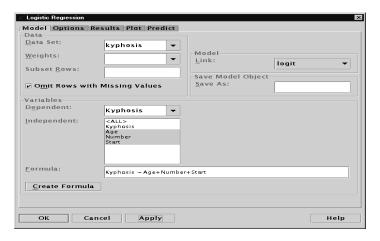
A summary of the log-linear regression appears in the **Report** window. The t-values in the resulting table of coefficients are all fairly large, indicating that all of the process variables have a significant influence upon the number of skips generated.

# Logistic Regression

Logistic regression models the relationship between a dichotomous response variable and one or more predictor variables. A linear combination of the predictor variables is found using maximum likelihood estimation, where the response variable is assumed to be generated by a binomial process whose probability parameter depends upon the values of the predictor variables.

## Fitting a logistic regression

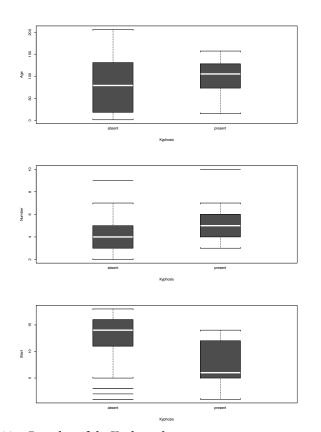
From the main menu, choose **Statistics** ▶ **Regression** ▶ **Logistic**. The **Logistic Regression** dialog opens, as shown in Figure 6.43.



**Figure 6.43:** The **Logistic Regression** dialog.

The data set kyphosis has 81 rows representing data on 81 children who have had corrective spinal surgery. The outcome Kyphosis is a binary variable, and the other three variables Age, Number, and Start, are numeric. Figure 6.44 displays box plots of Age, Number, and Start for each level of Kyphosis, as generated by the following commands:

```
> par(mfrow=c(3,1))
> boxplot(split(kyphosis$Age, kyphosis$Kyphosis),
+ xlab="Kyphosis", ylab="Age")
> boxplot(split(kyphosis$Number, kyphosis$Kyphosis),
+ xlab="Kyphosis", ylab="Number")
> boxplot(split(kyphosis$Start, kyphosis$Kyphosis),
+ xlab="Kyphosis", ylab="Start")
```



**Figure 6.44:** Box plots of the Kyphosis data.

Kyphosis is a postoperative spinal deformity. We are interested in exploring how the covariates influence whether or not the deformity occurs. Both Start and Number show strong location shifts with respect to the presence or absence of Kyphosis. The Age variable does not show such a shift in location. We can use logistic regression to quantify the influence of each covariate upon the likelihood of deformity.

- 1. Open the **Logistic Regression** dialog.
- 2. Type kyphosis in the **Data Set** field.
- 3. Specify Kyphosis~Age+Number+Start in the **Formula** field.
- 4. Click **OK**.

A summary of the logistic regression appears in the **Report** window. The summary contains information on the residuals, coefficients, and deviance. The high t-value for Start indicates it has a significant influence upon whether kyphosis occurs. The t-values for Age and Number are not large enough to display a significant influence upon the response.

```
*** Generalized Linear Model ***
Call: glm(formula = Kyphosis ~ Age + Number + Start,
  family = binomial(link = logit), data = kyphosis,
 na.action = na.exclude, control = list(
 epsilon = 0.0001, maxit = 50, trace = F))
Deviance Residuals:
      Min 10
                         Median
                                        30
                                               Max
-2.312363 -0.5484308 -0.3631876 -0.1658653 2.16133
Coefficients:
                 Value Std. Error t value
(Intercept) -2.03693225 1.44918287 -1.405573
       Age 0.01093048 0.00644419 1.696175
    Number 0.41060098 0.22478659 1.826626
     Start -0.20651000 0.06768504 -3.051043
```

```
(Dispersion Parameter for Binomial family taken to be 1 )

Null Deviance: 83.23447 on 80 degrees of freedom

Residual Deviance: 61.37993 on 77 degrees of freedom

Number of Fisher Scoring Iterations: 5
```

# Probit Regression

The **Probit Regression** dialog fits a probit response model. This is a variation of logistic regression suitable for binomial response data.

#### Fitting a probit regression model

From the main menu, choose **Statistics** ▶ **Regression** ▶ **Probit**. The **Probit Regression** dialog opens, as shown in Figure 6.45.

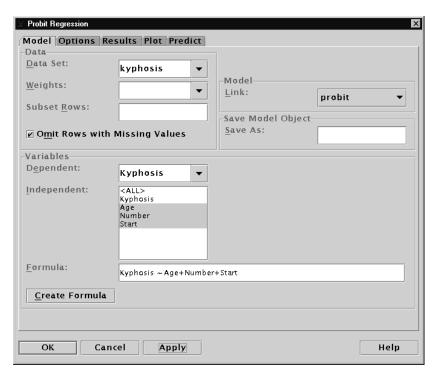


Figure 6.45: The Probit Regression dialog.

In this example, we fit a probit regression model to the kyphosis data set:

- 1. Open the **Probit Regression** dialog.
- 2. Type kyphosis in the **Data Set** field.
- 3. Specify Kyphosis~Age+Number+Start in the **Formula** field.
- 4. Click **OK**.

A summary of the model is printed in the **Report** window.

```
*** Generalized Linear Model ***
Call: glm(formula = Kyphosis ~ Age + Number + Start,
  family = binomial(link = probit), data = kyphosis,
 na.action = na.exclude, control = list(epsilon =
 0.0001, maxit = 50, trace = F))
Deviance Residuals:
      Min
                  1Q Median
                                       30
                                               Max
 -2.217301 -0.5440968 -0.3535132 -0.124005 2.149486
Coefficients:
                  Value Std. Error t value
(Intercept) -1.063353291 0.809886949 -1.312965
        Age 0.005984768 0.003507093 1.706475
    Number 0.215179016 0.121687912 1.768286
      Start -0.120214682 0.038512786 -3.121423
(Dispersion Parameter for Binomial family taken to be 1 )
    Null Deviance: 83.23447 on 80 degrees of freedom
Residual Deviance: 61.0795 on 77 degrees of freedom
Number of Fisher Scoring Iterations: 5
```

## **ANALYSIS OF VARIANCE**

Analysis of variance (ANOVA) is generally used to explore the influence of one or more categorical variables upon a continuous response.

# Fixed Effects ANOVA

The **ANOVA** dialog performs classical fixed effects analysis of variance.

## Fitting a fixed effects ANOVA model

From the main menu, choose **Statistics** ► **ANOVA** ► **Fixed Effects**. The **ANOVA** dialog opens, as shown in Figure 6.46.

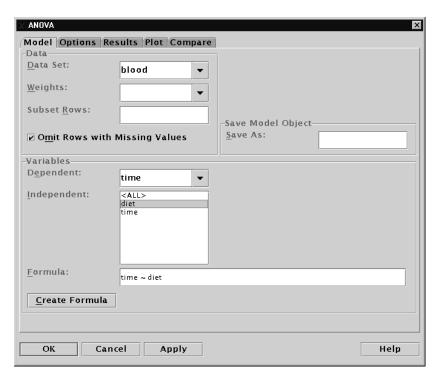


Figure 6.46: The ANOVA dialog.

In the section One-Way Analysis of Variance on page 245, we performed a simple one-way ANOVA on the blood data set listed in Table 6.2. These data give the blood coagulation times for four different diets. In general, the **ANOVA** dialog can handle far more complicated designs than the one-way ANOVA dialog. In addition, it generates diagnostic plots and provides more information on the results of the analysis. We use the **ANOVA** dialog to reproduce the results of the earlier example. We also generate some diagnostic plots to see how well our model suits our data.

- 1. If you have not done so already, create the blood data set with the instructions given on page 247.
- 2. Open the **ANOVA** dialog.
- 3. Enter blood as the **Data Set**.
- 4. Enter the formula time ~ diet for the one-way ANOVA we are going to perform. Alternatively, select time as the **Dependent** variable and diet as the **Independent** variable. As a third way of generating a formula, click the **Create Formula** button, select time as the **Response** variable and diet as a **Main Effect**. You can use the **Create Formula** button to create complicated linear models and learn the notation for model specifications. The on-line help discusses formula creation in detail.
- 5. Click on the **Plot** page and check all seven possible plots.
- 6. Click **OK** to do the analysis.

Spotfire S+ generates seven diagnostic plots. You can access these plots by clicking the seven page tabs at the bottom of the **Graph** window. The plots do not reveal any significant problems in our model. The **Report** window displays the results of the ANOVA.

# Random Effects ANOVA

Random effects ANOVA is used in balanced designed experiments where the treatment effects are taken to be random. The model must be balanced, and the model must be fully random. Only single strata designs are allowed.

For mixed effect models, use the **Linear Mixed Effects** dialog.

#### Fitting a random effects ANOVA model

From the main menu, choose **Statistics** ► **ANOVA** ► **Random Effects**. The **Random Effects Analysis of Variance** dialog opens, as shown in Figure 6.47.

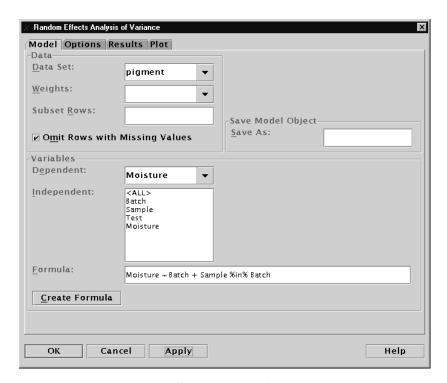


Figure 6.47: The Random Effects Analysis of Variance dialog.

## **Example**

The pigment data set has 60 rows and 4 columns. The rows represent 15 batches of pigment for which 2 samples were drawn from each batch, and 2 analyses were made on each sample. These data are from a designed experiment of moisture content where samples are nested within batch. We fit a random effects ANOVA model to assess the within-batch and between-batch variation.

- 1. Open the **Random Effects Analysis of Variance** dialog.
- 2. Type pigment in the **Data Set** field.

3. Enter the following **Formula**:

```
Moisture ~ Batch + Sample %in% Batch
```

4. Click **OK**.

A summary of the model is printed in the **Report** window.

# Multiple Comparisons

Analysis of variance models are typically used to compare the effects of several treatments upon some response. After an analysis of variance model has been fit, it is often of interest to determine whether any significant differences exist between the responses for the various treatment groups and, if so, to estimate the size of the differences. *Multiple comparisons* provides tests for equality of effects and also estimates treatment effects.

The **Multiple Comparisons** dialog calculates simultaneous or nonsimultaneous confidence intervals for any number of estimable linear combinations of the parameters of a fixed-effects linear model. It requires the name of an analysis of variance model (aov) or linear model (1m), and specification of which effects are of interest.

The Multiple Comparisons functionality is also available on the **Compare** page of the **ANOVA** dialog.

## Performing multiple comparisons

From the main menu, choose **Statistics** ► **ANOVA** ► **Multiple Comparisons**. The **Multiple Comparisons** dialog opens, as shown in Figure 6.48.

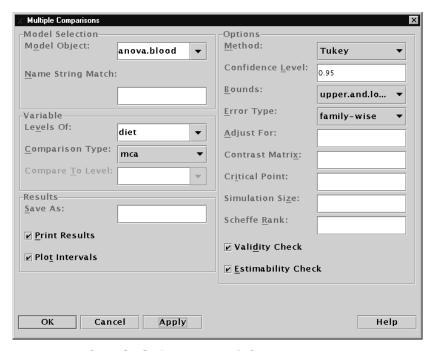


Figure 6.48: The Multiple Comparisons dialog.

In the section One-Way Analysis of Variance on page 245, we performed a simple one-way ANOVA on the blood data set listed in Table 6.2. These data give the blood coagulation times for four different diets. In the section Fixed Effects ANOVA on page 308, we revisited the blood data set and concluded that diet affects blood coagulation times. The next step is to generate multiple simultaneous confidence intervals to see which diets are different from each other. We can do this using either the **Compare** page on the **ANOVA** dialog or the **Multiple Comparisons** dialog.

- 1. If you have not done so already, create the blood data set with the instructions given on page 247.
- 2. If you have not done so already, perform the one-way analysis of variance on page 249 and save the results in the object anova.blood.
- 3. Open the **Multiple Comparisons** dialog.
- 4. Select anova.blood as the **Model Object** from the pull-down menu.
- 5. We want to compare the levels of diet using Tukey's multiple comparison procedure. Select diet from the pull-down menu for **Levels Of** and set the **Method** to **Tukey**.
- 6. Click **OK** to generate the multiple comparisons.

#### The **Report** window displays the result:

```
95 % simultaneous confidence intervals for specified
linear combinations, by the Tukey method
critical point: 2.7987
response variable: time
intervals excluding 0 are flagged by '****'
      Estimate Std.Error Lower Bound Upper Bound
A-B -5.00e+000
                    1.53
                               -9.28
                                          -0.725 ****
                                          -2.720 ****
A-C -7.00e+000
                    1.53
                              -11.30
A-D -8.93e-014
                    1.45
                               -4.06
                                           4.060
B-C -2.00e+000
                    1.37
                               -5.82
                                           1.820
                                           8.580 ****
B-D 5.00e+000
                    1.28
                                1.42
                                          10.600 ****
C-D 7.00e+000
                    1.28
                                3.42
```

From the above results and from the plot of the confidence intervals, we can see that diets A and D produce significantly different blood coagulation times than diets C and B.

## **MIXED EFFECTS**

Mixed effects models are regression or ANOVA models that include both fixed and random effects.

#### Linear

The **Linear Mixed Effects Models** dialog fits a linear mixed-effects model in the formulation of Laird and Ware (1982), but allows for nested random effects.

#### Fitting a linear mixed effects model

From the main menu, choose **Statistics** ▶ **Mixed Effects** ▶ **Linear**. The **Linear Mixed Effects Models** dialog opens, as shown in Figure 6.49.

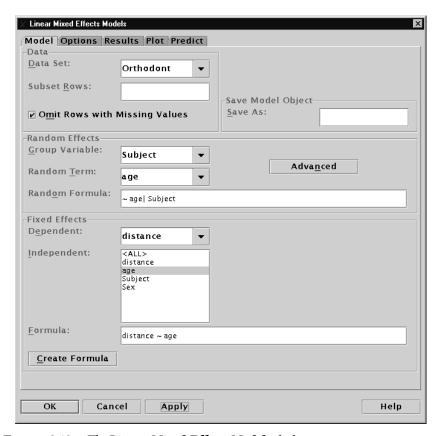


Figure 6.49: The Linear Mixed Effects Models dialog.

The Orthodont data set has 108 rows and four columns, and contains an orthodontic measurement on eleven girls and sixteen boys at four different ages. We use a linear mixed-effects model to determine the change in distance with age. The model includes fixed and random effects of age, with Subject indicating the grouping of measurements.

- 1. Open the **Linear Mixed Effects Models** dialog.
- 2. Type Orthodont in the **Data Set** field.
- 3. Specify distance~age in the Formula field.
- Select Subject as a Group Variable and age as a Random Term. The Random Formula field is automatically filled in as ~ age | Subject.
- Click **OK**.

A summary of the model is printed in the **Report** window.

#### **Nonlinear**

The **Nonlinear Mixed Effects Models** dialog fits a nonlinear mixed-effects model in the formulation described in Lindstrom and Bates (1990), but allows for nested random effects.

### Fitting a nonlinear mixed effects model

From the main menu, choose **Statistics** ▶ **Mixed Effects** ▶ **Nonlinear**. The **Nonlinear Mixed Effects Models** dialog opens, as shown in Figure 6.50.

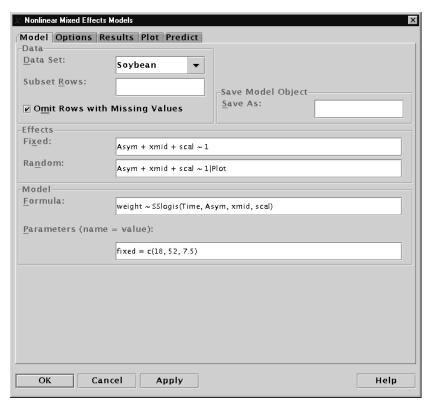


Figure 6.50: The Nonlinear Mixed Effects Models dialog.

The Soybean data comes from an experiment that compares growth patterns of two genotypes of soybeans. Variables include a factor giving a unique identifier for each plot (Plot), a factor indicating which variety of soybean is in the plot (Variety), the year the plot was planted (Year), the time each sample was taken (time), and the average leaf weight per plant (weight). We are interested in modeling weight as a function of Time in a logistic model with parameters Asym, xmid, and scal. These parameters have both fixed and random effects. The grouping variable is Plot.

- 1. Open the **Nonlinear Mixed Effects Models** dialog.
- 2. Type Soybean in the **Data Set** field.
- 3. Type the following **Formula**:

```
weight ~ SSlogis(Time, Asym, xmid, scal)
```

This specifies that we want to predict weight by a function SSlogis of the variables Time, Asym, xmid, and scal. The SSlogis function is a *self-starting* function used to specify the nonlinear model, as well as provide initial estimates to the solver.

4. Specify starting fixed effect parameter estimates in the **Parameters (name=value)** field:

```
fixed=c(18, 52, 7.5)
```

5. Specify that Asym, xmid, and scal are the fixed effects variables by typing the following formula in the **Fixed** field under **Effects**:

```
Asym + xmid + scal \sim 1
```

6. Specify that Asym, xmid, and scal are the random effects variables and that Plot is the grouping variable by typing the following formula in the **Random** field under **Effects**:

```
Asym + xmid + scal ~ 1 | Plot
```

7. Click **OK**.

A summary of the fitted model appears in the **Report** window.

# **GENERALIZED LEAST SQUARES**

Generalized least squares models are regression or ANOVA models in which the residuals have a nonstandard covariance structure. The covariance structures supported include correlated and heteroscedastic residuals.

#### Linear

The **Generalized Least Squares** dialog fits a linear model using generalized least squares. Errors are allowed to be correlated and/or have unequal variances.

#### Performing generalized least squares regression

From the main menu, choose **Statistics** ▶ **Generalized Least Squares** ▶ **Linear**. The **Generalized Least Squares** dialog opens, as shown in Figure 6.51.

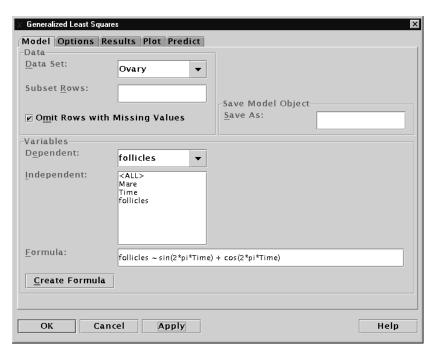


Figure 6.51: The Generalized Least Squares dialog.

The Ovary data set has 308 rows and three columns giving the number of ovarian follicles detected in different mares at different times in their estrus cycles. Biological models suggest that the number of follicles may be modeled as a linear combination of the sine and cosine of 2\*pi\*Time. We expect that the variation increases with Time, and hence use generalized least squares with a Power variance structure instead of standard linear regression. In a Power variance structure, the variance increases with a power of the absolute fitted values.

- 1. Open the **Generalized Least Squares** dialog.
- 2. Type Ovary in the **Data Set** field.
- 3. Enter the following **Formula**:

```
follicles ~ sin(2*pi*Time) + cos(2*pi*Time)
```

- 4. On the **Options** page of the dialog, select **Power** as the **Variance Structure Type**.
- 5. Click **OK**.

A summary of the fitted model appears in the **Report** window.

#### **Nonlinear**

The **Generalized Nonlinear Least Squares** dialog fits a nonlinear model using generalized least squares. The errors are allowed to be correlated and/or have unequal variances.

### Performing generalized nonlinear least squares regression

From the main menu, choose Statistics ▶ Generalized Least Squares ▶ Nonlinear. The Generalized Nonlinear Least Squares dialog opens, as shown in Figure 6.52.

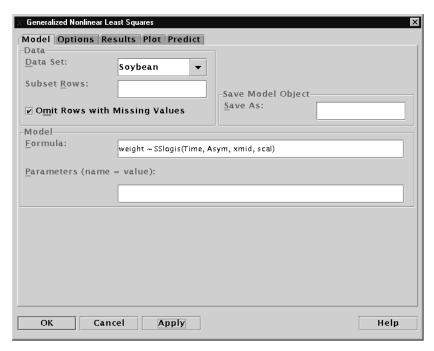


Figure 6.52: The Generalized Nonlinear Least Squares dialog.

The Soybean data comes from an experiment to compare growth patterns of two genotypes of soybeans. Variables include a factor giving a unique identifier for each plot (Plot), a factor indicating which variety of soybean is in the plot (Variety), the year the plot was planted (Year), the time each sample was taken (time), and the average leaf weight per plant (weight). We are interested in modeling weight as a function of Time in a logistic model with parameters Asym, xmid, and scal. We expect that the variation increases with time, and hence use generalized least squares with a Power variance structure instead of standard nonlinear regression. In a Power variance structure, the variance increases with a power of the absolute fitted values.

- 1. Open the **Generalized Nonlinear Least Squares** dialog.
- 2. Type Soybean in the **Data Set** field.
- 3. Enter the following **Formula**:

```
weight ~ SSlogis(Time, Asym, xmid, scal)
```

The SSlogis function is a *self-starting* function used to specify the nonlinear model, as well as provide initial estimates to the solver.

- 4. On the **Options** page of the dialog, select **Power** as the **Variance Structure Type**.
- 5. Click **OK**.

A summary of the fitted model appears in the **Report** window.

# **SURVIVAL**

Survival analysis is used for data in which censoring is present.

# Nonparametric Survival

Nonparametric survival curves are estimates of the probability of survival over time. They are used in situations such as medical trials where the response is time to failure, usually with some times lost to censoring. The most commonly used nonparametric survival curve is the Kaplan-Meier estimate. The **Nonparametric Survival** dialog fits a variety of nonparametric survival curves and allows the inclusion of grouping variables.

#### Fitting a nonparametric survival curve

From the main menu, choose **Statistics** ► **Survival** ► **Nonparametric Survival**. The **Nonparametric Survival** dialog opens, as shown in Figure 6.53.

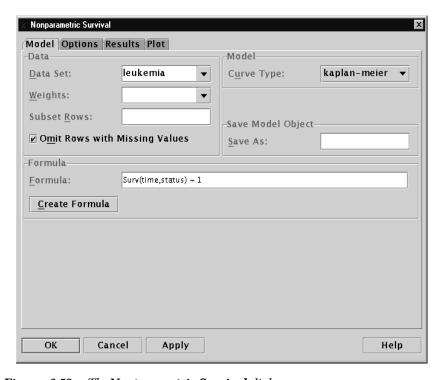


Figure 6.53: The Nonparametric Survival dialog.

The leukemia data set contains data from a trial to evaluate efficacy of maintenance chemotherapy for acute myelogenous leukemia. We fit a Kaplan-Meier survival curve to the full set of data.

- 1. Open the **Nonparametric Survival** dialog.
- 2. Type leukemia in the **Data Set** field.
- 3. Enter the Formula Surv(time, status)~1 or click on the Create Formula button to construct the formula. The Surv function creates a survival object, which is the appropriate response variable for a survival formula.
- 4. Click **OK**.

A summary of the fitted model appears in the **Report** window, and a plot of the survival curve with confidence intervals appears in a **Graph** window.

# Cox Proportional Hazards

The *Cox proportional hazards model* is the most commonly used regression model for survival data. It allows the estimation of nonparametric survival curves (such as Kaplan-Meier curves) in the presence of covariates. The effect of the covariates upon survival is usually of primary interest.

#### Fitting a Cox proportional hazards model

From the main menu, choose Statistics ▶ Survival ▶ Cox Proportional Hazards. The Cox Proportional Hazards dialog opens, as shown in Figure 6.54.

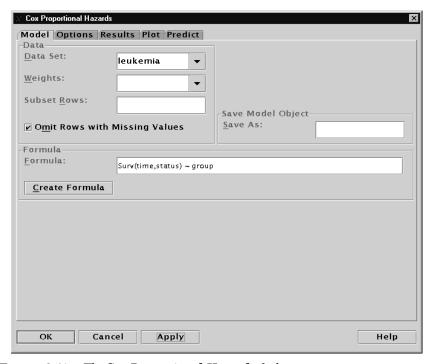


Figure 6.54: The Cox Proportional Hazards dialog.

We fit a Cox proportional hazards model to the leukemia data set with group used as a covariate.

- 1. Open the **Cox Proportional Hazards** dialog.
- 2. Type leukemia in the **Data Set** field.
- 3. Enter the Formula Surv(time, status)~group or click the Create Formula button to construct the formula. The Surv function creates a survival object, which is the appropriate response variable for a survival formula.
- 4. Select the **Survival Curves** check box on the **Plot** page.
- Click **OK**.

A summary of the fitted model appears in the **Report** window, and a plot of the survival curve with confidence intervals appears in a **Graph** window.

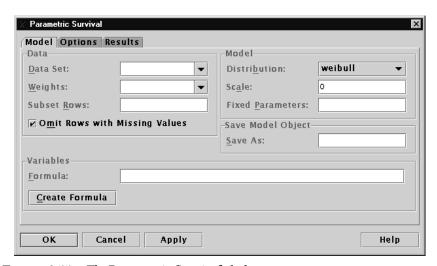
# Parametric Survival

Parametric regression models for censored data are used in a variety of contexts ranging from manufacturing to studies of environmental contaminants. Because of their frequent use for modeling failure time or survival data, they are often referred to as *parametric survival models*. In this context, they are used throughout engineering to discover reasons why engineered products fail. They are called *accelerated failure time models* or *accelerated testing models* when the product is tested under more extreme conditions than normal to accelerate its failure time.

The **Parametric Survival** and **Life Testing** dialogs fit the same type of model. The difference between the two dialogs is in the options available. The **Life Testing** dialog supports threshold estimation, truncated distributions, and offsets. In addition, it provides a variety of diagnostic plots and the ability to obtain predicted values. This functionality is not available in the **Parametric Survival** dialog. In contrast, the **Parametric Survival** dialog supports frailty and penalized likelihood models, which is not available in the **Life Testing** dialog.

#### Fitting a parametric survival model

From the main menu, choose Statistics ► Survival ► Parametric Survival. The Parametric Survival dialog opens, as shown in Figure 6.55.



**Figure 6.55:** The **Parametric Survival** dialog.

The capacitor data set contains measurements from a simulated accelerated life testing of capacitors. It includes time to failure (days), indicator of failure or censoring (event), and the voltage at which the test was run (voltage). We use a parametric survival model to examine how voltage influences the probability of failure.

- 1. Open the **Parametric Survival** dialog.
- 2. Type capacitor in the **Data Set** field.
- 3. Enter the **Formula** Surv(days, event)~voltage or click the **Create Formula** button to construct the formula. The Surv function creates a survival object, which is the appropriate response variable for a survival formula.
- 4. Click **OK**.

A summary of the fitted model appears in the **Report** window.

# Life Testing

The **Life Testing** dialog fits a parametric regression model for censored data. These models are used in a variety of contexts ranging from manufacturing to studies of environmental contaminants. Because of their frequent use for modeling failure time or survival data, they are often referred to as *parametric survival models*. In this context, they are used throughout engineering to discover reasons why engineered products fail. They are called *accelerated failure time models* or *accelerated testing models* when the product is tested under more extreme conditions than normal to accelerate its failure time.

The **Parametric Survival** and **Life Testing** dialogs fit the same type of model. The difference between the two dialogs is in the options available. The **Life Testing** dialog supports threshold estimation, truncated distributions, and offsets. In addition, it provides a variety of diagnostic plots and the ability to obtain predicted values. This functionality is not available in the **Parametric Survival** dialog. In contrast, the **Parametric Survival** dialog supports frailty and penalized likelihood models, which is not available in the **Life Testing** dialog.

## Performing life testing

From the main menu, choose **Statistics** ▶ **Survival** ▶ **Life Testing**. The **Life Testing** dialog opens, as shown in Figure 6.56.

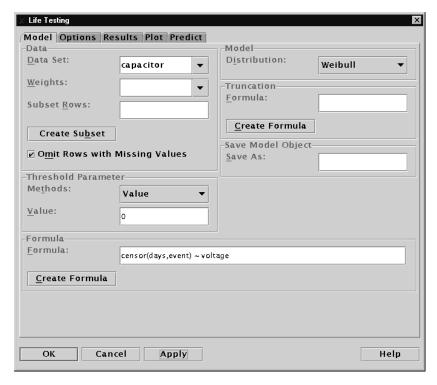


Figure 6.56: The Life Testing dialog.

We use the **Life Testing** dialog to examine how voltage influences the probability of failure in the capacitor data set.

- 1. Open the **Life Testing** dialog.
- 2. Type capacitor in the **Data Set** field.
- 3. Enter the Formula censor(days, event)~voltage or click the Create Formula button to construct the formula. The censor function creates a survival object, which is the appropriate response variable for a survival formula. It is similar to the Surv function, but provides more options for specifying censor codes.
- 4. Click **OK**.

A summary of the fitted model appears in the **Report** window.

# **TREE**

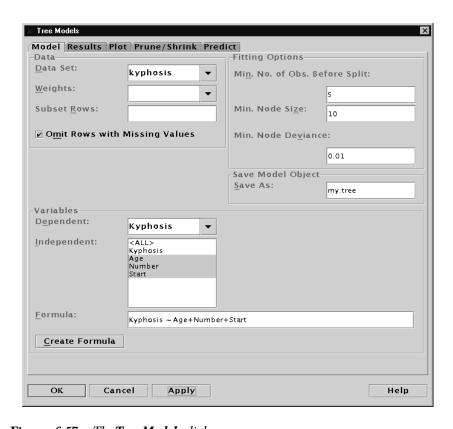
Tree-based models provide an alternative to linear and additive models for regression problems, and to linear and additive logistic models for classification problems. Tree models are fit by successively splitting the data to form homogeneous subsets. The result is a hierarchical tree of decision rules useful for prediction or classification.

#### **Tree Models**

The **Tree Models** dialog is used to fit a tree model.

#### Fitting a tree model

From the main menu, choose **Statistics** ► **Tree** ► **Tree Models**. The **Tree Models** dialog opens, as shown in Figure 6.57.



**Figure 6.57:** The **Tree Models** dialog.

The kyphosis data set has 81 rows representing data on 81 children who have had corrective spinal surgery. The outcome Kyphosis is a binary variable, and the other three columns Age, Number, and Start, are numeric. Kyphosis is a post-operative deformity which is present in some children receiving spinal surgery. We are interested in examining whether the child's age, the number of vertebrae operated on, or the starting vertebra influence the likelihood of the child having a deformity.

We fit a classification tree to the data, in which a tree structure is used to classify individuals as likely or unlikely to have kyphosis based on their values of Age, Number, and Start. The resulting classification tree divides individuals into groups based on these variables.

- 1. Open the **Tree Models** dialog.
- 2. Type kyphosis in the **Data Set** field.
- 3. Specify Kyphosis~Age+Number+Start in the **Formula** field.
- 4. Type my.tree in the **Save As** field. A tree model object is saved under this name, which we explore in a later example using **Tree Tools**.
- Click **OK**.

A summary of the model is printed in the **Report** window, and a tree plot is displayed in a **Graph** window.

#### **Tree Tools**

Spotfire S+ provides a rich suite of tools for interactively examining a regression tree. To use **Tree Tools**, first use the **Tree Models** dialog to create a tree model. Save the tree model by specifying a name in the **Save As** field of the dialog.

All of the **Tree Tools** begin by creating a plot of the specified tree model. The **Browse**, **Burl**, **Histogram**, **Identify**, and **Snip** tools let you select splits or nodes on the plot, and provide information on the selection. Click the left mouse button to make a selection, and click the right or center mouse button to leave the selection mode. With these tools, it may be necessary to arrange your windows prior to clicking **OK** or **Apply** so that the necessary **Graph** and **Report** windows are in view while making selections.

The tools behave in the following manner:

- **Browse**: select a node on the tree plot. Summary information on the node appears in the **Report** window. Right-click to leave the selection mode. Specify a name in the **Save As** field to save a list of the node information.
- **Burl**: select a split on the tree plot. Plots appear under the tree that display the change in deviance for all candidate splits. The actual split has the largest change in deviance. These plots are useful for examining whether other splits would produce an improvement in fit similar to the improvement from the actual split. Right-click to leave the selection mode. Specify a name in the **Save As** field to save a list with information on the candidate splits.
- **Histogram**: specify variables for which to draw histograms in the **Hist Variables** field. Select a split on the tree plot. Plots appear under the tree that display histograms of the specified variables, with separate histograms for the values in the two nodes resulting from the split. Right-click to leave the selection mode. Specify a name in the **Save As** field to save a list of the variable values corresponding to the histograms.
- **Identify**: select a node on the tree plot. The row names or numbers for the observations in that node appear in the **Report** window. Right-click to leave the selection mode. Specify a name in the **Save As** field to save a list of the observations in each node.
- **Rug**: specify the variable to plot in the **Rug/Tile Variable** field. A high-density plot that shows the average value of the specified variable for observations in each leaf is plotted beneath the tree plot. Specify a name in the **Save As** field to save a vector of the average values. This tool is not interactive.
- **Snip**: use this tool to create a new tree with some splits removed. Select a node on the tree plot to print the total tree deviance and what the total tree deviance would be if the subtree rooted at the node were removed. Click a second time on the same node to snip that subtree off and visually erase the subtree. This process may be repeated any number of times. Right-click to leave the selection mode. Specify a name in the **Save As** field to save the snipped tree.

• Tile: specify a variable to plot in the Rug/Tile Variable field. A vertical bar plot of the variable is plotted beneath the tree plot. Factor variables have one bar per level, and numeric variables are quantized into four equi-sized ordered levels. Specify a name in the Save As field to save a matrix of frequency counts for the observations in each leaf. This tool is not interactive.

#### Using the tree tools

From the main menu, choose **Statistics** ▶ **Tree** ▶ **Tree Tools**. The **Tree Tools** dialog opens, as shown in Figure 6.58.

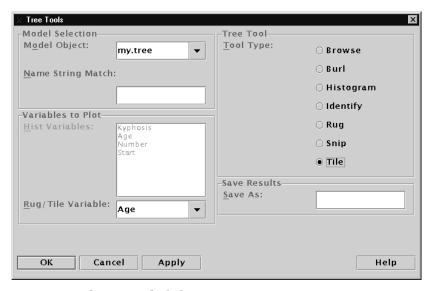


Figure 6.58: The Tree Tools dialog.

#### **Example**

In the section Tree Models on page 328, we fit a classification tree to the kyphosis data. We can use a tree tile plot to see histograms of Age within each group.

- 1. If you have not done so already, fit the classification tree and save the results in an object named my.tree. This process is outlined on page 329.
- 2. Open the **Tree Tools** dialog.

- 3. Select my.tree as the **Model Object**.
- 4. Select **Tile** as the **Tool Type**.
- 5. Select Age as the **Rug/Tile Variable**.
- 6. Click **OK**.

A tree tile plot is displayed in a **Graph** window. The top portion of the graph contains a plot of the tree. The bottom portion contains histograms of Age for each terminal node in the tree.

# **COMPARE MODELS**

In regression and ANOVA, the data analyst often has a variety of candidate models of interest. From these models, the data analyst usually chooses one which is thought to best describe the relationship between the predictors and the response.

Model selection typically involves making a trade-off between complexity and goodness-of-fit. A more complex model (one involving more variables or interactions of variables) is guaranteed to fit the observed data more closely than a simpler model. For example, a model with as many parameters as observations would fit the data perfectly. However, as the model grows more complex, it begins to reflect the random variation in the sample obtained rather than a more general relationship between the response and the predictors. This may make the model less useful than a simpler one for predicting new values or drawing conclusions regarding model structure.

The general strategy in regression is to choose a simpler model when doing so does not reduce the goodness-of-fit by a significant amount. In linear regression and ANOVA, an F-test may be used to compare two models. In logistic and log-linear regression, a chi-square test comparing deviances is appropriate.

The **Compare Models** dialog lets you compare the goodness-of-fit of two or more models. Typically, the models should be *nested*, in that the simpler model is a special case of the more complex model. Before using the **Compare Models** dialog, first save the models of interest as objects.

#### Comparing models

From the main menu, choose **Statistics Compare Models**. The **Compare Models** (**Likelihood Ratio Test**) dialog opens, as shown in Figure 6.59.

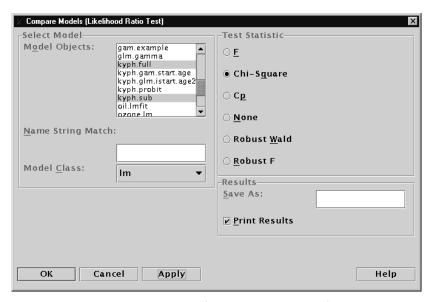


Figure 6.59: The Compare Models (Likelihood Ratio Test) dialog.

In the kyphosis analysis of the section Logistic Regression, we suggested that Start had a significant effect upon Kyphosis, but Age and Number did not. We can use a chi-square test to determine whether a model with just Start is sufficient.

- 1. Open the **Logistic Regression** dialog.
- 2. Type kyphosis in the **Data Set** field.
- Specify Kyphosis~Age+Number+Start in the Formula field. Type kyph.full in the Save As field and click Apply. Information describing this model is saved as an object named kyph.full.
- 4. Change the **Formula** field to Kyphosis~Start. Change the **Save As** name to kyph.sub, and click **OK**. Information describing this model is saved as an object named kyph.sub.
- 5. Open the **Compare Models** (**Likelihood Ratio Test**) dialog.

- 6. CTRL-click to select kyph.full and kyph.sub in the **Model Objects** list.
- 7. Select **Chi-Square** as the **Test Statistic**.
- 8. Click **OK**.

An analysis of deviance table appears in the **Report** window. The table displays the degrees of freedom and residual deviance for each model. Under the null hypothesis that the simpler model is appropriate, the difference in residual deviances is distributed as a chi-squared statistic. The Pr(Chi) column provides a p-value for the hypothesis that the simpler model is appropriate. If this value is less than a specific value, typically 0.05, then the more complex model causes a large enough change in deviance to warrant the inclusion of the additional terms. That is, the extra complexity is justified by an improvement in goodness-of-fit.

In our example the p-value of 0.035 suggests that Age and/or Number add extra information useful for predicting the outcome.

```
Analysis of Deviance Table

Response: Kyphosis

Terms Resid. Df Resid. Dev Test

1 Age + Number + Start 77 61.37993

2 Start 79 68.07218 -Age-Number
  Df Deviance Pr(Chi)

1
2 -2 -6.692253 0.03522052
```

# **CLUSTER ANALYSIS**

In cluster analysis, we search for groups (clusters) in the data in such a way that objects belonging to the same cluster resemble each other, whereas objects in different clusters are dissimilar.

# Compute Dissimilarities

A data set for clustering can consist of either rows of observations, or a dissimilarity object storing measures of dissimilarities between observations. K-means, partitioning around medoids using the large data algorithm, and monothetic clustering all operate on a data set. Partitioning around medoids, fuzzy clustering, and the hierarchical methods take either a data set or a dissimilarity object.

The clustering routines themselves do not accept nonnumeric variables. If a data set contains nonnumeric variables such as factors, they must either be converted to numeric variables, or dissimilarities must be used.

How we compute the dissimilarity between two objects depends on the type of the original variables. By default, numeric columns are treated as interval-scaled variables, factors are treated as nominal variables, and ordered factors are treated as ordinal variables. Other variable types should be specified as such through the fields in the **Special Variable Types** group.

### **Calculating dissimilarities**

From the main menu, choose **Statistics** ► **Cluster Analysis** ► **Compute Dissimilarities**. The **Compute Dissimilarities** dialog opens, as shown in Figure 6.60.

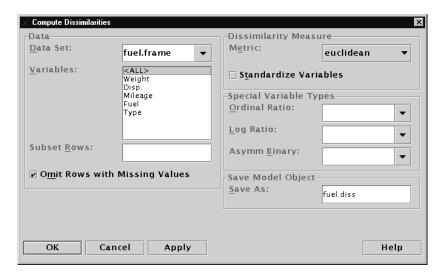


Figure 6.60: The Compute Dissimilarities dialog.

The data set fuel.frame is taken from the April 1990 issue of *Consumer Reports*. It contains 60 observations (rows) and 5 variables (columns). Observations of weight, engine displacement, mileage, type, and fuel were taken for each of sixty cars. In the fuel.frame data, we calculate dissimilarities as follows:

- 1. Open the Compute Dissimilarities dialog.
- 2. Type fuel.frame in the **Data Set** field.
- 3. Type fuel.diss in the Save As field.
- 4. Click OK.

The dissimilarities are calculated and saved in the object fuel.diss. We use this object in later examples of clustering dialogs.

# K-Means Clustering

One of the most well-known partitioning methods is k-means. In the k-means algorithm, observations are classified as belonging to one of k groups. Group membership is determined by calculating the centroid for each group (the multidimensional version of the mean) and assigning each observation to the group with the closest centroid.

#### Performing k-means clustering

From the main menu, choose **Statistics** ► **Cluster Analysis** ► **K-Means**. The **K-Means Clustering** dialog opens, as shown in Figure 6.61.

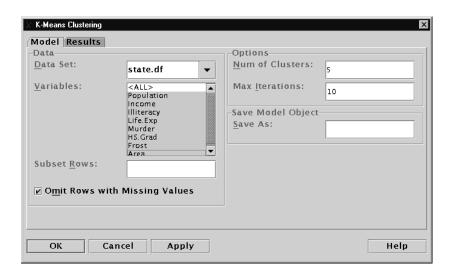


Figure 6.61: The K-Means Clustering dialog.

#### **Example**

We cluster the information in the state.x77 data set. These data describe various characteristics of the 50 states, including population, income, illiteracy, life expectancy, and education. By default, state.x77 is stored in an object of class "matrix". We must therefore convert it to class "data.frame" before it can be recognized by the dialogs. To do this, type the following in the **Commands** window:

```
> state.df <- data.frame(state.x77)</pre>
```

We can now proceed with the k-means clustering analysis on the state.df data frame:

- 1. Open the **K-Means Clustering** dialog.
- 2. Type state.df in the **Data Set** field.

- 3. CTRL-click to select the **Variables** Population through Area.
- 4. Click **OK**.

A summary of the clustering appears in the **Report** window.

# Partitioning Around Medoids

The partitioning around medoids algorithm is similar to k-means, but it uses medoids rather than centroids. Partitioning around medoids has the following advantages: it accepts a dissimilarity matrix; it is more robust because it minimizes a sum of dissimilarities instead of a sum of squared Euclidean distances; and it provides novel graphical displays (silhouette plots and clusplots).

#### Performing partitioning around medoids

From the main menu, choose **Statistics** ► **Cluster Analysis** ► **Partitioning Around Medoids**. The **Partitioning Around Medoids** dialog opens, as shown in Figure 6.62.

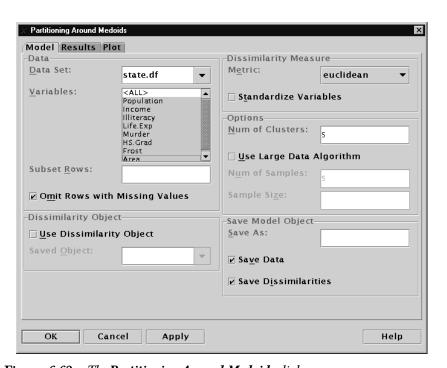


Figure 6.62: The Partitioning Around Medoids dialog.

#### Example I

In the section K-Means Clustering on page 337, we clustered the information in the state.df data set using the k-means algorithm. In this example, we use the partitioning around medoids algorithm.

- 1. If you have not already done so, create the state.df data frame from the state.x77 matrix. The instructions for doing this are located on page 338.
- 2. Open the **Partitioning Around Medoids** dialog.
- 3. Type state.df in the **Data Set** field.
- 4. CTRL-click to select the **Variables** Population through Area.
- 5. Click **OK**.

A summary of the clustering appears in the **Report** window.

#### Example 2

In the section Compute Dissimilarities on page 336, we calculated dissimilarities for the fuel.frame data set. In this example, we cluster the fuel.frame dissimilarities using the partitioning around medoids algorithm.

- 1. If you have not already done so, create the object fuel.diss from the instructions on page 337.
- 2. Open the **Partitioning Around Medoids** dialog.
- 3. Select the **Use Dissimilarity Object** check box.
- 4. Select fuel.diss as the Saved Object.
- 5. Click **OK**.

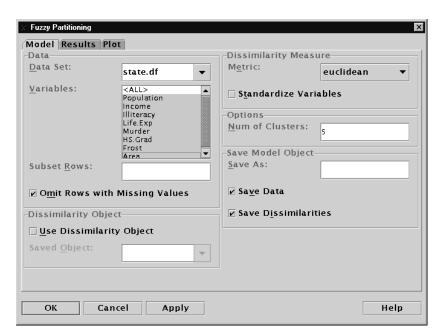
A summary of the clustering appears in the **Report** window.

# Fuzzy Partitioning

Most clustering algorithms are crisp clustering methods. This means that each object of the data set is assigned to exactly one cluster. For instance, an object lying between two clusters must be assigned to one of them. In *fuzzy clustering*, each observation is given fractional membership in multiple clusters.

#### Performing fuzzy partitioning

From the main menu, choose **Statistics** ▶ **Cluster Analysis** ▶ **Fuzzy Partitioning**. The **Fuzzy Partitioning** dialog opens, as shown in Figure 6.63.



**Figure 6.63:** The **Fuzzy Partitioning** dialog.

#### Example I

In the section K-Means Clustering on page 337, we clustered the information in the state.df data set using the k-means algorithm. In this example, we use fuzzy partitioning.

- 1. If you have not already done so, create the state.df data frame from the state.x77 matrix. The instructions for doing this are located on page 338.
- 2. Open the **Fuzzy Partitioning** dialog.
- 3. Type state.df in the **Data Set** field.
- 4. CTRL-click to select the **Variables** Population through Area, and click **OK**.

A summary of the clustering appears in the **Report** window.

In the section Compute Dissimilarities on page 336, we calculated dissimilarities for the fuel.frame data set. In this example, we cluster the fuel.frame dissimilarities using fuzzy partitioning.

- 1. If you have not already done so, create the object fuel.diss from the instructions on page 337.
- 2. Open the **Fuzzy Partitioning** dialog.
- 3. Select the **Use Dissimilarity Object** check box.
- 4. Select fuel.diss as the **Saved Object**.
- Click **OK**.

A summary of the clustering appears in the **Report** window.

# Agglomerative Hierarchical Clustering

Hierarchical algorithms proceed by combining or dividing existing groups, producing a hierarchical structure that displays the order in which groups are merged or divided. *Agglomerative* methods start with each observation in a separate group, and proceed until all observations are in a single group.

#### Performing agglomerative hierarchical clustering

From the main menu, choose Statistics Cluster Analysis Agglomerative Hierarchical. The Agglomerative Hierarchical Clustering dialog opens, as shown in Figure 6.64.

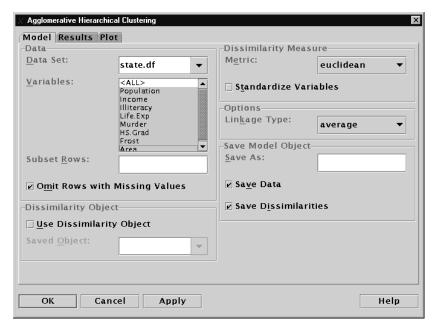


Figure 6.64: The Agglomerative Hierarchical Clustering dialog.

#### Example I

In the section K-Means Clustering on page 337, we clustered the information in the state.df data set using the k-means algorithm. In this example, we use an agglomerative hierarchical method.

- 1. If you have not already done so, create the state.df data frame from the state.x77 matrix. The instructions for doing this are located on page 338.
- 2. Open the **Agglomerative Hierarchical Clustering** dialog.
- 3. Type state.df in the **Data Set** field.
- 4. CTRL-click to select the **Variables** Population through Area.
- Click OK.

A summary of the clustering appears in the **Report** window.

In the section Compute Dissimilarities on page 336, we calculated dissimilarities for the fuel.frame data set. In this example, we cluster the fuel.frame dissimilarities using the agglomerative hierarchical algorithm.

- 1. If you have not already done so, create the object fuel.diss from the instructions on page 337.
- 2. Open the **Agglomerative Hierarchical Clustering** dialog.
- 3. Select the **Use Dissimilarity Object** check box.
- 4. Select fuel.diss as the Saved Object.
- Click **OK**.

A summary of the clustering appears in the **Report** window.

# Divisive Hierarchical Clustering

Hierarchical algorithms proceed by combining or dividing existing groups, producing a hierarchical structure that displays the order in which groups are merged or divided. *Divisive* methods start with all observations in a single group and proceed until each observation is in a separate group.

#### Performing divisive hierarchical clustering

From the main menu, choose Statistics ► Cluster Analysis ► Divisive Hierarchical. The Divisive Hierarchical Clustering dialog opens, as shown in Figure 6.65.

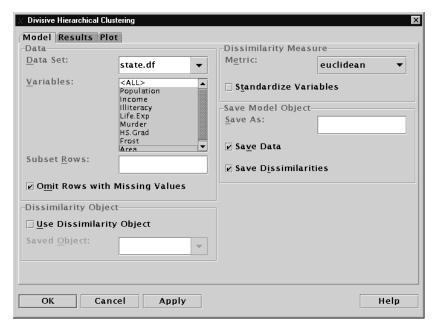


Figure 6.65: The Divisive Hierarchical Clustering dialog.

#### Example I

In the section K-Means Clustering on page 337, we clustered the information in the state.df data set using the k-means algorithm. In this example, we use a divisive hierarchical method.

- 1. If you have not already done so, create the state.df data frame from the state.x77 matrix. The instructions for doing this are located on page 338.
- 2. Open the **Divisive Hierarchical Clustering** dialog.
- 3. Type state.df in the **Data Set** field.
- 4. CTRL-click to select the **Variables** Population through Area.
- Click OK.

A summary of the clustering appears in the **Report** window.

In the section Compute Dissimilarities on page 336, we calculated dissimilarities for the fuel.frame data set. In this example, we cluster the fuel.frame dissimilarities using the divisive hierarchical algorithm.

- 1. If you have not already done so, create the object fuel.diss from the instructions on page 337.
- 2. Open the **Divisive Hierarchical Clustering** dialog.
- 3. Select the **Use Dissimilarity Object** check box.
- 4. Select fuel.diss as the Saved Object.
- Click **OK**.

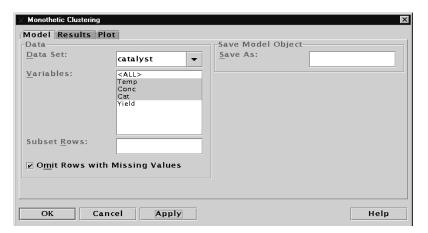
A summary of the clustering appears in the **Report** window.

# Monothetic Clustering

When all of the variables in a data set are binary, a natural way to divide the observations is by splitting the data into two groups based on the two values of a particular binary variable. *Monothetic analysis* produces a hierarchy of clusters in which a group is split in two at each step, based on the value of one of the binary variables.

#### Performing monothetic clustering

From the main menu, choose Statistics ► Cluster Analysis ► Monothetic (Binary Variables). The Monothetic Clustering dialog opens, as shown in Figure 6.66.



**Figure 6.66:** The **Monothetic Clustering** dialog.

The catalyst data set comes from a designed experiment. Its eight rows represent all possible combinations of two temperatures (Temp), two concentrations (Conc), and two catalysts (Cat). The fourth column represents the response variable Yield. We are interested in determining how temperature, concentration, and catalyst affect the Yield. Before fitting a model to these data, we can group observations according to the three binary predictors by using monothetic clustering.

- 1. Open the **Monothetic Clustering** dialog.
- 2. Type catalyst in the Data Set field.
- 3. CTRL-click to highlight the **Variables** Temp, Conc, and Cat.
- 4. Click OK.

A summary of the monothetic clustering appears in the **Report** window.

# **MULTIVARIATE**

Multivariate techniques summarize the structure of multivariate data based on certain classical models.

# Discriminant Analysis

The **Discriminant Analysis** dialog lets you fit a linear or quadratic discriminant function to a set of feature data.

#### Performing discriminant analysis

From the main menu, choose **Statistics** ► **Multivariate** ► **Discriminant Analysis**. The **Discriminant Analysis** dialog opens, as shown in Figure 6.67.

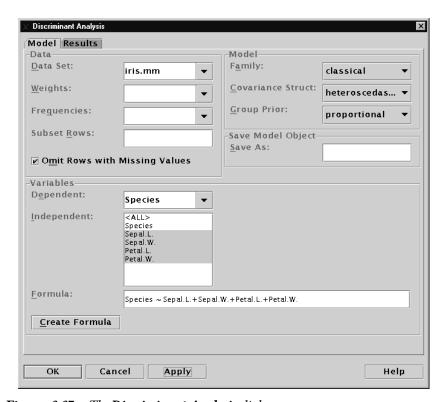


Figure 6.67: The Discriminant Analysis dialog.

We perform a discriminant analysis on Fisher's iris data. This data set is a three-dimensional array giving 4 measurements on 50 flowers from each of 3 species of iris. The measurements are in centimeters and include sepal length, sepal width, petal length, and petal width. The iris species are Setosa, Versicolor, and Virginica.

Before performing the discriminant analysis, we must create a twodimensional data frame that can be accepted by the dialogs. To do this, type the following in the **Commands** window:

```
> iris.mm <- data.frame(Species=factor(c(rep(1,50),</pre>
+ \text{ rep}(2,50), \text{ rep}(3,50)), \text{ labels=dimnames}(\text{iris})[[3]]),
+ rbind(iris[,,1], iris[,,2], iris[,,3])*10)
```

We can now use the **Discriminant Analysis** dialog on the iris.mm data frame:

- 1. Open the **Discriminant Analysis** dialog.
- 2. Type iris.mm in the **Data Set** field.
- 3. Choose Species as the **Dependent** variable.
- 4. CTRL-click to select Sepal.L., Sepal.W., Petal.L., and Petal.W. as the **Independent** variables.
- 5. Choose **heteroscedastic** as the **Covariance Struct**.
- 6. Click **OK**.

A summary of the fitted model appears in the **Report** window.

Factor Analysis In many scientific fields, notably psychology and other social sciences, you are often interested in quantities like intelligence or social status, which are not directly measurable. However, it is often possible to measure other quantities that reflect the underlying variable of interest. Factor analysis is an attempt to explain the correlations between observable variables in terms of underlying factors, which are themselves not directly observable. For example, measurable quantities, such as performance on a series of tests, can be explained in terms of an underlying factor, such as intelligence.

#### Performing factor analysis

From the main menu, choose **Statistics** ▶ **Multivariate** ▶ **Factor Analysis**. The **Factor Analysis** dialog opens, as shown in Figure 6.68.



**Figure 6.68:** The **Factor Analysis** dialog.

#### **Example**

The data set testscores contains five test scores for each of twenty-five students. We use factor analysis to look for structure in the scores. By default, testscores is stored in an object of class "matrix". We must therefore convert it to class "data.frame" before it can be recognized by the dialogs. To do this, type the following in the **Commands** window:

> testscores.df <- data.frame(testscores)</pre>

We can now proceed with the factor analysis on the testscores.df data frame:

- 1. Open the **Factor Analysis** dialog.
- 2. Type testscores.df in the **Data Set** field.
- 3. Specify that we want **2** factors in the **Number of Factors** field.
- 4. Select **<ALL>** in the **Variables** field.
- Click **OK**.

A summary of the factor analysis appears in the **Report** window.

# Principal Components

For investigations involving a large number of observed variables, it is often useful to simplify the analysis by considering a smaller number of linear combinations of the original variables. For example, scholastic achievement tests typically consist of a number of examinations in different subject areas. In attempting to rate students applying for admission, college administrators frequently reduce the scores from all subject areas to a single, overall score. *Principal components* is a standard technique for finding optimal linear combinations of the variables.

#### Performing principal components

From the main menu, choose **Statistics** ▶ **Multivariate** ▶ **Principal Components**. The **Principal Components** dialog opens, as shown in Figure 6.69.

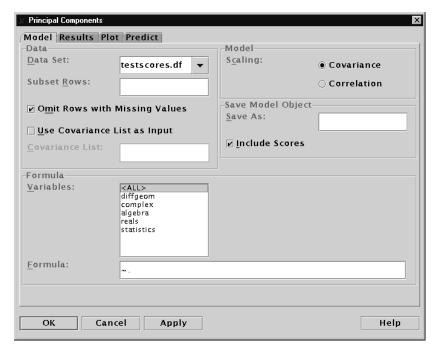


Figure 6.69: The Principal Components dialog.

#### Example

In the section Factor Analysis on page 349, we performed a factor analysis for the testscores.df data set. In this example, we perform a principal components analysis for these data.

- 1. If you have not done so already, create the testscores.df data frame with the instructions given on page 350.
- 1. Open the **Principal Components** dialog.
- 2. Type testscores.df in the **Data Set** field.
- 3. Select **<ALL>** in the **Variables** field.
- 4. Click **OK**.

A summary of the principal components analysis appears in the **Report** window.

#### **MANOVA**

Multivariate analysis of variance, known as MANOVA, is the extension of analysis of variance techniques to multiple responses. The responses for an observation are considered as one multivariate observation, rather than as a collection of univariate responses. If the responses are independent, then it is sensible to just perform univariate analyses. However, if the responses are correlated, then MANOVA can be more informative than the univariate analyses, as well as less repetitive.

#### **Performing MANOVA**

From the main menu, choose **Statistics** ▶ **Multivariate** ▶ **MANOVA**. The **Multivariate Analysis of Variance** dialog opens, as shown in Figure 6.70.

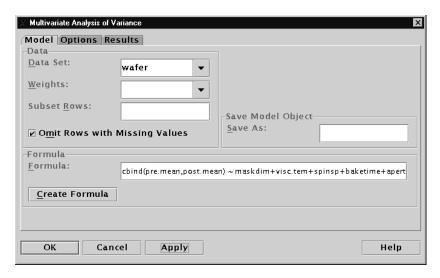


Figure 6.70: The Multivariate Analysis of Variance dialog.

#### **Example**

The data set wafer has eighteen rows and thirteen columns, of which eight contain factors, four contain responses, and one is the auxiliary variable N. It is a design object based on an orthogonal-array design for an experiment in which two integrated circuit wafers were made for each combination of factors. On each wafer, the pre- and post-etch line widths were measured five times. The response variables are the

mean and deviance of the measurements. As three of the wafers were broken, the auxiliary variable N gives the number of measurements actually made.

We are interested in treating the pre.mean and post.mean variables as a multivariate response, using MANOVA to explore the effect of each factor upon the response.

- 1. Open the **Multivariate Analysis of Variance** dialog.
- 2. Type wafer in the **Data Set** field.
- 3. Click the **Create Formula** button to open the **Formula** builder.
- 4. While holding down the CTRL key, select pre.mean and post.mean in the **Variables** list. Click the **Response** button to add these variables to the **Formula** as the response.
- 5. Select maskdim. Scroll through the Variables list until etchtime appears. Hold down Shift and select etchtime. This selects all columns between maskdim and etchtime. Click the Main Effect button to add these variables to the Formula as predictors.
- 6. Click **OK** to dismiss the **Formula** builder. The **Formula** field of the **MANOVA** dialog contains the formula you constructed.
- 7. Click **OK**.

A summary of the MANOVA appears in the **Report** window.

#### **QUALITY CONTROL CHARTS**

Quality control charts are useful for monitoring process data. *Continuous grouped* quality control charts monitor whether a process is staying within control limits. *Continuous ungrouped* charts are appropriate when variation is determined using sequential variation rather than group variation. It is also possible to create quality control charts for *counts* (the number of defective samples) and *proportions* (proportion of defective samples).

# Continuous Grouped

The Quality Control Charts (Continuous Grouped) dialog creates quality control charts of means (xbar), standard deviations (s), and ranges (r).

#### Creating quality control charts (continuous grouped)

From the main menu, choose Statistics ▶ Quality Control Charts ▶ Continuous Grouped. The Quality Control Charts (Continuous Grouped) dialog opens, as shown in Figure 6.71.

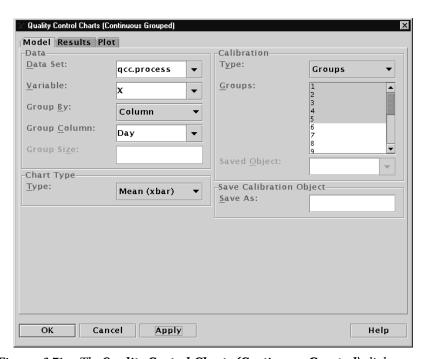


Figure 6.71: The Quality Control Charts (Continuous Grouped) dialog.

#### Example

In the section Kolmogorov-Smirnov Goodness-of-Fit on page 230, we created a data set called qcc.process that contains a simulated process with 200 measurements. Ten measurements per day were taken for a total of twenty days. In this example, we create an xbar Shewhart chart to monitor whether the process is staying within control limits. The first five days of observations are treated as calibration data for use in setting the control limits.

- 1. If you have not done so already, create the qcc.process data set with the instructions given on page 231.
- 2. Open the **Quality Control Charts (Continuous Grouped)** dialog.
- 3. Type qcc.process in the **Data Set** field.
- 4. Select X as the **Variable**.
- 5. Select Day as the **Group Column**.
- 6. Select **Groups** as the **Calibration Type**.
- 7. CTRL-click to select 1, 2, 3, 4, 5 from the **Groups** list box.
- 8. Click **OK**.

A Shewhart chart of the X data grouped by Day appears in a **Graph** window.

# Continuous Ungrouped

The Quality Control Charts (Continuous Ungrouped) dialog creates quality control charts of exponentially weighted moving averages (ewma), moving averages (ma), moving standard deviations (ms), and moving ranges (mr). These charts are appropriate when variation is determined using sequential variation rather than group variation.

#### Creating quality control charts (continuous ungrouped)

From the main menu, choose Statistics ▶ Quality Control Charts ▶ Continuous Ungrouped. The Quality Control Charts (Continuous Ungrouped) dialog opens, as shown in Figure 6.72.

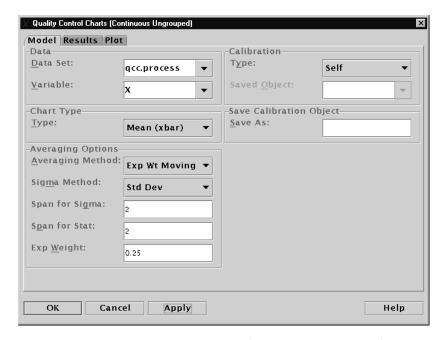


Figure 6.72: The Quality Control Charts (Continuous Ungrouped) dialog.

#### **Example**

For this example, we ignore the fact that qcc.process contains grouped data, and instead pretend that the 200 observations are taken at sequential time points. We create an exponentially weighted moving average Shewhart chart to monitor whether the process is staying within control limits.

- 1. If you have not done so already, create the qcc.process data set with the instructions given on page 231.
- 2. Open the **Quality Control Charts** (Continuous Ungrouped) dialog.
- 3. Type qcc.process in the **Data Set** field.
- 4. Select X as the **Variable**.
- Click **OK**.

A Shewhart chart appears in a **Graph** window.

# Counts and Proportions

The Quality Control Charts (Counts and Proportions) dialog creates quality control charts for counts (number of defective samples) and proportions (proportion of defective samples).

#### Creating quality control charts (counts and proportions)

From the main menu, choose Statistics ▶ Quality Control Charts ▶ Counts and Proportions. The Quality Control Charts (Counts and Proportions) dialog opens, as shown in Figure 6.73.

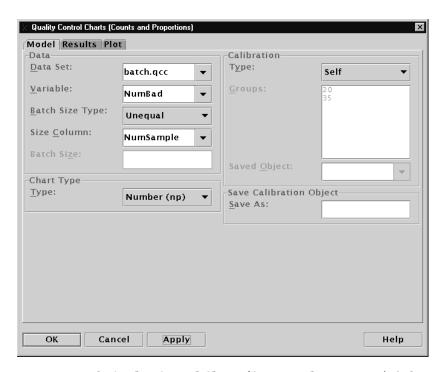


Figure 6.73: The Quality Control Charts (Counts and Proportions) dialog.

#### **Example**

We create a S-PLUS data set, batch.qcc, that contains simulated data representing the number of defective items in daily batches over 40 days. For the first 10 days the batches were of size 20, but for the remaining 30 days batches of 35 were taken. To create batch.qcc, type the following in the **Commands** window:

```
\rightarrow NumSample \leftarrow c(rep(20,times=10), rep(35,times=30))
```

```
> NumBad <- scan()</pre>
1: 3 2 7 4 5 4 4 8
9: 3 4 6 6 6 9 18 9
17: 7 11 11 9 10 10 14 5
25: 15 11 14 15 11 10 14 8
33: 11 13 16 14 19 13 15 23
41:
> batch.qcc <- data.frame(NumBad,NumSample)</pre>
> batch.qcc
   NumBad NumSample
         3
 1
                   20
 2
         2
                   20
 3
         7
                   20
 4
         4
                   20
                   20
 6
         4
                   20
 7
                   20
 8
        8
                   20
 9
                   20
10
                   20
         6
11
                   35
12
         6
                   35
13 . . .
```

The NumBad column encodes the number of defective items, and the NumSample column encodes the size of the batches.

We create a Number (np) Shewhart chart for these data.

- 1. Open the **Quality Control Charts (Counts and Proportions)** dialog.
- 2. Type batch.qcc in the **Data Set** field.
- 3. Select NumBad as the **Variable**.
- 4. Select NumSample as the **Size Column**.
- 5. Select **Number** (**np**) as the **Chart Type**.
- 6. Click **OK**.

A Shewhart chart of the NumBad data with group size indicated by NumSample appears in a **Graph** window.

#### **RESAMPLE**

In statistical analysis, the researcher is usually interested in obtaining not only a point estimate of a statistic, but also the variation in the point estimate, as well as confidence intervals for the true value of the parameter. For example, a researcher may calculate not only a sample mean, but also the standard error of the mean and a confidence interval for the mean.

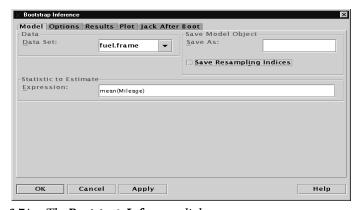
The traditional methods for calculating standard errors and confidence intervals generally rely upon a statistic, or some known transformation of it, being asymptotically normally distributed. If this normality assumption does not hold, the traditional methods may be inaccurate. Resampling techniques such as the bootstrap and jackknife provide estimates of the standard error, confidence intervals, and distributions for any statistic. To use these procedures, you must supply the name of the data set under examination and an S-PLUS function or expression that calculates the statistic of interest.

#### Bootstrap Inference

In the *bootstrap*, a specified number of new samples are drawn by sampling with replacement from the data set of interest. The statistic of interest is calculated for each set of data, and the resulting set of estimates is used as an empirical distribution for the statistic.

#### Performing bootstrap inference

From the main menu, choose **Statistics** ▶ **Resample** ▶ **Bootstrap**. The **Bootstrap Inference** dialog opens, as shown in Figure 6.74.



**Figure 6.74:** The **Bootstrap Inference** dialog.

#### Example I

The data set fuel.frame is taken from the April 1990 issue of *Consumer Reports*. It contains 60 observations (rows) and 5 variables (columns). Observations of weight, engine displacement, mileage, type, and fuel were taken for each of sixty cars. We obtain bootstrap estimates of mean and variation for the mean of the Mileage variable.

- 1. Open the **Bootstrap Inference** dialog.
- 2. Type fuel.frame in the **Data Set** field.
- 3. Type mean(Mileage) in the **Expression** field.
- 4. On the **Options** page, type **250** in the **Number of Resamples** field to perform fewer than the default number of resamples. This speeds up the computations required for this example.
- 5. Click on the **Plot** page, and notice that the **Distribution of Replicates** plot is selected by default.
- 6. Click **OK**.

A bootstrap summary appears in the **Report** window, and a histogram with a density line is plotted in a **Graph** window.

#### Example 2

In this example, we obtain bootstrap estimates of mean and variation for the coefficients of a linear model. The model we use predicts Mileage from Weight and Disp. in the fuel.frame data set.

- 1. Open the **Bootstrap Inference** dialog.
- 2. Type fuel.frame in the **Data Set** field.
- 3. Type
   coef(lm(Mileage ~ Weight+Disp., data=fuel.frame)) in
   the Expression field.
- 4. On the **Options** page, type **250** in the **Number of Resamples** field to perform fewer than the default number of resamples. This speeds up the computations required for this example.

- 5. Click on the **Plot** page, and notice that the **Distribution of Replicates** plot is selected by default.
- 6. Click **OK**.

A bootstrap summary appears in the **Report** window. In addition, three histograms with density lines (one for each coefficient) are plotted in a **Graph** window.

#### Jackknife Inference

In the jackknife, new samples are drawn by replicating the data, leaving out a single observation from each sample. The statistic of interest is calculated for each set of data, and this jackknife distribution is used to construct estimates.

#### Performing jackknife inference

From the main menu, choose **Statistics** ▶ **Resample** ▶ **Jackknife**. The **Jackknife Inference** dialog opens, as shown in Figure 6.75.



**Figure 6.75:** The **Jackknife Inference** dialog.

#### Example I

We obtain jackknife estimates of mean and variation for the mean of Mileage in the fuel.frame data.

- 1. Open the **Jackknife Inference** dialog.
- 2. Type fuel.frame in the **Data Set** field.
- 3. Type mean(Mileage) in the **Expression** field.

- 4. Click on the **Plot** page, and notice that the **Distribution of Replicates** plot is selected by default.
- 5. Click **OK**.

A jackknife summary appears in the **Report** window, and a histogram with a density line is plotted in a **Graph** window.

#### Example 2

In this example, we obtain jackknife estimates of mean and variation for the coefficients of a linear model. The model we use predicts Mileage from Weight and Disp. in the fuel.frame data set.

- 1. Open the **Jackknife Inference** dialog.
- 2. Type fuel.frame in the **Data Set** field.
- 3. Type
   coef(lm(Mileage ~ Weight+Disp., data=fuel.frame)) in
   the Expression field.
- 4. Click on the **Plot** page, and notice that the **Distribution of Replicates** plot is selected by default.
- 5. Click **OK**.

A jackknife summary appears in the **Report** window. In addition, three histograms with density lines (one for each coefficient) are plotted in a **Graph** window.

#### **SMOOTHING**

Smoothing techniques model a univariate response as a smooth function of a univariate predictor. With standard regression techniques, parametric functions are fit to scatter plot data. Frequently, you do not have enough prior information to determine what kind of parametric function to use. In such cases, you can fit a *nonparametric curve*, which does not assume a particular type of relationship.

Nonparametric curve fits are also called *smoothers* since they attempt to create a smooth curve showing the general trend in the data. The simplest smoothers use a *running average*, where the fit at a particular x value is calculated as a weighted average of the y values for nearby points. The weight given to each point decreases as the distance between its x value and the x value of interest increases. In the simplest kind of running average smoother, all points within a certain distance (or window) from the point of interest are weighted equally in the average for that point. The window width is called the *bandwidth* of the smoother, and is usually given as a percentage of the total number of data points. Increasing the bandwidth results in a smoother curve fit but may miss rapidly changing features. Decreasing the bandwidth allows the smoother to track rapidly changing features more accurately, but results in a rougher curve fit.

More sophisticated smoothers add variations to the running average approach. For example, smoothly decreasing weights or local linear fits may be used. However, all smoothers have some type of smoothness parameter (bandwidth) controlling the smoothness of the curve. The issue of good bandwidth selection is complicated and has been treated in many statistical research papers. You can, however, gain a good feeling for the practical consequences of varying the bandwidth by experimenting with smoothers on real data.

This section describes how to use four different types of smoothers.

- **Kernel Smoother**: a generalization of running averages in which different weight functions, or *kernels*, may be used. The weight functions provide transitions between points that are smoother than those in the simple running average approach.
- **Loess Smoother**: a noise-reduction approach that is based on local linear or quadratic fits to the data.

- **Spline Smoother**: a technique in which a sequence of polynomials is pieced together to obtain a smooth curve.
- **Supersmoother**: a highly automated variable span smoother. It obtains fitted values by taking weighted combinations of smoothers with varying bandwidths.

#### Kernel Smoother

A kernel smoother is a generalization of running averages in which different weight functions, or kernels, may be used. The weight functions provide transitions between points that are smoother than those in the simple running average approach. The default kernel is the normal or Gaussian kernel, in which the weights decrease with a Gaussian distribution away from the point of interest. Other choices include a triangle, a box, and the Parzen kernel. In a triangle kernel, the weights decrease linearly as the distance from the point of interest increases, so that the points on the edge of the smoothing window have a weight near zero. A box or boxcar smoother weighs each point within the smoothing window equally, and a Parzen kernel is a box convolved with a triangle.

#### Local Regression (Loess)

Local regression, or loess, was developed by W.S. Cleveland and others at Bell Laboratories. It is a clever approach to smoothing that is essentially a noise-reduction algorithm. Loess smoothing is based on local linear or quadratic fits to the data: at each point, a line or parabola is fit to the points within the smoothing window, and the predicted value is taken as the *y* value for the point of interest. Weighted least squares is used to compute the line or parabola in each window. Connecting the computed *y* values results in a smooth curve.

For loess smoothers, the bandwidth is referred to as the *span* of the smoother. The span is a number between 0 and 1, representing the percentage of points that should be included in the fit for a particular smoothing window. Smaller values result in less smoothing, and very small values close to 0 are not recommended. If the span is not specified, an appropriate value is computed using cross-validation. For small samples (n < 50), or if there are substantial serial correlations between observations close in x value, a prespecified fixed span smoother should be used.

#### Spline **Smoother**

Spline smoothers are computed by piecing together a sequence of polynomials. Cubic splines are the most widely used in this class of smoothers, and involve locally cubic polynomials. The local polynomials are computed by minimizing a penalized residual sum of squares. Smoothness is assured by having the value, slope, and curvature of neighboring polynomials match at the points where they meet. Connecting the polynomials results in a smooth fit to the data. The more accurately a smoothing spline fits the data values, the rougher the curve, and vice versa.

The smoothing parameter for splines is called the *degrees of freedom*. The degrees of freedom controls the amount of curvature in the fit, and corresponds to the degree of the local polynomials. The lower the degrees of freedom, the smoother the curve. The degrees of freedom automatically determines the smoothing window, by governing the trade-off between smoothness of the fit and fidelity to the data values. For n data points, the degrees of freedom should be between 1 and n-1. Specifying n-1 degrees of freedom results in a curve that passes through each of the data points exactly. If the degrees of freedom is not specified, a parameter estimate is computed by crossvalidation.

**Supersmoother** The *supersmoother* is a highly automated variable span smoother. It obtains fitted values by taking a weighted combination of smoothers The with varying bandwidths. smoothing parameter supersmoothers is called the *span*. The span is a number between 0 and 1, representing the percentage of points that should be included in the fit for a particular smoothing window. Smaller values result in less smoothing, and very small values close to 0 are not recommended. If the span is not specified, an appropriate value is computed using crossvalidation. For small samples (n < 50), or if there are substantial serial correlations between observations close in x value, a prespecified fixed span smoother should be used.

#### **Examples**

The air data set contains 111 observations (rows) and 4 variables (columns). It is taken from an environmental study that measured the four variables ozone, solar radiation, temperature, and wind speed for 111 consecutive days. We create smooth plots of ozone versus radiation.

- Choose Statistics ➤ Smoothing ➤ Kernel Smoother. Select air as the Data Set, radiation as the x Axis Value, and ozone as the y Axis Value. Click OK. A Graph window is created containing a plot of ozone versus radiation with a kernel smooth.
- 2. Choose Statistics ➤ Smoothing ➤ Loess Smoother. Select air as the Data Set, radiation as the x Axis Value, and ozone as the y Axis Value. Click OK. A Graph window is created containing a plot of ozone versus radiation with a loess smooth.
- 3. Choose Statistics ➤ Smoothing ➤ Spline Smoother. Select air as the Data Set, radiation as the x Axis Value, and ozone as the y Axis Value. Click OK. A Graph window is created containing a plot of ozone versus radiation with a smoothing spline smooth.
- 4. Choose Statistics ➤ Smoothing ➤ Supersmoother. Select air as the Data Set, radiation as the x Axis Value, and ozone as the y Axis Value. Click OK. A Graph window is created containing a plot of ozone versus radiation with a supersmoother smooth.

#### TIME SERIES

Time series techniques are applied to sequential observations, such as daily measurements. In most statistical techniques, such as linear regression, the organization of observations (rows) in the data is irrelevant. In contrast, time series techniques look for correlations between neighboring observations.

This section discusses the time series available from the **Statistics** Time Series menu:

- **Autocorrelations**: calculates autocorrelations, autocovariances, or partial autocorrelations for sequential observations.
- **ARIMA**: fits autoregressive integrated moving average models to sequential observations. These are very general models that allow inclusion of autoregressive, moving average, and seasonal components.
- **Lag plot:** plots a time series versus lags of the time series.
- **Spectrum plot:** plots the results of a spectrum estimation.

We use these techniques to examine the structure in an environmental data set.

#### Autocorrelations

The *autocovariance function* is an important tool for describing the serial (or temporal) dependence structure of a univariate time series. It reflects how much correlation is present between lagged observations.

#### Plotting autocorrelations

From the main menu, choose **Statistics** Time Series Autocorrelations. The Autocorrelations and Autocovariances dialog opens, as shown in Figure 6.76.

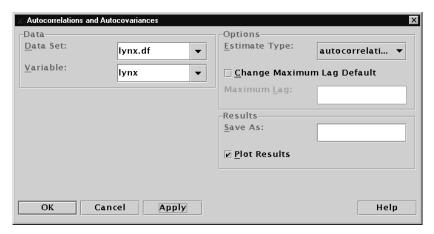
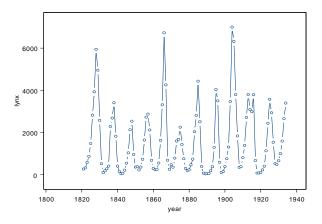


Figure 6.76: The Autocorrelations and Autocovariances dialog.

#### Example

The example data set lynx contains the annual number of lynx trappings in the Mackenzie River District of North-West Canada for the period 1821 to 1934. We can plot the data with the ts.plot command as follows:

```
> ts.plot(lynx, type="b", xlab="year", ylab="lynx", pch=1)
Figure 6.77 displays the graph.
```



**Figure 6.77:** Lynx trappings in the Mackenzie River District of North-West Canada.

A definite cycle is present in the data. We can use autocorrelations to explore the length of the cycle.

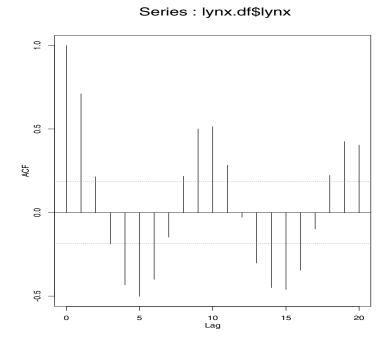
By default, lynx is stored in an object of class "ts". Before it can be recognized by the dialogs, we must store lynx as a column in a data frame. To do this, type the following in the **Commands** window:

#### > lynx.df <- data.frame(lynx)</pre>

We can now proceed with the autocorrelation analysis on the lynx.df data frame:

- 1. Open the **Autocorrelations and Autocovariances** dialog.
- 2. Type lynx.df in the **Data Set** field.
- 3. Select lynx as the **Variable**.
- 4. Click **OK**.

Figure 6.78 displays the resulting autocorrelation plot. The peaks at 10 and troughs at 5 reflect a ten-year cycle.



**Figure 6.78:** Autocorrelation plot of the 1 ynx data.

#### **ARIMA**

Autoregressive integrated moving-average (ARIMA) models are useful for a wide variety of time series analyses, including forecasting, quality control, seasonal adjustment, and spectral estimation, as well as providing summaries of the data.

#### Fitting an ARIMA model

From the main menu, choose **Statistics** ► **Time Series** ► **ARIMA Models**. The **ARIMA Modeling** dialog opens, as shown in Figure 6.79.

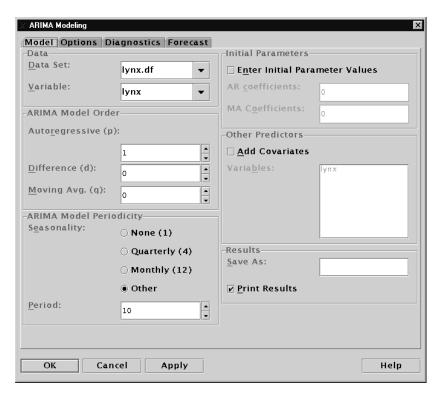


Figure 6.79: The ARIMA Modeling dialog.

#### Example

In the section Autocorrelations on page 368, we computed autocorrelations for the lynx time series. The autocorrelation plot in Figure 6.78 displays correlations between observations in the lynx data, with a ten-year cycle to the correlations. We can model this as an autoregressive model with a period of 10.

- 1. If you have not done so already, create the lynx.df data frame. The instructions for doing this are given on page 369.
- 2. Open the **ARIMA Modeling** dialog.
- 3. Type lynx.df in the **Data Set** field.
- 4. Select lynx as the **Variable**.
- 5. Specify an **Autoregressive Model Order** of 1.
- 6. Select **Other** as the **Seasonality**.
- 7. Specify a **Period** of 10.
- 8. Click OK.

Summaries for the ARIMA model are displayed in the **Report** window:

#### Lag Plot

The **Lag Plot** dialog plots a time series versus lags of the time series.

#### Creating a lag plot

From the main menu, choose **Statistics** ► **Time Series** ► **Lag Plot**. The **Lag Plot** dialog opens, as shown in Figure 6.80.

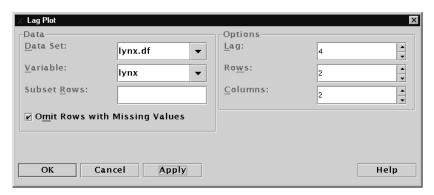


Figure 6.80: The Lag Plot dialog.

#### **Example**

In the section Autocorrelations on page 368, we computed autocorrelations for the lynx time series. In this example, we use a lag plot to example the correlation between observations at different lags.

- 1. If you have not done so already, create the lynx.df data frame with the instructions given on page 369.
- 2. Open the **Lag Plot** dialog.
- 3. Type lynx.df in the **Data Set** field.
- 4. Select lynx as the **Variable**.
- 5. Select a **Lag** of **4**.
- 6. Select a layout of 2 Rows by 2 Columns, and click OK.

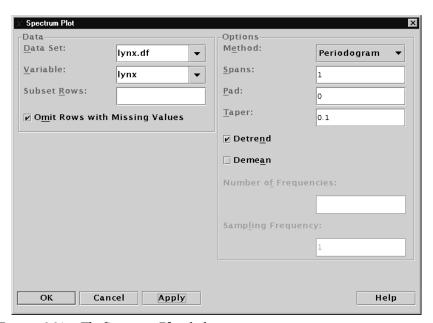
A lag plot of the lynx data appears in a **Graph** window.

#### **Spectrum Plot**

The **Spectrum Plot** dialog plots the results of a spectral estimation. This plot displays the estimated spectrum for a time series using either a smoothed periodogram or autoregressive parameters.

#### Creating a spectrum plot

From the main menu, choose **Statistics** ▶ **Time Series** ▶ **Spectrum Plot**. The **Spectrum Plot** dialog opens, as shown in Figure 6.81.



**Figure 6.81:** The **Spectrum Plot** dialog.

#### Example

In the section Autocorrelations on page 368, we computed autocorrelations for the lynx time series. In this example, we plot a smoothed periodogram of the lynx data to examine the periodicities in the series.

- 1. If you have not done so already, create the lynx.df data frame with the instructions given on page 369.
- 1. Open the **Spectrum Plot** dialog.
- 2. Type lynx.df in the **Data Set** field
- 3. Select lynx as the **Variable**, and click **OK**.

A spectrum plot of the lynx data appears in a **Graph** window.

#### **REFERENCES**

Box, G.E.P., Hunter, W.G., & Hunter, J.S. (1978). *Statistics for Experimenters*. New York: Wiley.

Chambers, J.M., Cleveland, W.S., Kleiner, B. & Tukey, P.A. (1983). *Graphical Methods for Data Analysis*. Belmont, California: Wadsworth.

Cleveland, W.S. (1979). Robust locally weighted regression and smoothing scatterplots. *Journal of the American Statistical Association*, 74: 829-836.

Cleveland, W.S. (1985). *The Elements of Graphing Data*. Monterrey, California: Wadsworth.

Fleiss, J.L. (1981). *Statistical Methods for Rates and Proportions* (2nd ed.). New York: Wiley.

Friedman, J.H. (1984). A Variable Span Smoother. Technical Report No. 5, Laboratory for Computational Statistics. Department of Statistics, Stanford University, California.

Laird, N.M. & Ware, J.H. (1982). Random-Effects Models for Longitudinal Data. *Biometrics*, 38: 963-974.

Lindstrom, M.J. & Bates, D.M. (1990). Nonlinear Mixed Effects Models for Repeated Measures Data. *Biometrics*, 46: 673-687.

Snedecor, G.W. & Cochran, W.G. (1980). *Statistical Methods* (7th ed.). Ames, Iowa: Iowa State University Press.

Venables, W.N. & Ripley B.D. (1999). *Modern Applied Statistics with S-PLUS* (3rd ed.). New York: Springer.

#### Chapter 6 Statistics

# CUSTOMIZING YOUR SPOTFIRE S+ SESSION



Introduction	378	
Setting Spotfire S+ Options		
Setting Environment Variables		
Customizing Your Session at Start-up and Closing	383	
Creating a .S.chapters File	384	
Creating a .S.init File	385	
Creating the .First Function	385	
Setting S_FIRST	385	
Customizing Your Session at Closing	386	
Using Personal Function Libraries		
Creating an S Chapter	387	
Placing the Chapter in Your Search Path	388	
Specifying Your Working Directory	389	
Specifying a Pager	390	
Environment Variables and printgraph	391	
Setting Up Your Window System		
Setting X11 Resources	393	
Spotfire S+ X11 Resources	394	
Common Resources for the Motif Graphics Device	394	

#### INTRODUCTION

Spotfire S+ offers a number of ways to customize your session. You can set options specifying how Spotfire S+ displays data and other information, create your own library of functions, or load C or Fortran code. You can even define a function to set these options each time you start Spotfire S+, and another function to "clean up" each time you end a session.

This chapter describes changes that apply only to your Spotfire S+ session. To install them for every user on your system, talk with your system administrator.

#### SETTING SPOTFIRE S+ OPTIONS

Options in Spotfire S+ serve much the same purpose as environment variables in Solaris/Linux: they determine the behavior of many aspects of the Spotfire S+ environment. You can set or modify these options with the options command. For example, to tell Spotfire S+ to echo back to the screen the commands you type in, use this expression:

```
> options(echo=T)
```

Table 7.1 lists some of the most useful options you can set. See the options help file for a complete description of the available options. If you want to set an option each time you start a session, see the section Customizing Your Session at Start-up and Closing (page 383).

You can also determine the value of any option with options. For example, to find the current value of the echo option, type the following expression at the > prompt:

```
> options("echo")
```

Spotfire S+ answers with the following:

```
options("echo")
$echo:
[1] T
```

Because echo is true (we set it in the first paragraph of this section), Spotfire S+ prints the command you type in before returning the requested value.

**Table 7.1:** Some of the options available with the options function.

echo	Specifies whether to repeat received commands on the screen. The default value is echo=F.
prompt	Specifies the character string to print when Spotfire S+ is ready for input. The default value is prompt=">".
continue	Specifies the character string to print when you press the return key before completing an S-PLUS expression. The default value is continue="+".

#### Chapter 7 Customizing Your Spotfire S+ Session

**Table 7.1:** Some of the options available with the options function.

width	Specifies the screen width. You can change this value to get the print command to create very wide or very narrow lines. The default value is width=80.	
length	Specifies the weight of the screen. This controls how frequently the print command prints out the summary of column names when printing a matrix. The default value is length=48.	
check	Specifies whether to perform automatic validity checking at various points in the evaluation. The default is false, or check=F.	
editor	Specifies the text editor to use in history and fix. The default is vi.	
digits	Specifies for the printing functions how many digits to use when printing numbers. The default value is digits=7.	
pager	Specifies the pager program to use in such places as the help and page functions. The default for pager is the value of environment variable S_PAGER, which in turn defaults to the value of environment variable PAGER, or "less" if that is not set.	

#### SETTING ENVIRONMENT VARIABLES

Table 7.2 is a list of the environment variables recognized by Spotfire S+. You are *not* required to set them.

Many of the variables in this section take effect if you set them to any value, and do not take effect if you do not set them, so you can leave them unset without harm. For example, to set **S\_SILENT\_STARTUP** type

#### setenv S\_SILENT\_STARTUP X

on the command line and Spotfire S+ does not print its copyright information on start-up, because the variable **S\_SILENT\_STARTUP** has a value (any value).

You can check the current values for these variables by using getenv from C or S code.

**Table 7.2:** Environment variables recognized by Spotfire S+.

Variable	Description
ALWAYS_PROMPT	Chiefly affects the actions of the parse function. Normally, parse prompts for input only when the input appears to be coming from a terminal. When ALWAYS_PROMPT is set (to anything at all), parse prompts even if the standard input and standard error streams are pipes or files. See the parse help file for more details.
EDITOR	Sets the command line editor to either <b>emacs</b> or <b>vi</b> . Overridden by <b>S_CLEDITOR</b> or <b>VISUAL</b> if either contains a valid value.
PATH	Specifies the directories which are searched when a command is issued to the shell. In particular, the <b>Splus</b> command should be installed in one of the listed directories.
S_CLEDITOR	Sets the command line editor to either <b>emacs</b> or <b>vi</b> .
S_CLHISTFILE	Sets the name of the command line editor's history file. The default is <b>\$HOME/.Splus_history</b> .
S_CLHISTSIZE	Specifies the maximum number of lines to put in the command line editor's history file.
S_CLNOHIST	Suppresses writing of the command line editor's history file.
S_EDITOR	Sets the value of options()\$editor. The specified editor is used by the fix function.
S_FIRST	S-PLUS function evaluated at start-up. See section Setting S_FIRST (page 385).

#### Chapter 7 Customizing Your Spotfire S+ Session

**Table 7.2:** Environment variables recognized by Spotfire S+.

SHELL	Specifies the command shell, which Spotfire S+ uses to determine the shell to use in shell escapes (1) if <b>S_SHELL</b> is not set.
SHOME	Specifies the directory where Spotfire S+ is installed. By default, this is set to the parent directory of the program executable.
S_PAGER	Specifies which pager to use. Sets the value of options()\$pager; the specified pager is used by the page, help, and? functions.
S_POSTSCRIPT_PRINT_COMMAND	Specifies the command ( <b>lp</b> , <b>lpr</b> , etc.) used to send files to a PostScript printer.
S_PRINTGRAPH_ONEFILE	Determines whether plots generated by the postscript function are accumulated in a single file (TRUE) or whether each plot is put in a separate EPS file. This environment variable sets the default for the onefile arguments to ps.options and postscript.
S_PRINT_ORIENTATION	Specifies the orientation of the graphic as landscape or portrait. Determines the default value of the horizontal argument to ps.options and printgraph.
S_SHELL	Specifies the shell used during shell escapes, that is, commands issued from the escape character (!). The default value is the value of <b>SHELL</b> .
S_SILENT_STARTUP	Disable printing of copyright/version messages.
S_WORK	Specifies the location of the <i>working</i> data directory, that is, the directory in which Spotfire S+ creates and reads data objects.
VISUAL	Sets the command line editor to either <b>emacs</b> or <b>vi</b> . Overridden by <b>S_CLEDITOR</b> if it contains a valid value.

# CUSTOMIZING YOUR SESSION AT START-UP AND CLOSING

If you set one or more options routinely each time you start Spotfire S+, or if you want to automatically attach library sections or Spotfire S+ chapters, you can store these choices and have Spotfire S+ set them automatically whenever it starts.

When you start Spotfire S+, the following initialization steps occur:

- 1. Basic initialization brings the evaluator to the point of being able to evaluate expressions.
- Spotfire S+ looks for the standard initialization file \$SHOME/ S.init. This is a text file containing S-PLUS expressions. The default initialization file performs the remaining steps in this list.
- 3. If your system administrator has performed any site customization in the file **\$SHOME/local/S.init**, the actions in that file are evaluated next.
- 4. Spotfire S+ looks for the file **\$SHOME**/.**S.chapters**, which is a text file containing paths of library sections or Spotfire S+ chapters to be attached for all users. By default, this file does not exist, since only the standard Spotfire S+ libraries are attached during the basic initialization.
- 5. Spotfire S+ looks for your personal **.S.chapters** file, first in the current directory, and then if not found, in your **MySwork** directory. You should list in this file any library sections or S-PLUS chapters you want attached at start-up.
- 6. Spotfire S+ determines your working data; see the section Specifying Your Working Directory for details.
- 7. Spotfire S+ evaluates the customization file .S.init if it is found in either the current directory or your MySwork directory. The .S.init file is a text file containing S-PLUS expressions that are executed at the start of your session. Note that this file is different than \$SHOME/S.init, which affects all users' sessions.

- 8. S-PLUS evaluates the function .First.Sys, which includes evaluating the local system initialization function .First.local if it exists.
- 9. S-PLUS evaluates the environment variable **S\_FIRST**, if set, or the first .First function found in the search paths set by steps 3–5.

In most cases, the initialization process includes only one of steps 6 and 8 above. Thus, you will probably use only one of the following mechanisms to set your start-up options:

- Create an S-PLUS function named .First containing the desired options.
- Create a text file of Spotfire S+ tasks named **.S.init** in either your current directory or your **MySwork** directory.
- Set the Spotfire S+ environment variable S\_FIRST as described below.

The .First function is the traditional Spotfire S+ initialization tool. The .S.init file has the advantage of being a text file that can easily be edited outside of Spotfire S+. The S\_FIRST variable is a convenient way to override .First for a specific Spotfire S+ session.

# Creating a .S.chapters File

If you want to attach specific Spotfire S+ chapters or library sections in your Spotfire S+ session, you can specify those directories using a **.S.chapters** file. Here is a sample **.S.chapters** file that attaches a specific users utility functions and also the maps library:

```
/homes/rich/Sstuff/utilities
maps
```

Paths beginning in "/" (including those using environment variables that evaluate to a path beginning in "/") are interpreted as absolute paths, those that begin with any other character are interpreted as paths relative to \$SHOME/library.

You can create a **.S.chapters** file in any directory in which you want to start up Spotfire S+. Spotfire S+ checks both the current directory and the default Spotfire S+ start-up directory **MySwork** to see whether this initialization file exists, and evaluates the first one it finds.

### Creating a .S.init File

Here is a sample **.S.init** file that sets the output width for the session as well as the default displayed precision:

```
{
  options(width=55, digits=4)
}
```

You can create a **.S.init** file in any directory in which you want to start up Spotfire S+. Spotfire S+ checks both the current directory and the default Spotfire S+ start-up directory **MySwork** to see whether this initialization file exists, and evaluates the first one it finds.

## Creating the .First Function

Here is a sample .First function that starts the Motif graphics device:

```
> .First <- function() motif()</pre>
```

After creating a .First function, you should always test it immediately to make sure it works. Otherwise Spotfire S+ does not execute it in subsequent sessions.

# Setting S\_FIRST

To store a sequence of commands in the **S\_FIRST** variable, use the following syntax:

For example, the following C shell command tells Spotfire S+ to start the Motif graphics device:

```
setenv S_FIRST 'motif()'
```

To avoid misinterpretation by the command line parser, it is safest to surround complex S-PLUS expressions with either single or double quotes (whichever you do *not* use in your S-PLUS expression).

You can also combine several commands into a single S-PLUS function, then set **S\_FIRST** to this function. For example:

```
> startup <- function() { options(digits=4)
+ options(expressions=128)}</pre>
```

You can call this function each time you start Spotfire S+ by setting **S\_FIRST** as follows:

```
setenv S_FIRST 'startup()'
```

Variables can only be defined at initialization, and not while Spotfire S+ is running. Any changes to **S\_FIRST** will take effect only upon restarting Spotfire S+.

#### Customizing Your Session at Closing

When Spotfire S+ quits, it looks in your data directory for a function called .Last. If .Last exists, Spotfire S+ runs it. A .Last function can be useful for cleaning up your directory by removing temporary objects or files.

# **USING PERSONAL FUNCTION LIBRARIES**

If you write functions that you want to use many times, you should not store them in your working directory, because objects in this directory are easily overwritten. Instead, to prevent yourself from inadvertently removing your functions, you should create a personal function library to hold them. A personal function library is simply an S chapter that you add to your Spotfire S+ search path, allowing you to access your functions from wherever you start Spotfire S+.

If you are working on a number of different projects, you can create personal function libraries for each project to store the functions developed for that project.

To set up your own library, there are two main steps:

- 1. Create an S chapter to hold your library of functions and help files.
- 2. Place the new directory in your Spotfire S+ search path.

We describe these steps in detail in the following subsections.

### Note

If your function library would be useful to many people on your system, you can ask your system administrator to create a system-wide version of your function library that everyone can access with the S-PLUS library function.

# Creating an S Chapter

To create a chapter, you use the **mkdir** command from the Solaris/ Linux prompt, followed by the S-PLUS utility **CHAPTER**. For example, to create a Spotfire S+ chapter called **mysplus** in your home directory, use the following commands:

```
% cd
% mkdir mysplus
% cd mysplus
% Splus CHAPTER
```

The **Splus CHAPTER** utility creates a **.Data** directory in the directory you created with **mkdir**; you will store your functions in this **.Data** subdirectory. The **.Data** subdirectory is created with two subdirectories, **\_\_Help** and **\_\_Meta**, which are used to store help files and object metadata, respectively.

### Note

You can create your S chapter directory anywhere you have write permission, and you can name it anything you like.

# Placing the Chapter in Your Search Path

To add an S chapter to your search path, use the S-PLUS attach function, which provides temporary access to a directory during a Spotfire S+ session. You name the directory to be added as a character-string argument to attach. For example, to add the chapter /usr/rich/mysplus to your search path with attach, use the following expression:

```
> attach("/usr/rich/mysplus")
```

When specifying directories to attach, you must specify the complete path name. Spotfire S+ does not expand such Solaris/Linux conventions as **-bob** or **\$HOME**.

Any directories you attach are detached when you quit Spotfire S+. In order to have your functions available at all times, you can specify the chapter as part of your **.S.chapters** file:

```
...other attached files
/spud/users/mysplus
...other attached files
```

You can also use either the **S.init** file or a .First function to attach mysplus to your Spotfire S+ search list, as in the following example:

```
> .First <- function(){
+ attach("/spud/users/mysplus")
+ }</pre>
```

Whenever you start Spotfire S+, mysplus is automatically attached, and your functions and help files are made available.

# SPECIFYING YOUR WORKING DIRECTORY

Whenever you assign the results of a S-PLUS expression to an object, using the <- or = operator within a Spotfire S+ session, Spotfire S+ creates the named object in your *working directory*. The working directory occupies position 1 in your Spotfire S+ search list, so it is also the first place Spotfire S+ looks for a S-PLUS object.

You specify the working directory with the environment variable **S\_WORK**, which can specify one directory or a colon-separated list of directories. The first valid directory in the list is used as the working directory, and the others are placed behind it in the search list. To be valid, a directory must be a valid Spotfire S+ chapter and be one for which you have write permission. If **S\_WORK** is set but contains no valid Spotfire S+ chapters, attempting to launch Spotfire S+ results in an error.

For example, to specify the chapter /usr/rich/mysplus as your working directory, set **S\_WORK** as follows:

```
setenv S_WORK /usr/rich/mysplus
```

If **S\_WORK** is not set, Spotfire S+ sets the working directory as follows:

- 1. If the current directory is a valid Spotfire S+ chapter, Spotfire S+ uses it as the working data.
- 2. Check for the existence of the directory \$HOME/MySwork.
  - If it exists and is a valid Spotfire S+ chapter, Spotfire S+ uses it as the working data.
  - If it exists but is not a valid Spotfire S+ chapter, Spotfire S+ prints a warning, then creates a directory in **\$HOME** with a name of the form **Schapter\$\$**, where **\$\$** is a number that guarantees the uniqueness of the chapter name, to use as the working data.
  - If it does not exist, Spotfire S+ creates it and initializes it as a Spotfire S+ chapter, then uses it as the working data.

# SPECIFYING A PAGER

A pager is a tool for viewing objects and files that are larger than can fit on your screen. They function much like editors for moving around files, but typically do not have actual editing functions. The most common uses for pagers in Spotfire S+ are to look at lengthy functions and data sets with the page function and to look at help files with the help function. The page function uses the pager specified in options()\$pager, while the help function uses the pager specified in options()\$help.pager.

The value of options()\$pager is initially specified by the **S\_PAGER** environment variable, if set, or to "less", if not. You can use the options function to specify a new default pager at any time during your Spotfire S+ session. Modifications to **S\_PAGER**, however, take effect only when you next start Spotfire S+.

Using options, usually in your .First function, is the preferred method for setting your pager. Simply use the following function call:

### > options(pager=pager)

where pager is a character string containing the command, with any necessary flags, used to start the pager.

The value of options()\$help.pager defaults to "slynx", which is a version of the lynx terminal-based Web browser. The help pager is used to display HTML text in a terminal window, as opposed to the JavaHelp window available via the help.start() command. Your help pager should therefore be an HTML-aware viewer, such as the default slynx browser. For more details, see the section Getting Help in Spotfire S+ on page 35.

# **ENVIRONMENT VARIABLES AND PRINTGRAPH**

Spotfire S+ uses environment variables to set defaults for the printgraph function. Your system administrator already set these variables system-wide, but if you would like to change the default values for your Spotfire S+ session, use your shell command to set a new value for the environment variable before you start Spotfire S+.

### Note

The printgraph function sets its defaults differently from the defaults for the *Print* button on graphics devices such as motif.

For example, to make printgraph produce plots with the *x*-axis on the short side of the paper, type the following from the C shell:

```
setenv S_PRINT_ORIENTATION portrait
```

Start Spotfire S+. Any plots made with printgraph are now produced in portrait mode.

Spotfire S+ uses the following environment variables with printgraph:

- **S\_PRINT\_ORIENTATION** controls the orientation of plots. It has two possible values: "portrait", which puts the *x*-axis along the short side of the paper, and "landscape", which puts the *y*-axis along the short side of the paper.
- **S\_PRINTGRAPH\_ONEFILE** controls whether Spotfire S+ writes printgraph output to one file or many. It has two possible values: "yes" and "no". If "yes", printgraph sends its output to **PostScript.out**. If "no", printgraph creates a separate file each time and tries to send it to the printer by executing the command specified in the variable **S\_POSTSCRIPT\_PRINT\_COMMAND**.
- **S\_POSTSCRIPT\_PRINT\_COMMAND** sets the Solaris/Linux PostScript printing command.

### Note

You cannot change the values of any environment variable once you start Spotfire S+. If you want to change a variable, you must stop Spotfire S+, change the variable, then start Spotfire S+ again. To change printgraph's behavior temporarily, see the printgraph help file for optional arguments.

You can also modify printgraph's behavior using options passed to ps.options.send. See the section Printing with PostScript Printers for details on how to control PostScript options.

# SETTING UP YOUR WINDOW SYSTEM

The motif graphics device has a control panel to help you pick the colors, fonts, and printing commands you want for your Spotfire S+graphics. When you save these settings, they are used each time you start one of these devices. You can also specify settings for these graphics devices by setting *X11 resources*.

The motif graphics device uses resources of the X Window System, Version 11, or X11. This section describes how to customize your graphics windows by setting X11 resources.

# Setting XII Resources

There are a number of ways you can set resources for X11 applications. You should talk with your system administrator about the way that is preferred on your system. This section describes one of the most flexible methods of setting X11 resources—using the **xrdb** command.

As with other X11 programs, before you can run the **xrdb** command, you must give it permission to access your display To do this, you need to first specify your *display server*, which controls the access to your display, and then explicitly give access to that server to the host on which you run **xrdb**. If you are running the C-shell, the network name of the computer or terminal you are sitting at is *displayserver*, and the network name of the machine on which you run **xrdb** is *remotehost*, you can give the appropriate permission with the following commands:

setenv DISPLAY displayserver:0 xhost + remotehost

The **setenv** command sets the **DISPLAY** environment variable to your window server so that every X11 program knows where to create windows. The **xhost** command gives the specified computer permission to create a window on your display.

The **xrdb** command takes a file of X11 resources as its argument and creates an *X11 Resource Database*. Whenever any X11 program tries to create a window on your display, the program first looks at your X11 resource data base to get default values. The **xrdb** command uses the C-preprocessor to set the defaults that are appropriate for your machine. See the **xrdb** manual page for more information.

# Spotfire S+ XII Resources

The file **SPlusMotif** in the directory **\$SHOME/splus/lib/X11/app-defaults** holds the system-wide default values for the motif graphics device. Many of the resources declared in the defaults file are discussed below.

When you specify a resource use the form:

### resource: value

where *resource* is the name of the resource you want to use and *value* is the value you want to give it. For example, set the resource which tells **xterm** windows to have a scrollbar with this command:

### xterm\*scrollBar : True

When you add this resource to your X11 resource data base, then create another window with the Solaris/Linux xterm command, the window has a scroll bar. In this example the name of the application for which you set defaults is xterm. When you want to set resources for your motif devices, you must use the proper application name, sgraphMotif.

For example, if you put the following resource into your resource data base:

### sgraphMotif\*copyScale: 0.75

you would specify the ratio of the size of your original graph to the size of any copies you created from it. When you create a copy of your motif graphics device, the copy is three-fourths the size of your current Spotfire S+ graphics window.

# Common Resources for the Motif Graphics Device

The following resources are commonly used with the motif graphics device:

• sgraphMotif\*copyScale sets the size ratio of the copy you produce when you click on the "Copy Graph" button. Spotfire S+ multiplies the height and the width of the canvas by the value in the copyScale resource to create the dimensions for the new window. The default resource declaration produces a copy with dimensions one half those of the current window:

## sgraphMotif\*copyScale: 0.5

• **sgraphMotif\*fonts** sets the fonts that the motif graphics device use for creating axis labels and plotting characters. The fonts must be named in order from smallest to largest. Use the Solaris/Linux command **xlsfonts** to see a complete list of the fonts available on your screen. As an example, the following resources tells the motif graphics device to use the **vg** family of fonts ranging in point size from 13 to 40:

sgraphMotif\*fonts: vg-13 vg-20 vg-25 vg-31 vg-40

### Note

If you select names that are too long to fit on one line, use multiple lines, and make sure that each line but the last ends with a backslash (\). Since these fonts are intended to list available sizes of the same font, the actual font used is controlled by the current value of par()\$cex and the size of the fonts relative to the **defaultFont** described below.

sgraphMotif\*defaultFont tells the motif graphics device which
font in the \*font resource list to use as the default font, when
cex=1.

### Note

The fonts are numbered from 0, so that the following resource tells the motif graphics devices to use the third font in the list given by **sgraphMotif\*fonts**: **sgraphMotif\*defaultFont**: 2

• sgraphMotif\*canvas.width and sgraphMotif\*canvas.height control the starting size of the drawing area of the graphics windows. The following resources set the size of the plotting area for the motif graphics device to 800 by 632 pixels.

sgraphMotif\*canvas.width: 800

sgraphMotif\*canvas.height: 632

### Note

When Spotfire S+ creates graphics to display in the graphics windows, it uses the initial values of \*canvas.width and \*canvas.height resources as the size of the drawing area. If you create a graphics device with a small drawing area and later resize the graphics window to a larger size, the resolution of the graphics image is reduced, so that your plots may look "blocky."

To set color resources for motif devices interactively, we recommend that you use the menus provided in the graphics windows. You can also use the **sgraphMotif\*colorSchemes** resource to define new color schemes. However, if you use **sgraphMotif\*colorSchemes** to define new color schemes, you must copy the existing resource completely before defining your new schemes, or the old color schemes will be unavailable.

# **INDEX**

operator 51	Binomial Power and Sample Size dialog 269, 271
	blood data 247
Symbols	bootstrap 360
•	box kernel 139, 153
First function 388	box plot 169
.Last function 386	for a single variable 170
	for multiple variables 171
A	Box Plot dialog 169
agglomerative hierarchical method 342	multiple variables 171 single variable 170
analysis of variance (ANOVA) 245, 308	C
one-way 245, 249	calling functions 49
random effects 309	candlestick plot 199
Apply button 124	c function 49
arguments	character strings
abbreviating 55	delimiting 49
ARIMA 371	chi-square goodness-of-fit test 232
Arithmetic, operators 50	chi-square test 218, 266
attach function 48, 388	class 41
autocovariance/correlation 368	cloud plot 184
autoregressive integrated moving-	Cloud Plot dialog 184
average (ARIMA) 371	cluster analysis
Axes page	agglomerative hierarchical 342
in graphics dialogs 121, 131	compute dissimilarities 336
_	divisive hierarchical 344
В	fuzzy analysis 340
bandwidth 138, 153, 364	k-means 337
span 142, 146	monothetic 346
bar chart 161	partitioning around medoids
Bar Chart dialog 161	339
tabulating data 163	coagulation data 246
batch command processing 27	command line editing 32
binomial power and sample size	command line editor 32
269, 271	command recall 34
	example 33
	startup 32

table of keystrokes 32	E
Commands window 124	editing
compute dissimilarities 336	command line 32
continuation 30	data objects 59
continuous response variable 246	editing data 57
contour plot 178	Editor 380
Contour Plot dialog 178	EDITOR environment variable 32
conventions, typographic 20	emacs 32
Correlations and Covariances	emacs_unixcom editor, table of
dialog 221	keystrokes 32
cosine kernel 153	emacs editor
counts and proportions 255	table of keystrokes 32
Cox proportional hazards 323	Environment variables
crosstabulations 218	PAGER 380
Crosstabulations dialog 218, 219	environment variables 381
custom application launcher 7	EDITOR 32
_	S_CLEDITOR 32
D	S_CMDFILE 383
data	S_WORK 389
editing 57	VISUAL 32
importing 57	error messages 29
with importData function	exact binomial test 255
57	examples
reading from a file 57	ANOVA of coagulation data
data objects	246
combining 49	one-sample speed of light data
editing 59	224
Data Set field 125, 214	two-sample weight gain data
Data Viewer 123	236
degrees of freedom 228	exploratory analysis, speed of light
delimiters	data 225, 237
for character strings 49	expressions
density plot 153	multiple line 30
bandwidth 153	
cosine kernel 153	F
kernel functions 153	factor analysis 240
normal (Gaussian) kernel 153	factor analysis 349 Factorial Design dialog 274
rectangle kernel 153	FASCII files
triangle kernel 153	notes on importing 103
Density Plot dialog 122	Fisher's exact test 259
divisive hierarchical method 344	formulas 214
dot plot 164	freedom, degrees of 228
Dot Plot dialog 164	Friedman rank test 252
tabulating data 166	THEGHIAH TAHK WSt 202

functions	Density Plot 122
calling 28, 49	Dot Plot 164
for hypothesis testing 73	Histogram 157
for statistical modeling 74	Level Plot 180
for summary statistics 71	Multipanel Conditioning page
high-level plotting 67	121, 147
importData 57	Parallel Plot 189
low-level plotting 68	Pie Chart 166
operators	Plot page 131
comparison 51	QQ Plot 175
logical 51	Scatter Plot 121, 127
precedence hierarchy of 53	Scatter Plot Matrix 186
qqnorm, for linear models 288	Strip Plot 173
fuzzy analysis 340	Subset Rows field 125
	Surface Plot 182
G	Time Series High-Low Plot 199
d	Time Series Line Plot 195
Gaussian kernel 139, 153	Titles page 121, 131
generalized models	graphics examples
linear 301	barley data 191
GNOME 7	djia data 200
graph dialogs	ethanol data 148
QQ Math Plot 159	exsurf data 179
graphical user interface	fuel.frame data 162
Apply button 124	kyphosis data 176
Commands window 124	lottery.payoff data 171
Data Viewer 123	main gain data 128
graphics dialogs 122	Michelson data 154
Graph menu 122	Puromycin data 133
Graph window 124	sensors data 139
OK button 124	sliced.ball data 184
Options menu 126	graphics options 126
Report window 124	Graph menu 122
graphics	Graph window 124
dialogs for 125	GUI See graphical user interface
Graph menu for 122	0 1
Graph window for 124	Н
Options menu for 126	11
graphics dialogs 122, 125	help 13
Axes page 121, 131	? function 16
Bar Chart 161	at the command line 16
Box Plot 169	from the graphical user
Cloud Plot 184	interface 13
Contour Plot 178	help.off function 13
Data Set field 125	help.start function 13

help function 16	K
Help menu 13 help window	KDE 7 kernel smoothers 139
navigation pane 13, 15	box kernel 139
Index page of 15	normal (Gaussian) kernel 139
Search page of 15 Table of Contents page	Parzen kernel 139
of 15	triangle kernel 139
toolbar 13, 14	keywords 15
buttons on 14	k-means method 337
topic pane 13, 15	Kolmogorov-Smirnov goodness-of- fit test 230, 243
keywords 15	Kruskal-Wallis rank sum test 250
Help, online	Kruskal-Wallis Rank Sum Test
manuals 16	dialog 251
help.off function 13 help.off function 35	G
help.start function 13	L
help.start function 35	loast squares line fits 125
help system 35	least squares line fits 135 in scatter plot matrices 188
high-low-open-close plot See high-	level plot 180
low plot	Level Plot dialog 180
high-low plot 199	levels, experimental factor 246
histogram 157	linear models
binning algorithms 158	diagnostic plots for 286, 287
Histogram dialog 157 hypothesis testing 72, 73	F-statistic for 285
nypothesis testing 72, 70	multiple R-squared for 285
I	standard error for 285 line plots 131, 195
	list function 46
importData function 57	lists
importing data 57	components 46
index plots 131	loess (local) regression 295
initialization, options function 379 installation 4	loess smoothers 142, 365
interquartile range 169	span 142
interrupting evaluation 30	
1 0	M
J	make.groups function 171
jackknife 362	MANOVA 353
Java	Mantel-Haenszel test 264
runtime environment 3	manuals, online 16
JavaHelp	matrix function 44
See help	McNemar's test 261
JRE 3, 4	Michaelis-Menten relationship 298
	modeling, statistical 73, 74

monothetic analysis 346 Multipanel Conditioning page in graphics dialogs 121, 147 multivariate analysis of variance (MANOVA) 353	P packages finding 28 parallel plot 189 Parallel Plot dialog 189 partitioning around medoids 339
N	Parzen kernel 139
navigation pane, help window 13, 15 Index page of 15 Search page of 15 Table of Contents page of 15 Nonlinear Least Squares Regression dialog 296, 297, 299, 300 nonlinear regression 296 nonparametric curve fits 138 normal (Gaussian) kernel 139, 153 normal power and sample size 269 Normal Power and Sample Size dialog 269	pie chart 166 Pie Chart dialog 166 tabulating data 168 Plot page in graphics dialogs 131 plots bar charts 161 box plots 169 cloud plots 184 contour plots 178 density plots 153 diagnostic, for linear models 286 dot plots 164 for linear models 287
O	high-level functions for 67
OK button 124 one-sample tests 223	high-low plots 199 histograms 157 index plots 131 least squares line fits 135 level plots 180 line plots 131, 195 low-level functions for 68 parallel plots 189 pie charts 166 qqplots 159, 175 robust line fits 136 scatter plot matrix 186 scatter plots 138 strip plots 173 surface plots 182 time series 195 time series plots 199 Trellis graphics 147, 191 using statistics dialogs 215 precedence of operators 54

principal components technique	Save As field 214
351	Save In field 214
probability distributions, skewed	SBATCH 27
225	Scatter Plot dialog 121, 127
Prompts, continuation 379	scatter plot matrix 186
proportions parameters test 257	Scatter Plot Matrix dialog 186
	least squares line fits 188
Q	scatter plots
•	least squares line fits 135, 188
QQ Math Plot dialog 159	multipanel conditioning 147
QQ Plot dialog 175	nonparametric curve fits for 138
qqplots 159	robust line fits 136
normal qqplot 159	smoothers 138
two-dimensional 175	three-dimensional 184
quantile-quantile plot See qqplots	Session options, continuation
	prompt 379
R	session options, echo 379
random affacts analysis of variance	Session options, editor 380
random effects analysis of variance 309	Session options, printing digits 380
	Session options, prompt 379
recalling previous commands 34	Session options, screen dimensions
rectangle kernel See box kernel regression 281	380
linear 282	smoothers 364
	for scatter plots 138
local (loess) 295 nonlinear 296	kernel smoothers 139
	loess smoothers 142
regression line 287 Report window 124	running averages 138
•	spline smoothers 144
resampling	supersmoothers 146
bootstrap 360 jackknife 362	span 142, 146
residuals	speed of light data 224
	exploratory analysis of 225
definition of 135, 282 normal plots 288	spline smoothers 144
plotting in linear models 288	degrees of freedom 144
resources 13	spotfire.tibco.com/support 17
rm function 48	Spotfire S+ 17
robust line fits 136	statistical modeling 73, 74
	statistical techniques
runtime environment, Java 3	analysis of variance
G	random effects 309
S	cluster analysis
S CLEDITOR environment	agglomerative hierarchical
variable 32	342
S_CMDFILE variable 383	compute dissimilarities 336
_	divisive hierarchical 344

fuzzy analysis 340	normal 269
k-means 337	principal components 351
monothetic 346	regression
partitioning around	linear 282
medoids 339	local (loess) 295
comparing samples	resampling 360
one-sample	bootstrap 360
chi-square goodness-of-	jackknife 362
fit test 232	smoothing
Kolmogorov-Smirnov	supersmoother 366
goodness-of-fit test	survival analysis
230	Cox proportional hazards
t-test 223	323
Wilcoxon signed-rank	time series
test 228	autocovariance/correlation
two-sample	368
Kolmogorov-Smirnov	autoregressive integrated
goodness-of-fit test	moving-average 371
$\overset{\circ}{2}43$	tree models 328
t-test 235	statistical tests
Wilcoxon rank sum test	analysis of variance (ANOVA)
241	245, 308
counts and proportions	one-sample 223
chi-square test 266	two-sample 234
exact binomial test 255	statistics
Fisher's exact test 259	dialogs for 213
Mantel-Haenszel test 264	Correlations and
McNemar's test 261	Covariances 221
proportions parameters test	Crosstabulations 218
$^{1}2\overline{57}$	Data Set field in 214
data summaries	formulas in 214
crosstabulations 218	Nonlinear Least Squares
summary statistics 216	Regression 296, 297, 299,
factor analysis 349	300
generalized linear models 301	plotting from 215
k samples	Save As field in 214
Friedman rank test 252	Save In field in 214
Kruskal-Wallis rank sum	Summary Statistics 216,
test 250	226
one-way analysis of	introduction to 210
variance 245	regression 281
multivariate analysis of variance	savings results from an analysis
353	215
power and sample size	Statistics menu for 211, 213
binomial 269, 271	summary 71, 216

common functions for 71	toolbar, help window 13, 14
Statistics menu 211, 213	buttons on 14
strip plot 173	topic pane, help window 13, 15
Strip Plot dialog 173	training courses 17
Student's t confidence intervals 227	treatment 246
Student's t significance test p-values	ANOVA models 249
227	tree-based models 328
Student's t-tests 227, 238	Trellis graphics 147, 191
Subset Rows field 125	functions for 121
summary statistics 71, 216	panels in 148
common functions for 71	triangle kernel 139, 153
Summary Statistics dialog 216, 226	two-sample tests 234
supersmoother 366	t-test 235
supersmoothers 146	Two-sample Wilcoxon Test dialog
span 146	242
surface plot 182	typographic conventions 20
Surface Plot dialog 182	71 6 1
survival analysis	U
Cox proportional hazards 323	_
syntax 29	unix function 56
case sensitivity 29	
continuation lines 30	V
continuation lines 30	variable, continuous response 246
continuation lines 30 spaces 29	variable, continuous response 246 vector arithmetic 53
continuation lines 30 spaces 29	variable, continuous response 246 vector arithmetic 53 vectors
continuation lines 30 spaces 29  T Technical Support 17	variable, continuous response 246 vector arithmetic 53 vectors creating 49
continuation lines 30 spaces 29  T  Technical Support 17 testing, hypothesis 72, 73	variable, continuous response 246 vector arithmetic 53 vectors creating 49 vi editor 32
continuation lines 30 spaces 29  T Technical Support 17 testing, hypothesis 72, 73 time series 195	variable, continuous response 246 vector arithmetic 53 vectors creating 49 vi editor 32 table of keystrokes 32
continuation lines 30 spaces 29  T Technical Support 17 testing, hypothesis 72, 73 time series 195 autocovariance/correlation 368	variable, continuous response 246 vector arithmetic 53 vectors creating 49 vi editor 32 table of keystrokes 32 vi function 59
continuation lines 30 spaces 29  T Technical Support 17 testing, hypothesis 72, 73 time series 195 autocovariance/correlation 368 autoregressive integrated	variable, continuous response 246 vector arithmetic 53 vectors creating 49 vi editor 32 table of keystrokes 32
continuation lines 30 spaces 29  T Technical Support 17 testing, hypothesis 72, 73 time series 195 autocovariance/correlation 368 autoregressive integrated moving-average 371	variable, continuous response 246 vector arithmetic 53 vectors creating 49 vi editor 32 table of keystrokes 32 vi function 59 VISUAL environment variable 32
continuation lines 30 spaces 29  T  Technical Support 17 testing, hypothesis 72, 73 time series 195 autocovariance/correlation 368 autoregressive integrated moving-average 371 candlestick plots 199	variable, continuous response 246 vector arithmetic 53 vectors creating 49 vi editor 32 table of keystrokes 32 vi function 59
continuation lines 30 spaces 29  T  Technical Support 17 testing, hypothesis 72, 73 time series 195 autocovariance/correlation 368 autoregressive integrated moving-average 371 candlestick plots 199 high-low plots 199	variable, continuous response 246 vector arithmetic 53 vectors creating 49 vi editor 32 table of keystrokes 32 vi function 59 VISUAL environment variable 32
continuation lines 30 spaces 29  T  Technical Support 17 testing, hypothesis 72, 73 time series 195 autocovariance/correlation 368 autoregressive integrated moving-average 371 candlestick plots 199 high-low plots 199 line plots 195	variable, continuous response 246 vector arithmetic 53 vectors creating 49 vi editor 32 table of keystrokes 32 vi function 59 VISUAL environment variable 32  W weight gain data 236
continuation lines 30 spaces 29  T Technical Support 17 testing, hypothesis 72, 73 time series 195 autocovariance/correlation 368 autoregressive integrated moving-average 371 candlestick plots 199 high-low plots 199 line plots 195 Time Series High-Low Plot dialog	variable, continuous response 246 vector arithmetic 53 vectors creating 49 vi editor 32 table of keystrokes 32 vi function 59 VISUAL environment variable 32  W weight gain data 236 Wilcoxon rank sum test 241
continuation lines 30 spaces 29  T  Technical Support 17 testing, hypothesis 72, 73 time series 195 autocovariance/correlation 368 autoregressive integrated moving-average 371 candlestick plots 199 high-low plots 199 line plots 195  Time Series High-Low Plot dialog 199	variable, continuous response 246 vector arithmetic 53 vectors creating 49 vi editor 32 table of keystrokes 32 vi function 59 VISUAL environment variable 32  W weight gain data 236 Wilcoxon rank sum test 241 Wilcoxon signed-rank test 228
continuation lines 30 spaces 29  T  Technical Support 17 testing, hypothesis 72, 73 time series 195 autocovariance/correlation 368 autoregressive integrated moving-average 371 candlestick plots 199 high-low plots 199 line plots 195  Time Series High-Low Plot dialog 199  Time Series Line Plot dialog 195	variable, continuous response 246 vector arithmetic 53 vectors creating 49 vi editor 32 table of keystrokes 32 vi function 59 VISUAL environment variable 32  W weight gain data 236 Wilcoxon rank sum test 241 Wilcoxon signed-rank test 228 working directory
continuation lines 30 spaces 29  T  Technical Support 17 testing, hypothesis 72, 73 time series 195 autocovariance/correlation 368 autoregressive integrated moving-average 371 candlestick plots 199 high-low plots 199 line plots 195  Time Series High-Low Plot dialog 199	variable, continuous response 246 vector arithmetic 53 vectors creating 49 vi editor 32 table of keystrokes 32 vi function 59 VISUAL environment variable 32  W weight gain data 236 Wilcoxon rank sum test 241 Wilcoxon signed-rank test 228