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SigmaPlot 14.5 & SigmaStat 4.0 Development and Testing Procedures

Systat Software Inc. is committed to developing state-of-the-art software that enhances and improves the quality of scientific research. Systat Software Inc. is the only scientific software company that offers a full range of scientific and engineering tools designed to meet the special needs of research scientists and engineers. Below is a summary of the procedures used by Systat Software Inc. for developing and assuring high quality software for SigmaPlot 14.5, SigmaStat 4.0 and related products.

Project

SigmaPlot 14.5 and SigmaStat 4.0 for Windows

Project Manager

Steve Rubenstein

Description of SigmaPlot

SigmaPlot goes beyond financially oriented spreadsheets and the "bells and whistles" of business graphing software by making technical features the highest priority. A user can choose from a full range of graphing options: technical axis scales, multiple axes, multiple intersecting 3D graphs, and much more.

SigmaPlot offers an intuitive Microsoft Office and Windows compatible interface. To start, users just need to click the graph type and style buttons on the Create Graph ribbon tab and select their data; SigmaPlot automatically creates a graph. For interactive graph creation, the Graph Wizard leads users quickly through each step. All graph attributes are customizable by double-clicking on the graph and choosing properties from the easy-to-read UI controls on the Graph Properties dialog box. To help users see complex interactions in their 3-D data, the program powerfully renders multiple intersecting 3-D graphs with hidden line removal. A Regression Wizard automatically determines initial parameters to help fit data.

New Features and Improvements Implemented in SigmaPlot 14.5

New Statistical Analysis Features:

- Additional numerical and graph results for contingency tables.
- Improvements in assumption checking and display formatting for correlation tests results.
- Expanded model selection criteria in Polynomial Regression.
- Easier access to setting of population mean and median population for Single Group tests.

New Statistical Graphs

- Quantile-Quantile Plot, Confidence and Prediction ellipses, and Jitter plots.

New Transforms and Mathematical Transforms:

- Added to Transform Language:
 - Function to compute product of matrices.

- Function to compute the eigenvalues/eigenvectors of real symmetric matrices.
- Function that both solves systems of linear equations and multilinear regression problems.
- Restructured transform library for easier navigation.
- Improvements in the random number generators when using a random seed.
- Added to transform library:
 - Transforms for Multilinear Orthogonal Regression and Regression with Equality Constraints.
 - Passing-Bablok Regression.
 - Chi-Square goodness of fit test for category data.

Histogram Result Graphs and Histogram Wizard:

- Added scaling options for histogram counts, options for left-edge or right-edge binning, user-defined bin counts, and automatic binning.

Macro Improvements:

- Enhanced options in the Polar and Parametric Equations macro for polar plots.

Smoothing:

- Option to generate reports when using the Smoothers, saving the settings for future reference.

Import and export options:

- Import multiple sheets from Excel files.

User interface improvements:

- Easily add value symbols to symbol and bar graphs with a new dialog available from the ribbon.
- Mini toolbar positions have been moved to make editing objects easier.
- Plots can be deleted directly from the Plot panel in Graph Properties.
- Changed the Add Axis default to be X Axis.
- Align objects now available from the right mouse menu.
- Greater access from a statistics report or a result graph to the statistics interface on the ribbon.

New Miscellaneous Features:

- Each section in a notebook can now contain one or more subsections.
- The Histogram Plus Kernel Density macro has been added to the toolbox.
- A system memory indicator has been added to the status bar showing the amount of remaining memory.
- Search in help has been improved.

Description of SigmaStat

SigmaStat provides a wide range of powerful, yet easy-to-use statistical analyses specifically designed to meet the needs of research scientists and engineers.

With the features in the program, you are guided through the process of choosing the appropriate test to analyze your data, running the test, and interpreting the results in the test report.

For many tests, graphs are available to summarize the test results.

The editing features in the program allow you to customize the appearance of reports and graphs. Your final results may be distributed using the large variety of file formats available for export.

New Features and Improvements Implemented in SigmaStat 4.0

- Principal Components Analysis (PCA) – Principal component analysis is a technique for reducing the complexity of high-dimensional data by approximating the data with fewer dimensions.
- Analysis of Covariance (ANCOVA) – Analysis of Covariance is an extension of ANOVA (Analysis of Variance) obtained by specifying one or more covariates as additional variables in the model.
- Cox Regression – This includes the proportional hazards model with stratification to study the impact of potential risk factors on the survival time of a population. The input data can be categorical.
- One-Sample T-test – Tests the hypothesis that the mean of a population equals a specified value.
- Odds Ratio and Relative Risk tests – Both tests the hypothesis that a treatment has no effect on the rate of occurrence of some specified event in a population. Odds Ratio is used in retrospective studies to determine the treatment effect after the event has been observed. Relative Risk is used in prospective studies where the treatment and control groups have been chosen before the event occurs.
- Shapiro-Wilk Normality test – A more accurate test than Kolmogorov-Smirnov for assessing the normality of sampled data. Used in assumption checking for many statistical tests but can also be used directly on worksheet data.
- New Result Graph – ANOVA Profile Plots: Used to analyze the main effects and higher-order interactions of factors in a multi-factor ANOVA design by comparing averages of the least square means.
- New Probability Transforms – Thirty-four new functions have been added to SigmaStat's Transform language for calculating probabilities and scores associated with distributions that arise in many fields of study.
- New Interface Change – Nonlinear Regression: An easy-to-use wizard interface and more detailed reports.
- New Interface Change – Quick Transforms: An easier way of performing computations in the worksheet.
- New Interface Change – New User Interface: Allows the user to work more easily with Excel worksheets.
- Yates correction added to the Mann-Whitney test – Yates correction for continuity, or Yates chi-square test is used when testing for independence in a contingency table when assessing whether two samples of observations come from the same distribution.
- Improved Error Messaging – Improved error messages have added information when assumption checking for ANOVA has failed.
- Deming Regression – Deming regression allows for errors in both X and Y variables – a technique for method comparison where the X data is from one method and the y data the other. The Deming regression method basically extends the normal linear regression, where the X values are considered to be error-free, to the case where both X and Y (both methods) have error. Hypotheses can then be tested, slope different from 1.0 for example, to determine if the methods are the same. For example, it might be used to compare two instruments designed to measure the same substance or to compare two algorithmic methods of detecting tumors in images. The graph compares the two methods to determine if they are different or the same. A report gives statistical results.

- Akaike Information Criterion (AICc) – The Akaike Information Criterion is now available in nonlinear regression reports. It is a goodness of fit criterion that also accounts for the number of parameters in the equation. It also is valid for non-nested equations that occur, for example, in enzyme kinetics analyses.
- New Probability Functions for Nonlinear Regression – A total of 24 probability functions have been added to the curve fit library. Automatic initial parameter estimate equations have been created for each.
- Nonlinear Regression Weighting – There are now seven different weighting functions built into each nonlinear regression equation (3D are slightly different). These functions are reciprocal y, reciprocal y squared, reciprocal x, reciprocal x squared, reciprocal predicted, reciprocal predicted squared and Cauchy. The iteratively reweighted least squares algorithm is used to allow the weights to change during each nonlinear regression iteration.
- Multiple Comparison Test Improvements – Two important improvements have been made. P values for the results of nonparametric ANOVA have been added. These did not exist before. Also, multiple comparison P values were limited to discrete choices (0.05, 0.01, etc.). This limitation no longer exists and any valid P value may be used.

SigmaPlot v14.5 & SigmaStat v4.0 21CFR11 Compliance

- SigmaPlot & SigmaStat provides password protection for project files, and an audit log to keep track of changes made to a project. It should be noted that in addition to the protection features offered by SigmaPlot & SigmaStat, the end user may need to implement additional controls and safety measures to meet the requirements set by FDA. As the regulations are revised periodically, Systat Software Inc., recommends that the end user contact FDA for the most up-to-date information
- [From the FDA:](#) "Software testing has limitations that must be recognized and considered when planning the testing of a particular software product. Except for the simplest of programs, software cannot be exhaustively tested. Generally, it is not feasible to test a software product with all possible inputs, nor is it possible to test all possible data processing paths that can occur during program execution. There is no one type of testing or testing methodology that can ensure a particular software product has been thoroughly tested. Testing of all program functionality does not mean all of the program has been tested. Testing of all of a program's code does not mean all necessary functionality is present in the program. Testing of all program functionality and all program code does not mean the program is 100% correct! Software testing that finds no errors should not be interpreted to mean that errors do not exist in the software product."
- If your company submits experimental results to the Food and Drug Administration (FDA) for approval, your company is required to comply with 21 CFR 11 (aka "Part 11"), a large set of regulations that includes extensive documentation and open records for auditors. Drug regulators in other countries tend to use principles and regulations similar to those of the FDA in the United States.
- SigmaPlot & SigmaStat organizes data, makes graphs and performs statistical analyses. Those analyses may be used in regulated research, but mostly are not. The FDA considers SigmaPlot to be "off the shelf software". For that reason, SigmaPlot is not directly responsible for compliance with FDA regulations. Instead, responsibility for compliance lies with the user. [Read the FDA policies on software.](#) [These policies seem to be written for software embedded in a medical device. We cannot find any statement from the FDA about software used to analyze data to be submitted to the FDA.]

Software Methodology

Software functionality is segmented into features and bug fixes. The most difficult features were implemented first, so we had time to test them.

From start to finish, the product planning and development cycle includes:

1. Concept (marketing and feasibility)

2. Requirements (Statement of Requirements, SOR)
3. Design (external and internal specifications)
4. Planning (Creation of Microsoft Project file)
5. Development (Tracking of the project using Microsoft Project)
6. Testing and documentation of features for each build
7. Beta Testing
8. Product release

Programming Languages Used

- Visual C++, Microsoft Visual Basic

Development Tools Used

- Microsoft Visual Studio 2010 using Microsoft Foundation Classes version 9
- Wise for Windows installer 6.0
- IBM/Rational ClearCase
- Elementool Bug Tracking System
- Oxygen 15.2
- MathType 6.9
- Fullshot 9.5.1.9

Product Compatibility

- Microsoft Windows 10
- Microsoft Windows 8
- Microsoft Windows 7
- MS Windows Vista
- Microsoft Office 2003 and up (paste to PowerPoint Slide, Insert Graphs into Word and other macros)
- SPSS (up to ver. 19)
- IE 6 and up, for use with the SigmaPlot WebViewer

Software Quality Assurance

Systat Software Inc. is committed to ensuring high quality software by using the SQA process, a planned and systematic set of activities that ensures that software processes and products conform to requirements, standards, and procedures. It includes the following disciplines:

- Quality assurance
- Quality engineering
- Verification and validation
- Error detection and reporting
- Error tracking, Corrective action and further error regression

Test Procedures

Manual tests are executed to exercise and evaluate SigmaPlot to demonstrate that it satisfies the specified requirements. These tests also identify differences between expected and actual results by using a broad set of test procedures.

Test procedures are derived from external specification documents and are guidelines to follow while testing the product.

The results of statistical procedures available in SigmaPlot and SigmaStat have been validated by using results in over 15 published works and other statistical software applications, including SPSS, SPLUS, R, and SYSTAT. The comparative studies with other statistical software were used to validate over 250 results. A SigmaStat notebook of sample data sets for each statistical procedure is maintained and used to check the consistency of the statistical results in over 190 test configurations as our software is modified over time.

A SigmaPlot macro is used to run the NIST (National Institute of Standards and Technology) nonlinear regression equations and data sets to compare to published results and our software results. The macro also has the capability to check the consistency of our software results over time as programming is modified. The NIST reference database consists of 27 data sets and models with various degrees of difficulty and with various starting conditions to test the global behavior and accuracy of the nonlinear regression algorithms in SigmaPlot and SigmaStat.

Applications Used for Verification

- SYSTAT
- SigmaStat
- SPSS
- Adobe Photoshop
- Adobe Illustrator
- GS Tools
- Corel Draw
- MS Office products (Word, Access, Excel)
- R

Hardware and Software Testing Platforms

- SigmaPlot 14.5 is tested on the QA Lab on Pentium 4 and higher personal computer systems.
- SigmaPlot 14.5 is designed and verified to work properly with the following operating systems:
- Windows 10
- Windows 8
- Windows 7
- Windows Vista

Independent Verification and Validation

Systat Software Inc. is committed to providing a beta testing process whereby the products of the software development life cycle phases are independently reviewed, verified, and validated by organizations that are completely independent of Systat Software Inc. Approximately 20 scientists and engineers have participated in beta testing of each release of SigmaPlot version 14.5 and SigmaStat version 4.0 and their feedback is invaluable for the increase of overall quality of the product.