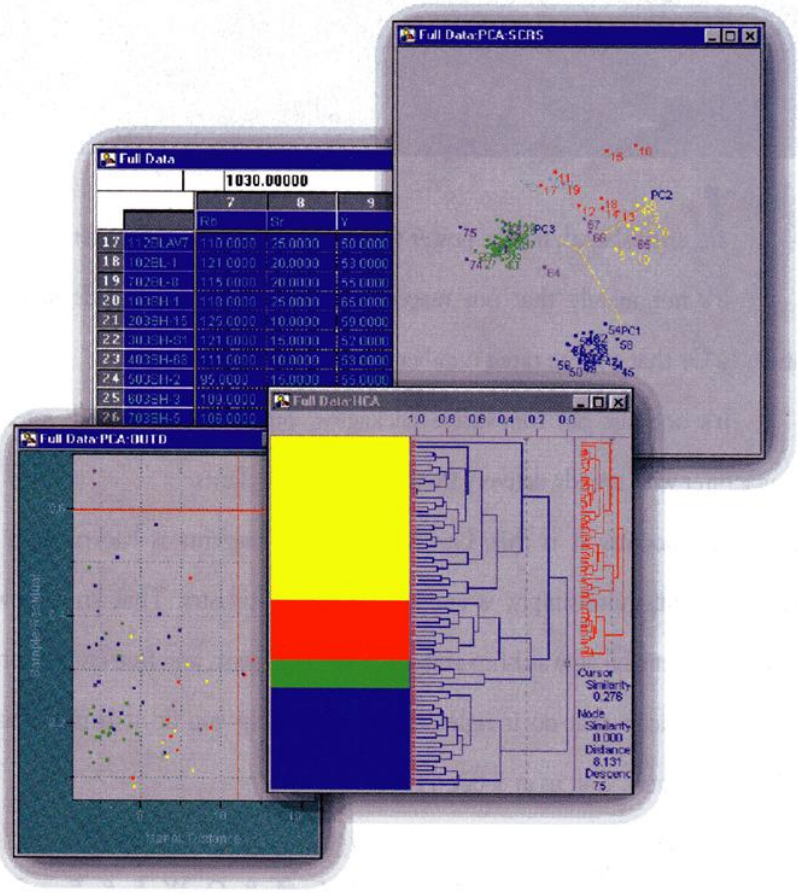
# A chemometrics toolbox


**Pirouette**
InfoMetrix
*P.O. Box 1528*
*17270 Wood-Red Rd., N.E., #777*
*Woodinville, WA 98072-1528*
*206-402-1450; fax 206-402-1040;*
*www.infometrix.com/infometrix*
*Version 2.02; $4000*

*Pirouette* is a versatile chemometrics toolbox for the Windows 95 and Windows NT operating systems. I evaluated it using two computer systems: a Pentium Pro 200-MHz machine with 64 MB of RAM running Windows NT 4.0 and a 100-MHz Pentium notebook computer with 16 MB of RAM running Windows 95. In terms of the look and feel, *Pirouette* uses the common Windows 3.1 dialog boxes for opening and saving files. This method can present a problem for networked computers because nodes in the network neighborhood are not recognized. Although *Pirouette* does not support Object Linking and Embedding (OLE), it does support cutting and pasting of tables as unformatted text and figures as device-independent bitmaps (DIBs). I evaluated *Pirouette* with Microsoft Word 7.0 and Excel 7.0 for transferring data and figures between applications.

*Pirouette* is easy to learn and use. Most of the basic chemometric methods, such as hierarchical cluster analysis (HCA), principal component analysis (PCA), K-nearest neighbors (KNN), Soft Independent Modeling for Class Analogies (SIMCA), partial least squares (PLS), and principal component regression (PCR), are readily available. These individual methods are all interfaced in an object-oriented fashion, which is the strength of *Pirouette*. For example, using HCA, the user can define class assignments for objects, and *Pirouette* automatically assigns colors for each class; these same colors will be mapped onto objects in other charts generated from separate chemometric analyses. *Pirouette* is missing a linear discriminant analysis (LDA) method, which is a standard classification method.

The object manager follows the same type of design with folders as the file manager in Windows uses for files, which allows the user to organize results and graphs of numerous methods. However, one cannot move to a chart by double clicking in the object manager, and multiple graphs in the same user-defined window cannot be manipulated together (e.g.,




Pirouette *includes all of the basic chemometric methods, including HCA.*

rotated). *Pirouette* does allow the user to add the calculations to a window and run multiple applications serially, which is another strong feature. *Pirouette* will not minimize while jobs are running, but other Windows programs can be used simultaneously.

*Pirouette* also allows manual rotation of three-dimensional charts around the axes. These charts are also automatically spun, which is an attractive—but not very useful—feature for data analysis. Another benefit of *Pirouette* is its built-in model validation. Models are all self-contained in that they store the preprocessing steps used during training, which are then automatically applied during prediction.

In addition to supporting ASCII, Lotus, and Excel formats, *Pirouette* supports several instrument formats, including the American Instrument Association (AIA) Standard, Beckman System Gold, Brimrose AOTF, Galactic Industries Lab Calc, Guided Wave Model 300, Hewlett Packard Model 8452, JCAMP-DX, KVB/Analect, LT Industries Model 1200, NIR-Systems, NSAS, Otsuka MCPD-1000, Perkin-Elmer Spectroscopy, PE Nelson Turbochrom, and Scientific Software EZChrom.

The data are manipulated by spreadsheet. Unlike stand-alone spreadsheet programs, this spreadsheet does not support a macro programming language or statistical and mathematical functions. However, data can be readily transferred between other spreadsheet programs via the Windows clipboard. The *Pirouette* spreadsheet supports basic operations such as file merging, inclusion, exclusion, and sorting by row and column. The software supports some of the basic data preprocessing functions; however, any sophisticated preprocessing, such as multiplicative scatter baseline correction, will have to be done before loading the data set into *Pirouette*.

*Pirouette* is copy-protected with a key device that plugs into the printer port. I never really cared for these devices because they typically involve getting down on your knees and climbing behind the computers to add and remove them. An advantage of the key, however, is that interim releases of the software can easily be obtained and installed from InfoMetrix's Internet site. Demonstration software can also be downloaded from this site.

Like most Windows programs, *Pirouette* generated the occasional crash and went through two interim releases during the review period. The technical support team for *Pirouette* is responsive and usually replies to problems by e-mail within the same day.

*Pirouette* is graphically oriented and automatically labels and colors graph objects. The charts are automatically converted to black and white for noncolor printers. Some charts, such as dendrograms, however, do not automatically map to the paper size and may be split among multiple pages. Another difficulty is that objects of different colors (e.g., points and lines) become indistinguishable when printed in black and white. A solution to this problem would be to map different colors to different symbols or lines. Also, legends would make the graphs more readable.

The chart configuration is fairly rigid, which may cause problems on large data sets with many points and observations. For example, in the PCA results, screen line plots of independent block residuals for every observation are drawn. The program did bog down with displaying line plots for large data sets (i.e., 340 objects and 1300 variables) on the notebook computer. (This problem was not noticeable on the Pentium Pro system.) Future releases are planned that will fix this problem.

In summary, for those interested in a versatile chemometric toolbox for a wide variety of data, *Pirouette* is perhaps the best software package around. The calculations were accurate, and they ran reasonably fast, although larger data sets will require faster computers. I recommend going to the Infometrix Web site and taking the demonstration version for a spin.

*Reviewed by Peter de B. Harrington, Ohio University, Athens*