Simfit

Tutorials and worked examples for simulation, curve fitting, statistical analysis, and plotting.
http://www.simfit.org.uk

There are numerous occasions in data analysis when it is useful to be able to examine data sets using numerical techniques in order to perform data transformations, or make calculations relevant to a particular problem. Typical examples would be to perform a singular value decomposition on a data matrix to estimate the rank, to locate the positive zeros of the Hessian of a binding polynomial to identify ligand concentrations separating regions of positive and negative cooperativity, or to calculate the zeros of the derivative of a polynomial used for data smoothing or calibration so as to locate turning points.

The following techniques are available from the numerical calculations option available from the SimFit program **simstat**.

Item	Action
Polynomial	Calculate zeros
Matrix	Determinant/eigenvalues/inverse
Matrix	Singular value decomposition
Matrix	Pseudo inverse and rank
Matrix	LU factorization/norms/condition number
Matrix	QR factorization
Matrix	Cholesky factorization of a positive definite matrix
Solve	$Ax = b$ (A nonsingular)
Solve	$Ax = b$ (L_1 norm over-determined)
Solve	$Ax = b$ (L_2 norm over-determined)
Solve	$Ax = b$ (L_∞ norm over-determined)
Calculate	$y^T Ay, \quad y^T A^{-1} y$
Calculate	$AB, \quad A^T B, \quad AB^T, \quad A^T B^T$
Calculate	$Ax = \lambda Bx$ (B positive definite)
Rotation	Orthomax
Rotation	Procrustes

In order to use one of these techniques the following procedure is recommended.

1. Open the [Statistics] option from the main SimFit menu, or alternatively use the [A/Z] option and open program **simstat**

2. Select the [Numerical analysis] option

3. Choose the procedure required

4. Study the default test file(s) provided to appreciate the data format required

5. Perform the calculations and view the results

6. Now try with your own data

Note that many SimFit test files have further information following on from the data section to help you understand the nature of the data set required, or to add information to assist in the interpretation of results.