Subject: On errors calculated by curve-fitting routines
Posted by Gernot Hassenpflug on Thu, 06 Mar 2008 03:08:49 GMT
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Hello all,

I'm using IDL 6.1, as well as Maple 11, Mathematica 6.0, Matlab 7.5 and the statistical language R. My goal is to calculate the covariance matrix of parameters of a second order polynomial curve fit. To clarify: I refer to this as linear fitting, since the parameters are linear; however, many books, papers and routines refer to this as non-linear fitting.

Matlab and Mathematica do not have built-in functions to do this (Mathematica has an add-on module which my institute has not bought) so I am comparing the parameter covariance matrix from IDL, Maple, R and my own programmed output learned from section 15.4 of Numerical Recipes, 2nd edition, and a paper by Keith Burrell in the American Journal of Physics Vol. 58, No. 2, pp 160--164 (1990) titled "Error analysis for parameters determined in nonlinear least-square fits", both describing the same method which uses the variances of the dependent data combined with the derivatives of the fitting function wrt the fitted parameters; i.e., the dependent data values themselves are not used, apparently.

I find that in IDL the routines POLY_FIT, LMFIT and CURVEFIT can all calculate the parameter covariance matrix and it is documented that LMFIT uses the method of Burrell and Numerical Recipes. I cannot tell what method the other two routines use.

Maple seems to use a different method apparently described on pp 197--198 of David M. Himmelblau's 1970 book titled "Process Analysis by Statistical Methods", which I have ordered used but not yet received.

I am hoping that contributors to this list could give their comments and opinions on what method of parameter variance and covariance is most sound, and which routines are therefore preferred for a polynomial fitting case (possibly over-determined).

Many thanks in advance,
Gernot Hassenpflug
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BOFH excuse #72:

Satan did it