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A NOTE ON GENERALIZED NONLINEAR LEAST-SQUARES DATA FITTING

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A convenient, accurate method for the solution of the generalized nonlinear least-squares data fitting problem which requires no input derivatives is compared with a recently published approach.

Wolberg and Isenberg recently published an article[1]) in this journal on applying symbolic formula manipulation to the problem of nonlinear least squares. They mention that a program which embodies this procedure is available through a commercial outlet. The main advantage of the Wolberg–Isenberg program is that the user need only enter the function to be fitted, but no partial derivatives required in the analysis need be calculated and entered since all such derivatives are automatically calculated internally by symbolic manipulation. For complicated functions the avoidance of input derivatives can save considerable work and possible grief.

It is worth emphasizing that an earlier[2,3]), more accurate, generalized least-squares program, which also avoids the need for any input derivatives, is available free from the author. The Powell–Macdonald program avoids the need for user-supplied input derivatives by automatically calculating all derivatives used in the analysis by numerical approximation. The use of approximate derivatives does not interfere with convergence of the program toward the exact least-squares solution provided a reasonable choice of the approximation interval (step-size) is made. No such choice need be made in the Wolberg–Isenberg program. Finally, the Powell–Macdonald method differs from the Wolberg–Isenberg approach in another important respect.

In the generalized situation, sometimes known as the errors-in-variables approach, one assumes that there are non-negligible random errors in the measurements of values of all variables. This is, in fact, the usual case[2]), although it has been customary to ignore or neglect all errors except those involved in dependent variable measurements. Wolberg and Isenberg use a method derived originally by Deming[4]) to solve this general case, where one uses weights derived from uncertainty measures for each variable at each measured point (*not* just weighting of the dependent variable). But it has been shown[2,5]) that the Deming iterative solution in only an approximation in this case and, on convergence, does not lead to a true least-squares solution. In fact, its final converged estimates do not lead to adequate satisfaction of the least squares minimization conditions[2]), necessary for a least sum of squares. The Wolberg–Isenberg method itself thus does not yield a *least*-squares solution in the generalized case.

The Powell–Macdonald program uses the Deming approach as a starting point in the generalized case and achieves a very rapid convergence to a true least-squares solution, even in situations where the variables and the parameters enter the fitting equation in strongly nonlinear fashion. Several detailed numerical examples have been presented earlier[2]) comparing results obtained with the Deming and Powell–Macdonald approaches for various linear and nonlinear fitting functions. As expected, the Powell–Macdonald sums of squares are always less than those following from the Deming method when all variables are weighted. At least a relative minimum *least*-squares solution is ensured in the Powell–Macdonald method because iteration only ceases when the minimization conditions are very well satisfied. When uncertainties are considered to occur only in the dependent variable measurement, the Powell–Macdonald program reduces to just the Deming solution, which is exact in this special case. Thus, the program applies to both generalized and ordinary, linear and nonlinear, least-squares fitting situations.

References

1) J. R. Wolberg and J. Isenberg, Nucl. Instr. and Meth. **112** (1973) 533.

2) D. R. Powell and J. R. Macdonald, Computer J. **15** (1972) 148; **16** (1973) 51. It appears that the expression for estimates of parameter variances given in this paper is too small by a factor of two in the full generalized case.

3) J. R. Macdonald, J. Comp. Phys. **11** (1973) 620.

4) W. E. Deming, *Statistical adjustment of data* (J. Wiley, New York, 1943).

5) H. I. Britt and R. H. Luecke, Technometrics **15** (1973) 233.