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Letter to the Editor

Comment on "The Equivalence and Numerical Solution of Regression Optimal Policy and Boundary Value Problems Involving Differential Equations

The article by Wnek and Haas [1] contains two errors. First, the interpretation of covariance terms [1, p. 338] is incorrect and can lead to serious errors if implemented in the suggested manner. Second, the formulas for the variances and covariances of the parameters [1, p. 337] are in error.

The authors explain the "significance of the covariances" cov (k_i, k_j) between the parameters k_i and k_j of a least squares problem by stating that "...each correlation coefficient should ideally be unity if all the parameters belong in the model." On [p. 339], this interpretation is apparently used as a criterion to reject parameters with small correlation coefficients.

The argument used by Wnek and Haas for this interpretation is that due to a linearization process in the solution algorithm, the relation between the observations and small changes of parameters is linear and therefore, the correlation coefficients between the parameters should be ± 1. In reality the covariances between the parameters are independent of the observations in a linear model. They depend mainly on the spread pattern of the independent variables τ_j and on the formulation of the model. This well known property of data fitting problems, is exploited, e.g., when orthogonal functions are used for fitting [2, p. 144, 166]. Being independent of the observations, the covariances do not provide any information about the importance of the parameters for the model. The cov(k_i, k_j) are, however, needed when the parameters are used for the calculation of other quantities, such as the functionals $Y_j(k_1, ..., k_M, \tau)$. Estimates of the accuracies of such quantities depend on the covariances between the parameters [2, p. 59]. The significance assigned by Wnek and Haas to cov(k_i, k_j) should have been assigned to the covariances cov(Y_i^D, k_j). Formulas for the computation of these covariances in the linear case are given, e.g., in [2, p. 168].

In the nonlinear case considered by Wnek and Haas the cov(k_i, k_j) depend on the observations, too, because the least squares values of the parameters depend on the observations. However, even in this case small correlation coefficients between parameters do not indicate that the corresponding parameters do not belong to the model, but rather that a (desirable) model formulation resembling orthogonal functions has been used.

The formula (40) for the cov(k_i, k_j) given by Wnek and Haas is correct only if the functionals Y_i are linear functions of the parameters. Variance formulas for nonlinear problems necessarily contain second order derivatives, as has been shown in [3, 4, 5]. The complete formula for the variance-covariance matrix $\mathscr{V}$ is in the present case

$$\mathscr{V} = \sigma^2 \mathscr{B}^{-1} \mathscr{A} (\mathscr{B}^{-1})^T$$

where

$$\mathscr{A} = \alpha_{hl},$$

$$\mathscr{B} = \alpha_{hl} - \sum_{j=1}^{N_D} \sum_{i=1}^{N} w_{ij} c_{ij} (\partial^2 Y_{ij} / \partial k_h \partial k_l),$$

and

$$c_{ij} = Y_{ij}^D - Y_i(k_1, \ldots, k_M, \tau_j).$$

Obviously $\mathscr{V}$ reduces to [1, Eq. (40)] only if the second-order derivatives of the Y_{ij} are zero, i.e., in the linear case. It has been shown in [4] that neglecting the second-order derivatives can produce a significant effect on the variances and covariances and on corresponding error estimates. Therefore, those terms should be kept in the variance formulas not only for theoretical but also for practical reasons.

References

1. W. J. Wnek and W. R. Haas, *J. Comput. Phys.* **18** (1975), 326–341.
2. P. R. Bevington, "Data Reduction and Error Analysis for the Physical Sciences," McGraw–Hill, New York, 1969.
3. R. E. Barieau and B. J. Dalton, Non-linear regression and the principle of least squares, Bureau of Mines Report of Investigations, No. 6900, 1966.
4. A. Celmiņš, Least squares adjustment with finite residuals for nonlinear constraints and partially correlated data, Ballistic Research Laboratories Report No. 1658, July 1973.
5. A. J. Pope, Modern trends in adjustment calculus, International Symposium on Problems Related to the Redefinition of North American Geodetic Networks, Frederictown, New Brunswick, May 1974.

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Aivars Celmiņš

Chief, Fluid Mechanics Branch,
Applied Mathematics and Sciences Laboratory,
USABRL, Aberdeen Proving Ground, MD 21005