STATISTICS OF NON-LINEAR REGRESSION

As you've seen, the Solver finds the set of least-squares regression coefficients very quickly and efficiently. However, it does not provide the standard deviations of the coefficients. Without these, the Solver's solution is essentially useless. The following illustrates how to obtain the standard deviations of the regression coefficients after obtaining the coefficients by using the Solver.

The standard deviation of the regression coefficient a_i is given by*

$$\sigma_i = \sqrt{\mathbf{P}_{ii}^{-1}} \; SE(y) \tag{12-11}$$

where $\mathbf{P}_{ii}^{-1}$ is the i^{th} diagonal element of the inverse of the $\mathbf{P}_{ij}$ matrix,

$$\mathbf{P}_{ij} = \sum_{n=1}^{N} \frac{\delta F_n}{\delta a_i} \frac{\delta F_n}{\delta a_j} \tag{12-12}$$

$\delta F_n/\delta a_i$ is the partial derivative of the function with respect to a_i evaluated at x_n and

$$SE(y) = \sqrt{\frac{SS_{resid}}{N-k}} \tag{12-13}$$

The quantities SS_{resid}, N and k are as defined in Chapter 11.

The $\delta F/\delta a_i$ terms can be calculated for each data point by numerical differentiation. The term a_i is varied by a small amount from its optimized value while the other a_j terms are held constant. The differential $\delta F/\delta a_i = \Delta F/\Delta a_i = (F_{new} - F_{opt})/(a_{new} - a_{opt})$ is calculated for each data point. Since Excel carries 15 significant figures, the change in a_i can be made very small, so that $\delta F/\delta a_i =$

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* K. J. Johnson, *Numerical Methods in Chemistry*, Marcel Dekker, New York, 1980, p. 278.