To: VSRT Group  
From: Alan E.E. Rogers  
Subject: Least squares fitting of a curve to the ozone spectrum

If we assume that a theoretical spectrum of a fixed shape can adequately represent the data when adjusted in amplitude and offset the problem is mathematically similar to finding the slope and intercept of a straight line fit to data. The algebra is most compact using the following matrix notation:

\( y \) is a column vector representing the spectrum  
\( x \) is a column vector with 2 elements, the first representing the amplitude and the second the offset.  
\( A \) is a “design” matrix  
\( \varepsilon \) is column vector of errors  

so that  
\[
y = Ax + \varepsilon
\]

The least squares solution is the result of minimizing  
\[
Q = \varepsilon^T \varepsilon = (y - Ax)^T (y - Ax) = y^T y - x^T A^T y - y^T A x + x^T A^T A x
\]

setting the derivative of \( Q \) with respect to \( x \) to zero  
\[
A^T A x = A^T y
\]

and we obtain the estimate, \( \hat{x} \),  
\[
\hat{x} = \left( A^T A \right)^{-1} A^T y
\]

an error estimate is obtained from  
\[
\left\langle (\hat{x} - x)(\hat{x} - x)^T \right\rangle^{1/2} = \left( A^T A \right)^{-1} A^T \varepsilon \varepsilon^T A \left( A^T A \right)^{-1} = \left[ \left( A^T A \right)^{-1} \right]^{1/2} \sigma
\]

when the errors are uncorrelated and have a standard deviation of \( \sigma \). The \( \left\langle \right\rangle \) brackets denote a statistical average.  

If the theoretic spectrum is \( z_i \) and the measured spectrum \( y_i \) the amplitude estimate is  
\[
\left( a_4 a_9 - a_1 a_5 \right)/d
\]
where \( a_4 = \sum_{i=0}^{N-1} z_i y_i \)

\( a_0 = N \)

\( a_1 = \sum z_i \)

\( a_3 = \sum y_i \)

\( d = a_0 a_2 - a_1^2 \)

The error estimate in amplitude

\( d^{1/2} \sigma \)

Reference: