Least Squares Fits

In analyzing the results of an experiment, a common desire is to compare the results with an analytical expression and to evaluate how closely the results conform to that expectation. One procedure used in doing this is known as a "least squares fit". The simplest form of this procedure is to compare a set of processed measurements that we will denote by (x_i, y_i) where y_i is the measurement made at the condition $x = x_i$ and the index $i = 1, 2, 3...I$ denotes the set of those data points, I in number. A simple least squares fit to this data consists of evaluating the difference between this data and an analytical or empirical expression, $Y(x)$, which contains one or more adjustable parameters that will be denoted by a_j, $j = 1, 2, 3..J$ where J is a small number that must be much less than I.

The first step in this procedure is to evaluate the sum of the squares of the discrepancies between the data and the analytical expectation. This is denoted by $S(a_1, a_2, ...)$ where

$$S \;=\; \sum_{i=1}^{I} \{y_i - Y(x_i)\}^2 \tag{Kcc1}$$

The procedure seeks the values of the parameters, a_j, that produce the smallest value of the sum, S. This occurs when

$$\frac{\partial S}{\partial a_j} \;=\; 0 \tag{Kcc2}$$

Denoting the function $\partial Y/\partial a_j$ by Y' the relation (Kcc2) can be written as

$$\sum_{i=1}^{I} \{y_i - Y(x_i)\}\, Y'(x_i) \;=\; 0 \tag{Kcc3}$$

This represents an equation for the parameter, a_j, that can then be solved (at least numerically) to find the value of that parameter that best fits the data assuming there is just one parameter a_j $(J = 1)$ or that all the other a_j values are fixed. If there are multiple adjustable parameters $(J > 1)$ then there are J simultaneous equations of the form (Kcc3) which must be solved to obtain the values of the parameters a_j, $j = 1 \rightarrow J$.

Sometimes the expressions $Y(x)$ are linear in all the adjustable parameters, a_j, in which case the values of Y' are independent of the values of a_j and the equations (Kcc3) can be written as

$$\sum_{i=1}^{I} \{Y(x_i)\}\, Y'(x_i) \;=\; \sum_{i=1}^{I} \; y_i Y'(x_i) \tag{Kcc4}$$

and since the a_j only appear on the left-hand side of these equations in the functions $Y(x_i)$ and they only appear linearly, these equations can be written in matrix form and solved using a matrix inversion procedure. Indeed this is a common process used in data analysis.

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There are many variants of this procedure and often it is exercised for a range of choices of the analytical expression $Y(x)$ and its parameters, a_j.

As another example it may be useful to delineate the following procedure. Sometimes experiments are conducted to evaluate the transfer matrix representing the linear relationship between flow variables at one location or time and the same variables at another location or time. If the state of the system is defined by two independent variables (for example the pressure, p, and flow rate, m) then the transfer matrix, $[T]$, is described by

$$\begin{Bmatrix} p_2 \\ m_2 \end{Bmatrix} = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} \begin{Bmatrix} p_1 \\ m_1 \end{Bmatrix} \tag{Kcc6}$$

where the subscripts 1 and 2 denote the two locations or times. Furthermore the variables p and m may be complex in order to represent both their magnitude and phase. In order to determine the components of the transfer matrix, $[T]$, it is necessary to obtain at least two (and often many more) linearly independent "sets" of data for each experimental condition. We will denote the number of sets by I and the sets therefore represent a data block comprising complex values of the fluctuating variables, namely,

$$p_1 \quad , \quad p_2 \quad , \quad m_1 \quad , \quad m_2 \quad \text{for} \quad i \;=\; 1,\; 2\;, 3\; ...I \tag{Kcc7}$$

A least squares procedure is then needed that minimizes the sum of the squares of the spectral radii of the residues in the two equations (Kcc6) and leads to the transfer function that best fits the data. This procedure leads to the following relations:

$$T_{11} \;=\; S_8(S_5\; S_2 - S_3\; S_6) \quad \text{and} \quad T_{12} \;=\; S_8(S_6\; S_1 - S_2\; \overline{S}_3) \tag{Kcc8}$$

and

$$T_{21} \;=\; S_8(S_5\; S_4 - S_3\; S_7) \quad \text{and} \quad T_{22} \;=\; S_8(S_7\; S_1 - S_4\; \overline{S}_3) \tag{Kcc9}$$

where

$$S_1 = \sum_{i=1}^{I} p_1\, \overline{p_1} \quad , \quad S_2 = \sum_{i=1}^{I} p_2\, \overline{p_1} \quad , \quad S_3 = \sum_{i=1}^{I} m_1\, \overline{p_1}$$

$$S_4 = \sum_{i=1}^{I} \overline{p_1}\, m_2 \quad , \quad S_5 = \sum_{i=1}^{I} m_1\, \overline{m_1} \quad , \quad S_6 = \sum_{i=1}^{I} p_2\, \overline{m_1}$$

$$S_7 = \sum_{i=1}^{I} m_2\, \overline{m_1} \quad , \quad S_8 = \frac{1}{S_5\; S_1 - S_3\; \overline{S}_3} \tag{Kcc10}$$

where the bar denotes the complex conjugate.