TOOL: A regression fit of a chosen function form to a set of data is obtained by picking coefficients that minimize the total squared difference (or error) between the function and the data. (If the function form is a polynomial, for example, the parameters are the coefficients of the polynomial.) The data points, $(\vec{x}_i, y_i)$, are located at points $\vec{x}_i$ in an N-dimensional space. We denote the function fit as $(\vec{x}_i, f(\vec{a},\vec{x}_i))$, where $\vec{a}$ contains the coefficients of f.

$E \equiv SSE \equiv$ Sum of Squared Errors of all observations

$$E = \sum_{i=1}^{N}(y_i - f(\vec{a},\vec{x}_i))^2$$

From calculus, the least squares solution is to set the derivatives of the total squared error with respect to a_1, ..., a_M equal to zero.

$$\frac{dE}{da_j} = 2\left\{\sum_{i=1}^{N}[y_i - f(\vec{a},\vec{x}_i)]\left.\frac{df(\vec{a},\vec{x})}{da_j}\right|_{\vec{x}=\vec{x}_i}\right\} = 0$$

NOTE: The sum is over i, but the derivative is with respect to j.

NOT'N: $f_i \equiv f(\vec{a},\vec{x}_i)$

$$f_{ji} \equiv \left.\frac{df(\vec{a},\vec{x})}{da_j}\right|_{\vec{x}=\vec{x}_i}$$

Using this notation, we find a_1, ..., a_M by solving the following equation:

$$\sum_{i=1}^{N}\left\{[y_i - f_i]f_{ji}\right\} = 0, \quad j = 1,\ldots,M$$

or

$$\sum_{i=1}^{N} y_i f_{ji} = \sum_{i=1}^{N} f_i f_{ji}, \quad j = 1,\ldots,M$$

NOTE: We get M equations in M unknowns—one for each a_j.