A Basic Explanation of the Least Squares Method

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A common task in numerical analysis is the determination of a function of a predetermined type which provides the “best fit” for a given set of data, the data being specified as a set of ordered pairs of domain and range values. With the type of the function having already been determined, what remains is the determination of the various coefficients in that function.

In its most general form, the desired function has the form

$$F=\sum_{\mathrm{i=1}}^{n} a_i f_i$$

where n is the number of terms in the function, the values a_1, a_2, ... a_n are the desired coefficients, and the functions f_1, f_2,... f_n are simpler functions of a pre-determined type (often integral powers of the argument) which comprise F.

The least squares technique takes the value of F for each of the domain values in the data set and subtracts from each result the corresponding range value. Each such difference is squared, and all of the squares are summed:

$$\sum_{j=1}^{m} (F(x_j)-y_j)^2 \quad (2)$$

where x_1, x_2, ... x_m are the domain values in the data set, and y_1, y_2, ... y_m are the range values of the data, and m is the number of data.

The method then determines the values of a_1, a_2, ... a_n for which this sum has the smallest value. This is accomplished by differentiating the sum over each of the coefficients, and solving each such derivative for zero. This results in an system of n equations in n unknowns.

(2) is expanded somewhat to yield

$$\sum_{j=1}^{m} (F(x_j)^2-2y_jF(x_j)+y_j^2)$$

and we differentiate over each of a_1, a_2, ... a_n, and solve for zero,

$$\frac{d}{da_i}\sum_{j=1}^{m} (F(x_j)^2-2y_jF(x_j)+y_j^2)=0$$

$$\frac{d}{da_i}\sum_{j=1}^{m} F(x_j)^2-2\frac{d}{da_i}\sum_{j=1}^{m} y_jF(x_j)+\frac{d}{da_i}\sum_{j=1}^{m} y_j^2=0$$

$$\sum_{j=1}^{m}\frac{d}{da_i}F(x_j)^2-2\sum_{j=1}^{m}\frac{d}{da_i}y_jF(x_j)+\sum_{j=1}^{m}\frac{d}{da_i}y_j^2=0$$
$$\sum_{j=1}^{m}\frac{d}{da_i}\Big(\sum_{k=1}^{n}a_kf_k(x_j)\Big)^2-2\sum_{j=1}^{m}\frac{d}{da_i}y_j\Big(\sum_{k=1}^{n}a_kf_k(x_j)\Big)+\sum_{j=1}^{m}\frac{d}{da_i}y_j^2=0$$

giving

$$2\sum_{j=1}^{m}\Big(f_i(x_j)\sum_{k=1}^{n}a_kf_k(x_j)\Big)-2\sum_{j=1}^{m}y_jf_i(x_j)=0$$
$$\sum_{j=1}^{m}\Big(f_i(x_j)\sum_{k=1}^{n}a_kf_k(x_j)\Big)=\sum_{j=1}^{m}y_jf_i(x_j)$$

which results in the equation

$$a_1\sum_{j=1}^{m}f_1(x_j)f_i(x_j)+a_2\sum_{j=1}^{m}f_2(x_j)f_i(x_j)+\ldots+a_n\sum_{j=1}^{m}f_n(x_j)f_i(x_j)=\sum_{j=1}^{m}y_jf_i(x_j)$$

for each i from 1 to n. The characteristic matrix is

$$\begin{bmatrix}
\sum_{k=1}^{m}f_1(x_k)f_1(x_k) & \sum_{k=1}^{m}f_1(x_k)f_2(x_k) & \cdots & \sum_{k=1}^{m}f_1(x_k)f_n(x_k)\\
\sum_{k=1}^{m}f_2(x_k)f_1(x_k) & \sum_{k=1}^{m}f_2(x_k)f_2(x_k) & \cdots & \sum_{k=1}^{m}f_2(x_k)f_n(x_k)\\
\vdots & \vdots & \ddots & \vdots\\
\sum_{k=1}^{m}f_n(x_k)f_1(x_k) & \sum_{k=1}^{m}f_n(x_k)f_2(x_k) & \cdots & \sum_{k=1}^{m}f_n(x_k)f_n(x_k)
\end{bmatrix}$$

and multiplying its inverse by

$$\begin{bmatrix}
\sum_{j=1}^{m}y_jf_1(x_j)\\
\sum_{j=1}^{m}y_jf_2(x_j)\\
\vdots\\
\sum_{j=1}^{m}y_jf_n(x_j)
\end{bmatrix}$$

will yield the desired coefficients.

Note that where the determinant of the characteristic matrix is zero, the data set is inadequate in some way (generally, the cause is an insufficient number of data samples).

It is important to remember that the size of the matrix representing the system of equations is dependent on the number of coefficients sought, and not on the number of items in the data set. If only five coefficients are needed, but the data set numbers in the thousands, the characteristic matrix is still five by five; however, determining the contents of the matrix will involve a lot of calculating.