Appendix A: Least Squares Method

The process of determination of a mathematical model for a group of variables is known as the parameter estimation process. One of the more popular approaches used in parameter estimation is the ***Least Squares Method***.

In its simplest form the least squares method will be illustrated in this section. Suppose that the relationship between two group of variables $\boldsymbol{x}$ and $\boldsymbol{y}$ can be best described by the equation of a straight line:

$$\boldsymbol{y} = \boldsymbol{a}_1 \boldsymbol{x} + \boldsymbol{a}_0 \tag{A-1}$$

One could arbitrarily choose two sets of $\boldsymbol{x}$ and $\boldsymbol{y}$ quantities and solve for the two unknown parameters $\boldsymbol{a}_1$ and $\boldsymbol{a}_0$. Yet, the line constructed by the computed $\boldsymbol{a}_1$ and $\boldsymbol{a}_0$ parameters might not pass through some sets of $\boldsymbol{x}$ and $\boldsymbol{y}$, since the information associated with those points were not used in computing $\boldsymbol{a}_1$ and $\boldsymbol{a}_0$.

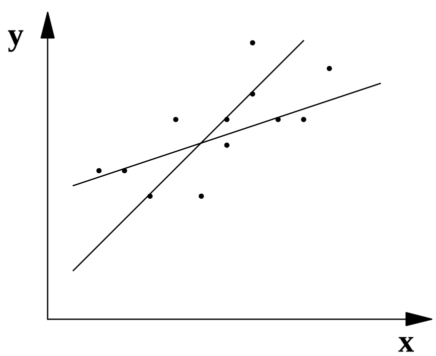

Figure A-1. Straight Lines Fitting the Data

The reasons for all the points not being located on one straight line could be:

- Errors in data set
- Inaccurate model for the data set.

The least squares criterion requires that the sum of the squares of the deviations separating the data points from the curve will be minimum. These deviations are simply the difference between the estimated values of $\boldsymbol{y}$ (hereafter denoted by $\hat{\boldsymbol{y}}_r$) from Eq. (A-1) and the actual measured values of $\boldsymbol{y}$ ($\boldsymbol{y}_r$). In other words, the deviations are the errors associated with the value of $\boldsymbol{y}$ predicted by the model and the actual measured data. The least squares method approach will use information associated with all of the $\boldsymbol{x}$ and $\boldsymbol{y}$ sets, to determine the "best" estimates of $\boldsymbol{a_1}$ and $\boldsymbol{a_0}$.

$$E = \sum_{r=1}^{N} e_r^2 = \sum_{r=1}^{N} \left[\boldsymbol{y}_r - \hat{\boldsymbol{y}}_r \right]^2 = \sum_{r=1}^{N} \left[\boldsymbol{y}_r - \left(\boldsymbol{a_1} \boldsymbol{x}_r + \boldsymbol{a_0} \right) \right]^2 \tag{A-2}$$

Minimization of error, Eq. (A-2), with respect to $\boldsymbol{a_1}$ and $\boldsymbol{a_0}$ results in the following equations which are called the ***normal equations*** for the least squares problem:

$$\frac{\partial E}{\partial \boldsymbol{a_1}} = \sum_{r=1}^{N} 2 \left[\boldsymbol{y}_r - \left(\boldsymbol{a_1} \boldsymbol{x}_r + \boldsymbol{a_0} \right) \right] \left[-\boldsymbol{x}_r \right] = 0 \tag{A-3}$$

$$\frac{\partial E}{\partial \boldsymbol{a_0}} = \sum_{r=1}^{N} 2 \left[\boldsymbol{y}_r - \left(\boldsymbol{a_1} \boldsymbol{x}_r + \boldsymbol{a_0} \right) \right] \left[-1 \right] = 0 \tag{A-4}$$

Equations (A-3) and (A-4) can be solved for the unknown parameters $\boldsymbol{a_1}$ and $\boldsymbol{a_0}$.

$$\boldsymbol{a_1} = \frac{N \sum_{r=1}^{N} \boldsymbol{x}_r \boldsymbol{y}_r - \left(\sum_{r=1}^{N} \boldsymbol{x}_r \right) \left(\sum_{r=1}^{N} \boldsymbol{y}_r \right)}{N \sum_{r=1}^{N} \boldsymbol{x}_r^2 - \left(\sum_{r=1}^{N} \boldsymbol{x}_r \right)^2} \tag{A-5}$$

$$\boldsymbol{a_0} = \frac{\left(\sum_{r=1}^{N} \boldsymbol{y}_r \right) \left(\sum_{r=1}^{N} \boldsymbol{x}_r^2 \right) - \left(\sum_{r=1}^{N} \boldsymbol{x}_r \right) \left(\sum_{r=1}^{N} \boldsymbol{x}_r \boldsymbol{y}_r \right)}{N \sum_{r=1}^{N} \boldsymbol{x}_r^2 - \left(\sum_{r=1}^{N} \boldsymbol{x}_r \right)^2} \tag{A-6}$$

The $\boldsymbol{a_1}$ and $\boldsymbol{a_0}$ values computed from Eqs. (A-5) and (A-6) represent the characteristics of a straight line which would "best" describe the $\boldsymbol{x}$ and $\boldsymbol{y}$ sets of values.

Similarly, one could compute $\boldsymbol{a_1}$ and $\boldsymbol{a_0}$ parameters with the criterion that the sum of the square of errors in the $\boldsymbol{x}$ ($e_{\boldsymbol{x}}$) would be minimum. Another approach could be the minimization of the sum of the square of errors in the $\boldsymbol{x}$ and $\boldsymbol{y}$ ($e_{\boldsymbol{v}}$).

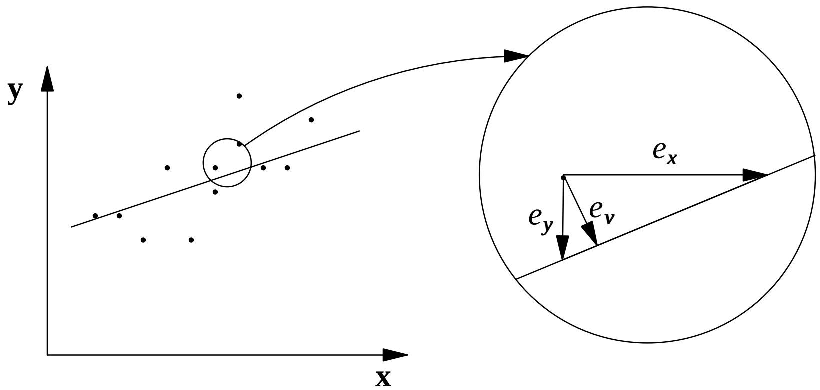

Figure A-2. Errors in Least Squares Estimation

The least squares problem can be formulated in matrix notation as:

$$\{Y\} = [X]\,\{A\} \tag{A-7}$$

where,

$$\{Y\} = \begin{Bmatrix} \boldsymbol{y}_1 \\ \boldsymbol{y}_2 \\ . \\ . \\ . \\ \boldsymbol{y}_N \end{Bmatrix} \quad [X] = \begin{bmatrix} \boldsymbol{x}_1 & 1 \\ \boldsymbol{x}_2 & 1 \\ . & . \\ . & . \\ . & . \\ \boldsymbol{x}_N & 1 \end{bmatrix} \quad \{A\} = \begin{Bmatrix} \boldsymbol{a_1} \\ \boldsymbol{a_0} \end{Bmatrix}$$

The equations presented by matrix Eq. (A-7) are in general a set of inconsistent and overdetermined equations. Inconsistent, since it is not usually possible to find {A} that would satisfy all the individual equations of Eq. (A-7), and overdetermined, since the number of equations is larger than the number of unknowns. The least square solution of Eq. (A-7) is:

$$[X]^T\{Y\} = [X]^T[X]\{A\} \tag{A-8}$$

and solving for unknown vector {A}

$$\{A\} = \left([X]^T[X]\right)^{-1}[X]^T\{Y\} \tag{A-9}$$

provided that $([X]^T[X])^{-1}$ exists. In the case that the inverse of $([X]^T[X])$ does not exist, one could use numerical techniques to solve for vector {A}.

In a more general case where matrices A, X, and Y are complex valued, the transpose notation, T, must be replaced with hermitian notation, H, in Eqs. (A-8) and (A-9). Where the hermitian operator, H, is the complex conjugate transpose. Hence, the unknown vector {A} is given by:

$$\{A\} = \left([X]^H[X]\right)^{-1}[X]^H\{Y\} \tag{A-10}$$

Individual equations in matrix Eq. (A-7) could be multiplied by a weighting factor to give that equation more or less weight in the computation. The weighting factors could be presented in form of a diagonal (N$\times$N) matrix, W. The diagonal element in row i represents the weighting factor corresponding to equation i, and the off diagonal terms are all zero. Matrix W is pre-multiplied to both sides of Eq. (A-7):

$$[W]\{Y\} = [W][X]\{A\} \tag{A-11}$$

where:

$$[W] = \begin{bmatrix} w_1 & 0 & . & 0 \\ 0 & w_2 & . & 0 \\ . & . & . & . \\ 0 & 0 & . & w_N \end{bmatrix}$$

Solving for vector {A} in Eq. (A-11):

$$\{A\} = \left([X]^H [W]^H [W][X] \right)^{-1} [X]^H [W]^H [W] \{Y\} \tag{A-12}$$

In general the relationship of Eq. (A-1) could be in the form of:

$$\boldsymbol{y} = \boldsymbol{a}_N \, \boldsymbol{x}^N + \boldsymbol{a}_{N-1} \, \boldsymbol{x}^{N-1} + \cdots + \boldsymbol{a}_{\mathbf{1}} \boldsymbol{x} + \boldsymbol{a}_{\mathbf{0}} \tag{A-13}$$

A set of equations similar to the formulation above could be written and solved to obtain the least squares estimation of unknown parameters $\boldsymbol{a}_N$, $\boldsymbol{a}_{N-1}$, ..., $\boldsymbol{a}_{\mathbf{1}}$, $\boldsymbol{a}_{\mathbf{0}}$.

The least squares method stated above could easily be extended to problems involving more than one independent variable. For example, $\boldsymbol{z}$ could be expressed in terms of $\boldsymbol{x}$ and $\boldsymbol{y}$:

$$\boldsymbol{z} = \boldsymbol{a}_{\mathbf{2}} \, \boldsymbol{y} + \boldsymbol{a}_{\mathbf{1}} \, \boldsymbol{x} + \boldsymbol{a}_{\mathbf{0}} \tag{A-14}$$

The corresponding normal equations for the least squares problem of Eq. (A-14) are:

$$\frac{\partial E}{\partial \boldsymbol{a}_{\mathbf{2}}} = \sum_{r=1}^{N} 2 \left[\boldsymbol{z}_r - \left(\boldsymbol{a}_{\mathbf{2}} \, \boldsymbol{y}_r + \boldsymbol{a}_{\mathbf{1}} \, \boldsymbol{x}_r + \boldsymbol{a}_{\mathbf{0}} \right) \right] \left[-\boldsymbol{y}_r \right] = 0 \tag{A-15}$$

$$\frac{\partial E}{\partial \boldsymbol{a}_{\mathbf{1}}} = \sum_{r=1}^{N} 2 \left[\boldsymbol{z}_r - \left(\boldsymbol{a}_{\mathbf{2}} \, \boldsymbol{y}_r + \boldsymbol{a}_{\mathbf{1}} \, \boldsymbol{x}_r + \boldsymbol{a}_{\mathbf{0}} \right) \right] \left[-\boldsymbol{x}_r \right] = 0 \tag{A-16}$$

$$\frac{\partial E}{\partial \boldsymbol{a}_{\mathbf{0}}} = \sum_{r=1}^{N} 2 \left[\boldsymbol{z}_r - \left(\boldsymbol{a}_{\mathbf{2}} \, \boldsymbol{y}_r + \boldsymbol{a}_{\mathbf{1}} \, \boldsymbol{x}_r + \boldsymbol{a}_{\mathbf{0}} \right) \right] \left[-1 \right] = 0 \tag{A-17}$$

Equations (A-15) - (A-17) can be solved for the unknown parameters $\boldsymbol{a}_{\mathbf{2}}$, $\boldsymbol{a}_{\mathbf{1}}$, and $\boldsymbol{a}_{\mathbf{0}}$. The computed values $\boldsymbol{a}_{\mathbf{2}}$, $\boldsymbol{a}_{\mathbf{1}}$, and $\boldsymbol{a}_{\mathbf{0}}$ represent the characteristics of a plane which would "best" describe the $\boldsymbol{x}$, $\boldsymbol{y}$, and $\boldsymbol{z}$ sets of values.

The above theory and formulation could be expanded to least squares estimation of a surface and eventually to higher order dimensions.

A.1 Correlation Coefficient

The "goodness" of the least squares estimation process is measured by the coefficient of correlation parameter which is defined in terms of ***total variation*** and ***explained variation***. The total variation of $\boldsymbol{y}$ is defined as $\sum_{r=1}^{N}(\boldsymbol{y}_r - \bar{\boldsymbol{y}})^2$, which is the sum of the squares of the deviations of $\boldsymbol{y}_r$ from the mean value, $\bar{\boldsymbol{y}}$. Total variation consists of two parts: (1) the explained variation, $\sum_{r=1}^{N}(\hat{\boldsymbol{y}}_r - \bar{\boldsymbol{y}})^2$; and (2) the unexplained variation, $\sum_{r=1}^{N}(\boldsymbol{y}_r - \hat{\boldsymbol{y}}_r)^2$. The terms explained variation and unexplained variation are used to denote the fact that the deviations $\hat{\boldsymbol{y}}_r - \bar{\boldsymbol{y}}$ have a definite pattern, while, the deviations $\boldsymbol{y}_r - \hat{\boldsymbol{y}}_r$ are random and unpredictable.

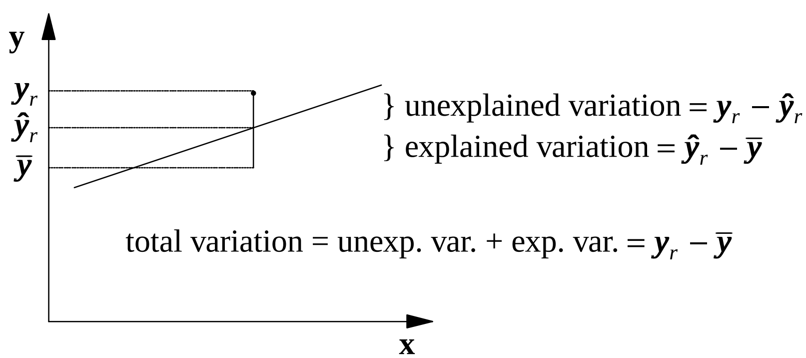

Figure A-3. Variations in Data

Therefore, the coefficient of correlation $\boldsymbol{\gamma}^2$, is defined as:

$$\boldsymbol{\gamma}^2 = \left(\frac{\sum_{r=1}^{N}(\hat{\boldsymbol{y}}_r - \bar{\boldsymbol{y}})^2}{\sum_{r=1}^{N}(\boldsymbol{y}_r - \bar{\boldsymbol{y}})^2} \right) \tag{A-18}$$

The magnitude of $\boldsymbol{\gamma}^2$ varies between 0 and 1. A value of 0 indicates no correlation between dependent and independent variable(s), while a value of 1 indicates perfect correlation.

It should be pointed out that the coefficient of correlation computed for a set of data and a assumed model, only indicates the relationship of data based on the assumed model. That is, the coefficient of correlation measures the degree to which the assumed model describes the relationship for a set of data.

A.2 Examples

A.2.1 Example 1

For the data given in Table A-1 and the assumed model equation:

$$\boldsymbol{y} = \boldsymbol{a_1 x} + \boldsymbol{a_0} \tag{A-19}$$

x	65	63	67	64	68	62	70	66	68	67	69	71
y	68	66	68	65	69	66	68	65	71	67	68	70

Table A-12. x and y Values for Least Squares Fit

a) Find the least squares solution of $\boldsymbol{a_1}$ and $\boldsymbol{a_0}$.
b) Find the coefficient of correlation.

Solution:

a) The following normal equations must be solved for $\boldsymbol{a_1}$ and $\boldsymbol{a_0}$

$$\boldsymbol{a_0}\, N + \boldsymbol{a_1} \sum_{r=1}^{N} \boldsymbol{x}_r = \sum_{r=1}^{N} \boldsymbol{y}_r \tag{A-20}$$

$$\boldsymbol{a_0} \sum_{r=1}^{N} \boldsymbol{x}_r + \boldsymbol{a_1} \sum_{r=1}^{N} \boldsymbol{x}_r^2 = \sum_{r=1}^{N} \boldsymbol{x}_r\, \boldsymbol{y}_r \tag{A-21}$$

substituting the appropriate terms in Eqs. (A-20) and (A-21):

$$12\,\boldsymbol{a_0} + 800\,\boldsymbol{a_1} = 811$$
$$800\,\boldsymbol{a_0} + 53418\,\boldsymbol{a_1} = 54107$$

from which we find $\boldsymbol{a_1} = 0.476$ and $\boldsymbol{a_0} = 35.82$ or

$$\boldsymbol{y} = 0.476\,\boldsymbol{x} + 35.82 \tag{A-22}$$

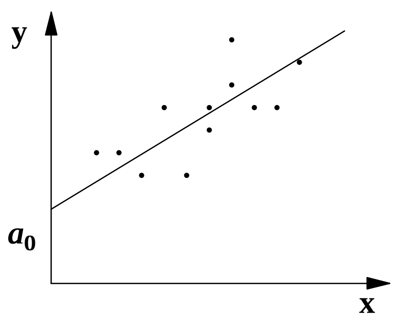

Figure A-4. Least Squares Fit of Data

b) Explained variation $= \sum_{r=1}^{N} (\hat{\boldsymbol{y}}_r - \bar{\boldsymbol{y}})^2 = 19.22$

Total variation $= \sum_{r=1}^{N} (\boldsymbol{y}_r - \bar{\boldsymbol{y}})^2 = 38.92$

Coefficient of correlation $= \boldsymbol{\gamma}^2 = \dfrac{19.22}{38.92} = 0.7027$

A.2.2 Example 2

Given the model for the sampled impulse response function between two points on a structure as,

$$h(t_k) = \sum_{r=1}^{2N} A_r e^{\lambda_r k \Delta t} \tag{A-23}$$

where,

$k = 0, 1, 2, \cdots, 2N$

$\Delta t =$ value of time subinterval

$t_k = k \Delta t$

and the known pole information λ_r, formulate the least squares solution of estimating the residues, A_r.

Solution:

For simplicity and conciseness let,

$$\mathbf{z}_r = e^{\lambda_r \Delta t}$$

and therefore Eq. (A-23) can be rewritten as,

$$h(t_k) = \sum_{r=1}^{2N} A_r \mathbf{z}_r^k \tag{A-24}$$

expanding Eq. (A-24) for time values of t_0 to t_{2N-1} will result in the following 2N equations

$$\begin{gathered} h(t_0) = A_1 + A_2 + \cdots + A_{2N} \\ h(t_1) = A_1\, \mathbf{z}_1 + A_2\, \mathbf{z}_2 + \cdots + A_{2N}\, \mathbf{z}_{2N} \\ h(t_2) = A_1\, \mathbf{z}_1^2 + A_2\, \mathbf{z}_2^2 + \cdots + A_{2N}\, \mathbf{z}_{2N}^2 \\ . \end{gathered} \tag{A-25}$$

$$\vdots$$

$$h(t_{2N-1}) = A_1\, \mathbf{z}_1^{2N-1} + A_2\, \mathbf{z}_2^{2N-1} + \cdots + A_{2N}\, \mathbf{z}_{2N}^{2N-1}$$

presenting the 2N equations of Eq. (A-25) in matrix form gives,

$$\begin{bmatrix} 1 & 1 & . & 1 \\ \mathbf{z}_1 & \mathbf{z}_2 & . & \mathbf{z}_{2N} \\ \mathbf{z}_1^2 & \mathbf{z}_2^2 & . & \mathbf{z}_{2N}^2 \\ . & . & . & . \\ \mathbf{z}_1^{2N-1} & \mathbf{z}_2^{2N-1} & . & \mathbf{z}_{2N}^{2N-1} \end{bmatrix} \begin{Bmatrix} A_1 \\ A_2 \\ . \\ A_{2N} \end{Bmatrix} = \begin{Bmatrix} h(t_0) \\ h(t_1) \\ h(t_2) \\ . \\ h(t_{2N-1}) \end{Bmatrix} \tag{A-26}$$

or,

$$[z]\{A\} = \{h\} \quad .$$

Solving Eq. (A-26) with more than 2N rows for vector {h} and matrix [z] will result in the least squares solution of the residues. Using the $\bar{\ }$ notation to denote that vector {h} and matrix [z] have been expanded (more rows):

$$[\, \bar{\mathbf{z}}\,]^H\, [\, \bar{\mathbf{z}}\,]\{A\} = [\, \bar{\mathbf{z}}\,]^H \{\, \bar{h}\, \} \quad . \tag{A-27}$$

A.3 References

[1] Ben Nobel, James W. Daniel, **Applied Linear Algebra**, Prentice-Hall, Inc., 1977.

[2] Gibert Strang, **Introduction to Applied Mathematics**, Wellesley-Cambridge Press, 1986.

[3] Murray R. Spiegel, **Schaum's Outline Series "Statistics"**, McGraw-Hill Book, 1961.