An Introduction to the Math of Design of Experiments and Response Surface Methodology Preview

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Thank you,

Bill Kappele

An Introduction to the Math of DOE

By William D. Kappele

An Introduction to the Math of DOE

Math Options Inc.

336 36th St. # 179

Bellingham, WA, 98225

(888) 764-3958

www.ObjectiveDOE.com

How You Will Learn

- Through examples and exercises
- From real data
- No homework

Mathematical Preliminaries

- Objectives-
  - You will be able to define the term "matrix."
  - You will be able to calculate the following using matrices:
    - Transpose
    - Scalar-Matrix Product
    - Matrix-Matrix Product
    - Determinant
    - Inverse
    - Condition Number
    - Trace

Definitions

- A Matrix
  is a rectangular array of elements.

1	-1	-1	1
1	-1	1	-1
1	1	-1	-1
1	1	1	1
1	-1	-1	1
1	-1	1	-1
1	1	-1	-1
1	1	1	1

- The Identity Matrix
  is a matrix with all main diagonal elements equal to one and all off-diagonal elements equal to 0

1	0	0	0	0
0	1	0	0	0
0	0	1	0	0
0	0	0	1	0
0	0	0	0	1

Matrix Transpose

- The transpose of a matrix is a matrix with the rows of the original matrix as its columns.

X=

1	-1	-1	1
1	-1	1	-1
1	1	-1	-1

X'=

1	1	1
-1	-1	1
-1	1	-1
1	-1	-1

- If a matrix is denoted by X, its transpose is denoted by X'.

Matrix Addition

- Matrices of the same dimensions can be added.
- $C = A + B$ means $c_{ij} = a_{ij} + b_{ij}$
- Matrices of the same dimension can be subtracted.
- $C = A - B$ means $c_{ij} = a_{ij} - b_{ij}$

Scalar Multiplication

- Multiplying a matrix by a number is called "scalar multiplication."
- Each element in the matrix is multiplied by the "scalar."

8*I=

8	0	0	0
0	8	0	0
0	0	8	0
0	0	0	8

Matrix Multiplication

- To multiply one matrix by another, the first matrix must have the same number of columns as the number of rows in the second matrix.
- The resulting matrix will have as many rows as the first matrix and as many columns as the second matrix.
- AB=C means $c_{ij}=\sum_{k=1}^{n} a_{ik}*b_{kj}$

Matrix Multiplication Example

- Multiply A by B:

A=

1	2
3	4
5	6

B=

1	2	3
4	5	6

AB=

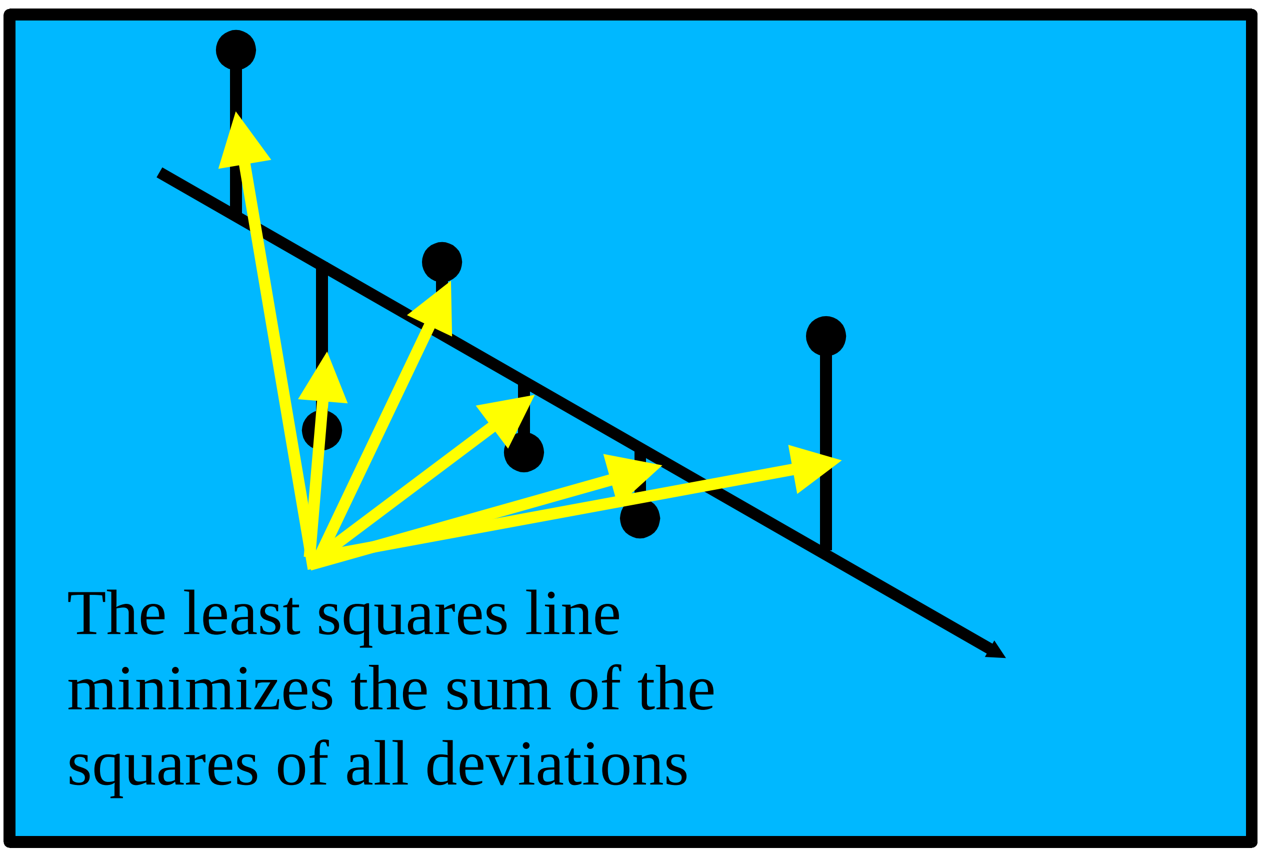
1*1+2*4	1*2+2*5	1*3+2*6
3*1+4*4	3*2+4*5	3*3+4*6
5*1+6*4	5*2+6*5	5*3+6*6

Least Squares Regression

- Objectives:
  - You will be able to calculate b-coefficients for a model.
  - You will understand the principle of Least Squares

The Principle of Least Squares

- The sum of the squares of the deviations from the best fit line is a minimum.



Matrix Form of Least Squares

- First, write the problem down:

$$b_0+b_1X_1(1)+b_2X_2(1)+\ldots+b_{12}X_1(1)X_2(1)+\ldots=Y(1)$$
$$b_0+b_1X_1(2)+b_2X_2(2)+\ldots+b_{12}X_1(2)X_2(2)+\ldots=Y(2)$$
$$\vdots$$
$$b_0+b_1X_1(n)+b_2X_2(n)+\ldots+b_{12}X_1(n)X_2(n)+\ldots=Y(n)$$

- Second, express the problem in matrix form:

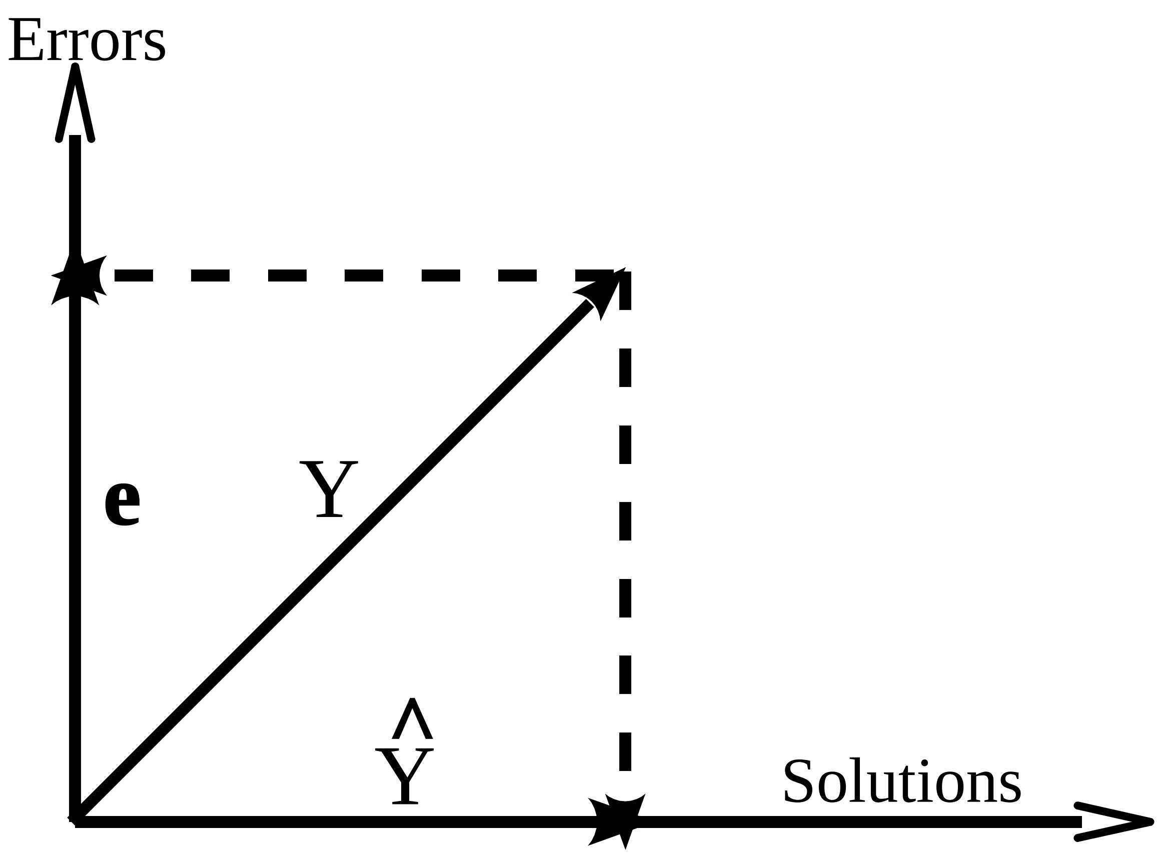
$$\underbrace{\begin{bmatrix} 1 & X1(1) & X2(1) & \ldots & X1(1)X2(1) & \ldots \\ 1 & X1(2) & X2(2) & \ldots & X1(2)X2(2) & \ldots \\ & \vdots & & \vdots & \vdots & \\ 1 & X1(n) & X2(n) & \ldots & X1(n)X2(n) & \ldots \end{bmatrix}}_{X} \underbrace{\begin{bmatrix} b0 \\ b1 \\ b2 \\ \vdots \\ b12 \\ \vdots \end{bmatrix}}_{b} \underbrace{\begin{bmatrix} Y(1) \\ Y(2) \\ \vdots \\ Y(n) \end{bmatrix}}_{Y}$$

Minimizing the Error

- To include the response variation in the data, write the matrix form of the problem as:
  - $Xb + e = Y$
  - e is a vector of errors
- The best estimate of Y possible in light of the response variation is $\hat{Y}$
  - $Xb = \hat{Y}$
- So,
  - $e = Y - Xb = Y - \hat{Y}$

What Does the Error Look Like?

- The drawing below illustrates how we can find $\hat{Y}$ to minimize e.



e is smallest when it is perpendicular to $\hat{Y}$, or $\hat{Y}'e = 0$.

Finding b for $\hat{Y}$

$$\hat{Y}'e = 0$$

$$(Xb)'(Y-Xb) = 0$$

$$b'X'(Y-Xb) = 0$$

We are looking for a non-zero b, so

$$X'(Y-Xb) = 0$$

$$X'Y - X'Xb = 0$$

$$X'Xb = X'Y$$

These are called the Normal Equations.

If X'X is not singular, then

$$(X'X)^{-1}(X'X)b = (X'X)^{-1}X'Y$$

$$b = (X'X)^{-1}X'Y$$

Least Squares Example

- Analyze the data for Acmyxil analysis in the following design:

pH	ML Kcl	Abs
6.4	1.0	0.6974
5.8	1.0	0.7097
6.4	0.5	0.6848
5.8	1.0	0.7225
5.2	0.5	0.5752
5.8	1.0	0.7463
5.8	1.5	0.6540
5.2	1.0	0.6146
5.8	1.0	0.6937
6.4	1.5	0.6116
5.8	0.5	0.6725
5.2	1.5	0.5180

End of Preview

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