Note Title 10/19/2007

Polynomial regression (Least squares)

LSC $S = \sum_i (f(x_i) - y_i)^2$

Assume $f(x) = a_0 + a_1 x$

$$S = \sum_i (a_0 + a_1 x_i - y_i)^2$$

$$= \sum_i (a_0 + a_1 x_i)^2 + y_i^2 - 2 y_i (a_0 + a_1 x_i)$$

$$= \sum_i a_0^2 + 2 a_0 a_1 x_i + a_1^2 x_i^2 + y_i^2 - 2 a_0 y_i - 2 a_1 x_i y_i$$

$$= \sum_i a_0^2 + 2 a_0 a_1 x_i - 2 a_0 y_i + a_1^2 x_i^2 - 2 a_1 x_i y_i + y_i^2$$

To minimize S, take derivatives w/ respect to a_0 + a_1 and set equal = 0

$$\frac{dS}{da_0} = 0 = \sum (2 a_0 + 2 a_1 x_i + 2 y_i)$$

or $n a_0 + a_1 \Sigma x_i = \Sigma y_i$

$$\frac{dS}{da_1} = 0 = \sum (2 a_0 x_i + 2 a_1 x_i^2 - 2 x_i y_i)$$

or $a_0 \Sigma x_i + a_1 \Sigma x_i^2 = \Sigma x_i y_i$

This gives 2 eqn's & 2 unknowns,

$$n a_0 + (\Sigma x_i) a_1 = \Sigma y_i$$
$$(\Sigma x_i) a_0 + (\Sigma x_i^2) a_1 = \Sigma x_i y_i$$

These are called the characteristic equations for a 1st order polynomial LSC mode fit

In matrix form

$$\begin{bmatrix} n & \Sigma x_i \\ \Sigma x_i & \Sigma x_i^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} \Sigma y_i \\ \Sigma x_i y_i \end{bmatrix}$$

solving algebraically,

$$a_0 = \frac{\Sigma y_i - a_1 \Sigma x_i}{n} \qquad a_1 = \frac{n \Sigma x_i y_i - \Sigma x_i \Sigma y_i}{n \Sigma x_i^2 - (\Sigma x_i)^2}$$

Now consider a 2nd order polynomial

$$a_0 + a_1 x + a_2 x^2 = f(x)$$

Plugging into LSC

$$S = \Sigma \left[(a_0 + a_1 x_i + a_2 x_i^2) - y_i \right]^2$$

(Note: To simplify writing, I will drop i subscript in derivation and restore it in final eqns)

$$S = \Sigma (a_0 + a_1 x + a_2 x^2)^2 - 2(a_0 + a_1 x + a_2 x^2) y + y^2$$

$$= \Sigma a_0^2 + 2a_0 a_1 x + 2a_0 a_2 x^2 + 2a_1 a_2 x^3 + a_1^2 x^2 + a_2^2 x^4 - 2a_0 y - 2a_1 xy - 2a_2 x^2 y + y^2$$

Taking derivatives of S w/respect to a_0, a_1, a_2 gives characteristic eqns

$$\frac{\partial S}{\partial a_0} = \Sigma\, 2a_0 n + 2a_1 x + 2a_2 x^2 - 2y = 0$$

$$\Rightarrow n a_0 + (\Sigma x) a_1 + (\Sigma x^2) a_2 - \Sigma y = 0$$

$$\frac{\partial S}{\partial a_1} = \Sigma\, 2a_0 x + 2a_2 x^3 + 2a_1 x^2 - 2xy = 0$$

$$\Rightarrow \Sigma x\, a_0 + (\Sigma x^2) a_1 + (\Sigma x^3) a_2 = \Sigma xy$$

$$\frac{\partial S}{\partial a_2} = \Sigma\, 2a_0 x^2 + 2a_1 x^3 + 2a_2 x^4 - 2x^2 y = 0$$

$$\Rightarrow (\Sigma x_i^2) a_0 + (\Sigma x_i^3) a_1 + (\Sigma x_i^4) a_2 = \Sigma x_i^2 y_i$$

in matrix format

$$\begin{bmatrix} n & \Sigma x_i & \Sigma x_i^2 \\ \Sigma x_i & \Sigma x_i^2 & \Sigma x_i^3 \\ \Sigma x_i^2 & \Sigma x_i^3 & \Sigma x_i^4 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \Sigma y_i \\ \Sigma x_i y_i \\ \Sigma x_i^2 y_i \end{bmatrix}$$

Given 3 eqns, can solve for 3 unknowns, a_0, a_1, and a_2

Note that there is a pattern here that will help you set up the characteristic eqns for any n^{th} order polynomial without doing all the algebra of multiplying terms

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For an n^{th} order polynomial,

$$a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots a_n x^n = f(x)$$

The characteristic eqn's can directly be written in matrix format as

$$\begin{bmatrix} n & \Sigma x & \Sigma x^2 & \Sigma x^3 \cdots & \Sigma x^n \\ \Sigma x & \Sigma x^2 & \Sigma x^3 & \Sigma x^4 \cdots & \Sigma x^{n+1} \\ \Sigma x^2 & \Sigma x^3 & \Sigma x^4 & \Sigma x^5 \cdots & \Sigma x^{n+1} \\ \vdots & & & & \\ \Sigma x^n & \Sigma x^{n+1} & \cdot & \cdot & \Sigma x^{2n} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} \Sigma y \\ \Sigma x y \\ \Sigma x^2 y \\ \vdots \\ \Sigma x^n y \end{bmatrix}$$

Given n eqns and n unknowns you can always solve for a_i.