Lecture 9

Interpolation and Curve Fitting III

Nonlinear Data, Curve Fitting

Ceng375 *Numerical Computations* at December 21, 2010

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Contents

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- We can develop normal equations to the preceding development for a least-squares line by setting the partial derivatives equal to zero.
- Such *nonlinear* simultaneous equations are much more difficult to solve than *linear* equations.

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- In effect, this amounts to minimizing the squares of the percentage errors, which itself may be a desirable feature.

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- In effect, this amounts to minimizing the squares of the percentage errors, which itself may be a desirable feature.
- An added advantage of the linearized forms is that plots of the data on either log-log or semilog graph paper show at a glance whether these forms are suitable, by whether a straight line represents the data when so plotted.

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- such as by plotting against $1/x, 1/(ax+b), 1/x^2$,
- and other polynomial forms of the argument may give curves with gentle enough changes in slope to allow a smooth curve to be drawn.

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- The constants a, b, and c are determined by special procedures.
- Another relation that fits data to an S-shaped curve is

$$\frac{1}{y} = a + be^{-x}$$

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- With errors defined by

$$e_i = Y_i - y_i = Y_i - a_0 - a_1 x_i - a_2 x_i^2 - \ldots - a_n x_i^n$$

Least-Squares Polynomials II

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$$S = \sum_{i=1}^{N} e_i^2 = \sum_{i=1}^{N} (Y_i - a_0 - a_1 x_i - a_2 x_i^2 - \ldots - a_n x_i^n)^2$$

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- At the minimum, all the partial derivatives $\partial S / \partial a_0, \partial S / \partial a_n$ vanish.
- Writing the equations for these gives $n + 1$ equations:

$$\frac{\partial S}{\partial a_0} = 0 = \sum_{i=1}^{N} 2(Y_i - a_0 - a_1 x_i - a_2 x_i^2 - \ldots - a_i x_i^n)(-1)$$
$$\frac{\partial S}{\partial a_1} = 0 = \sum_{i=1}^{N} 2(Y_i - a_0 - a_1 x_i - a_2 x_i^2 - \ldots - a_i x_i^n)(-x_i)$$
$$\vdots$$
$$\frac{\partial S}{\partial a_n} = 0 = \sum_{i=1}^{N} 2(Y_i - a_0 - a_1 x_i - a_2 x_i^2 - \ldots - a_i x_i^n)(-x_i^n)$$

Least-Squares Polynomials III

- Dividing each by -2 and rearranging gives the $n+1$ *normal equations* to be solved simultaneously:

$$
\begin{aligned}
a_0 N + a_1 \sum x_i + a_2 \sum x_i^2 + \ldots + a_n \sum x_i^n &= \sum Y_i \\
a_0 \sum x_i + a_1 \sum x_i^2 + a_2 \sum x_i^3 + \ldots + a_n \sum x_i^{n+1} &= \sum x_i Y_i \\
a_0 \sum x_i^2 + a_1 \sum x_i^3 + a_2 \sum x_i^4 + \ldots + a_n \sum x_i^{n+2} &= \sum x_i^2 Y_i \\
&\vdots \\
a_0 \sum x_i^n + a_1 \sum x_i^{n+1} + a_2 \sum x_i^{n+2} + \ldots + a_n \sum x_i^{2n} &= \sum x_i^n Y_i
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\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
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\end{bmatrix}}^{B}
\overbrace{\begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}}^{a}
=
\begin{bmatrix} \sum Y_i \\ \sum x_i Y_i \\ \sum x_i^2 Y_i \\ \vdots \\ \sum x_i^n Y_i \end{bmatrix} \qquad (3)
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All the summations in Eqs. 2 and 3 run from 1 to N.

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- Special methods that use **orthogonal** polynomials are a remedy.
- Degrees higher than 4 are used very infrequently.
- It is often better to fit a series of lower-degree polynomials to subsets of the data.
- Matrix B of Eq. 3 is called the **normal matrix** for the least-squares problem.

Least-Squares Polynomials V

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$$A = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & \dots & x_N \\ x_1^2 & x_2^2 & x_3^2 & \dots & x_N^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_1^n & x_2^n & x_3^n & \dots & x_N^n \end{bmatrix}$$

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- AA^T is just the coefficient matrix of Eq. 3.
- It is easy to see that Ay, where y is the column vector of y-values, gives the right-hand side of Eq. 3.

$$\overbrace{\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & \dots & x_N \\ x_1^2 & x_2^2 & x_3^2 & \dots & x_N^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_1^n & x_2^n & x_3^n & \dots & x_N^n \end{bmatrix}}^{A} \overbrace{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}}^{y} = \begin{bmatrix} \sum Y_i \\ \sum x_i Y_i \\ \sum x_i^2 Y_i \\ \vdots \\ \sum x_i^n Y_i \end{bmatrix} \quad (4)$$

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$$\overbrace{\begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ x_1 & x_2 & x_3 & \dots & x_N \\ x_1^2 & x_2^2 & x_3^2 & \dots & x_N^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_1^n & x_2^n & x_3^n & \dots & x_N^n \end{bmatrix}}^{A} * \overbrace{\begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^n \\ 1 & x_2 & x_2^2 & \dots & x_2^n \\ 1 & x_3 & x_3^2 & \dots & x_3^n \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_N & x_N^2 & \dots & x_N^n \end{bmatrix}}^{A^T} =$$

$$\underbrace{\begin{bmatrix} N & \sum x_i & \sum x_i^2 & \sum x_i^3 & \dots & \sum x_i^n \\ \sum x_i & \sum x_i^2 & \sum x_i^3 & \sum x_i^4 & \dots & \sum x_i^{n+1} \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 & \sum x_i^5 & \dots & \sum x_i^{n+2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum x_i^n & \sum x_i^{n+1} & \sum x_i^{n+2} & \sum x_i^{n+3} & \dots & \sum x_i^{2n} \end{bmatrix}}_{B}$$

Least-Squares Polynomials VII

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- Least-squares polynomials with all x-values (from given xy-pair data) are inserted.

Least-Squares Polynomials VIII

- It is illustrated the use of Eqs. 2 to fit a quadratic to the data of Table 1.

x_i	0.05	0.11	0.15	0.31	0.46	0.52	0.70	0.74	0.82	0.98	1.171
Y_i	0.956	0.890	0.832	0.717	0.571	0.539	0.378	0.370	0.306	0.242	0.104

$\Sigma x_i = 6.01$	$N = 11$
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Table: Data to illustrate curve fitting.

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- To set up the normal equations, we need the sums tabulated in Table 1. The equations to be solved are:

$$\begin{aligned} 11a_0 + 6.01a_1 + 4.6545a_2 &= 5.905 \\ 6.01a_0 + 4.6545a_1 + 4.1150a_2 &= 2.1839 \\ 4.6545a_0 + 4.1150a_1 + 3.9161a_2 &= 1.3357 \end{aligned}$$

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- The result is $a_0 = 0.998$, $a_2 = -1.018$,$a_3 = 0.225$, so the least- squares method gives

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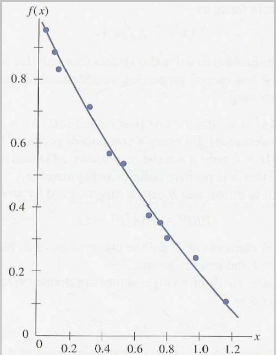

Figure: Figure for the data to illustrate curve fitting.

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- Setting $S_\lambda = S_A = 0$ gives the following equations:

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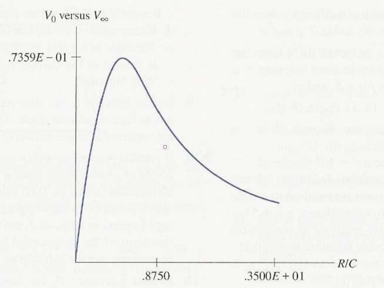

Figure: The graph of V_θ/V_∞ vs R/C.

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