2. Least Squares Polynomials

Theorem (Least-Squares Polynomial Curve Fitting). Given the n data points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, the least squares polynomial of degree m of the form

$$P_m(x) = c_1 + c_2 x + c_3 x^2 + \ldots + c_m x^{m-1} + c_{m+1} x^m$$

that fits the n data points is obtained by solving the following linear system

$$\begin{pmatrix} n & \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 & \cdots & \sum_{i=1}^{n} x_i^m \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 & \sum_{i=1}^{n} x_i^3 & \cdots & \sum_{i=1}^{n} x_i^{m+1} \\ \sum_{i=1}^{n} x_i^2 & \sum_{i=1}^{n} x_i^3 & \sum_{i=1}^{n} x_i^4 & \cdots & \sum_{i=1}^{n} x_i^{m+2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^{n} x_i^m & \sum_{i=1}^{n} x_i^{m+1} & \sum_{i=1}^{n} x_i^{m+2} & \cdots & \sum_{i=1}^{n} x_i^{2m} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_{m+1} \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i y_i \\ \sum_{i=1}^{n} x_i^2 y_i \\ \vdots \\ \sum_{i=1}^{n} x_i^m y_i \end{pmatrix}$$

for the m+1 coefficients $\{c_1, c_2, \ldots, c_m, c_{m+1}\}$. These equations are referred to as the "normal equations".

Example 1. Find the standard "least squares parabola" $a + b x + c x^2$ for the data points $(-1, 10), (0, 9), (1, 7), (2, 5), (3, 4), (4, 3), (5, 0), (6, -1)$.

Solution 1.

Linear Least Squares

The linear least-squares problem is stated as follows. Suppose that n data points $\{(x_i, y_i)\}_{i=1}^{n}$ and a set of m linearly independent functions $\{f_j[x]\}_{j=1}^{m}$ are given. We want to fine m coefficients $\{c_j\}_{j=1}^{m}$ so that the function $f[x]$ given by the linear combination

$$f[x] = \sum_{j=1}^{m} c_j f_j[x]$$

will minimize the sum of the squares of the errors

$$E[c_1, c_2, \ldots, c_m] = \sum_{i=1}^{n} (f[x_i] - y_i)^2 = \sum_{i=1}^{n} \left(\sum_{j=1}^{m} c_j f_j[x_i] - y_i \right)^2.$$

Theorem (Linear Least Squares). The solution to the linear least squares problem is found by creating the matrix $\mathbf{F}$ whose elements are $F_{i,j} = f_j[x_i]$

$$\mathbf{F} = \{F_{i,j}\}$$

The coefficients $\{c_j\}_{j=1}^{m}$ are found by solving the linear system

$$\mathbf{F}^T \mathbf{F}\, \mathbf{C} = \mathbf{F}^T \mathbf{Y}$$

where $\mathbf{C} = \text{Transpose}[\{c_1, c_2, \ldots, c_m\}]$ and $\mathbf{Y} = \text{Transpose}[\{y_1, y_2, \ldots, y_n\}]$.

Example 2. Use the linear least squares method to find the polynomial curve fit of degree = 3 for the points $(-4.5, 0.7)$, $(-3.2, 2.3)$, $(-1.4, 3.8)$, $(0.8, 5.0)$, $(2.5, 5.5)$, $(4.1, 5.6)$.

Solution 2.

Example 1. Find the standard "least squares parabola" $a + b\,x + c\,x^2$ for the data points $(-1, 10), (0, 9), (1, 7), (2, 5), (3, 4), (4, 3), (5, 0), (6, -1)$.

Solution 1.

Let's peek at the linear system that was solved.

$y = a + b\,x + c\,x^2$

The normal equations for finding the coefficients a and b are:

$$\begin{pmatrix} 8 & 20 & 92 \\ 20 & 92 & 440 \\ 92 & 440 & 2276 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 32 \\ 64 \\ 400 \end{pmatrix}$$

The solution is

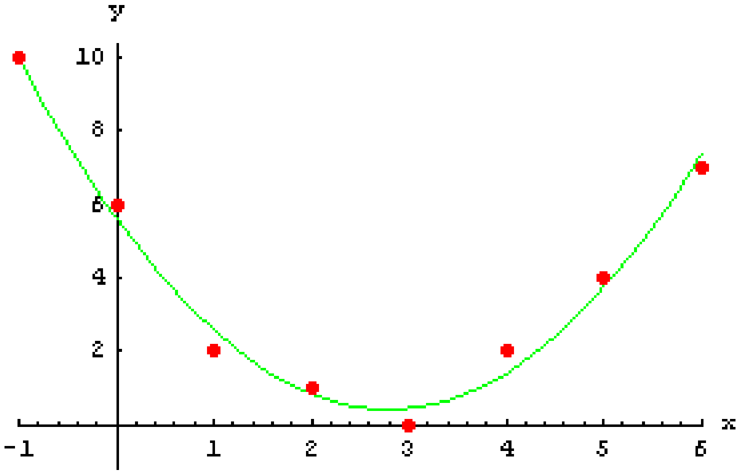
$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} \frac{118}{21} \\ -\frac{26}{7} \\ \frac{2}{3} \end{pmatrix}$$

$$a = \frac{118}{21}$$
$$b = -\frac{26}{7}$$
$$c = \frac{2}{3}$$

The `least squares parabola` is

$$y = \frac{118}{21} - \frac{26\,x}{7} + \frac{2\,x^2}{3} = 5.61905 - 3.71429\,x + 0.666667\,x^2$$

Of course we want a graph.



Points = {{-1, 10}, {0, 6}, {1, 2}, {2, 1}, {3, 0}, {4, 2}, {5, 4}, {6, 7}}

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Example 2. Use the linear least squares method to find the polynomial curve fit of degree = 3 for the points $(-4.5, 0.7), (-3.2, 2.3), (-1.4, 3.8), (0.8, 5.0), (2.5, 5.5), (4.1, 5.6)$.
Solution 2.

Construct the polynomial of degree = 3

$$p[x] = c_1 + x\,c_2 + x^2\,c_3 + x^3\,c_4$$

Construct the matrices $\mathbf{F}$, $\mathbf{F}^T$, and $\mathbf{F}^T\mathbf{F}$, and the vector $\mathbf{F}^T\mathbf{Y}$

$$Y = \begin{pmatrix} 0.7 \\ 2.3 \\ 3.8 \\ 5. \\ 5.5 \\ 5.6 \end{pmatrix}$$

$$F = \begin{pmatrix} 1 & -4.5 & 20.25 & -91.125 \\ 1 & -3.2 & 10.24 & -32.768 \\ 1 & -1.4 & 1.96 & -2.744 \\ 1 & 0.8 & 0.64 & 0.512 \\ 1 & 2.5 & 6.25 & 15.625 \\ 1 & 4.1 & 16.81 & 68.921 \end{pmatrix}$$

$$F^T = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ -4.5 & -3.2 & -1.4 & 0.8 & 2.5 & 4.1 \\ 20.25 & 10.24 & 1.96 & 0.64 & 6.25 & 16.81 \\ -91.125 & -32.768 & -2.744 & 0.512 & 15.625 & 68.921 \end{pmatrix}$$

We will use the following matrix and vector.

$$F^T F = \begin{pmatrix} 6. & -1.7 & 56.15 & -41.579 \\ -1.7 & 56.15 & -41.579 & 840.81 \\ 56.15 & -41.579 & 840.81 & -929.658 \\ -41.579 & 840.81 & -929.658 & 14379.5 \end{pmatrix}$$

$$F^T Y = \begin{pmatrix} 22.9 \\ 24.88 \\ 176.886 \\ 324.874 \end{pmatrix}$$

Solve the linear system $\mathbf{F}^T\mathbf{F}\,\mathbf{C} = \mathbf{F}^T\mathbf{Y}$.

Solve

$F^T F\ C = F^T F$

$$F^T F = \begin{pmatrix} 6. & -1.7 & 56.15 & -41.579 \\ -1.7 & 56.15 & -41.579 & 840.81 \\ 56.15 & -41.579 & 840.81 & -929.658 \\ -41.579 & 840.81 & -929.658 & 14379.5 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} 22.9 \\ 24.88 \\ 176.886 \\ 324.874 \end{pmatrix}$$

Get

$$\{c_j\}_{j==1}^{4} = \{4.66863, 0.489392, -0.0742387, 0.00267659\}$$

Construct the polynomial.

$$p[x] = 4.66863 + 0.489392\,x - 0.0742387\,x^2 + 0.00267659\,x^3$$