Least Squares

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This note will explain the method of least squares applied to polynomial approximation. Suppose we have $m+1$ data points $(x_j, y_j),\ j = 0, \dots, m$ and want to find a polynomial fit to the data. One way is to use method of least squares. Let the polynomial be expressed as $a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$. We consider the equations

$$\begin{aligned} a_0 + a_1 x_0 + a_2 x_0^2 + \cdots + a_n x_0^n =& y_0 \\ a_0 + a_1 x_1 + a_2 x_1^2 + \cdots + a_n x_1^n =& y_1 \\ & \cdots \\ a_0 + a_1 x_m + a_2 x_m^2 + \cdots + a_n x_m^n =& y_m. \end{aligned}$$

Rewrite these equations as

$$\begin{bmatrix} 1 & x_0 & x_0^2 & \dots & x_0^n \\ 1 & x_1 & x_1^2 & \dots & x_1^n \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & x_m & x_m^2 & \dots & x_m^n \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_m \end{bmatrix}.$$

Let X denote

$$X = \begin{bmatrix} 1 & x_0 & x_0^2 & \dots & x_0^n \\ 1 & x_1 & x_1^2 & \dots & x_1^n \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & x_m & x_m^2 & \dots & x_m^n \end{bmatrix},$$

and

$$a = \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{bmatrix},\ y = \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_m \end{bmatrix}.$$

Then the normal equations are

$$X^T X a = X^T y.$$

This can be written symbolically as

$$\begin{bmatrix} m+1 & \sum x & \dots & \sum x^n \\ \sum x & \sum x^2 & \dots & \sum x^{n+1} \\ \vdots & \vdots & \vdots & \vdots \\ \sum x^n & \sum x^{n+1} & \dots & \sum x^{2n} \end{bmatrix} a = \begin{bmatrix} \sum y \\ \sum xy \\ \dots \\ \sum x^n y \end{bmatrix}.$$

If all x_i are distinct and $m \geq n$ then X is nonsingular. The proof is as follows. Suppose there is a vector a so that $Xa = 0$. Then the polynomial $a_0 + a_1 x + a_2 x^2 + \ldots a_n x^n$ vanishes at $m + 1$ distinct points $x_0, x_1, x_2, \ldots, x_m$. Since $m \geq n$, the polynomial is the zero polynomial, *i.e.* $a = 0$.

This implies that $X^T X$ is a square nonsingular matrix. For if $X^T X a = 0$ then then $a^T X^T X a = ||Xa||^2 = 0$. Hence $Xa = 0$, so $a = 0$.