In a nutshell: Least-squares best-fitting polynomial

Least-squares best-fitting linear polynomials

Given $n + 1$ points $(x_0, y_0), \ldots, (x_n, y_n)$ with at least two different x values, we can find a least-squares best-fitting linear polynomial that passes as closely as possible to the $n + 1$ points as follows:

1. Create the Vandermonde matrix $V = \begin{pmatrix} x_0 & 1 \\ x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_{n-1} & 1 \\ x_n & 1 \end{pmatrix}$ and the vector $\mathbf{y} = \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_{n-1} \\ y_n \end{pmatrix}$.
2. Solve the system $V^\mathrm{T} V\mathbf{a} = V^\mathrm{T}\mathbf{y}$. This can be simplified to solving $\begin{pmatrix} \sum_{k=0}^{n} x_k^2 & \sum_{k=0}^{n} x_k \\ \sum_{k=0}^{n} x_k & n+1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_0 \end{pmatrix} = \begin{pmatrix} \sum_{k=0}^{n} x_k y_k \\ \sum_{k=0}^{n} y_k \end{pmatrix}$.
3. The first entry is the coefficient of x and the second is the constant coefficient.

If these $n + 1$ x-values are equally spaced, we can shift and scale them so that the x-values line up with the points $-n$, $1 - n$, $2 - n$, …, –2, –1, 0, in which case, the system of two linear equations in two unknowns simplifies to:

$$\begin{pmatrix} \frac{n(n+1)(2n+1)}{6} & -\frac{n(n+1)}{2} \\ -\frac{n(n+1)}{2} & n+1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_0 \end{pmatrix} = \begin{pmatrix} -\sum_{k=0}^{n} k y_k \\ \sum_{k=0}^{n} y_k \end{pmatrix}$$

Least-squares best-fitting quadratic polynomials

Assuming there are at least three different x values, we can find a least-squares best-fitting quadratic polynomial that passes as closely as possible to the $n + 1$ points as follows:

1. Create the Vandermonde matrix $V = \begin{pmatrix} x_0^2 & x_0 & 1 \\ x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ \vdots & \vdots & \vdots \\ x_{n-1}^2 & x_{n-1} & 1 \\ x_n^2 & x_n & 1 \end{pmatrix}$ and the vector $\mathbf{y} = \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_{n-1} \\ y_n \end{pmatrix}$.
2. Solve the system $V^T V\mathbf{a} = V^T\mathbf{y}$. This can be simplified to solving
$$\begin{pmatrix} \sum_{k=0}^n x_k^4 & \sum_{k=0}^n x_k^3 & \sum_{k=0}^n x_k^2 \\ \sum_{k=0}^n x_k^3 & \sum_{k=0}^n x_k^2 & \sum_{k=0}^n x_k \\ \sum_{k=0}^n x_k^2 & \sum_{k=0}^n x_k & n+1 \end{pmatrix} \begin{pmatrix} a_2 \\ a_1 \\ a_0 \end{pmatrix} = \begin{pmatrix} \sum_{k=0}^n x_k^2 y_k \\ \sum_{k=0}^n x_k y_k \\ \sum_{k=0}^n y_k \end{pmatrix}.$$
3. The first entry is the coefficient of x^2, the second the coefficient of x, and the last is the constant coefficient.

If these $n + 1$ x-values are equally spaced, we can shift and scale them so that the x-values line up with the points $-n$, $1 - n$, $2 - n$, …, -2, -1, 0, in which case, the system of three linear equations in three unknowns simplifies to:

$$\begin{pmatrix} \frac{n(n+1)(2n+1)(3n^2+3n-1)}{30} & -\frac{n^2(n+1)^2}{2} & \frac{n(n+1)(2n+1)}{6} \\ -\frac{n^2(n+1)^2}{2} & \frac{n(n+1)(2n+1)}{6} & -\frac{n(n+1)}{2} \\ \frac{n(n+1)(2n+1)}{6} & -\frac{n(n+1)}{2} & n+1 \end{pmatrix} \begin{pmatrix} a_2 \\ a_1 \\ a_0 \end{pmatrix} = \begin{pmatrix} \sum_{k=0}^n k^2 y_k \\ -\sum_{k=0}^n k y_k \\ \sum_{k=0}^n y_k \end{pmatrix}$$