In a nutshell: Approximating derivatives using least-squares best-fitting polynomials

Least-squares best-fitting linear polynomials

Given equally-spaced points (x_0, y_0), (x_1, y_1), (x_2, y_2), …, where the x values are equally spaced by a value h, we can approximate the derivative at $x_k + \delta h$ as follows:

1. Create the Vandermonde matrix $V = \begin{pmatrix} -n & 1 \\ 1-n & 1 \\ \vdots & \vdots \\ -2 & 1 \\ -1 & 1 \\ 0 & 1 \end{pmatrix}$ and the vector $\mathbf{y} = \begin{pmatrix} y_{k-n} \\ y_{k-n+1} \\ \vdots \\ y_{k-2} \\ y_{k-1} \\ y_k \end{pmatrix}$.
2. Find $(V^\mathrm{T}V)^{-1}V^\mathrm{T}$ which can be done most succinctly by calculating $\det(V^\mathrm{T}V)$, which must be an integer, and then $\det(V^\mathrm{T}V)(V^\mathrm{T}V)^{-1}V^\mathrm{T}$ must be an $(n + 1) \times 2$ integer matrix.
3. Thus, we note that $(V^\mathrm{T}V)^{-1}V^\mathrm{T}\mathbf{y}$ defines a_1 and a_0 as linear combinations of the y-values.
4. The derivative of this interpolating polynomial is a_1.

For example, if we want to find the coefficients a_1 and a_0 for eight points, we have

$$\begin{pmatrix} a_1 \\ a_0 \end{pmatrix} = \frac{1}{\det\left(V^T V\right)}\left(\det\left(V^T V\right)\left(V^T V\right)^{-1} V^T\right)\mathbf{y} = \frac{1}{336}\begin{pmatrix} -28 & -20 & -12 & -4 & 4 & 12 & 20 & 28 \\ -56 & -28 & 0 & 28 & 56 & 84 & 112 & 140 \end{pmatrix}\mathbf{y}$$

and thus, our approximation of the derivative at $x_k + \delta h$ would be a_1.

Least-squares best-fitting quadratic polynomials

Given equally-spaced points (x_0, y_0), (x_1, y_1), (x_2, y_2), …, where the x values are equally spaced by a value h, we can find the linear polynomial that approximates the value at $x_k + \delta h$ as follows:

1. Create the Vandermonde matrix $V = \begin{pmatrix} n^2 & -n & 1 \\ (1-n)^2 & 1-n & 1 \\ \vdots & \vdots & \vdots \\ 4 & -2 & 1 \\ 1 & -1 & 1 \\ 0 & 0 & 1 \end{pmatrix}$ and the vector $\mathbf{y} = \begin{pmatrix} y_{k-n} \\ y_{k-n+1} \\ \vdots \\ y_{k-2} \\ y_{k-1} \\ y_k \end{pmatrix}$.
2. Find $(V^{\mathrm{T}}V)^{-1}V^{\mathrm{T}}$ which can be done most succinctly by calculating $\det(V^{\mathrm{T}}V)$, which must be an integer, and then $\det(V^{\mathrm{T}}V)(V^{\mathrm{T}}V)^{-1}V^{\mathrm{T}}$ must be an $(n + 1) \times 3$ integer matrix.
3. Thus, we note that $(V^{\mathrm{T}}V)^{-1}V^{\mathrm{T}}\mathbf{y}$ defines a_2, a_1 and a_0 as linear combinations of the y-values.
4. The derivative of this interpolating polynomial is $2a_2\delta + a_1$ and the second derivative is $2a_2$.

For example, if we want to find the coefficients a_2, a_1 and a_0 for eight points, we have

$$\begin{pmatrix} a_2 \\ a_1 \\ a_0 \end{pmatrix} = \left(\left(V^T V \right)^{-1} V^T \right) \mathbf{y} = \frac{1}{56448} \begin{pmatrix} 2352 & 336 & -1008 & -1680 & -1680 & -1008 & 336 & 3252 \\ 11760 & -1008 & -9072 & -12432 & -11088 & -5040 & 5712 & 21168 \\ 7056 & -2352 & -7056 & -7056 & -2352 & 7056 & 21168 & 39984 \end{pmatrix} \mathbf{y}$$

and thus, our approximation of the derivative at $x_k + \delta h$ would be $2a_2\delta + a_1$.

Our approximation of the second derivative at $x_k + \delta h$ would be $2a_2$.