Computational Science:
Computational Methods in Engineering

Polynomial Technique for Deriving Finite-Difference Approximations

Outline

- Polynomial technique
- Examples

2

Polynomial Technique for Deriving Finite-Difference Approximations

Concept of Using Polynomials

An Nth-order polynomial can be fit to a set of $N + 1$ points.

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_N x^N$$

After the curve fit, the function or any of its derivatives can be interpolated at any point from the polynomial.

$$\begin{aligned}
f(x) &= a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + \cdots + a_N x^N \\
f'(x) &= a_1 + 2a_2 x + 3a_3 x^2 + 4a_4 x^3 + \cdots + N a_N x^{N-1} \\
f''(x) &= 2a_2 + 6a_3 x + 12a_4 x^2 + \cdots + N(N-1) a_N x^{N-2} \\
f'''(x) &= 6a_3 + 24a_4 x + \cdots + N(N-1)(N-2) a_N x^{N-3} \\
&\vdots
\end{aligned}$$

Easiest Point x for Evaluating $f(x)$

Recall the equations that will be used to evaluate $f(x)$ or one of its derivatives:

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + \cdots + a_N x^N$$
$$f'(x) = a_1 + 2a_2 x + 3a_3 x^2 + 4a_4 x^3 + \cdots + N a_N x^{N-1}$$
$$f''(x) = 2a_2 + 6a_3 x + 12a_4 x^2 + \cdots + N(N-1) a_N x^{N-2}$$

These are most easily evaluated at $x = 0$ because the above equations reduce to

$$f(0) = a_0$$
$$f'(0) = a_1$$
$$f''(0) = 2a_2$$
$$f'''(0) = 6a_3$$
$$\vdots$$

How can this be made to happen every time?

How to Make Any Point Easy

Suppose it is desired to evaluate $f(x)$ or one of its derivatives at the general point $x = x_{\text{fd}}$.

To do this, translate the x-axis by x_{fd} before fitting the polynomial.

Recall that the finite-difference coefficients depend only on the relative position of the points. An offset will not affect their values.

Now write the polynomial at each shifted point.

$$f(\tilde{x}_1) = a_0 + a_1 \tilde{x}_1 + a_2 \tilde{x}_1^2 + \cdots + a_N \tilde{x}_1^N$$
$$f(\tilde{x}_2) = a_0 + a_1 \tilde{x}_2 + a_2 \tilde{x}_2^2 + \cdots + a_N \tilde{x}_2^N$$
$$\vdots$$
$$f(\tilde{x}_{N+1}) = a_0 + a_1 \tilde{x}_{N+1} + a_2 \tilde{x}_{N+1}^2 + \cdots + a_N \tilde{x}_{N+1}^N$$

$$\tilde{x}_n = x_n - x_{\text{fd}}$$

In the shifted coordinate system, the finite-difference is being evaluated at $\tilde{x} = 0$.

$$f(0) = a_0 \qquad f'(0) = a_1 \qquad f''(0) = 2a_2 \qquad f'''(0) = 6a_3 \qquad \cdots$$

Four-Step Procedure to Derive Finite-Difference Approximations

Step 1 – Identify set of points x_1, x_2, …, to x_N from which to derive a finite-difference approximation.

Step 2 – Shift coordinates so that $\tilde{x} = 0$ corresponds to where the function or one of its derivatives is being calculated.

$$\tilde{x}_i = x_i - x_{\text{fd}}$$

Step 3 – Fit shifted points to a polynomial.

$$f(\tilde{x}) = a_0 + a_1\tilde{x} + a_2\tilde{x}^2 + \cdots + a_N\tilde{x}^N$$

Step 4 – Write finite-difference approximation directly from one of the derivatives of the polynomial.

$$f(0) = a_0$$
$$f'(0) = a_1$$
$$f''(0) = 2a_2$$
$$\vdots$$

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Slide 7

Step 1 – Choose x Coordinates

Identify the x-coordinates of the points from which a derivate is to be approximated.

Store these values of x in a column vector.

$$[x] = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{N+1} \end{bmatrix}$$

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8

Step 2 – Shift x-Axis

Shift the function across the x-axis until $\tilde{x} = 0$ corresponds to the point where the derivative is to be approximated.

$$\frac{d^a}{dx^a} f\left(x = x_{\text{fd}}\right) = \frac{d^a}{dx^a} f\left(\tilde{x} = 0\right)$$

Subtract x_{fd} from the column vector $[x]$ to shift the coordinates.

$$[\tilde{x}] = [x] - x_{\text{fd}} = \begin{bmatrix} x_1 - x_{\text{fd}} \\ x_2 - x_{\text{fd}} \\ \vdots \\ x_{N+1} - x_{\text{fd}} \end{bmatrix} = \begin{bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \\ \vdots \\ \tilde{x}_{N+1} \end{bmatrix}$$

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9

Step 3 – Fit Points to Polynomial (1 of 3)

Use the column vector $[\tilde{x}]$ to build matrix $[\tilde{X}]$.

$$\left[\tilde{X}\right] = \begin{bmatrix} [\tilde{x}]^0 & [\tilde{x}]^1 & \cdots & [\tilde{x}]^N \end{bmatrix}$$

$$= \begin{bmatrix} 1 & \tilde{x}_1 & \cdots & \tilde{x}_1^N \\ 1 & \tilde{x}_2 & \cdots & \tilde{x}_2^N \\ \vdots & \vdots & \ddots & \\ 1 & \tilde{x}_{N+1} & & \tilde{x}_{N+1}^N \end{bmatrix} = \begin{bmatrix} 1 & x_1 - x_{\text{fd}} & \cdots & \left(x_1 - x_{\text{fd}}\right)^N \\ 1 & x_2 - x_{\text{fd}} & \cdots & \left(x_2 - x_{\text{fd}}\right)^N \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N+1} - x_{\text{fd}} & \cdots & \left(x_{N+1} - x_{\text{fd}}\right)^N \end{bmatrix}$$

Insert 1's instead of $[\tilde{x}]^0$.

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10

Step 3 – Fit Points to Polynomial (2 of 3)

Invert the matrix $[\tilde{X}]$.

$$[\tilde{Y}] = [\tilde{X}]^{-1} = \begin{bmatrix} \tilde{y}_{11} & \tilde{y}_{12} & \cdots & \tilde{y}_{1,N+1} \\ \tilde{y}_{21} & \tilde{y}_{22} & \cdots & \tilde{y}_{2,N+1} \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{y}_{N+1,1} & \tilde{y}_{N+1,2} & \cdots & \tilde{y}_{N+1,N+1} \end{bmatrix}$$

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11

Step 3 – Fit Points to Polynomial (3 of 3)

Calculate the polynomial coefficients.

$$[a] = [\tilde{X}]^{-1}[f] = [\tilde{Y}][f] \quad \rightarrow \quad \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_N \end{bmatrix} = \begin{bmatrix} \tilde{y}_{11} & \tilde{y}_{12} & \tilde{y}_{13} & \cdots & \tilde{y}_{1,N+1} \\ \tilde{y}_{21} & \tilde{y}_{22} & \tilde{y}_{23} & \cdots & \tilde{y}_{2,N+1} \\ \tilde{y}_{31} & \tilde{y}_{32} & \tilde{y}_{33} & \cdots & \tilde{y}_{3,N+1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \tilde{y}_{N+1,1} & \tilde{y}_{N+1,2} & \tilde{y}_{N+1,3} & \cdots & \tilde{y}_{N+1,N+1} \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_{N+1} \end{bmatrix}$$

$$\begin{aligned} a_0 &= \tilde{y}_{11} f_1 + \tilde{y}_{12} f_2 + \tilde{y}_{13} f_3 + \cdots + \tilde{y}_{1,N+1} f_{N+1} \\ a_1 &= \tilde{y}_{21} f_1 + \tilde{y}_{22} f_2 + \tilde{y}_{23} f_3 + \cdots + \tilde{y}_{2,N+1} f_{N+1} \\ a_2 &= \tilde{y}_{31} f_1 + \tilde{y}_{32} f_2 + \tilde{y}_{33} f_3 + \cdots + \tilde{y}_{3,N+1} f_{N+1} \\ &\vdots \\ a_N &= \tilde{y}_{N+1,1} f_1 + \tilde{y}_{N+1,2} f_2 + \tilde{y}_{N+1,3} f_3 + \cdots + \tilde{y}_{1,N+1} f_{N+1} \end{aligned}$$

At this point, f_1 to f_{N+1} will be symbolic.

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12

Step 4 – Write Finite-Difference Approximation

Recall how the function or one of it’s derivatives is interpolated given the polynomial…

$$f(\tilde{x}=0)=a_0$$
$$\frac{d}{dx}f(\tilde{x}=0)=a_1$$
$$\frac{d^2}{dx^2}f(\tilde{x}=0)=2a_2$$
$$\vdots$$

$$\begin{aligned} a_0 &= \tilde{y}_{11}f_1+\tilde{y}_{12}f_2+\tilde{y}_{13}f_3+\cdots+\tilde{y}_{1,N+1}f_{N+1} \\ a_1 &= \tilde{y}_{21}f_1+\tilde{y}_{22}f_2+\tilde{y}_{23}f_3+\cdots+\tilde{y}_{2,N+1}f_{N+1} \\ a_2 &= \tilde{y}_{31}f_1+\tilde{y}_{32}f_2+\tilde{y}_{33}f_3+\cdots+\tilde{y}_{3,N+1}f_{N+1} \\ &\vdots \\ a_N &= \tilde{y}_{N+1,1}f_1+\tilde{y}_{N+1,2}f_2+\tilde{y}_{N+1,3}f_3+\cdots+\tilde{y}_{1,N+1}f_{N+1} \end{aligned}$$

$$f(\tilde{x}=0)=\tilde{y}_{11}f_1+\tilde{y}_{12}f_2+\tilde{y}_{13}f_3+\cdots+\tilde{y}_{1,N+1}f_{N+1}$$
$$\frac{d}{dx}f(\tilde{x}=0)=\tilde{y}_{21}f_1+\tilde{y}_{22}f_2+\tilde{y}_{23}f_3+\cdots+\tilde{y}_{2,N+1}f_{N+1}$$
$$\frac{d^2}{dx^2}f(\tilde{x}=0)=\boxed{2}\tilde{y}_{N+1,1}f_1+\boxed{2}\tilde{y}_{N+1,2}f_2+\boxed{2}\tilde{y}_{N+1,3}f_3+\cdots+\boxed{2}\tilde{y}_{1,N+1}f_{N+1}$$

The rows of $[\tilde{Y}]$ are essentially the finite-difference coefficients.

Exception

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13

Examples Using Polynomial Technique

14

Example #1

Derive first-order and second-order finite-difference approximations that span across three evenly spaced points. The approximations should be evaluated at the midpoint.

$$[\tilde{x}] = \begin{bmatrix} -h \\ 0 \\ h \end{bmatrix} \qquad [\tilde{X}] = \left[[\tilde{x}]^0 \;\; [\tilde{x}]^1 \;\; [\tilde{x}]^2 \right] = \begin{bmatrix} 1 & -h & h^2 \\ 1 & 0 & 0 \\ 1 & h & h^2 \end{bmatrix} \qquad [\tilde{Y}] = [\tilde{X}]^{-1} = \begin{bmatrix} 0 & 1 & 0 \\ -1/2h & 0 & 1/2h \\ 1/2h^2 & -1/h^2 & 1/2h^2 \end{bmatrix}$$

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ -1/2h & 0 & 1/2h \\ 1/2h^2 & -1/h^2 & 1/2h^2 \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} \Rightarrow \begin{aligned} a_0 &= 0 \cdot f_1 + 1 \cdot f_2 + 0 \cdot f_3 = f_2 \\ a_1 &= (-1/2h) \cdot f_1 + 0 \cdot f_2 + (1/2h) \cdot f_3 = \frac{-f_1 + f_3}{2h} \\ a_2 &= (1/2h^2) \cdot f_1 + (-1/h^2) \cdot f_2 + (1/2h^2) \cdot f_3 = \frac{f_1 - 2f_2 + f_3}{2h^2} \end{aligned}$$

$$\begin{aligned} f(x_{\text{fd}}) &= a_0 = f_2 \\ \frac{df(x_{\text{fd}})}{dx} &= a_1 = \frac{f_3 - f_1}{2h} \\ \frac{d^2 f(x_{\text{fd}})}{dx^2} &= 2a_2 = \frac{f_1 - 2f_2 + f_3}{h^2} \end{aligned}$$

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Example #2

Derive first-order and second-order finite-difference approximations that span across three evenly spaced points. The approximations should be evaluated at the first point.

$$[\tilde{x}] = \begin{bmatrix} 0 \\ h \\ 2h \end{bmatrix} \qquad [\tilde{X}] = \left[[\tilde{x}]^0 \;\; [\tilde{x}]^1 \;\; [\tilde{x}]^2 \right] = \begin{bmatrix} 1 & 0 & 0 \\ 1 & h & h^2 \\ 1 & 2h & (2h)^2 \end{bmatrix} \qquad [\tilde{Y}] = [\tilde{X}]^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ -3/(2h) & 2/h & -1/2h \\ 1/(2h^2) & -1/h^2 & 1/(2h^2) \end{bmatrix}$$

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ -3/(2h) & 2/h & -1/2h \\ 1/(2h^2) & -1/h^2 & 1/(2h^2) \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} \Rightarrow \begin{aligned} a_0 &= 1 \cdot f_1 + 0 \cdot f_2 + 0 \cdot f_3 = f_1 \\ a_1 &= (-3/2h) \cdot f_1 + (2/h) \cdot f_2 + (-1/2h) \cdot f_3 = \frac{-1.5f_1 + 2f_2 - 0.5f_3}{h} \\ a_2 &= (1/2h^2) \cdot f_1 + (-1/h^2) \cdot f_2 + (1/2h^2) \cdot f_3 = \frac{f_1 - 2f_2 + f_3}{2h^2} \end{aligned}$$

$$\begin{aligned} f(x_{\text{fd}}) &= a_0 = f_1 \\ \frac{df(x_{\text{fd}})}{dx} &= a_1 = \frac{-1.5f_1 + 2f_2 - 0.5f_3}{h} \\ \frac{d^2 f(x_{\text{fd}})}{dx^2} &= 2a_2 = \frac{f_1 - 2f_2 + f_3}{h^2} \end{aligned}$$

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Example #3 – Higher Order Accuracy (1 of 2)

Let's evaluate some derivatives at the midpoint of four discrete points.

$$[\tilde{x}] = \begin{bmatrix} -3h/2 \\ -h/2 \\ h/2 \\ 3h/2 \end{bmatrix} \qquad [\tilde{X}] = \left[[\tilde{x}]^0 \quad [\tilde{x}]^1 \quad [\tilde{x}]^2 \quad [\tilde{x}]^3 \right] = \begin{bmatrix} 1 & -\frac{3h}{2} & \frac{9h^2}{4} & -\frac{27h^3}{8} \\ 1 & -\frac{h}{2} & \frac{h^2}{4} & -\frac{h^3}{8} \\ 1 & \frac{h}{2} & \frac{h^2}{4} & \frac{h^3}{8} \\ 1 & \frac{3h}{2} & \frac{9h^2}{4} & \frac{27h^3}{8} \end{bmatrix}$$

$$[\tilde{Y}] = [\tilde{X}]^{-1} = \begin{bmatrix} -\frac{1}{16} & \frac{9}{16} & \frac{9}{16} & -\frac{1}{16} \\ \frac{1}{24h} & -\frac{9}{8h} & \frac{9}{8h} & -\frac{1}{24h} \\ \frac{1}{4h^2} & -\frac{1}{4h^2} & -\frac{1}{4h^2} & \frac{1}{4h^2} \\ -\frac{1}{6h^3} & \frac{1}{2h^3} & -\frac{1}{2h^3} & \frac{1}{6h^3} \end{bmatrix}$$

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17

Example #3 – Higher Order Accuracy (2 of 2)

The coefficients are then

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} = \underbrace{\begin{bmatrix} -\frac{1}{16} & \frac{9}{16} & \frac{9}{16} & -\frac{1}{16} \\ \frac{1}{24h} & -\frac{9}{8h} & \frac{9}{8h} & -\frac{1}{24h} \\ \frac{1}{4h^2} & -\frac{1}{4h^2} & -\frac{1}{4h^2} & \frac{1}{4h^2} \\ -\frac{1}{6h^3} & \frac{1}{2h^3} & -\frac{1}{2h^3} & \frac{1}{6h^3} \end{bmatrix}}_{[\tilde{Y}]} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix} \Rightarrow$$

$$a_0 = -\frac{1}{16} f_1 + \frac{9}{16} f_2 + \frac{9}{16} f_3 - \frac{1}{16} f_4$$

$$a_1 = \frac{1}{24h} f_1 - \frac{9}{8h} f_2 + \frac{9}{8h} f_3 - \frac{1}{24h} f_4$$

$$a_2 = \frac{1}{4h^2} f_1 - \frac{1}{4h^2} f_2 - \frac{1}{4h^2} f_3 + \frac{1}{4h^2} f_4$$

$$a_3 = -\frac{1}{6h^3} f_1 + \frac{1}{2h^3} f_2 - \frac{1}{2h^3} f_3 + \frac{1}{6h^3} f_4$$

$$f(x_{2.5}) = a_0 = \frac{-f_1 + 9f_2 + 9f_3 - f_4}{16}$$

$$\frac{df(x_{2.5})}{dx} = a_1 = \frac{f_1 - 27f_2 + 27f_3 - f_4}{24\Delta x}$$

$$\frac{d^2 f(x_{2.5})}{dx^2} = 2a_2 = \frac{f_1 - f_2 - f_3 + f_4}{2(\Delta x)^2}$$

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18