



Computational Science:
Computational Methods in Engineering

Implementing the Polynomial Technique in MATLAB



Outline

- Implementing the Polynomial Technique in MATLAB
- Examples



Implementing the Polynomial Technique in MATLAB



General Form of the Polynomial Fit

So far, the finite-difference approximations were derived analytically.

What if a 6th-order accurate finite-difference is desired?

This is unreasonable to do analytically.

Recall the matrix equation representing the polynomial written at each discrete point. It always had the following form where the w 's were just numerical constants. The h 's were symbolic.

$$\begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{N+1} \end{bmatrix} = \begin{bmatrix} 1 & w_{12}h & w_{13}h^2 & \cdots & w_{1N}h^N \\ 1 & w_{22}h & w_{23}h^2 & \cdots & w_{2N}h^N \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & w_{N+1,2}h & w_{N+1,3}h^2 & \cdots & w_{N+1,N}h^N \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_N \end{bmatrix}$$

Factor Out Symbolic Term h

It is possible to separate the w terms from the h terms.

$$\begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{N+1} \end{bmatrix} = \begin{bmatrix} 1 & w_{12} & w_{13} & \cdots & w_{1N} \\ 1 & w_{22} & w_{23} & \cdots & w_{2N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & w_{N+1,2} & w_{N+1,3} & \cdots & w_{N+1,N} \end{bmatrix} \begin{bmatrix} 1 \\ h \\ h^2 \\ \vdots \\ h^N \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_N \end{bmatrix}$$

It was possible to assign numbers to all of these coefficients. This is a fully numerical matrix. It does not contain any symbolic variables.

These are the symbolic variables.

Hint: $[W] = [\tilde{X}]$ when $h = 1$

So build $[W]$ by building $[\tilde{X}]$ while pretending $h = 1$.

Solve Matrix Equation for $[a]$

Solving the matrix equation for $[a]$ gives

$$\begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_N \end{bmatrix} = \begin{bmatrix} 1 & & & & \\ & h & & & \\ & & h^2 & & \\ & & & \ddots & \\ & & & & h^N \end{bmatrix}^{-1} \begin{bmatrix} 1 & w_{12} & w_{13} & \cdots & w_{1N} \\ 1 & w_{22} & w_{23} & \cdots & w_{2N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & w_{N+1,2} & w_{N+1,3} & \cdots & w_{N+1,N} \end{bmatrix}^{-1} \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{N+1} \end{bmatrix}$$

$$\downarrow$$

$$\begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_N \end{bmatrix} = \begin{bmatrix} 1 & & & & \\ & \frac{1}{h} & & & \\ & & \frac{1}{h^2} & & \\ & & & \ddots & \\ & & & & \frac{1}{h^N} \end{bmatrix} \begin{bmatrix} v_{11} & v_{12} & v_{13} & \cdots & v_{1N} \\ v_{21} & v_{22} & v_{23} & \cdots & v_{2N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ v_{N+1,1} & v_{N+1,2} & v_{N+1,3} & \cdots & v_{N+1,N} \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{N+1} \end{bmatrix}$$

$$[V] = [W]^{-1}$$

The key aspect here is that $[W]$ will be completely numerical so it is easily inverted using MATLAB. This accommodates large matrices and avoids symbolic manipulation.

Incorporate Symbolic h Again

Next, reincorporate symbolic h by multiplying the matrices.

$$\begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_N \end{bmatrix} = \begin{bmatrix} 1 \\ \frac{1}{h} \\ \frac{1}{h^2} \\ \vdots \\ \frac{1}{h^N} \end{bmatrix} \begin{bmatrix} v_{11} & v_{12} & v_{13} & \cdots & v_{1,N} \\ v_{21} & v_{22} & v_{23} & \cdots & v_{2,N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ v_{N+1,1} & v_{N+1,2} & v_{N+1,3} & \cdots & v_{N+1,N} \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{N+1} \end{bmatrix}$$

$$\downarrow$$

$$\begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_N \end{bmatrix} = \begin{bmatrix} 1 \cdot v_{11} & 1 \cdot v_{12} & 1 \cdot v_{13} & \cdots & 1 \cdot v_{1,N} \\ \frac{1}{h} \cdot v_{21} & \frac{1}{h} \cdot v_{22} & \frac{1}{h} \cdot v_{23} & \cdots & \frac{1}{h} \cdot v_{2,N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{h^N} \cdot v_{N+1,1} & \frac{1}{h^N} \cdot v_{N+1,2} & \frac{1}{h^N} \cdot v_{N+1,3} & \cdots & \frac{1}{h^N} \cdot v_{N+1,N} \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{N+1} \end{bmatrix}$$

Extract Polynomial Coefficients

Next, read off the polynomial coefficients from the matrix equation.

$$\begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_N \end{bmatrix} = \begin{bmatrix} 1 \cdot v_{11} & 1 \cdot v_{12} & 1 \cdot v_{13} & \cdots & 1 \cdot v_{1,N} \\ \frac{1}{h} \cdot v_{21} & \frac{1}{h} \cdot v_{22} & \frac{1}{h} \cdot v_{23} & \cdots & \frac{1}{h} \cdot v_{2,N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{h^N} \cdot v_{N+1,1} & \frac{1}{h^N} \cdot v_{N+1,2} & \frac{1}{h^N} \cdot v_{N+1,3} & \cdots & \frac{1}{h^N} \cdot v_{N+1,N} \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{N+1} \end{bmatrix}$$

$$\downarrow$$

$$a_0 = v_{11}f_1 + v_{12}f_2 + \cdots + v_{1,N}f_{N+1}$$

$$a_1 = \frac{v_{21}f_1 + v_{22}f_2 + \cdots + v_{2,N}f_{N+1}}{h}$$

$$\vdots$$

$$a_N = \frac{v_{N+1,1}f_1 + v_{N+1,2}f_2 + \cdots + v_{N+1,N}f_{N+1}}{h^N}$$

Write Finite-Difference Approximations

Last, write the finite-difference approximations from the polynomial coefficients.

$$f = a_0 = v_{11}f_1 + v_{12}f_2 + \cdots + v_{1N}f_{N+1}$$

$$\frac{df}{dx} = a_1 = \frac{v_{21}f_1 + v_{22}f_2 + \cdots + v_{2N}f_{N+1}}{h}$$

$$\frac{d^2f}{dx^2} = 2a_2 = 2 \frac{v_{31}f_1 + v_{32}f_2 + \cdots + v_{3N}f_{N+1}}{h^2}$$

Staring at these equations long enough, it can be seen that the v_{ij} coefficients are determined completely numerically. Just remember to divide by h^α and perhaps multiply the finite-difference expression by a constant.

Examples

Example #1 – 6th Order Accurate Finite-Differences (1 of 2)

1. Here seven points are needed to calculate seven polynomial coefficients.

$$[\hat{x}] = [-3h \quad -2h \quad -h \quad 0 \quad h \quad 2h \quad 3h]^T$$

There is not actually a transpose operation happening here. This is just a notation to write a column vector as a row vector.

2. To build the $[W]$ matrix, think $h = 1$ for now.

$$[\hat{x}] = [-3 \quad -2 \quad -1 \quad 0 \quad 1 \quad 2 \quad 3]^T$$

$$[W] = \begin{bmatrix} [\hat{x}]^0 & [\hat{x}]^1 & [\hat{x}]^2 & [\hat{x}]^3 & [\hat{x}]^4 & [\hat{x}]^5 & [\hat{x}]^6 \end{bmatrix} = \begin{bmatrix} 1 & -3 & 9 & -27 & 81 & -243 & 729 \\ 1 & -2 & 4 & -8 & 16 & -32 & 64 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 4 & 8 & 16 & 32 & 64 \\ 1 & 3 & 9 & 27 & 81 & 243 & 729 \end{bmatrix}$$

Example #1 – 6th Order Accurate Finite-Differences (2 of 2)

3. Invert $[W]$.

$$[V] = [W]^{-1} = \begin{bmatrix} 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 \\ -0.0167 & 0.1500 & -0.7500 & -0.0000 & 0.7500 & -0.1500 & 0.0167 \\ 0.0056 & -0.0750 & 0.7500 & -1.3611 & 0.7500 & -0.0750 & 0.0056 \\ 0.0208 & -0.1667 & 0.2708 & 0.0000 & -0.2708 & 0.1667 & -0.0208 \\ -0.0069 & 0.0833 & -0.2708 & 0.3889 & -0.2708 & 0.0833 & -0.0069 \\ -0.0042 & 0.0167 & -0.0208 & -0.0000 & 0.0208 & -0.0167 & 0.0042 \\ 0.0014 & -0.0083 & 0.0208 & -0.0278 & 0.0208 & -0.0083 & 0.0014 \end{bmatrix}$$

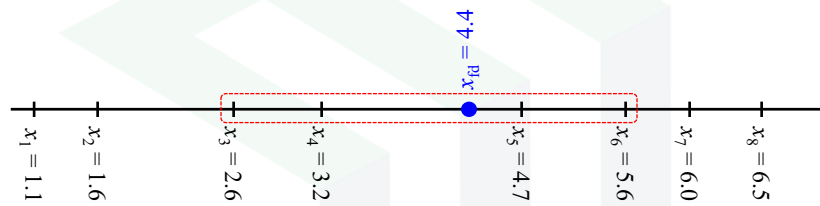
4. Write the finite-difference approximations, remembering to incorporate the symbolic h 's back in.

$$f \approx a_0 = \frac{0 \cdot f_1 + 0 \cdot f_2 + 0 \cdot f_3 + 1 \cdot f_4 + 0 \cdot f_5 - 0 \cdot f_6 + 0 \cdot f_7}{1}$$

$$\frac{\partial f}{\partial x} \approx a_1 = \frac{-0.0167 f_1 + 0.15 f_2 - 0.75 f_3 - 0 \cdot f_4 + 0.75 f_5 - 0.15 f_6 + 0.0167 f_7}{h}$$

$$\frac{\partial^2 f}{\partial x^2} \approx 2a_2 = \frac{2 \cdot 0.0056 f_1 - 2 \cdot 0.0750 f_2 + 2 \cdot 0.7500 f_3 - 2 \cdot 1.3611 f_4 + 2 \cdot 0.7500 f_5 - 2 \cdot 0.0750 f_6 + 2 \cdot 0.0056 f_7}{h^2}$$

Example #2 – Nonuniform Grid (1 of 3)



Derive the finite-difference equations for first- and second-order derivatives at the point x_{fid} .

1. Choose range of points.

$$[x] = [2.6 \ 3.2 \ 4.7 \ 5.6]^T$$

Example #2 – Nonuniform Grid (2 of 3)

2. Shift x axis.

$$\begin{aligned} [\tilde{x}] &= [x] - x_{fid} \\ &= [2.6 \ 3.2 \ 4.7 \ 5.6]^T - 4.4 \\ &= [-1.8 \ -1.2 \ 0.3 \ 1.2]^T \end{aligned}$$

3. Build $[\tilde{X}]$ matrix.

$$[\tilde{X}] = \begin{bmatrix} [\hat{x}]^0 & [\hat{x}]^1 & [\hat{x}]^2 & [\hat{x}]^3 \end{bmatrix} = \begin{bmatrix} 1 & -1.8 & 3.24 & -5.832 \\ 1 & -1.2 & 1.44 & -1.728 \\ 1 & 0.3 & 0.09 & 0.027 \\ 1 & 1.2 & 1.44 & 1.728 \end{bmatrix}$$

Note: This is not called the “[W] matrix” because the symbolic h term did not have to be factored out.

Example #2 – Nonuniform Grid (3 of 3)

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

$$[\tilde{Y}] = [\tilde{X}]^{-1} = \begin{bmatrix} -0.1143 & 0.3000 & 0.9143 & -0.1000 \\ 0.3810 & -1.0833 & 0.5079 & 0.1944 \\ 0.0794 & 0.1389 & -0.6349 & 0.4167 \\ -0.2646 & 0.4630 & -0.3527 & 0.1543 \end{bmatrix}$$

5. Write the finite-difference approximations directly from the rows of $[\tilde{Y}]$.

$$f \approx a_0 = -0.1143f_1 + 0.3f_2 + 0.9143f_3 - 0.1f_4$$

$$\frac{\partial f}{\partial x} \approx a_1 = 0.3810f_1 - 1.0833f_2 + 0.5079f_3 + 0.1944f_4$$

$$\frac{\partial^2 f}{\partial x^2} \approx 2a_2 = 2 \cdot 0.0794f_1 + 2 \cdot 0.1389f_2 - 2 \cdot 0.6349f_3 + 2 \cdot 0.4167f_4$$

Note: The symbolic variable h did not appear in $[\tilde{x}]$ so it does not need to be incorporated here.