Computational Science:
Computational Methods in Engineering

Implementing the Polynomial Technique in MATLAB

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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.

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

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Factor Out Symbolic Term h

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

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

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 $h = 1$.

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Solve Matrix Equation for $[a]$

Solving the matrix equation for $[a]$ gives

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

$\downarrow$

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

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

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.

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Incorporate Symbolic h Again

Next, reincorporate symbolic h by multiplying the matrices.

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

$$\downarrow$$

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

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Extract Polynomial Coefficients

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

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

$$\downarrow$$

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

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

$$\vdots$$

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

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Write Finite-Difference Approximations

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

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

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

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

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.

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Examples

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

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

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

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.

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

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

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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.

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

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

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

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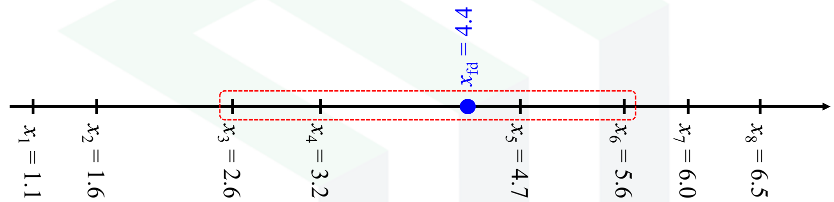
Example #2 – Nonuniform Grid (1 of 3)



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

1. Choose range of points.

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

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Example #2 – Nonuniform Grid (2 of 3)

2. Shift x axis.

$$[\tilde{x}] = [x] - x_{fd}$$
$$= [2.6 \quad 3.2 \quad 4.7 \quad 5.6]^T - 4.4$$
$$= [-1.8 \quad -1.2 \quad 0.3 \quad 1.2]^T$$

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

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

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

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Example #2 – Nonuniform Grid (3 of 3)

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

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

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

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

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

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

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

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