Computational Science:
Computational Methods in Engineering

Matrix Operators

Outline

- One-Dimensional Matrix Operators
- Incorporating Boundary Conditions

One-Dimensional Matrix Operators

Functions Vs. Operations (1 of 2)

$$a(x)\frac{\partial^2}{\partial x^2}f(x)+\gamma b(x)\frac{\partial}{\partial x}f(x)+c(x)f(x)=g(x)$$

Operations

Everything else in a differential equation is something that operates on a function.

$a(x),b(x),c(x) \equiv$ point-by-point multiplication on $f(x)$

$\frac{\partial}{\partial x},\frac{\partial^2}{\partial x^2} \equiv$ calculates derivatives of $f(x)$

$\gamma \equiv$ scales entire $f(x)$

Functions

Functions only appear in a differential equation as the unknown or as the excitation.

$f(x) \equiv$ unknown

$g(x) \equiv$ excitation

EMPossible

Functions Vs. Operations (2 of 2)

$$[A][D_x^2][f]+\gamma[B][D_x][f]+[C][f]=[g]$$

Operations

Operations are always stored in square matrices. Any linear operation can be put into matrix form.

$$[L]=\begin{bmatrix} l_{11} & l_{12} & & l_{1M} \\ l_{21} & l_{22} & \cdots & l_{2M} \\ & \vdots & & \\ l_{M1} & l_{M2} & & l_{MM} \end{bmatrix}$$

Functions

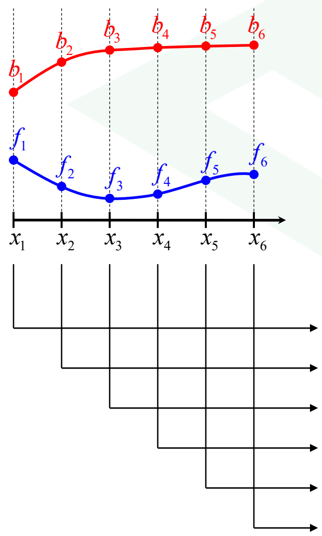
Functions are stored as column vectors.

$$[f]=\begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_M \end{bmatrix} \qquad [g]=\begin{bmatrix} g_1 \\ g_2 \\ \vdots \\ g_M \end{bmatrix}$$

EMPossible

Slide 5

Point-by-Point Multiplication (1 of 2)



Since the functions are stored in in column-vector form, how are point-by-point multiplications performed using a square matrix?

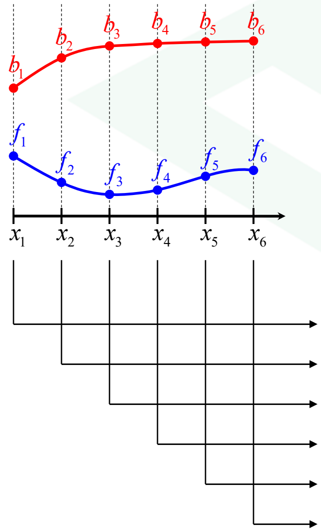
$$b(x)f(x) \rightarrow [\mathbf{B}][\mathbf{f}]$$

$$\underbrace{\begin{bmatrix} & & \\ & ? & \\ & & \end{bmatrix}}_{[\mathbf{B}]}\underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix}}_{[\mathbf{f}]}=\underbrace{\begin{bmatrix} b_1 f_1 \\ b_2 f_2 \\ b_3 f_3 \\ b_4 f_4 \\ b_5 f_5 \\ b_6 f_6 \end{bmatrix}}_{[\mathbf{B}][\mathbf{f}]}$$

EMPossible

Slide 6

Point-by-Point Multiplication (2 of 2)



Since the functions are stored in in column-vector form, how are point-by-point multiplications performed using a square matrix?

$$b(x)f(x) \rightarrow [\mathbf{B}][\mathbf{f}]$$

$$\underbrace{\begin{bmatrix} b_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & b_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & b_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & b_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & b_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & b_6 \end{bmatrix}}_{[\mathbf{B}]} \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix}}_{[\mathbf{f}]} = \underbrace{\begin{bmatrix} b_1 f_1 \\ b_2 f_2 \\ b_3 f_3 \\ b_4 f_4 \\ b_5 f_5 \\ b_6 f_6 \end{bmatrix}}_{[\mathbf{B}][\mathbf{f}]}$$

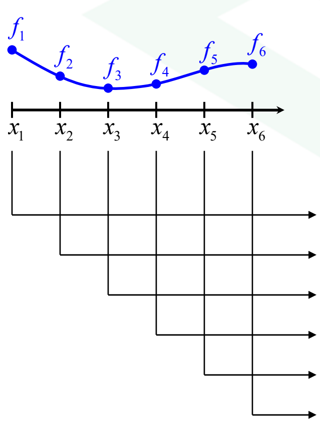
EMPossible

Slide 7

First-Order Partial Derivative (1 of 2)

How can a square matrix be constructed so that when it premultiplies a vector it calcualtes a vector containing the first-order partial derivative?

$$\frac{\partial}{\partial x} f(x) \rightarrow [D_x][f]$$



$$\underbrace{\begin{bmatrix} & & \\ & ? & \\ & & \end{bmatrix}}_{[D_x]} \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix}}_{[f]} = \underbrace{\frac{1}{2\Delta_x} \begin{bmatrix} f_2 - f_0 \\ f_3 - f_1 \\ f_4 - f_2 \\ f_5 - f_3 \\ f_6 - f_4 \\ f_7 - f_5 \end{bmatrix}}_{[D_x][f]}$$

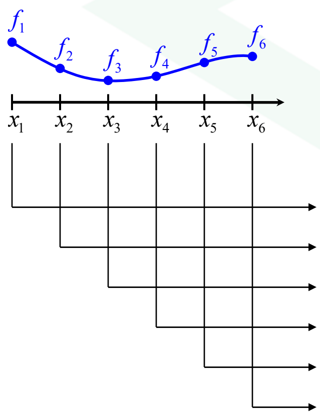
EMPossible

Slide 8

First-Order Partial Derivative (2 of 2)

How can a square matrix be constructed so that when it premultiplies a vector it calcualtes a vector containing the first-order partial derivative?

$$\frac{\partial}{\partial x} f(x) \rightarrow [D_x][f]$$



$$\underbrace{\frac{1}{2\Delta_x}\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{bmatrix}}_{[D_x]} \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix}}_{[f]} = \underbrace{\frac{1}{2\Delta_x}\begin{bmatrix} f_2 - f_0 \\ f_3 - f_1 \\ f_4 - f_2 \\ f_5 - f_3 \\ f_6 - f_4 \\ f_7 - f_5 \end{bmatrix}}_{[D_x][f]}$$

?

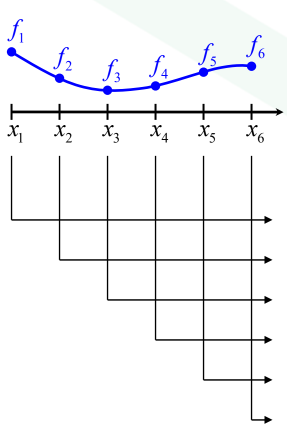
EMPossible

Slide 9

Second-Order Partial Derivative (1 of 2)

How can a square matrix be constructed so that when it premultiplies a vector it calculates a vector containing the second-order partial derivative?

$$\frac{\partial^2}{\partial x^2} f(x) \rightarrow [D_x^2][f]$$



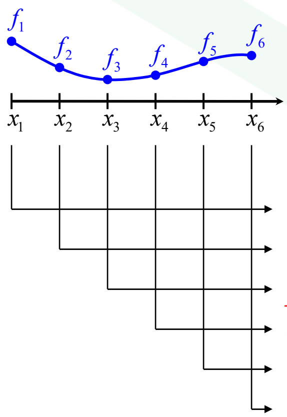
$$\underbrace{\begin{bmatrix} & & \\ & ? & \\ & & \end{bmatrix}}_{[D_x^2]} \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix}}_{[f]} = \underbrace{\frac{1}{\Delta_x^2}\begin{bmatrix} f_2 - 2f_1 + f_0 \\ f_3 - 2f_2 + f_1 \\ f_4 - 2f_3 + f_2 \\ f_5 - 2f_4 + f_3 \\ f_6 - 2f_5 + f_4 \\ f_7 - 2f_6 + f_5 \end{bmatrix}}_{[D_x^2][f]}$$

EMPossible

Slide 10

Second-Order Partial Derivative (2 of 2)

How can a square matrix be constructed so that when it premultiplies a vector it calculates a vector containing the second-order partial derivative?



$$\frac{\partial^2}{\partial x^2} f(x) \rightarrow [D_x^2][f]$$

$$\underbrace{\frac{1}{\Delta_x^2}\begin{bmatrix} -2 & 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 1 & -2 \end{bmatrix}}_{[D_x^2]} \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix}}_{[f]} = \underbrace{\frac{1}{\Delta_x^2}\begin{bmatrix} f_2 - 2f_1 + f_0 \\ f_3 - 2f_2 + f_1 \\ f_4 - 2f_3 + f_2 \\ f_5 - 2f_4 + f_3 \\ f_6 - 2f_5 + f_4 \\ f_7 - 2f_6 + f_5 \end{bmatrix}}_{[D_x^2][f]}$$

?

EMPossible

Why Are Separate Derivative Matrices Needed for 1st and 2nd-Order Derivative Matrices?

It is known that,

$$\frac{\partial^2}{\partial x^2} = \frac{\partial}{\partial x}\frac{\partial}{\partial x}$$

So why can can't $\mathbf{D}_x^{(2)}$ simply be calculated as $\mathbf{D}_x^{(2)} = \mathbf{D}_x^{(1)}\,\mathbf{D}_x^{(1)}$?

It turns out this does not make efficient use of the grid. For a 5-point, 1D grid, this would be

$$\mathbf{D}_x^{(1)}\mathbf{D}_x^{(1)} = \frac{1}{(2\Delta_x)^2}\begin{bmatrix} -1 & 0 & 1 & 0 & 0 \\ 0 & -2 & 0 & 1 & 0 \\ 1 & 0 & -2 & 0 & 1 \\ 0 & 1 & 0 & -2 & 0 \\ 0 & 0 & 1 & 0 & -1 \end{bmatrix}$$

This is not as accurate because it calculates the derivative with poorer grid resolution than is available.

$$\mathbf{D}_x^{(2)} = \frac{1}{\Delta_x^2}\begin{bmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{bmatrix}$$

This derivate matrix makes optimal use of the available grid resolution.

EMPossible

USE SPARSE MATRICES!!!!!!!

WARNING !!

The derivative operators will be **EXTREMELY** large matrices.

For a small grid that is just 100×200 points:

Total Number of Points:	20,000
Size of Derivate Operators:	20,000 × 20,000
Total Elements in Matrices:	400,000,000
Memory to Store One Full Matrix:	6 Gb
Memory to Store One Sparse Matrix:	1 Mb

NEVER AT ANY POINT should you use **FULL MATRICES** in the finite-difference method. Not even for intermediate steps. **NEVER!**

EMPossible

Slide 13

Placing Diagonals into Sparse Matrices in MATLAB

```
M = 6;
Z = sparse(M,M);
d = ones(M,1);
A = spdiags(d,0,Z);
```

⇨

```
A =
[ 1  0  0  0  0  0  ]
[ 0  1  0  0  0  0  ]
[ 0  0  1  0  0  0  ]
[ 0  0  0  1  0  0  ]
[ 0  0  0  0  1  0  ]
[ 0  0  0  0  0  1  ]
```

```
M = 6;
Z = sparse(M,M);
d = ones(M,1);
A = spdiags(-d,-1,Z);
A = spdiags(+d,+1,A);
```

⇨

```
A =
[  0   1   0   0   0   0  ]
[ -1   0   1   0   0   0  ]
[  0  -1   0   1   0   0  ]
[  0   0  -1   0   1   0  ]
[  0   0   0  -1   0   1  ]
[  0   0   0   0  -1   0  ]
```

EMPossible

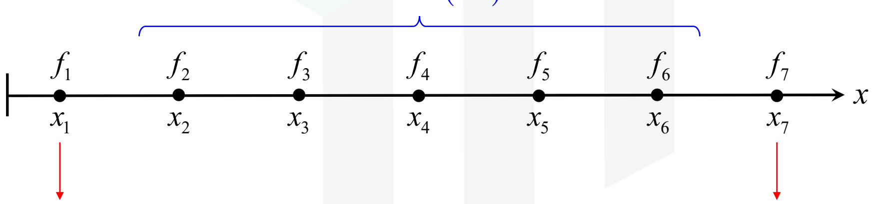
14

Incorporating Boundary Conditions

Dirichlet Boundary Conditions (1 of 2)

The simplest boundary condition is to assume all function values outside of the grid are zero.

$$\frac{d^2 f_i}{dx^2} \cong \frac{f_{i-1} - 2f_i + f_{i+1}}{(\Delta x)^2}$$

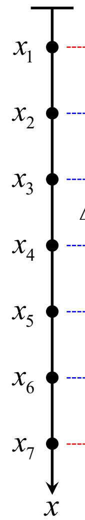


$$\frac{d^2 f_1}{dx^2} \cong \frac{0 - 2f_1 + f_2}{(\Delta x)^2}$$

$$\frac{d^2 f_7}{dx^2} \cong \frac{f_6 - 2f_7 + 0}{(\Delta x)^2}$$

EMPossible

Dirichlet Boundary Conditions (2 of 2)



$$\frac{d^2 f_1}{dx^2} \cong \frac{0 - 2f_1 + f_2}{(\Delta x)^2}$$
$$\frac{d^2 f_2}{dx^2} \cong \frac{f_1 - 2f_2 + f_3}{(\Delta x)^2}$$
$$\frac{d^2 f_3}{dx^2} \cong \frac{f_2 - 2f_3 + f_4}{(\Delta x)^2}$$
$$\frac{d^2 f_4}{dx^2} \cong \frac{f_3 - 2f_4 + f_5}{(\Delta x)^2}$$
$$\frac{d^2 f_5}{dx^2} \cong \frac{f_4 - 2f_5 + f_6}{(\Delta x)^2}$$
$$\frac{d^2 f_6}{dx^2} \cong \frac{f_5 - 2f_6 + f_7}{(\Delta x)^2}$$
$$\frac{d^2 f_7}{dx^2} \cong \frac{f_6 - 2f_7 + 0}{(\Delta x)^2}$$

$$\Rightarrow \underbrace{\frac{1}{(\Delta x)^2}\begin{bmatrix} -2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -2 \end{bmatrix}}_{[D_x^2]} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \end{bmatrix}$$

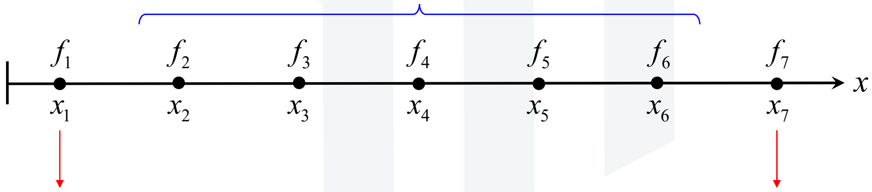
EMPossible

17

Periodic Boundary Conditions (1 of 2)

If the problem is periodic (i.e. keeps repeating), then the value outside of the grid is the same as the value at the opposite side of the grid.

$$\frac{d^2 f_i}{dx^2} \cong \frac{f_{i-1} - 2f_i + f_{i+1}}{(\Delta x)^2}$$

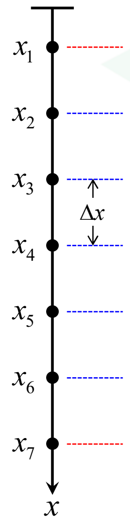


$$\frac{d^2 f_1}{dx^2} \cong \frac{f_7 - 2f_1 + f_2}{(\Delta x)^2} \qquad \frac{d^2 f_7}{dx^2} \cong \frac{f_6 - 2f_7 + f_1}{(\Delta x)^2}$$

EMPossible

18

Periodic Boundary Conditions (2 of 2)



$$\frac{d^2 f_1}{dx^2} \cong \frac{f_7 - 2f_1 + f_2}{(\Delta x)^2}$$
$$\frac{d^2 f_2}{dx^2} \cong \frac{f_1 - 2f_2 + f_3}{(\Delta x)^2}$$
$$\frac{d^2 f_3}{dx^2} \cong \frac{f_2 - 2f_3 + f_4}{(\Delta x)^2}$$
$$\frac{d^2 f_4}{dx^2} \cong \frac{f_3 - 2f_4 + f_5}{(\Delta x)^2}$$
$$\frac{d^2 f_5}{dx^2} \cong \frac{f_4 - 2f_5 + f_6}{(\Delta x)^2}$$
$$\frac{d^2 f_6}{dx^2} \cong \frac{f_5 - 2f_6 + f_7}{(\Delta x)^2}$$
$$\frac{d^2 f_7}{dx^2} \cong \frac{f_6 - 2f_7 + f_1}{(\Delta x)^2}$$

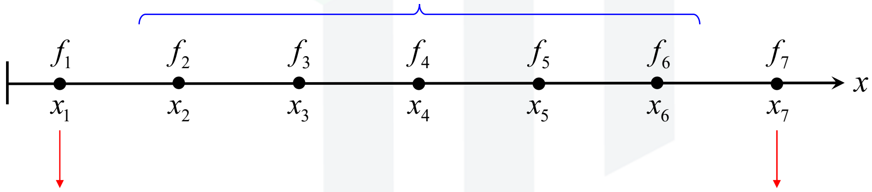
$$\Rightarrow \underbrace{\frac{1}{(\Delta x)^2}\begin{bmatrix} -2 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & -2 \end{bmatrix}}_{[D_x^2]} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \end{bmatrix}$$

19

Neuman Boundary Conditions (1 of 3)

The Neuman boundary condition allows functions to continue linearly off of the grid as if to infinity.

$$\frac{df_i}{dx} \cong \frac{f_{i+1} - f_{i-1}}{2\Delta x} \qquad \frac{d^2 f_i}{dx^2} \cong \frac{f_{i-1} - 2f_i + f_{i+1}}{(\Delta x)^2}$$



$$\frac{df_1}{dx} \cong \frac{f_2 - f_1}{\Delta x} \qquad \frac{d^2 f_1}{dx^2} \cong 0 \qquad \frac{df_7}{dx} \cong \frac{f_7 - f_6}{\Delta x} \qquad \frac{d^2 f_7}{dx^2} \cong 0$$

20

Neuman Boundary Conditions (2 of 3)

x_1: $\frac{df_1}{dx} \cong \frac{2f_2 - 2f_1}{2\Delta x}$

x_2: $\frac{df_2}{dx} \cong \frac{f_3 - f_1}{2\Delta x}$

x_3: $\frac{df_3}{dx} \cong \frac{f_4 - f_2}{2\Delta x}$

Δx

x_4: $\frac{df_4}{dx} \cong \frac{f_5 - f_3}{2\Delta x}$

x_5: $\frac{df_5}{dx} \cong \frac{f_6 - f_4}{2\Delta x}$

x_6: $\frac{df_6}{dx} \cong \frac{f_7 - f_5}{2\Delta x}$

x_7: $\frac{df_7}{dx} \cong \frac{2f_7 - 2f_6}{2\Delta x}$

x

$$\Rightarrow \underbrace{\frac{1}{2\Delta x}\begin{bmatrix} -2 & 2 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & -2 & 2 \end{bmatrix}}_{[D_x]} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \end{bmatrix}$$

EMPossible

21

Neuman Boundary Conditions (3 of 3)

x_1: $\frac{d^2 f_1}{dx^2} \cong 0$

x_2: $\frac{d^2 f_2}{dx^2} \cong \frac{f_1 - 2f_2 + f_3}{(\Delta x)^2}$

x_3: $\frac{d^2 f_3}{dx^2} \cong \frac{f_2 - 2f_3 + f_4}{(\Delta x)^2}$

Δx

x_4: $\frac{d^2 f_4}{dx^2} \cong \frac{f_3 - 2f_4 + f_5}{(\Delta x)^2}$

x_5: $\frac{d^2 f_5}{dx^2} \cong \frac{f_4 - 2f_5 + f_6}{(\Delta x)^2}$

x_6: $\frac{d^2 f_6}{dx^2} \cong \frac{f_5 - 2f_6 + f_7}{(\Delta x)^2}$

x_7: $\frac{d^2 f_7}{dx^2} \cong 0$

x

$$\Rightarrow \underbrace{\frac{1}{(\Delta x)^2}\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}}_{[D_x^2]} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \end{bmatrix}$$

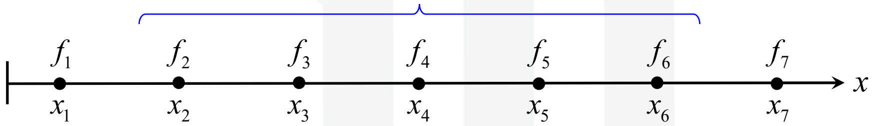
EMPossible

22

High-Order Boundary Conditions (1 of 2)

Here we estimate the derivative at the boundaries using special finite-difference equations derived specifically for these points.

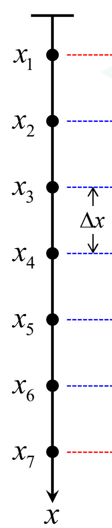
$$\frac{d^2 f_i}{dx^2} \cong \frac{f_{i-1} - 2f_i + f_{i+1}}{h^2}$$



$$\frac{d^2 f_1}{dx^2} \cong \frac{2f_1 - 5f_2 + 4f_3 - f_4}{h^2} \qquad \frac{d^2 f_7}{dx^2} \cong \frac{-f_4 + 4f_5 - 5f_6 + 2f_7}{h^2}$$

EMPossible

High-Order Boundary Conditions (2 of 2)



$$\frac{d^2 f_1}{dx^2} \cong \frac{2f_1 - 5f_2 + 4f_3 - f_4}{(\Delta x)^2}$$

$$\frac{d^2 f_2}{dx^2} \cong \frac{f_1 - 2f_2 + f_3}{(\Delta x)^2}$$

$$\frac{d^2 f_3}{dx^2} \cong \frac{f_2 - 2f_3 + f_4}{(\Delta x)^2}$$

$$\frac{d^2 f_4}{dx^2} \cong \frac{f_3 - 2f_4 + f_5}{(\Delta x)^2}$$

$$\frac{d^2 f_5}{dx^2} \cong \frac{f_4 - 2f_5 + f_6}{(\Delta x)^2}$$

$$\frac{d^2 f_6}{dx^2} \cong \frac{f_5 - 2f_6 + f_7}{(\Delta x)^2}$$

$$\frac{d^2 f_7}{dx^2} \cong \frac{-f_4 + 4f_5 - 5f_6 + 2f_7}{(\Delta x)^2}$$

$$\Rightarrow \underbrace{\frac{1}{(\Delta x)^2}\begin{bmatrix} 2 & -5 & 4 & -1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & -1 & 4 & -5 & 2 \end{bmatrix}}_{\left[D_x^2\right]} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \end{bmatrix}$$

EMPossible