Computational Science:
Computational Methods in Engineering

Matrix Operators

1

Outline

- Introduction to the Topic
- Matrix Operators for One-Dimensional Problems
- Building Matrix Operators
- Incorporating Boundary Conditions

2

2

Introduction to Matrix Operators

Slide 3

3

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 $f(x)$

Functions

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

$f(x) \equiv$ unknown

$g(x) \equiv$ excitation

EMPossible

Slide 4

4

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

5

The Derivative Matrix

Recall numerical differentiation,

```
fd(1) = (2*f(1) - 5*f(2) + 4*f(3) - f(4))/h^2;
for nx = 2 : Nx-1
   fd(nx) = (f(nx-1) - 2*f(nx) + f(nx+1))/h^2;
end
fd(Nx) = (-f(Nx-3) + 4*f(Nx-2) - 5*f(Nx-1) + 2*f(Nx))/h^2;
```

$$\frac{d^2 f_i}{dx^2} \approx \begin{cases} \dfrac{2f_1-5f_2+4f_3-f_4}{\Delta x^2} & i=1 \\ \dfrac{f_{i+1}-2f_i+f_{i-1}}{\Delta x^2} & 2\le i\le N \\ \dfrac{2f_{N-3}-5f_{N-2}+4f_{N-1}-f_N}{\Delta x^2} & i=N \end{cases}$$

It is possible build a matrix $[D_x^2]$ that performs a numerical differentiation on column vector $[f]$.

$$\left[\frac{d^2 f}{dx^2}\right] \approx [D_x^2][f]$$

$$[D_x^2]=\frac{1}{\Delta x^2}\begin{bmatrix} 2 & -5 & 4 & -1 & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & & \ddots & & \\ & 2 & -5 & 4 & -1 & \end{bmatrix} \qquad [f]=\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_N \end{bmatrix}$$

EMPossible

Slide 6

6

Generalization of Matrix Operators

In fact, any linear operation can be expressed as a matrix and performed by matrix multiplication.

$$\frac{d^a}{dx^a} f(x) \rightarrow \left[D_x^a\right][f]$$ Derivatives

$$\text{DFT}\left[f(x)\right] \rightarrow [\text{DFT}][f]$$ Discrete Fourier transforms

$$\int_a^b f(x)\,dx \rightarrow \left[\int dx\right][f]$$ Integrals

$$g(x) * f(x) \rightarrow [g\,*][f]$$ Convolutions

EMPossible

Slide 7

7

Procedure to Determine Matrix Operators

Step 1 – Write big blank matrix equation.

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

$$\begin{bmatrix} & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix} = \begin{bmatrix} \\ \\ \\ \\ \\ \\ \end{bmatrix}$$

EMPossible

Slide 8

8

Procedure to Determine Matrix Operators

Step 2 – Write the desired answer in the final column vector.

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

$$\begin{bmatrix} & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \end{bmatrix}\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix} = \frac{1}{2\Delta_x}\begin{bmatrix} f_2 - 0 \\ f_3 - f_1 \\ f_4 - f_2 \\ f_5 - f_3 \\ f_6 - f_4 \\ 0 - f_5 \end{bmatrix}$$

EMPossible

Slide 9

9

Procedure to Determine Matrix Operators

Step 3 – Fill in the square matrix with values that will give the answer.

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

$$\frac{1}{2\Delta_x}\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{bmatrix}\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix} = \frac{1}{2\Delta_x}\begin{bmatrix} f_2 - 0 \\ f_3 - f_1 \\ f_4 - f_2 \\ f_5 - f_3 \\ f_6 - f_4 \\ 0 - f_5 \end{bmatrix}$$

EMPossible

Slide 10

10

Procedure to Determine Matrix Operators

Step 4 – Read off the matrix operator.

$$\frac{d}{dx}f(x) \rightarrow \boxed{[D_x]}[f]$$

$$\boxed{\frac{1}{2\Delta_x}\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{bmatrix}}\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix} = \frac{1}{2\Delta_x}\begin{bmatrix} f_2 - 0 \\ f_3 - f_1 \\ f_4 - f_2 \\ f_5 - f_3 \\ f_6 - f_4 \\ 0 - f_5 \end{bmatrix}$$

EMPossible

Slide 11

11

Procedure to Determine Matrix Operators

Step 5 – Done!

$$[D_x] = \frac{1}{2\Delta_x}\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{bmatrix}$$

EMPossible

Slide 12

12

Note About Numerical Differentiation with Derivative Matrices

Derivative matrices are fully capable of calculating numerical derivatives.

```
fd(1) = (2*f(1) - 5*f(2) + 4*f(3) - f(4))/h^2;
for nx = 2 : Nx-1
   fd(nx) = (f(nx-1) - 2*f(nx) + f(nx+1))/h^2;
end
fd(Nx) = (-f(Nx-3) + 4*f(Nx-2) - 5*f(Nx-1) + 2*f(Nx))/h^2;
```

$$\left[f'\right]=\left[D_x^2\right]\left[f\right]$$

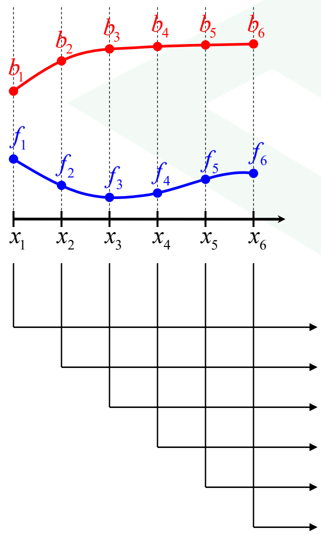
However, it is usually very inefficient to use them this way because it is necessary to build and store the derivative matrices in memory. Derivative matrices are more intended to implement the finite-difference method to solve differential equations.

If numerical differentiation is the only purpose, use a for loop instead of derivative matrices.

If the derivative matrices have already been constructed for the finite-difference method, it is good practice to use them to perform numerical differentiation in post-processing steps. It is also good practice to test your derivative matrices by performing numerical differentiation with them.

Matrix Operators for One-Dimensional Problems

Point-by-Point Multiplication (1 of 2)



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

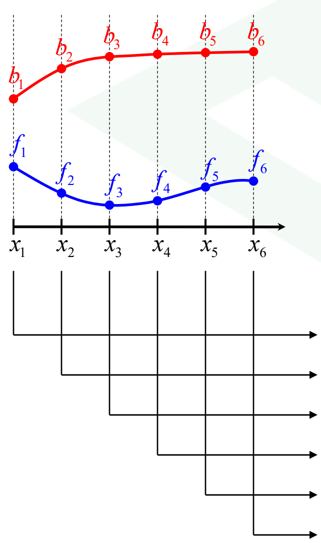
$$b(x)\,f(x) \quad \rightarrow \quad [\mathbf{B}][\mathbf{f}]$$

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

Slide 15

15

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?

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

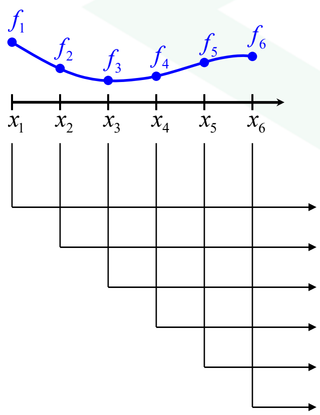
$$\underbrace{\begin{bmatrix} b_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & b_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & b_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & b_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & b_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & b_6 \end{bmatrix}}_{[\mathbf{B}]}\underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix}}_{[\mathbf{f}]}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

Slide 16

16

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?



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

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

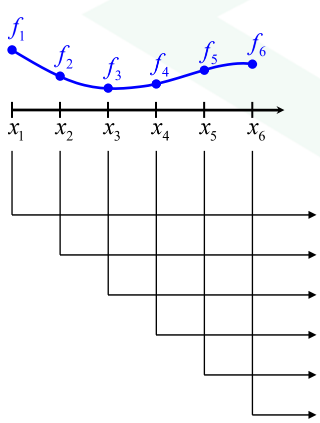
EMPossible

Slide 17

17

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?



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

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

?

EMPossible

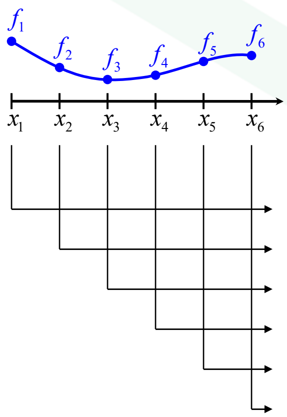
Slide 18

18

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?

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



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

EMPossible

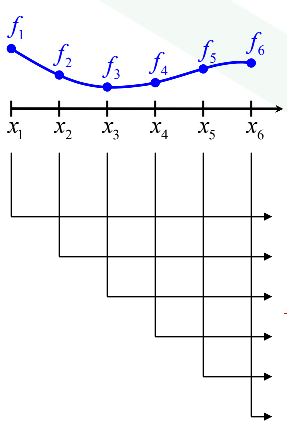
Slide 19

19

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?

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



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

?

EMPossible

Slide 20

20

Building Matrix Operators

21

Does $[D_x][D_x]$= $\left[D_x^2\right]$?

It is known that,

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

Is it possible to multiply derivative matrices together to get a higher-order derivative matrix?

This is what $[D_x][D_x]$ gives...

$$[D_x][D_x] = \frac{1}{(2\Delta_x)^2}\begin{bmatrix} -1 & 0 & 1 & 0 & 0 \\ 0 & -2 & 0 & 1 & 0 \\ 1 & 0 & -2 & 0 & 1 \\ 0 & 1 & 0 & -2 & 0 \\ 0 & 0 & 1 & 0 & -1 \end{bmatrix}$$

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

This is what the answer should be...

$$\left[D_x^2\right] = \frac{1}{\Delta_x^2}\begin{bmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{bmatrix}$$

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

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 23

23

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

24

24

Incorporating Boundary Conditions

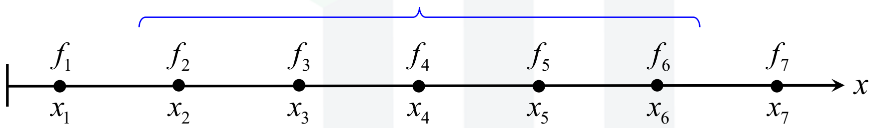
Slide 25

25

Dirichlet Boundary Conditions (1 of 2)

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

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

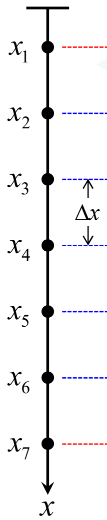


$$\frac{d^2 f_1}{dx^2} \cong \frac{0 - 2f_1 + f_2}{(\Delta x)^2} \qquad \frac{d^2 f_7}{dx^2} \cong \frac{f_6 - 2f_7 + 0}{(\Delta x)^2}$$

EMPossible

26

Dirichlet Boundary Conditions (2 of 2)



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

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

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

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

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

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

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

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

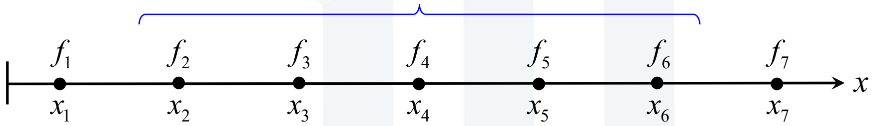
EMPossible

27

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.

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

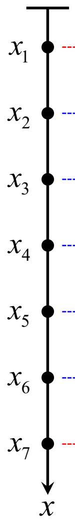


$$\frac{d^2 f_1}{dx^2} \cong \frac{f_7 - 2f_1 + f_2}{(\Delta x)^2} \qquad \frac{d^2 f_7}{dx^2} \cong \frac{f_6 - 2f_7 + f_1}{(\Delta x)^2}$$

EMPossible

28

Periodic Boundary Conditions (2 of 2)



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

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

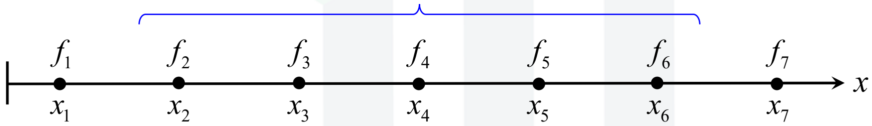
EMPossible

29

Neuman Boundary Conditions (1 of 3)

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

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



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

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

EMPossible

30

Neuman Boundary Conditions (2 of 3)

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

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

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

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

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

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

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

$x_1, x_2, x_3, x_4, x_5, x_6, x_7$, Δx, 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

31

Neuman Boundary Conditions (3 of 3)

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

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

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

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

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

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

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

$x_1, x_2, x_3, x_4, x_5, x_6, x_7$, Δx, x

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

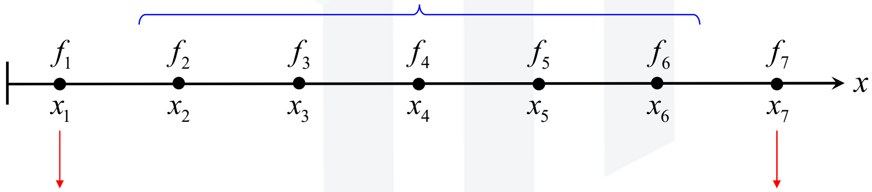
EMPossible

32

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

33

High-Order Boundary Conditions (2 of 2)

x_1: $\frac{d^2 f_1}{dx^2} \cong \frac{2f_1 - 5f_2 + 4f_3 - f_4}{(\Delta x)^2}$

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

x

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

EMPossible

34

35