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Computational Methods in EE

Topic 6c – Numerical Differentiation

EE 4386/5301 Computational Methods in EE

Outline

Computational Methods in EE

- Numerical Differentiation
- Numerical Differentiation Using MATLAB
- Boundary Conditions

Computational Methods in EE

Numerical Differentiation

The Problem

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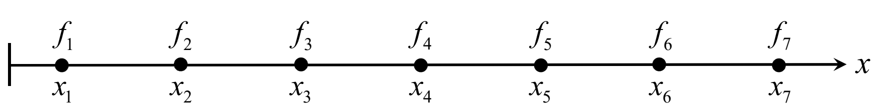
Suppose we wish to calculate the second-order derivative of some function that is known only at seven discrete points.

$$\frac{d^2 f(x)}{dx^2} \cong ?$$

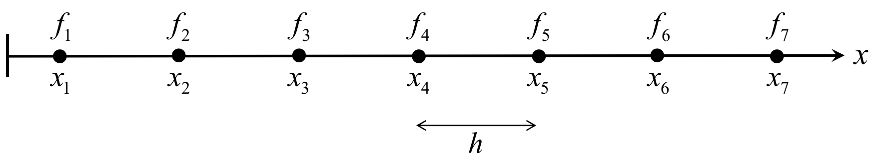


The Finite-Difference Approximation

Computational Methods in EE

We can estimate the second-order derivative with a 3-point finite-difference approximation.

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



The Middle Points

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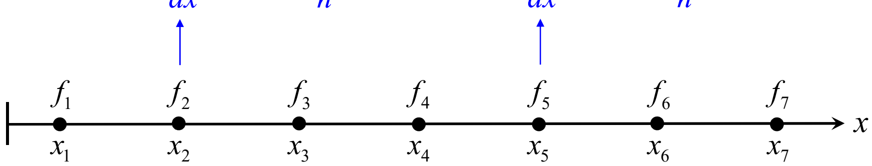
We can calculate the derivatives at each intermediate point by applying our finite-difference approximation using the surrounding points.

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



Problem at the Boundaries

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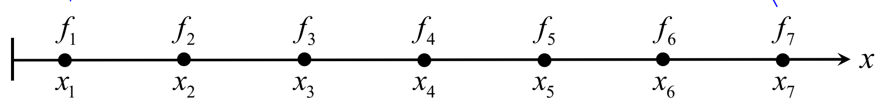
How do we evaluate the finite-differences at $i = 1$ and $i = 7$?

$$\frac{d^2 f_1}{dx^2} \cong \frac{f_0 - 2f_1 + f_2}{h^2}$$

Does not exist (f_0)

$$\frac{d^2 f_7}{dx^2} \cong \frac{f_6 - 2f_7 + f_8}{h^2}$$

Does not exist (f_8)



The finite-difference equations at the boundaries of the grid contain terms that do not exist because they are outside of the grid and so they are not stored in memory.

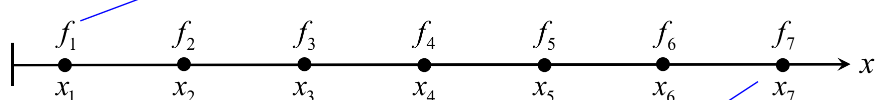
The Boundary Fix

Computational Methods in EE

We must derive new finite-difference approximations for each boundary point.

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

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



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

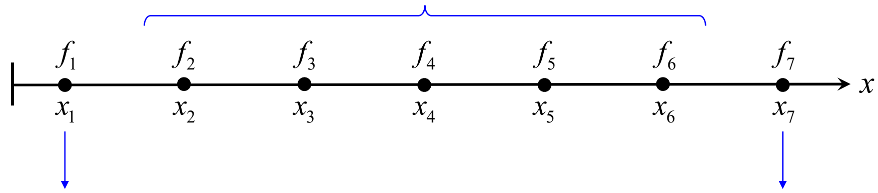
$$\frac{d^2 f_7}{dx^2} \cong \frac{-f_4 + 4f_5 - 5f_6 + 2f_7}{h^2}$$

Summary of Finite-Difference Approximations

Computational Methods in EE

Below are all of the equations across the entire grid to numerically calculate the second-order derivative. The boundary points get their own special equations.

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



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

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

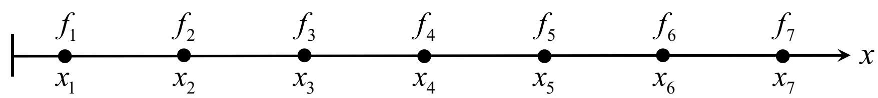
Computational Methods in EE

Numerical Differentiation Using MATLAB

MATLAB Code for Numerical Differentiation

Computational Methods in EE

```
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;
```

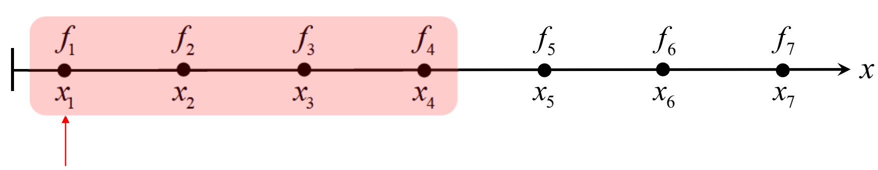


Calculation at Point 1

Computational Methods in EE

```
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;
```

```
fd(1) = (2*f(1) - 5*f(2) + 4*f(3) - f(4))/h^2;
```



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

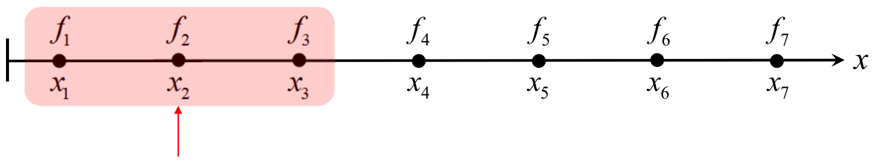
$$\frac{d^2 f_1}{dx^2} \cong \frac{2f_1 - 5f_2 + 4f_3 - f_4}{h^2}$$

Calculation at Point 2

Computational Methods in EE

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

```
fd(2) = (f(1) - 2*f(2) + f(3))/h^2;
```



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

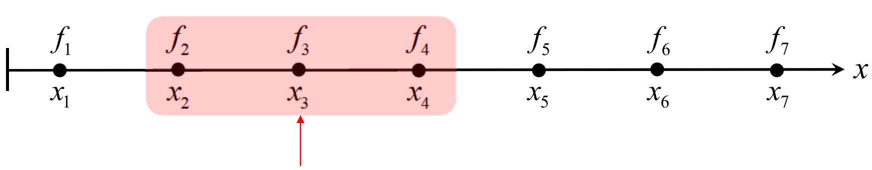
$$\frac{d^2 f_2}{dx^2} \cong \frac{f_1 - 2f_2 + f_3}{h^2}$$

Calculation at Point 3

Computational Methods in EE

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

```
fd(3) = (f(2) - 2*f(3) + f(4))/h^2;
```



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

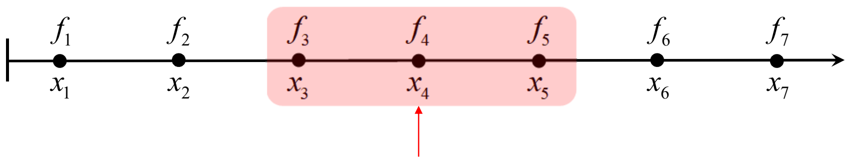
$$\frac{d^2 f_3}{dx^2} \cong \frac{f_2 - 2f_3 + f_4}{h^2}$$

Calculation at Point 4

Computational Methods in EE

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

```
fd(4) = (f(3) - 2*f(4) + f(5))/h^2;
```



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

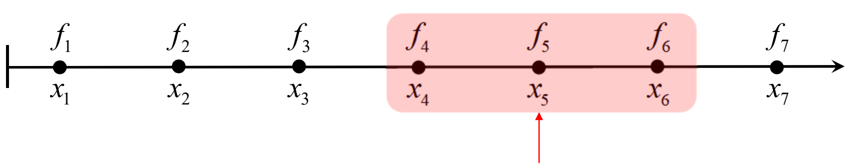
$$\frac{d^2 f_4}{dx^2} \cong \frac{f_3 - 2f_4 + f_5}{h^2}$$

Calculation at Point 5

Computational Methods in EE

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

```
fd(5) = (f(4) - 2*f(5) + f(6))/h^2;
```



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

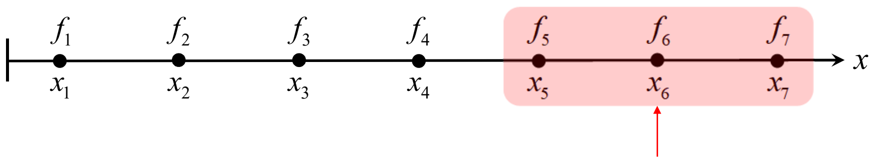
$$\frac{d^2 f_5}{dx^2} \cong \frac{f_4 - 2f_5 + f_6}{h^2}$$

Calculation at Point 6

Computational Methods in EE

```
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;            nx = 6
end
fd(Nx) = (-f(Nx-3) + 4*f(Nx-2) - 5*f(Nx-1) + 2*f(Nx))/h^2;
```

```
fd(6) = (f(5) - 2*f(6) + f(7))/h^2;
```



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

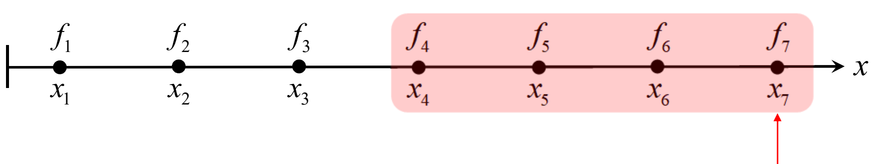
$$\frac{d^2 f_6}{dx^2} \cong \frac{f_5 - 2f_6 + f_7}{h^2}$$

Calculation at Point 7

Computational Methods in EE

```
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;
```

```
fd(7) = (-f(4) + 4*f(5) - 5*f(6) + 2*f(7))/h^2;
```



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

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

Computational Methods in EE

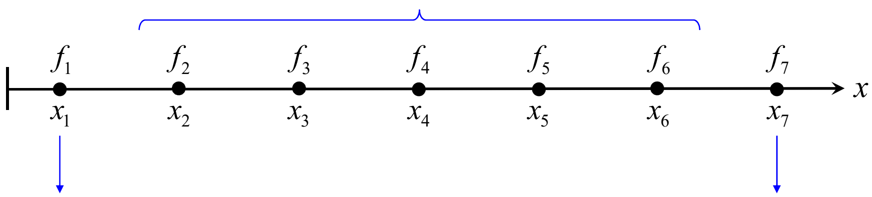
Boundary Conditions

High-Order Boundary Conditions

Computational Methods in EE

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

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



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

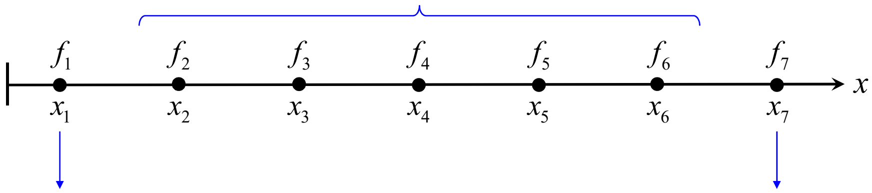
$$\frac{d^2 f_7}{dx^2} \cong \frac{-f_4 + 4f_5 - 5f_6 + 2f_7}{h^2}$$

Dirichlet Boundary Conditions

Computational Methods in EE

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

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



$$\frac{d^2 f_1}{dx^2} \cong \frac{0 - 2f_1 + f_2}{h^2}$$

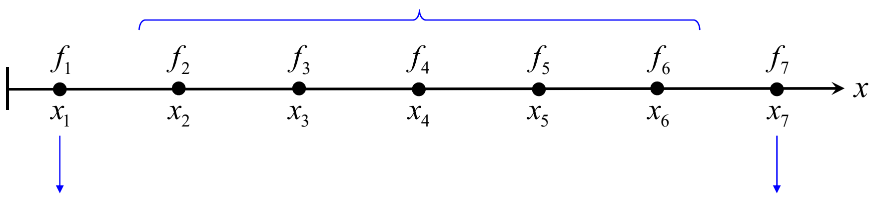
$$\frac{d^2 f_7}{dx^2} \cong \frac{f_6 - 2f_7 + 0}{h^2}$$

Periodic Boundary Conditions

Computational Methods in EE

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.

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



$$\frac{d^2 f_1}{dx^2} \cong \frac{f_7 - 2f_1 + f_2}{h^2}$$

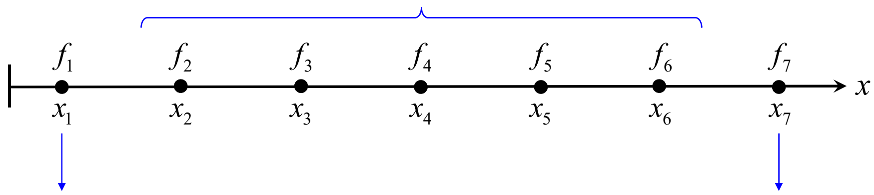
$$\frac{d^2 f_7}{dx^2} \cong \frac{f_6 - 2f_7 + f_1}{h^2}$$

Neuman Boundary Conditions

Computational Methods in EE

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

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



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