



Computational Science:  
Computational Methods in Engineering

# One-Dimensional Finite-Difference Method

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## Outline

- Introduction & Problem Setup
- Conventional Finite-Difference Method
- Improved Finite-Difference Method
- Matrix Operators
- Incorporating Boundary Conditions
- Solving ODE's

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# Introduction & Problem Setup

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## The Finite-Difference Method

The finite-difference method is a way of obtaining a numerical solution to differential equations. It does not give a symbolic solution.

### Governing Equation

$$\frac{d^2 y}{dx^2} - \frac{dy}{dx} + y = 0 \quad 0 \leq x \leq 10$$

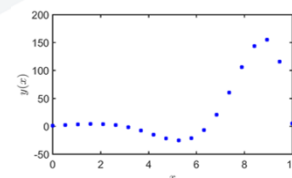
$$y(0) = 1, y(10) = 5$$

### Matrix Equation

$$[A][y] = [b]$$

### Numerical Solution

$$[y] = [A]^{-1}[b]$$

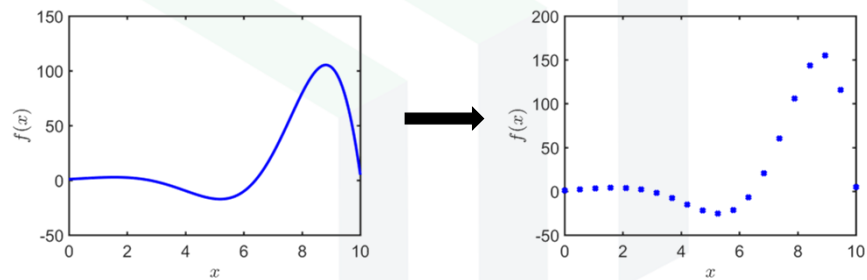


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## Functions are Discrete

To obtain a numerical solution using the finite-difference method, functions are stored as arrays of discrete points.

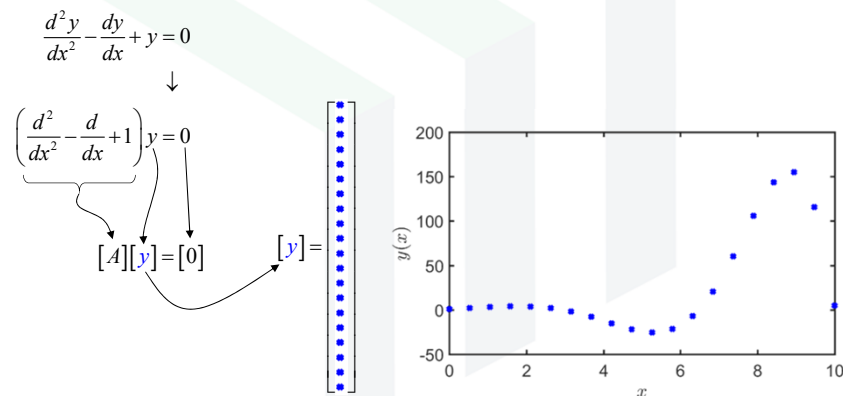


The function can be resolved more accurately using more points, but the solution will be more computationally intensive to obtain. This is a fundamental tradeoff.

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## Discrete Functions are Stored as Column Vectors

Discrete functions are stored as a 1D array of numbers in a column vector.



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# Conventional Finite-Difference Method

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## Step 1 – Identify Governing Equation & Boundary Values

Governing Equation

$$\frac{d^2 y}{dx^2} - \frac{dy}{dx} + y = 0 \quad 0 \leq x \leq 10$$

Boundary Values

$$y(0) = 1$$

$$y(10) = 5$$

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## Step 2 – Approximate Derivatives with Finite-Differences (1 of 3)

First, let the function be discrete.

This allows us to approximate the derivatives with finite-differences.

$$\frac{d^2 y}{dx^2} - \frac{dy}{dx} + y = 0$$

$$\frac{y(x + \Delta x) - 2y(x) + y(x - \Delta x)}{\Delta x^2} - \frac{y(x) - y(x - \Delta x)}{\Delta x} + y(x) = 0$$

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## Step 2 – Approximate Derivatives with Finite-Differences (2 of 3)

It is critical to ensure that each term in the finite-difference equation exists at the same point.

$$\frac{y(x + \Delta x) - 2y(x) + y(x - \Delta x)}{\Delta x^2} - \frac{y(x) - y(x - \Delta x)}{\Delta x} + y(x) = 0$$

This is not a healthy or stable formulation because not all of the terms exist at the same point.

Exists at  $x$

Exists at  $x$

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## Step 2 – Approximate Derivatives with Finite-Differences (3 of 3)

This is the correct finite-difference equation.

$$\begin{aligned} \frac{d^2 y}{dx^2} - \frac{dy}{dx} + y &= 0 \\ \downarrow \\ \frac{y(x + \Delta x) - 2y(x) + y(x - \Delta x)}{\Delta x^2} - \frac{y(x + \Delta x) - y(x - \Delta x)}{2\Delta x} + y(x) &= 0 \end{aligned}$$

All terms exist at  $x$ .

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## Step 3 – Write Finite-Difference Equation Using Array Indices

$$\begin{aligned} \frac{d^2 y}{dx^2} - \frac{dy}{dx} + y &= 0 \\ \downarrow \\ \frac{y(x + \Delta x) - 2y(x) + y(x - \Delta x)}{\Delta x^2} - \frac{y(x + \Delta x) - y(x - \Delta x)}{2\Delta x} + y(x) &= 0 \\ \downarrow \\ \frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} - \frac{y_{i+1} - y_{i-1}}{2\Delta x} + y_i &= 0 \end{aligned}$$

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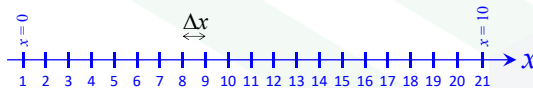
## Step 4 – Rearrange Finite-Difference Equation

The finite-difference equation is rearranged so as to collect the  $y$  terms.

$$\begin{aligned} \frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} - \frac{y_{i+1} - y_{i-1}}{2\Delta x} + y_i &= 0 \\ \downarrow \\ \frac{1}{\Delta x^2} y_{i+1} - \frac{2}{\Delta x^2} y_i + \frac{1}{\Delta x^2} y_{i-1} - \frac{1}{2\Delta x} y_{i+1} + \frac{1}{2\Delta x} y_{i-1} + y_i &= 0 \\ \downarrow \\ \left( \frac{1}{\Delta x^2} + \frac{1}{2\Delta x} \right) y_{i-1} + \left( 1 - \frac{2}{\Delta x^2} \right) y_i + \left( \frac{1}{\Delta x^2} - \frac{1}{2\Delta x} \right) y_{i+1} &= 0 \end{aligned}$$

## Step 5 – Setup Grid

Let's solve this problem using 21 points.



The grid spacing  $\Delta x$  is then

$$\Delta x = \frac{x_b - x_a}{N - 1} = \frac{10 - 0}{21 - 1} = 0.5$$

## Step 6 – Revise Finite-Difference Equation

Substituting  $\Delta x = 0.5$  into our finite-difference equation gives

$$\left(\frac{1}{\Delta x^2} + \frac{1}{2\Delta x}\right)y_{i-1} + \left(1 - \frac{2}{\Delta x^2}\right)y_i + \left(\frac{1}{\Delta x^2} - \frac{1}{2\Delta x}\right)y_{i+1} = 0$$

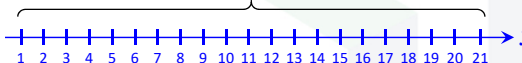
$$\downarrow$$

$$\left(\frac{1}{0.5^2} + \frac{1}{2 \cdot 0.5}\right)y_{i-1} + \left(1 - \frac{2}{0.5^2}\right)y_i + \left(\frac{1}{0.5^2} - \frac{1}{2 \cdot 0.5}\right)y_{i+1} = 0$$

$$\downarrow$$

$$5y_{i-1} - 7y_i + 3y_{i+1} = 0$$

## Step 7 – Write Finite-Difference Equation at Each Point on Grid

$$5y_{i-1} - 7y_i + 3y_{i+1} = 0$$


$$\begin{aligned} 5y_0 - 7y_1 + 3y_2 &= 0 \\ 5y_1 - 7y_2 + 3y_3 &= 0 \\ 5y_2 - 7y_3 + 3y_4 &= 0 \\ 5y_3 - 7y_4 + 3y_5 &= 0 \\ 5y_4 - 7y_5 + 3y_6 &= 0 \\ 5y_5 - 7y_6 + 3y_7 &= 0 \\ 5y_6 - 7y_7 + 3y_8 &= 0 \\ 5y_7 - 7y_8 + 3y_9 &= 0 \\ 5y_8 - 7y_9 + 3y_{10} &= 0 \\ 5y_9 - 7y_{10} + 3y_{11} &= 0 \\ 5y_{10} - 7y_{11} + 3y_{12} &= 0 \\ 5y_{11} - 7y_{12} + 3y_{13} &= 0 \\ 5y_{12} - 7y_{13} + 3y_{14} &= 0 \\ 5y_{13} - 7y_{14} + 3y_{15} &= 0 \\ 5y_{14} - 7y_{15} + 3y_{16} &= 0 \\ 5y_{15} - 7y_{16} + 3y_{17} &= 0 \\ 5y_{16} - 7y_{17} + 3y_{18} &= 0 \\ 5y_{17} - 7y_{18} + 3y_{19} &= 0 \\ 5y_{18} - 7y_{19} + 3y_{20} &= 0 \\ 5y_{19} - 7y_{20} + 3y_{21} &= 0 \\ 5y_{20} - 7y_{21} + 3y_{22} &= 0 \end{aligned}$$

These terms exist  
outside of the grid.





# Improved Finite-Difference Method

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## Step 1 – Identify Governing Equation & Boundary Values

Governing Equation

$$\frac{d^2 y}{dx^2} - \frac{dy}{dx} + y = 0 \quad 0 \leq x \leq 10$$

Boundary Values

$$y(0) = 1$$

$$y(10) = 5$$

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## Step 2 – Write Equation in Matrix Form Going Term-by-Term

$$\frac{d^2}{dx^2}y(x) - \frac{d}{dx}y(x) + y(x) = 0$$

$$[D_x^2][y] - [D_x][y] + [y] = [0]$$

## Step 3 – Factor Out $[y]$ To Put in Standard Form

$$[D_x^2][y] - [D_x][y] + [y] = [0]$$

↓

$$\left([D_x^2] - [D_x] + [I]\right)[y] = [0]$$

↓

$$[A][y] = [0] \quad \text{standard form}$$

$$[A] = [D_x^2] - [D_x] + [I]$$

$$A = DX^2 - DX + I;$$







# Matrix Operators

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## 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

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## 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.

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

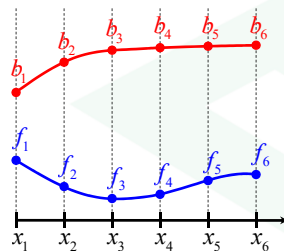
### Functions

Functions are stored as column vectors.

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

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## Point-by-Point Multiplication (1 of 2)



Since we are storing our "functions" in vector form, how do we perform a point-by-point multiplication using a square matrix?

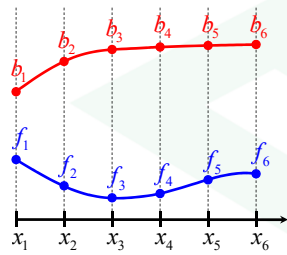
$$b(x)f(x) \rightarrow [B][f]$$

$$\begin{bmatrix} ? \\ ? \\ ? \\ ? \\ ? \\ ? \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix} = \begin{bmatrix} b_1 f_1 \\ b_2 f_2 \\ b_3 f_3 \\ b_4 f_4 \\ b_5 f_5 \\ b_6 f_6 \end{bmatrix}$$

[B]                  [f]                  [B][f]

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## Point-by-Point Multiplication (2 of 2)



Since we are storing our "functions" in vector form, how do we perform a point-by-point multiplication using a square matrix?

$$b(x)f(x) \rightarrow [B][f]$$

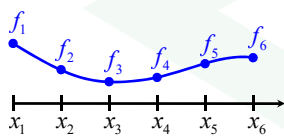
$$\begin{bmatrix} b_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & b_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & b_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & b_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & b_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & b_6 \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix} = \begin{bmatrix} b_1 f_1 \\ b_2 f_2 \\ b_3 f_3 \\ b_4 f_4 \\ b_5 f_5 \\ b_6 f_6 \end{bmatrix}$$

[B] [f] [B][f]

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## First-Order Partial Derivative (1 of 2)

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



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

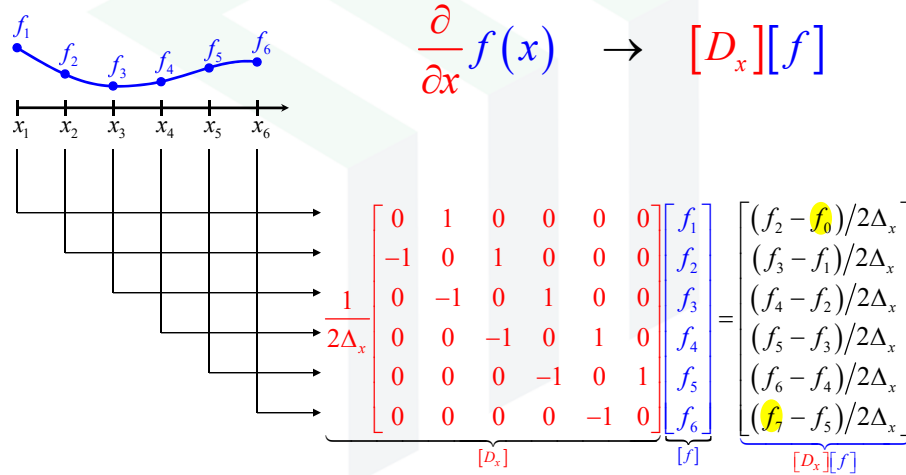
$$\begin{bmatrix} ? \\ ? \\ ? \\ ? \\ ? \\ ? \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix} = \begin{bmatrix} (f_2 - f_1)/2\Delta_x \\ (f_3 - f_2)/2\Delta_x \\ (f_4 - f_3)/2\Delta_x \\ (f_5 - f_4)/2\Delta_x \\ (f_6 - f_5)/2\Delta_x \\ (f_1 - f_2)/2\Delta_x \end{bmatrix}$$

[D<sub>x</sub>] [f] [D<sub>x</sub>][f]

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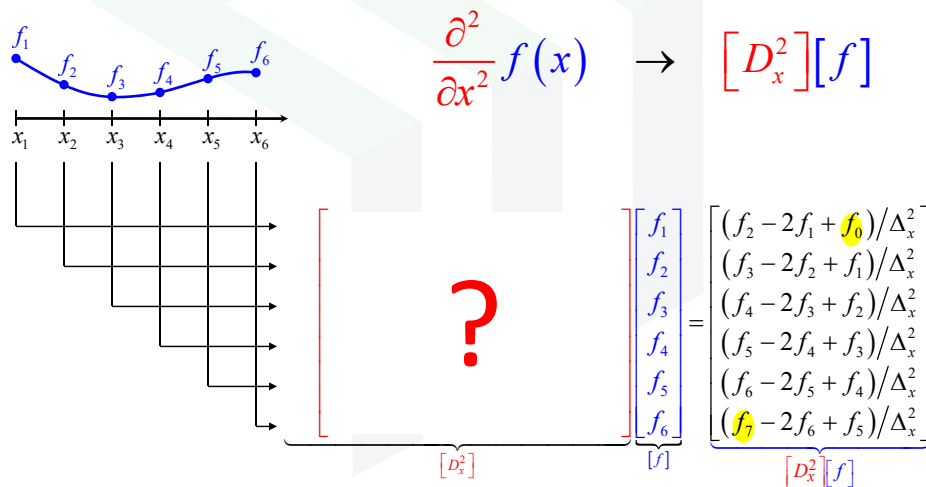
## First-Order Partial Derivative (2 of 2)

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



## Second-Order Partial Derivative (1 of 2)

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



## Second-Order Partial Derivative (2 of 2)

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

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

$$\frac{1}{\Delta_x^2} \begin{bmatrix} -2 & 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix} = \begin{bmatrix} (f_2 - 2f_1 + f_0)/\Delta_x^2 \\ (f_3 - 2f_2 + f_1)/\Delta_x^2 \\ (f_4 - 2f_3 + f_2)/\Delta_x^2 \\ (f_5 - 2f_4 + f_3)/\Delta_x^2 \\ (f_6 - 2f_5 + f_4)/\Delta_x^2 \\ (f_7 - 2f_6 + f_5)/\Delta_x^2 \end{bmatrix}$$

## Why Do We Need Separate Derivative Matrices for First- and Second-Order Derivatives?

It is known that,

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

Can we just calculate  $\mathbf{D}^{(2)}$  from  $\mathbf{D}^{(1)}$ ?  $\mathbf{D}_x^{(2)} = \mathbf{D}_x^{(1)} \mathbf{D}_x^{(1)}$

Yes, but this does not make efficient use of the grid. For a 5-point, 1D grid, we have

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

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 derivative 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!**

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## 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 ]
    
```

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# Incorporating Boundary Conditions

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## Dirichlet Boundary Conditions (1 of 2)

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

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

The diagram shows a horizontal axis labeled  $x$  with seven nodes marked by black dots and labeled  $x_1$  through  $x_7$ . Above each node is a function value  $f_1$  through  $f_7$ . A blue bracket spans from  $x_2$  to  $x_6$ , with the general finite difference formula  $\frac{d^2 f_i}{dx^2} \cong \frac{f_{i-1} - 2f_i + f_{i+1}}{(\Delta x)^2}$  centered above it. Below the axis, two red arrows point downwards from  $x_1$  and  $x_7$  to their respective modified formulas:

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

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

EMPossible

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## Dirichlet Boundary Conditions (2 of 2)

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

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

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

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

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

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

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

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

$[D_x^2]$

## 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.

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

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

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

## Periodic Boundary Conditions (2 of 2)

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

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

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

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

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

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

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

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

$[D_x^2]$

## Neuman Boundary Conditions (1 of 3)

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

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

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

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

## Neuman Boundary Conditions (2 of 3)

$x_1$  .....  $\frac{df_1}{dx} \cong \frac{2f_2 - 2f_1}{2\Delta x}$   
 $x_2$  .....  $\frac{df_2}{dx} \cong \frac{f_3 - f_1}{2\Delta x}$   
 $x_3$  .....  $\frac{df_3}{dx} \cong \frac{f_4 - f_2}{2\Delta x}$   
 $x_4$  .....  $\frac{df_4}{dx} \cong \frac{f_5 - f_3}{2\Delta x}$   
 $x_5$  .....  $\frac{df_5}{dx} \cong \frac{f_6 - f_4}{2\Delta x}$   
 $x_6$  .....  $\frac{df_6}{dx} \cong \frac{f_7 - f_5}{2\Delta x}$   
 $x_7$  .....  $\frac{df_7}{dx} \cong \frac{2f_7 - 2f_6}{2\Delta x}$

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

$[D_x]$

## Neuman Boundary Conditions (3 of 3)

$x_1$  .....  $\frac{d^2 f_1}{dx^2} \cong 0$   
 $x_2$  .....  $\frac{d^2 f_2}{dx^2} \cong \frac{f_1 - 2f_2 + f_3}{(\Delta x)^2}$   
 $x_3$  .....  $\frac{d^2 f_3}{dx^2} \cong \frac{f_2 - 2f_3 + f_4}{(\Delta x)^2}$   
 $x_4$  .....  $\frac{d^2 f_4}{dx^2} \cong \frac{f_3 - 2f_4 + f_5}{(\Delta x)^2}$   
 $x_5$  .....  $\frac{d^2 f_5}{dx^2} \cong \frac{f_4 - 2f_5 + f_6}{(\Delta x)^2}$   
 $x_6$  .....  $\frac{d^2 f_6}{dx^2} \cong \frac{f_5 - 2f_6 + f_7}{(\Delta x)^2}$   
 $x_7$  .....  $\frac{d^2 f_7}{dx^2} \cong 0$

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

$[D_x^2]$

## 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.

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

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

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

## High-Order Boundary Conditions (2 of 2)

$$\frac{1}{(\Delta x)^2} \begin{bmatrix} 2 & -5 & 4 & -1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & -1 & 4 & -5 & 2 \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \end{bmatrix}$$

$[D_x^2]$

# Solving Ordinary Differential Equations

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## Boundary Values

Many differential equations give boundary values, or initial conditions, that must be incorporated into the matrix equation in order to obtain a numerical solution.

For example, a problem may be stated as...

$$\frac{d^2 f(x)}{dx^2} + 5 \frac{df(x)}{dx} + 6f(x) = 0 \quad 0 \leq x \leq 2$$

$$f(0) = 2$$

$$f(2) = 0.2$$

Boundary values

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## Why are Boundary Values Needed?

To solve the differential equation, it is first converted to matrix form.

$$\frac{d^2}{dx^2} f(x) + 5 \frac{d}{dx} f(x) + 6f(x) = 0$$

$$\downarrow \quad \downarrow \quad \downarrow \quad \downarrow \quad \downarrow \quad \downarrow \quad \downarrow$$

$$[D_x^2][f] + 5[D_x][f] + 6[f] = [0]$$

Next, this is rearranged into standard form  $\mathbf{Ax} = \mathbf{b}$ .

$$[A][f] = [0] \quad [A] = [D_x^2] + 5[D_x] + 6[I]$$

This is not solvable.

$$[f] = [A]^{-1}[0] = [0]$$

The boundary values have to be incorporated in order to obtain a nontrivial solution. When this is done, the matrix equation will become

$$[A'][f] = [b]$$

## Incorporating Boundary Values

It is possible to incorporate the boundary values into the matrix operators that we used to build  $[A]$ . However, it is usually easier to incorporate these directly into the final matrix equation.

The steps are:

1. Build direct matrix equation  $[A][f]=[0]$ .
2. For each row in  $[A]$  that corresponds to a boundary point:
  1. Replace entire row with 0's.
  2. Insert a '1' into the diagonal, or pivot, position.
  3. Place the boundary value in the same row of  $[b]$ .

## Solve Matrix Equation

This matrix equation is now in the form

$$[A][f]=[b]$$

This is solved for  $[f]$  as follows.

$$[f]=[A]^{-1}[b]$$

For small to moderate size problems, this can be solved directly using LU decomposition, or just backward division in MATLAB.

`f = A\b;`      **DO NOT USE `f = inv(A)*b`**

For large problems, iterative methods are preferred, but the conditioning of  $[A]$  becomes important and a solution is not guaranteed.

## Example (1 of 10)

Solve the following ordinary differential equation.

$$\frac{d^2 f(x)}{dx^2} + 5 \frac{df(x)}{dx} + 6f(x) = 0 \quad 0 \leq x \leq 2$$

$$f(0) = 2 \quad f(2) = 0.2$$

```
% DEFINE BOUNDARY VALUES
xa = 0;
xb = 2;
fa = 2;
fb = 0.2;
```

## Example (2 of 10)

Step 1 – Formulate the matrix equation  $[A][f] = [0]$ .

$$\frac{d^2}{dx^2} f(x) + 5 \frac{d}{dx} f(x) + 6f(x) = 0$$

$$\downarrow \quad \downarrow \quad \downarrow \quad \downarrow \quad \downarrow \quad \downarrow$$

$$[D_x^2][f] + 5[D_x][f] + 6[f] = [0]$$

$$([D_x^2] + 5[D_x] + 6[I])[f] = [0]$$

$$[A][f] = [0]$$

$$[A] = [D_x^2] + 5[D_x] + 6[I]$$

## Example (3 of 10)

Step 2 – Calculate grid parameters  $N$  and  $\Delta x$ .

Choose  $N = 11$ . *This is just a first guess!*

Calculate  $\Delta x$ .

$$\Delta x = \frac{b-a}{N-1} = \frac{2-0}{11-1} = 0.2$$

```
% GRID PARAMETERS
```

```
Nx = 11;
```

```
dx = (xb - xa) / (Nx - 1);
```

## Example (4 of 10)

Step 3 – Build Matrix Operators  $[D_x^2]$ ,  $[D_x]$ ,  $[I]$ .

$$[D_x^2] = \begin{bmatrix} -50 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 25 & -50 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 25 & -50 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 25 & -50 & 25 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 25 & -50 & 25 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 25 & -50 & 25 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 25 & -50 & 25 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 25 & -50 & 25 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & -50 & 25 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & -50 & 25 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & -50 \end{bmatrix}$$

$$[D_x] = \begin{bmatrix} 0 & 2.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -2.5 & 0 & 2.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2.5 & 0 & 2.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2.5 & 0 & 2.5 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2.5 & 0 & 2.5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2.5 & 0 & 2.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -2.5 & 0 & 2.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -2.5 & 0 & 2.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2.5 & 0 & 2.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2.5 & 0 & 2.5 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2.5 & 0 \end{bmatrix}$$

$$[I] = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

```
% BUILD MATRIX OPERATORS
I = speye(Nx,Nx);
[DX,DX2] = fdder1d(Nx,dx);
```

## Example (5 of 10)

Step 4 – Calculate  $[A]$  and  $[b]$ .

$$[A] = [D_x^2] + 5[D_x] + 6[I] = \begin{bmatrix} -44 & 37.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 12.5 & -44 & 37.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 12.5 & -44 & 37.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 12.5 & -44 & 37.5 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 12.5 & -44 & 37.5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 12.5 & -44 & 37.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 12.5 & -44 & 37.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 12.5 & -44 & 37.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 12.5 & -44 & 37.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 12.5 & -44 & 37.5 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 12.5 & -44 \end{bmatrix}$$

$$[b] = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

```
% CALCULATE [A] AND [b]
A = DX2 + 5*DX + 6*I;
b = sparse(Nx,1);
```

## Example (6 of 10)

Step 5 – Incorporate Boundary Values into  $[A]$  and  $[b]$ .

$$[A] = [D_x^2] + 5[D_x] + 6[I] = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 12.5 & -44 & 37.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 12.5 & -44 & 37.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 12.5 & -44 & 37.5 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 12.5 & -44 & 37.5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 12.5 & -44 & 37.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 12.5 & -44 & 37.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 12.5 & -44 & 37.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 12.5 & -44 & 37.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 12.5 & -44 & 37.5 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$[b] = \begin{bmatrix} 2 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0.2 \end{bmatrix}$$

```
% INCORPORATE BOUNDARY VALUES
```

```
A([1 Nx], :) = 0;
```

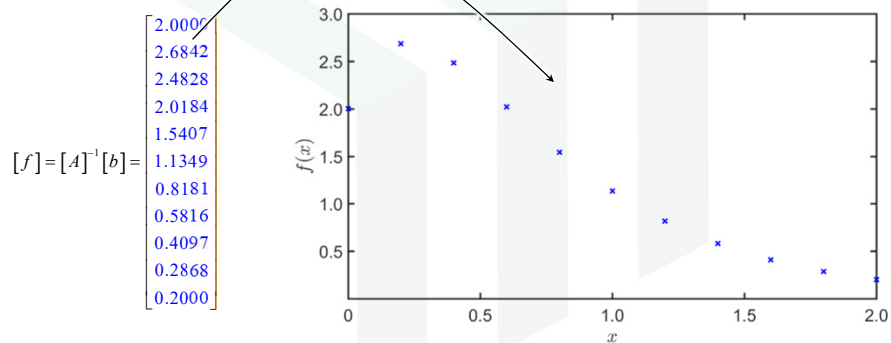
```
A(1,1) = 1;
```

```
A(Nx,Nx) = 1;
```

```
b([1 Nx]) = [ fa fb ];
```

## Example (7 of 10)

Step 6 – Solve for  $[f]$ .



```
% SOLVE FOR [f]
```

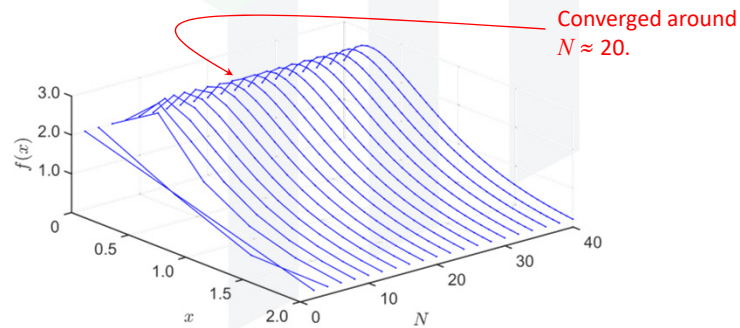
```
f = A\b;
```

## Example (8 of 10)

### Step 7 – Check for Convergence

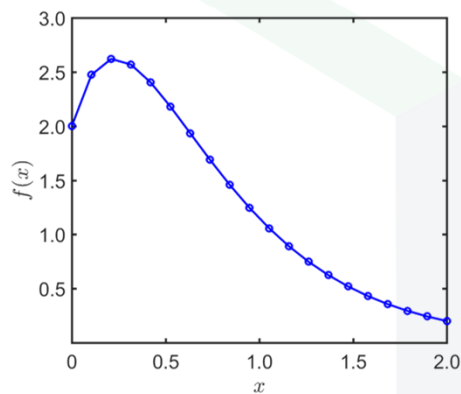
A solution was obtained, but it was all based on a guess for how many points  $N$  to use on the grid.

It is critical to check for convergence by increasing the value of  $N$  until the changes in the solution are negligible.



## Example (9 of 10)

### Step 8 – Obtain the final answer at convergence (i.e. $N = 20$ ).



```
% PLOT RESULT
h = plot(x,F,'-ob','LineWidth',2);
h2 = get(h,'Parent');
set(h2,'LineWidth',2,'FontSize',18);
xlabel('$x$', 'Interpreter', 'LaTeX');
ylabel('$f(x)$', 'Interpreter', 'LaTeX');
T = [0 0.5 1 1.5 2];
L = {'0' '0.5' '1.0' '1.5' '2.0'};
set(gca,'XTick',T,'XTickLabel',L);
T = [0.5 1 1.5 2 2.5 3];
L = {'0.5' '1.0' '1.5' '2.0' '2.5' '3.0'};
set(gca,'YTick',T,'YTickLabel',L);
```

## Example (10 of 10)

Step 9 – Post process the data.

The finite-difference method is complete.

Usually, after obtaining a solution, the results are analyzed further.

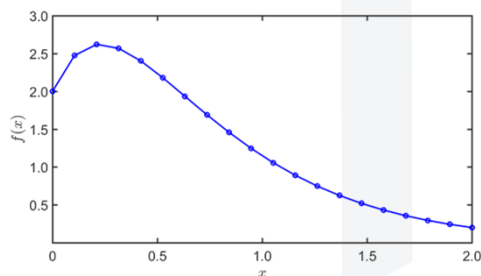
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## Code Altogether

$$\frac{d^2 f(x)}{dx^2} + 5 \frac{df(x)}{dx} + 6f(x) = 0$$

$$0 \leq x \leq 2$$

$$f(0) = 2 \quad f(2) = 0.2$$



```

% DEFINE BOUNDARY VALUES
xa = 0;
xb = 2;
fa = 2;
fb = 0.2;

% GRID PARAMETERS
Nx = 20;
dx = (xb - xa)/(Nx - 1);

% BUILD MATRIX OPERATORS
I = speye(Nx,Nx);
[DX,DX2] = fdder1d(Nx,dx);

% CALCULATE [A] AND [b]
A = DX2 + 5*DX + 6*I;
b = sparse(Nx,1);

% INCORPORATE BOUNDARY VALUES
A([1 Nx],:) = 0;
A(1,1) = 1;
A(Nx,Nx) = 1;
b([1 Nx]) = [ fa fb ];

% SOLVE PROBLEM
f = A\b;

```

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