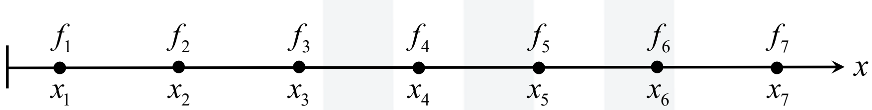
Computational Science:
Computational Methods in Engineering

Introduction to Numerical Differentiation

The Problem

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

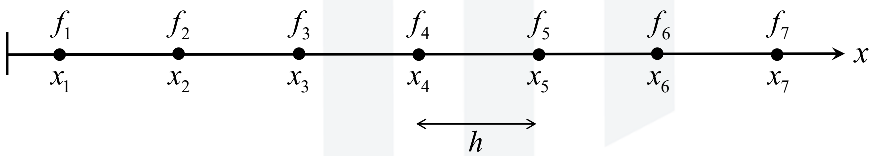
$$\frac{d^2 f(x)}{dx^2} \cong ?$$



The Finite-Difference Approximation

The second-order derivative can be estimated with a 3-point finite-difference approximation.

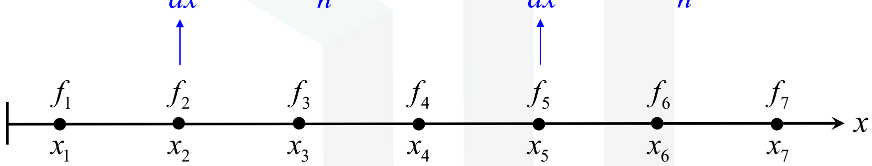
$$\frac{d^2 f_i}{dx^2} \cong \frac{f_{i-1} - 2f_i + f_{i+1}}{h^2}$$



The Middle Points

The derivatives are approximated at each intermediate point by applying the 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

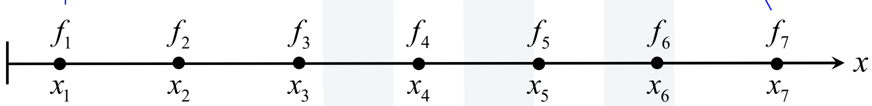
How are the finite-differences evaluated at $i = 1$ and $i = 7$?

Does not exist

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

Does not exist

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



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.

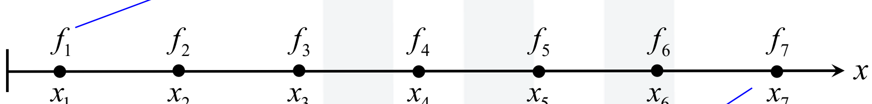
EMPossible

One Possible Boundary Fix

New finite-difference approximations must be derived for each boundary point.

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

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



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

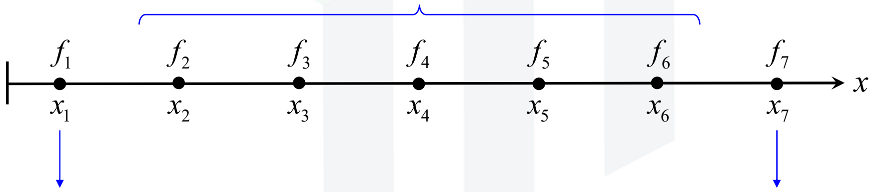
$$\frac{d^2 f_7}{dx^2} \cong \frac{-f_4 + 4f_5 - 5f_6 + 2f_7}{h^2}$$

EMPossible

Summary of Finite-Difference Approximations

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.

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



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

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