Computational Science:
Computational Methods in Engineering

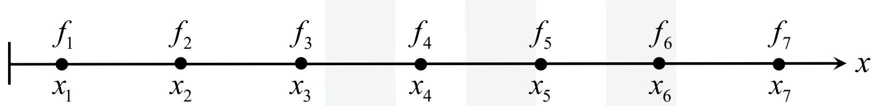
Introduction to Numerical Differentiation

1

The Problem

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

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

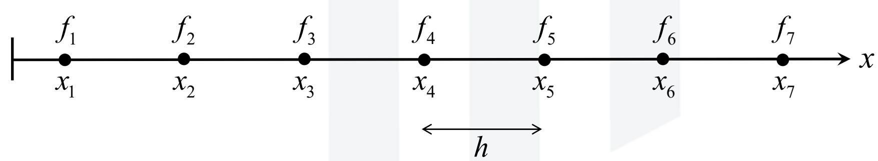


2

The Finite-Difference Approximation

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

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

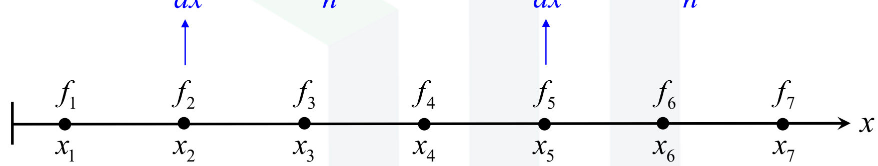


3

The Middle Points

The derivatives are approximated at each intermediate point by applying the finite-difference approximation using the surrounding points.

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



4

Problem at the Boundaries

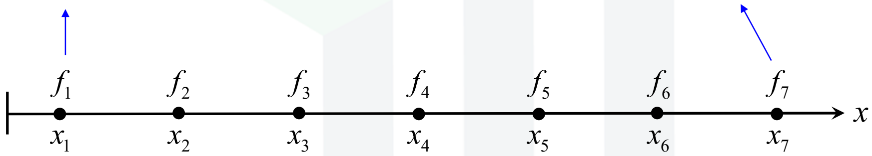
How are the finite-differences evaluated at the end points $i = 1$ and $i = 7$?

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

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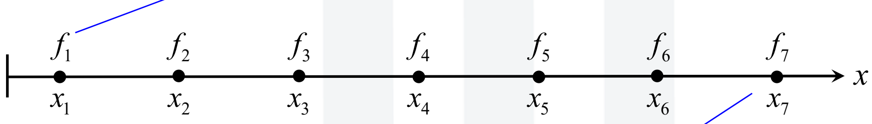
One Possible Boundary Fix

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

$$[\tilde{x}] = [0 \quad h \quad 2h \quad 3h]^T \qquad \frac{d^2 f_1}{dx^2} \cong \frac{2f_1 - 5f_2 + 4f_3 - f_4}{h^2}$$



$$[\tilde{x}] = [-3h \quad -2h \quad -h \quad 0]^T \qquad \frac{d^2 f_7}{dx^2} \cong \frac{-f_4 + 4f_5 - 5f_6 + 2f_7}{h^2}$$

EMPossible

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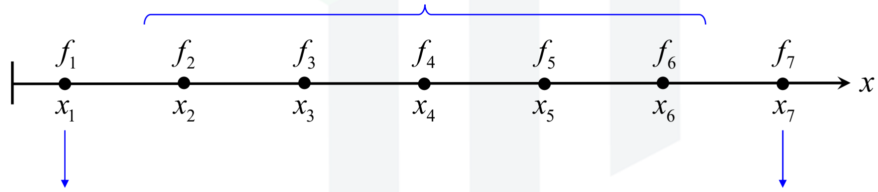
Summary of Finite-Difference Approximations

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.

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



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

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

EMPossible

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