



Computational Science:
Computational Methods in Engineering

Introduction to Numerical Differentiation

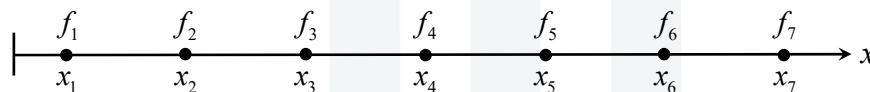


1

The Problem

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

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

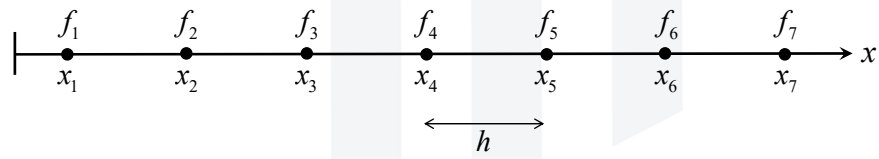


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The Finite-Difference Approximation

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

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

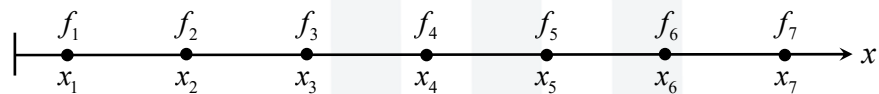


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The Middle Points

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

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



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Problem at the Boundaries

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

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

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

The diagram shows a horizontal axis labeled x with points $x_1, x_2, x_3, x_4, x_5, x_6, x_7$ marked. Above each point is a function value $f_1, f_2, f_3, f_4, f_5, f_6, f_7$. A blue arrow points from the f_0 term in the first equation to the point x_1 . Another blue arrow points from the f_8 term in the second equation to the point x_7 . Red circles are drawn around f_0 and f_8 , with red text "Does not exist" pointing to them.

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.

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One Possible Boundary Fix

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

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

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

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

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

The diagram shows a horizontal axis labeled x with points $x_1, x_2, x_3, x_4, x_5, x_6, x_7$ marked. Above each point is a function value $f_1, f_2, f_3, f_4, f_5, f_6, f_7$. A blue arrow points from the f_4 term in the first equation to the point x_4 . Another blue arrow points from the f_4 term in the second equation to the point x_4 .

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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.

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

The diagram shows a horizontal axis labeled x with seven points marked x_1 through x_7 . Above each point is a function value f_1 through f_7 . A blue bracket spans from x_2 to x_6 , with the central difference formula $\frac{d^2 f_i}{dx^2} \cong \frac{f_{i-1} - 2f_i + f_{i+1}}{h^2}$ positioned above it. Below the axis, two special boundary formulas are shown: $\frac{d^2 f_1}{dx^2} \cong \frac{2f_1 - 5f_2 + 4f_3 - f_4}{h^2}$ and $\frac{d^2 f_7}{dx^2} \cong \frac{-f_4 + 4f_5 - 5f_6 + 2f_7}{h^2}$. Blue arrows point from x_1 and x_7 on the axis to their respective formulas.

