Quiz

1) Name three numerical integration methods
2) 2 x 2 + 2 x 2 + 2 – 2 x 2 = ?

Write your name and today's date

Numerical Differentiation

Taylor Series Review

If we expand f around x_i and f is $(n+1)$-times continuously differentiable on an open interval containing x_i, Taylor's theorem with the remainder term says that if x_{i+1} is another point in this interval, then:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \ldots + \frac{f^{(n)}(x_i)}{n!}h^n + R_n \quad \textbf{(7.1)}$$

where:

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1}$$

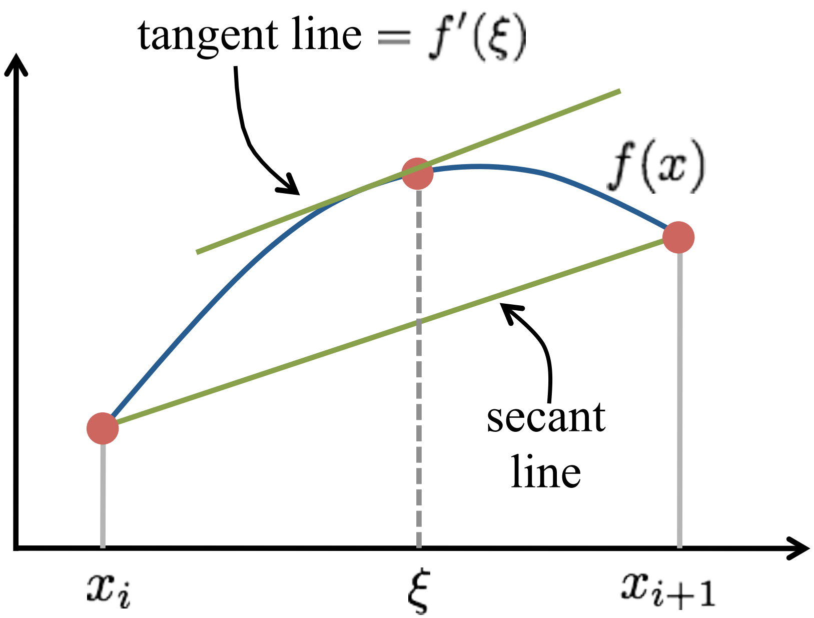
ξ is a number in the open interval between x_i and x_{i+1}

$$h = x_{i+1} - x_i$$

$$f(x_{i+1}) = f(x_i + h)$$

Mean Value Theorem

The appearance of ξ, a point between x_i and x_{i+1}, suggests that there is a connection between this result and the Mean Value Theorem,



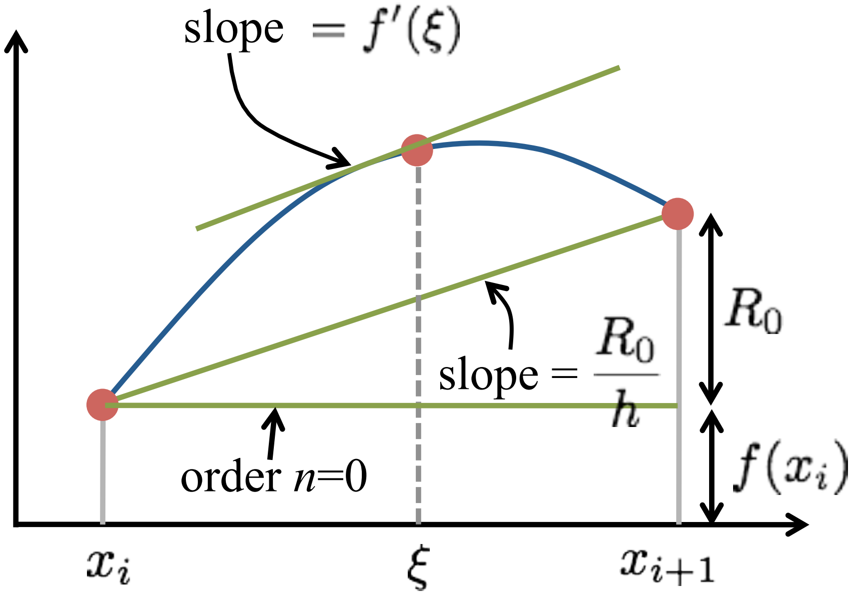
which states that given a planar arc between two endpoints, there is at least one point at which the tangent to the arc is parallel to the secant through its endpoints.

If a function f is continuous on $[x_i, x_{i+1}]$ and differentiable on (x_i, x_{i+1}), then there exists a point ξ such that:

$$f'(\xi) = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

Mean Value Theorem & Taylor's Theorem

Back to the Taylor series, for $n = 0$:



$$f(x_{i+1}) \cong f(x_i) + R_0 \qquad \textbf{(7.2)}$$

where

$$R_0 = f'(\xi)h$$

$$h = x_{i+1} - x_i$$

Then

$$f(x_{i+1}) = f(x_i) + f'(\xi)(x_{i+1} - x_i) \qquad \textbf{(7.3)}$$

where ξ is between x_i and x_{i+1}. This is the Mean Value Theorem, which is used to prove Taylor's theorem. We can also regard a Taylor expansion as an extension of the Mean Value Theorem.

Approximation of 1st Order Derivative by Forward Difference

If we truncate the Taylor series after the 1st derivative:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + R_1 \qquad \textbf{(7.4)}$$

where

$$R_1 = \frac{f''(\xi)}{2}h^2 \quad \text{or} \quad \frac{R_1}{h} = \frac{f''(\xi)}{2}h \qquad \textbf{(7.5)}$$

Rearranging eqn. (7.4) gives us

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{R_1}{h}$$

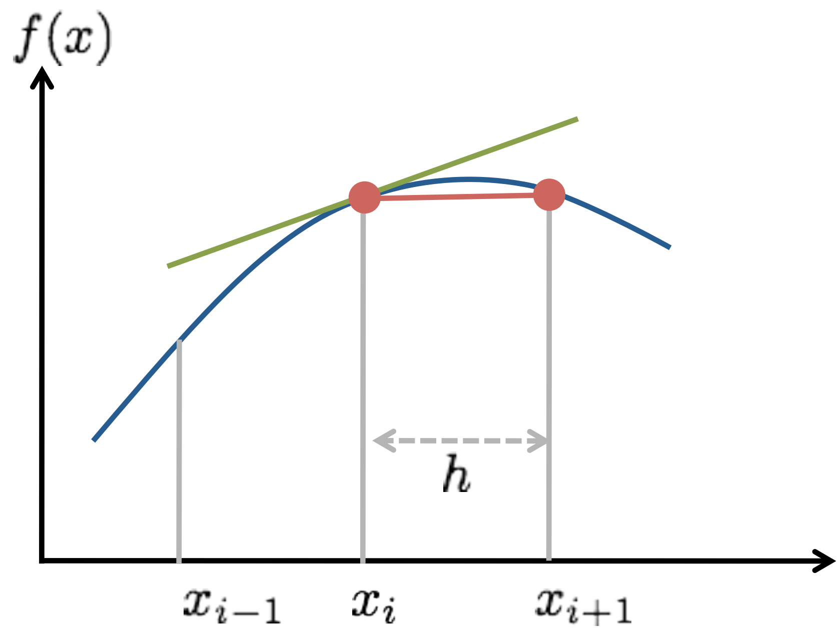
or

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + \mathcal{O}(h) \qquad \textbf{(7.6)}$$

Approximation of 1st Order Derivative by Forward Difference

Graphical illustration of forward difference approximation:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + \mathcal{O}(h)$$



Big O Notation

Big O notation, also called Landau's symbol, is a symbolism used in complexity theory, computer science, and mathematics to describe the asymptotic behavior of functions. Basically it tells us how fast a function grows or declines.

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + \mathcal{O}(h)$$

tells that the error of the 1st derivative approximation is proportional to the step size *h*. Consequently, if we halve the step size, we would expect to halve the error of the derivative.

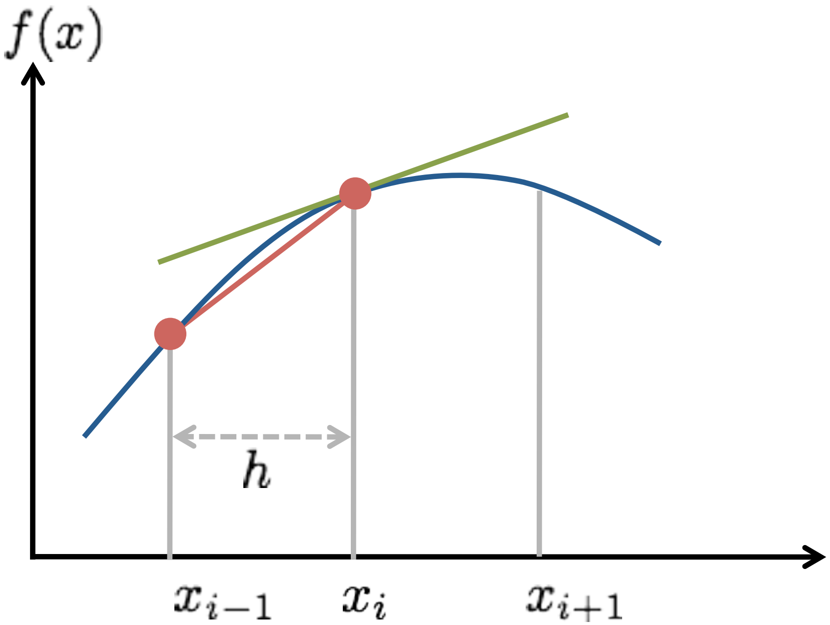
Big O Notation

Here is a list of classes of functions that are commonly encountered when analyzing algorithm. The slower growing functions are listed first, c is some arbitrary constant.

Notation	Name
$O(1)$	Constant
$O(\log(n))$	Logarithmic
$O((\log(n))^c)$	Polylogarithmic
$O(n)$	Linear
$O(n^2)$	Quadratic
$O(n^c)$	Polynomial
$O(c^n)$	Exponential

Approximation of 1st Order Derivative by Backward Difference

The Taylor series can be expanded backward to calculate a previous value on the basis of a present value.



$$h = x_i - x_{i-1}$$

$$x_{i-1} = x_i - h$$

$$f(x_{i-1}) = f(x_i - h)$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \ldots \quad \textbf{(7.7)}$$

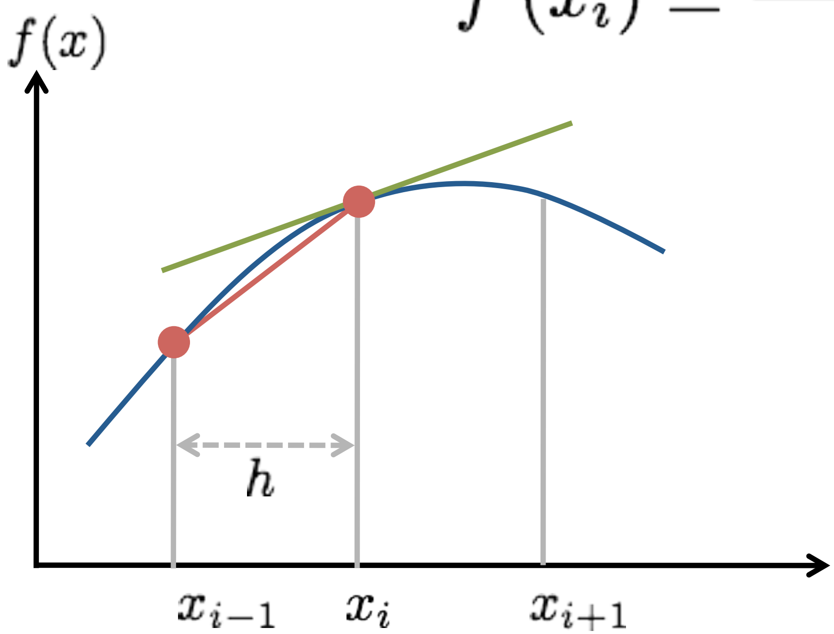
Approximation of 1st Order Derivative by Backward Difference

Truncating the expansion in eqn. (7.7) after the first derivative gives:

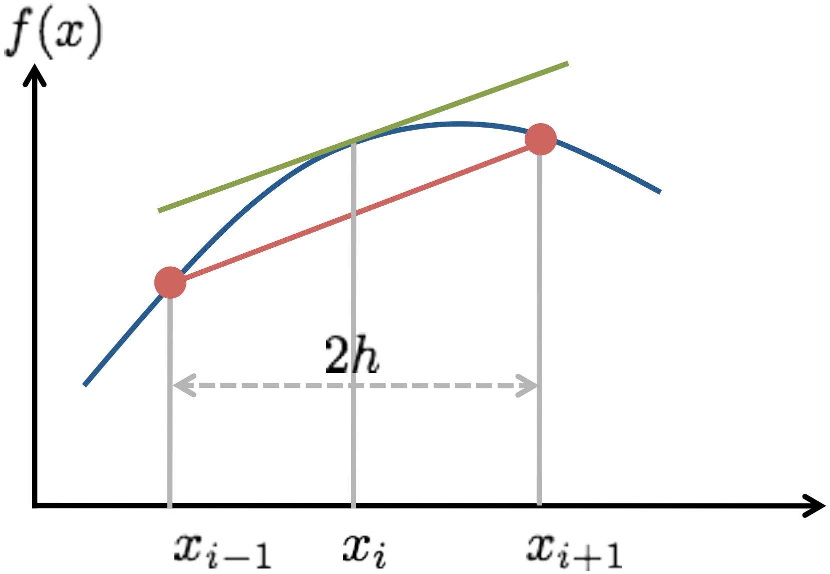
$$f(x_{i-1}) \cong f(x_i) - f'(x_i)h + R_1$$

Rearranging:

$$f'(x_i) \cong \frac{f(x_i) - f(x_{i-1})}{h} + \mathcal{O}(h) \qquad \textbf{(7.8)}$$



Approximation of 1st Order Derivative by Central Difference



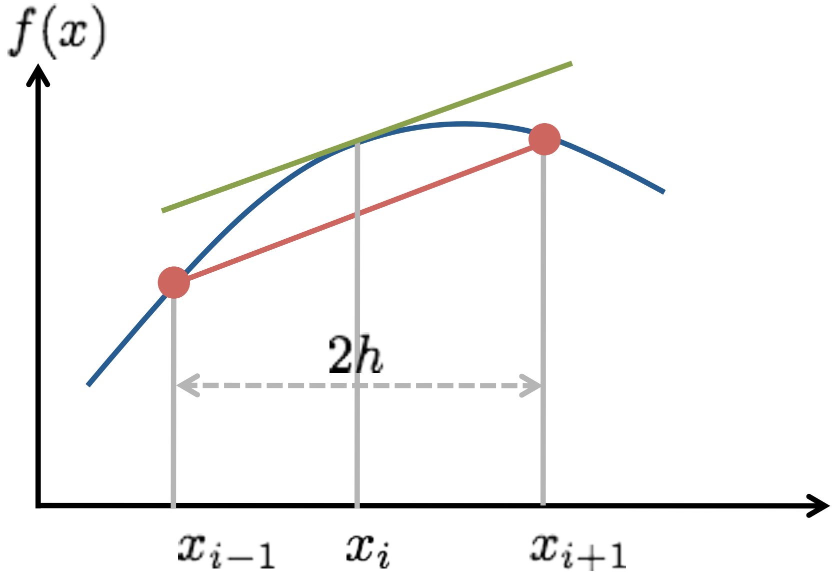
The third way to approximate the first derivative is by subtracting backward difference from forward difference:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \dots$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \dots$$

$$f(x_{i+1}) - f(x_{i-1}) = 2f'(x_i)h + \frac{2f'''(x_i)}{3!}h^3 + \dots \qquad \textbf{(7.9)}$$

Approximation of 1st Order Derivative by Central Difference



For the central difference method, the error can be found from the 3rd degree Taylor polynomial with remainder:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(c_1)}{3!}h^3$$

and

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(c_2)}{3!}h^3$$

where $x_i \leq c_1 \leq x_{i+1}$ and $x_{i-1} \leq c_2 \leq x_i$

Approximation of 1st Order Derivative by Central Difference

Subtracting these two equations gives:

$$f(x_{i+1}) - f(x_{i-1}) = 2f'(x_i)h + \frac{h^3}{3!}\left(f'''(c_1) + f'''(c_2)\right) \quad \textbf{(7.10)}$$

Since $f''(x)$ is continuous, the intermediate value theorem can be used to find a value c, so that

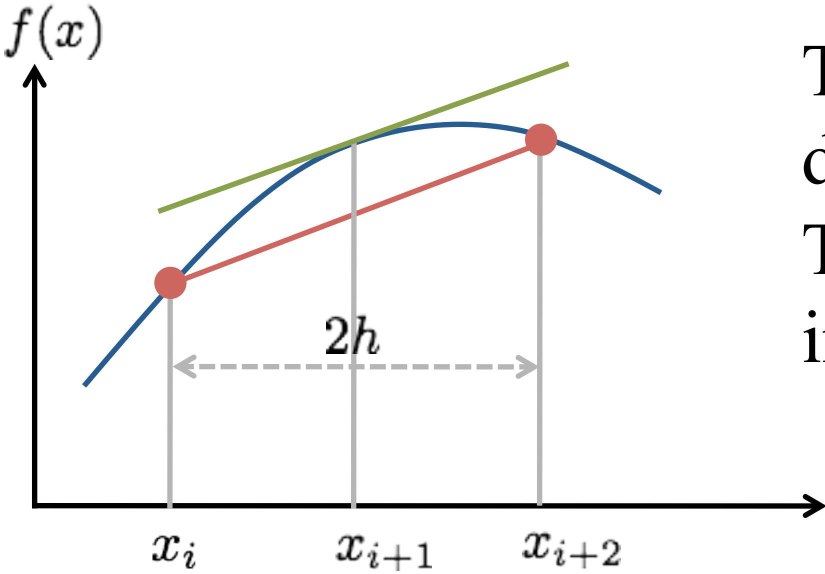
$$\frac{f'''(c_1) + f'''(c_2)}{2} = f'''(c) \quad \textbf{(7.11)}$$

Substituting (7.11) into (7.10) and rearranging:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + \mathcal{O}(h^2) \quad \textbf{(7.12)}$$

The central difference is more accurate as the error is $O(h^2)$.

2nd Order Forward Difference



To approximate 2nd order derivatives, we write a forward Taylor series expansion for $f(x_{i+2})$ in terms of $f(x_i)$:

$$f(x_{i+2}) = f(x_i) + f'(x_i)(2h) + \frac{f''(x_i)}{2!}(2h)^2 + \ldots$$

If we truncate after the 2nd order:

$$f(x_{i+2}) \cong f(x_i) + 2f'(x_i)h + 2f''(x_i)h^2 + R_2 \qquad \textbf{(7.12)}$$

2^{nd} Order Forward Difference

Truncating the forward difference after the 2^{nd} order and multiplying by 2 gives:

$$2f(x_{i+1}) \cong 2f(x_i) + 2f'(x_i)h + f''(x_i)h^2 + 2R_2 \quad \textbf{(7.13)}$$

Subtracting eqn. (7.13) from (7.12) yields

$$f(x_{i+2}) - 2f(x_{i+1}) \cong -f(x_i) + f''(x_i)h^2 - R_2$$

Rearranging:

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + \frac{R_2}{h^2}$$

2^{nd} Order Forward Difference

The 2^{nd} order remainder can be written

$$R_2 = \frac{f'''(\xi)}{3!}h^3$$

or

$$\frac{R_2}{h^2} = \frac{f'''(\xi)}{3!}h = \mathcal{O}(h)$$

Hence:

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + \mathcal{O}(h) \qquad \textbf{(7.14)}$$

2nd Order Backward and Central Differences

The same manipulations can be employed to derive a 2nd order backward difference:

$$f''(x_i) = \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2} + \mathcal{O}(h) \qquad \textbf{(7.15)}$$

and a 2nd order central difference:

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} + \mathcal{O}(h^2) \qquad \textbf{(7.16)}$$

As was the case with the 1st-derivative approximations, the central difference is more accurate.

Forward Difference

First derivative | Error

$$f'(x) = \frac{f(x_{i+1}) - f(x_i)}{h} \qquad \mathcal{O}(h)$$

$$f'(x) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} \qquad \mathcal{O}(h^2)$$

Second derivative

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} \qquad \mathcal{O}(h)$$

$$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2} \qquad \mathcal{O}(h^2)$$

Forward Difference

Third derivative | Error

$$f'''(x_i) = \frac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3} \qquad \mathcal{O}(h)$$

$$f'''(x_i) = \frac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3} \qquad \mathcal{O}(h^2)$$

Fourth derivative

$$f''''(x_i) = \frac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4} \qquad \mathcal{O}(h)$$

$$f''''(x_i) = \frac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4} \qquad \mathcal{O}(h^2)$$

Backward Difference

First derivative | Error

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} \qquad \mathcal{O}(h)$$

$$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h} \qquad \mathcal{O}(h^2)$$

Second derivative

$$f''(x_i) = \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2} \qquad \mathcal{O}(h)$$

$$f''(x_i) = \frac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2} \qquad \mathcal{O}(h^2)$$

Central Difference

First derivative — Error

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} \qquad \mathcal{O}(h^2)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} \qquad \mathcal{O}(h^4)$$

Second derivative

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) - f(x_{i-1})}{h^2} \qquad \mathcal{O}(h^2)$$

$$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}$$

$$\mathcal{O}(h^4)$$

Example 7.1

Approximate the first-order derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at x = 0.5 using finite differences and a step size of $h = 0.25$ with accuracy $O(h^2)$.

Example 7.1

Solution:

The derivative can be calculated analytically as

$$f'(x) = -0.4x^3 - 0.45x^2 - 1.0x - 0.25$$

and its true value at x=0.5 is $f'(0.5)$ = -0.9125. The data that we need is

$$x_{i-2} = 0 \qquad f(x_{i-2}) = 1.2$$

$$x_{i-1} = 0.25 \qquad f(x_{i-1}) = 1.1035156$$

$$x_i = 0.5 \qquad f(x_i) = 0.925$$

$$x_{i+1} = 0.75 \qquad f(x_{i+1}) = 0.6363281$$

$$x_{i+2} = 1 \qquad f(x_{i+2}) = 0.2$$

Example 7.1

The forward difference of accuracy $O(h^2)$ is computed as

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$$

$$f'(0.5) = \frac{-0.2 + (4)(0.6363281) - (3)(0.925)}{(2)(0.25)}$$

$$= -0.859375$$

and percentage relative error

$$\varepsilon = \frac{|-0.9125 - (-0.859375)|}{|-0.9125|} \times 100\% = 5.82\%$$

Example 7.1

The backward difference of accuracy $O(h^2)$ is computed as

$$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i+2})}{2h}$$

$$f'(0.5) = \frac{(3)(0.925) - (4)(1.1035156) + 1.2}{(2)(0.25)}$$

$$= -0.878125$$

and percentage relative error

$$\varepsilon = \frac{|-0.9125 - (-0.878125)|}{|-0.9125|} \times 100\% = 3.77\%$$

Example 7.1

The central difference of accuracy $O(h^2)$ is computed as

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$$

$$f'(0.5) = \frac{-0.2 + (8)(0.6363281) - (8)(1.1035156) + 1.2}{(12)(0.25)}$$

$$= -0.9125$$

and percentage relative error

$$\varepsilon = 0\%$$

Richardson Extrapolation

Two ways to improve derivative estimates when using finite divided differences:

(1) Decrease the step size

(2) Use a higher-order formula that employs more points

The third approach is based on Richardson extrapolation, where we could use two derivative estimates to compute a third, more accurate approximation. Recall the formula in Lecture 6 for Romberg integration:

$$I \cong \frac{4}{3}I(h) - \frac{1}{3}I(2h)$$

In a similar fashion:

$$D \cong \frac{4}{3}D(h) - \frac{1}{3}D(2h) \qquad \textbf{(7.17)}$$

Example 7.2

Using Richardson extrapolation estimate the derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x = 0.5$ employing step sizes of 0.5 and 0.25.

Using central difference with $h = x_i - x_{i-1} = x_{i+1} - x_i$ or $2h = x_{i+1} - x_{i-1}$ thus with $h = 0.5$ at $x_i = 0.5$ the function values at points

$$x_{i-1} = 0 \qquad f(0) = 1.2$$

$$x_{i+1} = 1 \qquad f(1) = 0.2$$

the derivative

$$D(0.5) = \frac{0.2 - 1.2}{2(0.5)} = -1$$

Example 7.2

If we halve the step size to $h = 0.25$, where now

$$x_{i+1} = 0.75 \qquad f(0.75) = 0.6363$$

$$x_i = 0.5$$

$$x_{i-1} = 0.25 \qquad f(0.25) = 1.1035$$

the derivative

$$D(0.25) = \frac{0.6363 - 1.1035}{2(0.25)} = -0.9344$$

The improved estimate can be determined now by

$$D = \frac{4}{3}D(0.25) - \frac{1}{3}D(0.5) = -0.9125$$

with error (compared to true value) $\epsilon_r = 0\%$

Derivatives of Unequally Spaced Data

One way to handle non-equispaced data is to fit a second-order Lagrange interpolating polynomial to each set of the three adjacent points. The 2nd order polynomial can be differentiated to give:

$$f'(x) = f(x_{i-1})\frac{2x - x_i - x_{i+1}}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})}$$

$$+f(x_i)\frac{2x - x_{i-1} - x_{i+1}}{(x_i - x_{i-1})(x_i - x_{i+1})}$$

$$+f(x_{i+1})\frac{2x - x_{i-1} - x_i}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} \qquad \textbf{(7.18)}$$