Numerical Analysis

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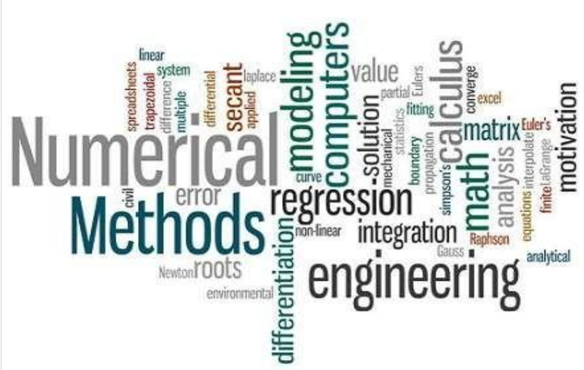
Week 12, Lecture-I-II



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Course Syllabus

- **Introduction:** Numerical analysis and background, definitions of computer number systems, floating point representation, representation of numbers in different bases, and round-off errors.
- **Root Finding:** Bisection method, fixed-point iteration, Newton's method, the secant method and their error analysis and order of convergence (Newton’s method and Secant method).
- **Direct Methods for Solving Linear Systems:** Gaussian elimination, LU decomposition, pivoting strategies, and PA=LU-factorization,…..
- **Polynomial:** Polynomial interpolation, Lagrange interpolation, Piecewise interpolation, divided differences interpolation, and curve fitting in interpolation (Application: Regression)…...
- **Integration:** Numerical differentiation, numerical integration, and composite numerical integration…….
- **Ordinary Differential Equations:** Euler's Method, and Runge-Kutta methods…..

- **Numerical Differentiation**

- **Richardson Extrapolation**

- **Numerical Integration**

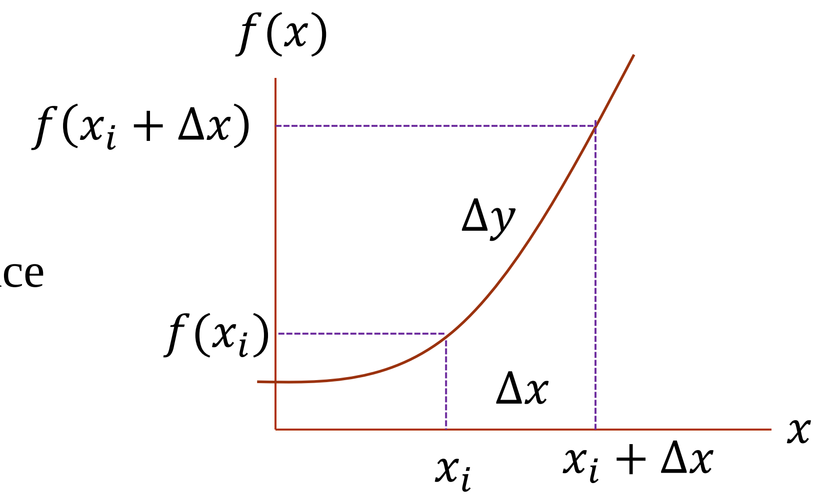
Numerical Differentiation

Numerical differentiation

❑ Definition of differentiation

The mathematical definition of a derivative begins with a difference approximation:

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$



And as Δx is allowed to approach zero, the difference becomes a derivative

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

❑ Numerical Differentiation

In numerical differentiation, we find estimate for the derivative or slope of a function by using the function values at only a set of discrete points.

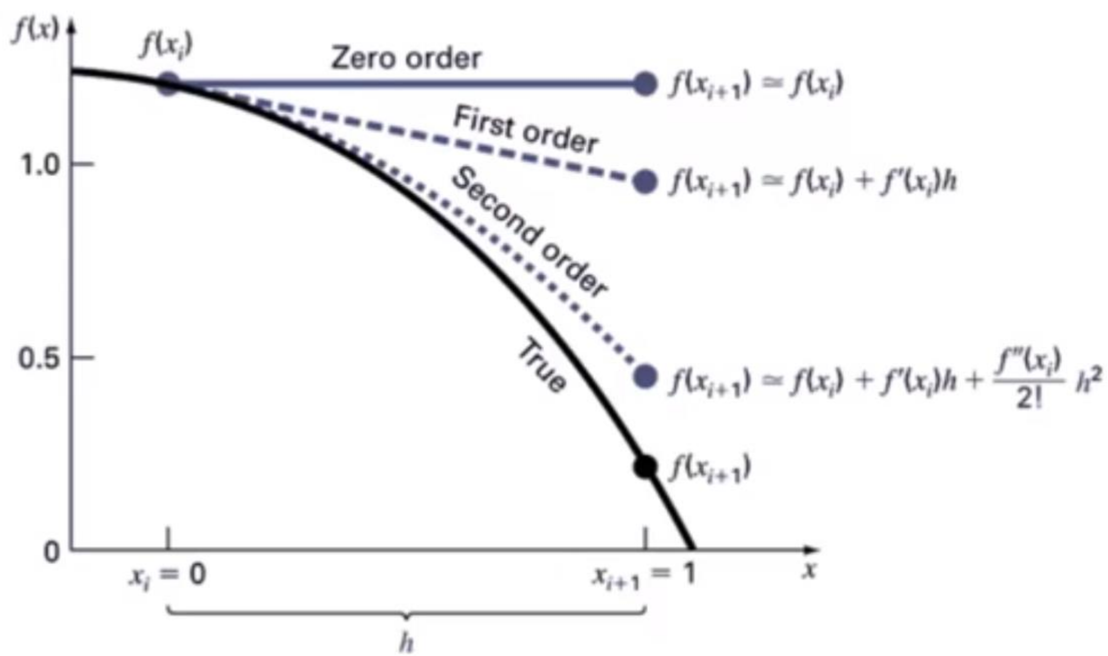
Simplest approach $\Delta x = h = finite$

$$\frac{dy}{dx} = \frac{f(x_i+h)-f(x_i)}{h} + error$$

Numerical differentiation

We can use the Taylor series to predict the next value of a function

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

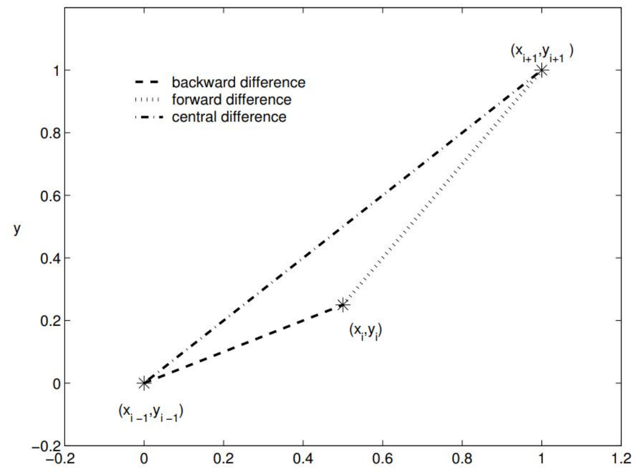


So we can use the Taylor series to understand going backwards that what type of error we are going to have when we take this derivative.

Numerical differentiation

❑ First Derivative

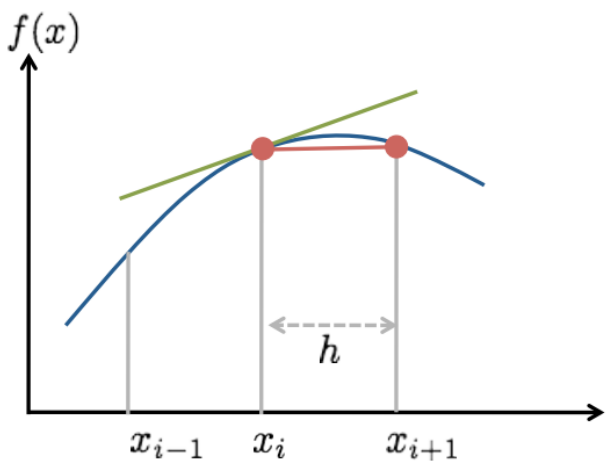
Suppose that a variable y_i and y_{i+1} depends on another variable x_i and x_{i+1}, i.e. $y_i = f(x_i)$ and $y_{i+1} = f(x_{i+1})$ but we only know the values of f at a finite set of points, e.g., as data from an experiment



$$(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$$

- **Forward Difference Formula (FDF)**

Suppose then that we need information about the derivative of $f(x)$. One obvious idea would be to approximate $f'(x_i)$ by the **Forward Difference**



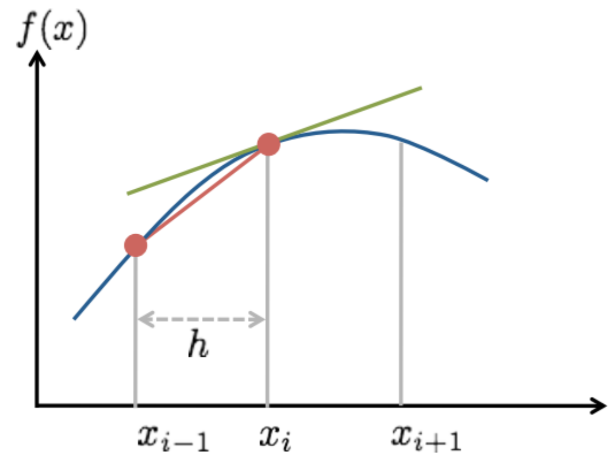
$$f'(x_i) = y_i' \approx \frac{y_{i+1} - y_i}{x_{i+1} - x_i}. = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

Numerical differentiation

- **Backward Difference Formula (BDF)**

This formula follows directly from the definition of the derivative in calculus. An alternative would be to use a **Backward Difference**

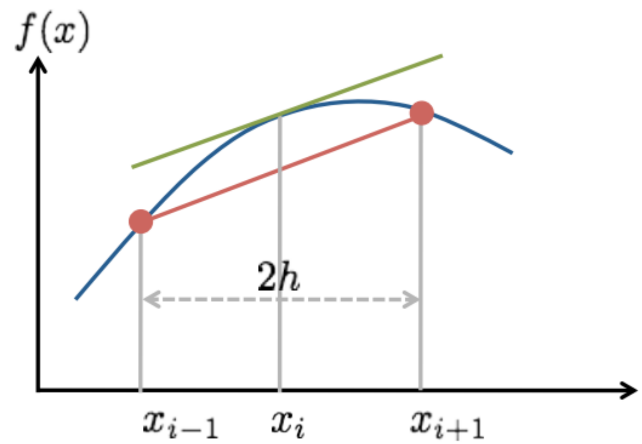
$$f'(x_i) \approx \frac{y_i - y_{i-1}}{x_i - x_{i-1}} = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$



- **Central Difference Formula (CDF)**

Since the errors for the forward difference and backward difference tend to have opposite signs, it would seem likely that averaging the two methods would give a better result than either alone. If the points are evenly spaced, i.e. $x_{i+1} - x_i = x_i - x_{i-1} = h$, then averaging the forward and backward differences leads to a symmetric expression called the **Central Difference**

$$f'(x_i) = y_i' \approx \frac{y_{i+1} - y_{i-1}}{2h} = \frac{f(x_{i+1}) - f(x_{i-1})}{2h}$$



Numerical differentiation

❑ Error of approximation (Truncation error)

We can use Taylor polynomials to derive the accuracy of the forward, backward and central difference formulas. For example the usual form of the Taylor polynomial with remainder (sometimes called Taylor's Theorem) is

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(c)\,,$$

where c is some (unknown) number between x and $x+h$. Letting $x = x_i, x+h = x_{i+1}$ and solving for $f'(x_i)$ leads to

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

Notice that the quotient in this equation is exactly the forward difference formula. Thus the error of the forward difference is $-(h/2)f''(c)$ which means it is $O(h)$. Replacing h in the above calculation by $-h$ gives the error for the backward difference formula; it is also $O(h)$

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

Numerical differentiation

Error of approximation ((Truncation error))

For the central difference, the error can be found from the third degree Taylor polynomials with remainder

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

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

where $x_i \leq c_1 \leq x_{i+1}$ and $x_{i-1} \leq c_2 \leq x_i$. Subtracting these two equations and solving for $f'(x_i)$ leads to

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

This shows that the error for the central difference formula is $O(h^2)$. Thus, central differences are significantly better and so: **It is best to use central differences whenever possible.**

Numerical differentiation

❑ Higher order approximation

- We can also interpolate the data by a polynomial rather than a straight line. This can be done by using 3 data points. These data points must be evenly spaced.

$$x_{i-2}, \quad x_{i-1}, \quad x_i, \quad x_{i+1}, \quad x_{i+2}$$

Three points FDF

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

Three points BDF

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

$$= \frac{3y_i - 4y_{i-1} + y_{i-2}}{2h}$$

Numerical differentiation

Example

Approximate the derivative of $f(x) = x^2 + 2x$ at $x = 3$ using the forward, backward, and central difference method and step size 1.

Solution We have

$x_{i-1} = 2$ $x_i = 3$ $x_{i+1} = 4$ $\Delta x = h = 1$

$f(2) = 8$ $f(3) = 15$ $f(4) = 24$

Forward Difference Formula (FDF)

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} = \frac{f(4) - f(3)}{4 - 3} = \frac{24 - 15}{1} = 9$$

$f'(3) = 9$

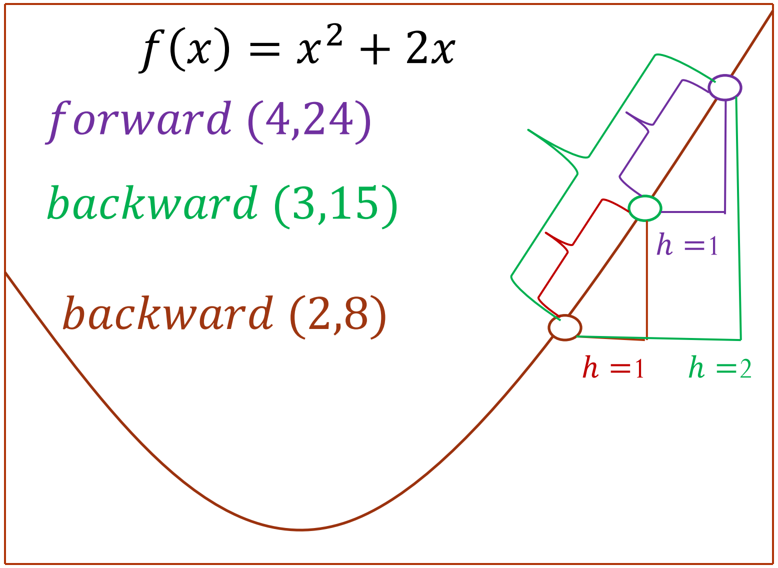
Numerical differentiation

Example

Backward Difference Formula (BDF)

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

$$= \frac{15 - 8}{1} = 7 \qquad f'(3) = 7$$



Central Difference Formula (CDF)

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

$$= \frac{24 - 8}{2} = \frac{16}{2} = 8 \qquad f'(3) = 8$$

Now take the derivatives of the given function

$$f(x) = x^2 + 2x \qquad f'(x) = 2x + 2$$

$$f'(3) = 2(3) + 2 = 8$$

Numerical differentiation

Example

Estimate $f'(x_2)$ using forwards backward and central differences, given function is $f'(x) = 2^x \ln|2|$

x :	1	2	3	4	5
$f(x)$:	2	4	8	16	32

Solution

$$f'(x) = 2^x \ln|2|$$

Forward Difference Formula (FDF)

$$f'(x_2) = \frac{f(x_3) - f(x_2)}{x_3 - x_2} = \frac{16 - 8}{4 - 3} = 8$$

$$f'(3) = 2^3 \ln|2|$$

$$f'(3) = 5.544$$

Backward Difference Formula (BDF)

$$f'(x_2) = \frac{f(x_2) - f(x_1)}{x_2 - x_1} = \frac{8 - 4}{3 - 2} = 4$$

Central Difference Formula (CDF)

$$f'(x_2) = \frac{f(x_3) - f(x_1)}{x_3 - x_1} = \frac{16 - 4}{4 - 2} = \frac{12}{2} = 6$$

Richardson Extrapolation

Richardson Extrapolation

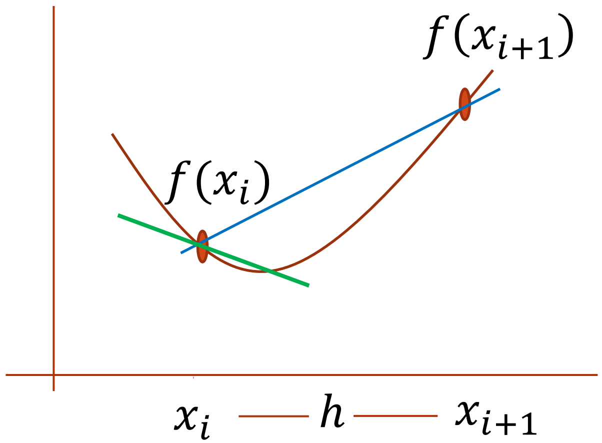
❑ Numerical difference

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

- We already know that how to extract/ find numerical differences with the help of discrete data points using various difference formulas.

- We can find numerical differences from two methods straight line interpolation and polynomial interpolation.

- The accuracy of methods for computing derivative or integrals of a function f(x) depends on the spacing between points at which f is evaluated and that the approximation tends to the exact value as this spacing tends to zero.



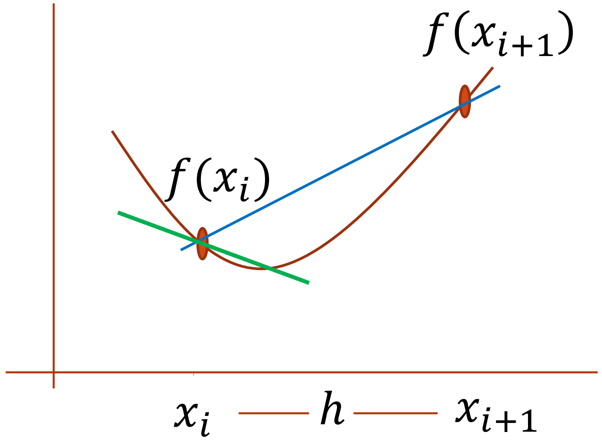
Richardson Extrapolation

❑ Numerical difference

- We have called uniform spacing to h

- Approximated value by using CDF with step size h is called $D(h)$.

- Approximated value by using CDF with step size $\frac{h}{2}$ is called $D(\frac{h}{2})$.



$$D(h) = f'(x_i) = \frac{1}{2h}[f(x_i + h) - f(x_i - h)] - \frac{h^2}{6}f''(x) + O(h^4)$$

$$D\left(\frac{h}{2}\right) = f'(x_i) = \frac{1}{2\frac{h}{2}}\left[f\left(x_i + \frac{h}{2}\right) - f\left(x_i - \frac{h}{2}\right)\right] - \frac{h^2}{24}f''(x) + O(h^4)$$

Richardson Extrapolation

❑ Numerical difference

- We can solve these two equations to obtain an approximations that is 4th order accurate.

$$\mathrm{D} = \frac{4D\left(\frac{h}{2}\right) - D(h)}{3}$$

D- improved estimate or true value

- This process of extrapolating from $D(h)$ and $D\left(\frac{h}{2}\right)$ to approximate D with a higher order of accuracy is called Richardson Extrapolation.

Richardson Extrapolation

Example

By use of Richardson extrapolation find $f'(x_2)$ with h=2, given function is $f'(x) = 2^x \ln|2|$

x :	1	2	3	4	5
$f(x)$:	2	4	8	16	32

Solution

We know that

$$D = \frac{4D\left(\frac{h}{2}\right) - D(h)}{3}$$

$$f'(x) = 2^x \ln|2|$$

$$f'(3) = 2^3 \ln|2|$$

$$f'(3) = 5.544$$

For this formula we have to find $D(h)$ and $D\left(\frac{h}{2}\right)$

$$D(h) = f'(x_2) = \frac{1}{2h}[f(x_2 + h) - f(x_2 - h)]$$

$$= \frac{1}{2(2)}[f(5) - f(1)] = \frac{1}{4}[32 - 2] = \frac{30}{4} = 7.5$$

Richardson Extrapolation

$$D\left(\frac{h}{2}\right) = f'(x_2) = \frac{1}{2\frac{h}{2}}\left[f\left(x_2 + \frac{h}{2}\right) - f\left(x_2 - \frac{h}{2}\right)\right]$$

$$D\left(\frac{h}{2}\right) = \frac{1}{2\frac{2}{2}}\left[f\left(x_2 + \frac{2}{2}\right) - f\left(x_2 - \frac{2}{2}\right)\right] = \frac{1}{2}[f(3+1) - f(3-1)] = \frac{1}{2}[f(4) - f(2)]$$

$$D\left(\frac{h}{2}\right) = \frac{1}{2}[16-4] = \frac{12}{2} = 6$$

$$\mathrm{D} = \frac{4D\left(\frac{h}{2}\right) - D(h)}{3} = \frac{4(6) - (7.5)}{3} = \frac{16.5}{3} = 5.5$$

Richardson Extrapolation

Greater accuracy

- This method can be further extended to achieve greater accuracy i.e accuracy of $o(h^6)$, $o(h^8)$ etc.
- To achieve accuracy of $o(h^6)$ we combine two $o(h^4)$ values.
- Suppose we have given two values of h 4 and 2

h	$D(h)$	$D'(h)(O(h^4))$	$D^2(h)(O(h^6))$
4	$D(h)$	$D'(h) = \dfrac{4D\left(\frac{h}{2}\right) - D(h)}{3}$	$D^2(h) = \dfrac{4^2 D'\left(\frac{h}{2}\right) - D'(h)}{4^2 - 1}$
2	$D\left(\frac{h}{2}\right)$		
1	$D\left(\frac{h}{2}\right)$	$D'(h) = \dfrac{4D\left(\frac{h}{2}\right) - D(h)}{3}$	

$$D^3(h) = \frac{4^3 D^2\left(\frac{h}{2}\right) - D^2(h)}{4^3 - 1}$$

$$D^k(h) = \frac{4^k D^{k-1}\left(\frac{h}{2}\right) - D^{k-1}(h)}{4^k - 1}$$

Richardson Extrapolation

Example By use of Richardson extrapolation find $f'(1)$ using the approximation formula

$$f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h}$$

with h=0.4, 0.2, and 0.1 from the following values

x :	0.6	0.8	0.9	1.0	1.1	1.2	1.4
$f(x)$:	0.707178	0.859892	0.925863	0.984007	1.033743	1.074575	1.127986

Solution First we have to take $h = 0.4$

$$D(h) = f'(1) = \frac{f(1+h) - f(1-h)}{2h} = \frac{f(1.4) - f(0.6)}{2(0.4)} = 0.52601$$

Now let us take $h = 0.2$

$$D(h) = f'(1) = \frac{f(1+h) - f(1-h)}{2h} = \frac{f(1.2) - f(0.8)}{2(0.2)} = 0.5367075$$

Now let us take $h = 0.1$

$$D(h) = f'(1) = \frac{f(1+h) - f(1-h)}{2h} = \frac{f(1.1) - f(0.9)}{2(0.1)} = 0.5394$$

Richardson Extrapolation

h	$D(h)$	$D'(h)(O(h^4))$	$D^2(h)(O(h^6))$
0.4	0.52601	$D'(h) = \dfrac{4D\left(\frac{h}{2}\right) - D(h)}{3}$ $D'(0.4) = \dfrac{4D(0.2) - D(0.4)}{3}$ $D'(0.4) = \dfrac{4(0.5367075) - (0.52601)}{3}$ $D'(0.4) = 0.5402733$	$D^2(h) = \dfrac{4^2 D'\left(\frac{h}{2}\right) - D'(h)}{4^2 - 1}$ $D^2(h) = \dfrac{16D'\left(\frac{h}{2}\right) - D'(h)}{15}$ $D^2(0.4) = \dfrac{16D'(0.2) - D'(0.4)}{15}$ $D^2(0.4) = 0.540299$
0.2	0.5367075	$D'(h) = \dfrac{4D\left(\frac{h}{2}\right) - D(h)}{3}$ $D'(0.2) = \dfrac{4D(0.1) - D(0.2)}{3}$ $D'(0.2) = \dfrac{4(0.5394) - (0.5367075)}{3}$ $D'(0.2) = 0.5402975$	
0.1	0.5394		

Thank You !