NUMERICAL METHODS

$$U^{n+1} = U^n + \Delta t\, f(U^n)$$

$$\frac{\partial v}{\partial t} + V \cdot \nabla v = \nabla \cdot (k \nabla v) + g(v)$$

$$(\lambda + \mu)\nabla(\nabla \cdot u) + \mu \nabla^2 u = \alpha(3\lambda + 2\mu)\nabla T - \rho b$$

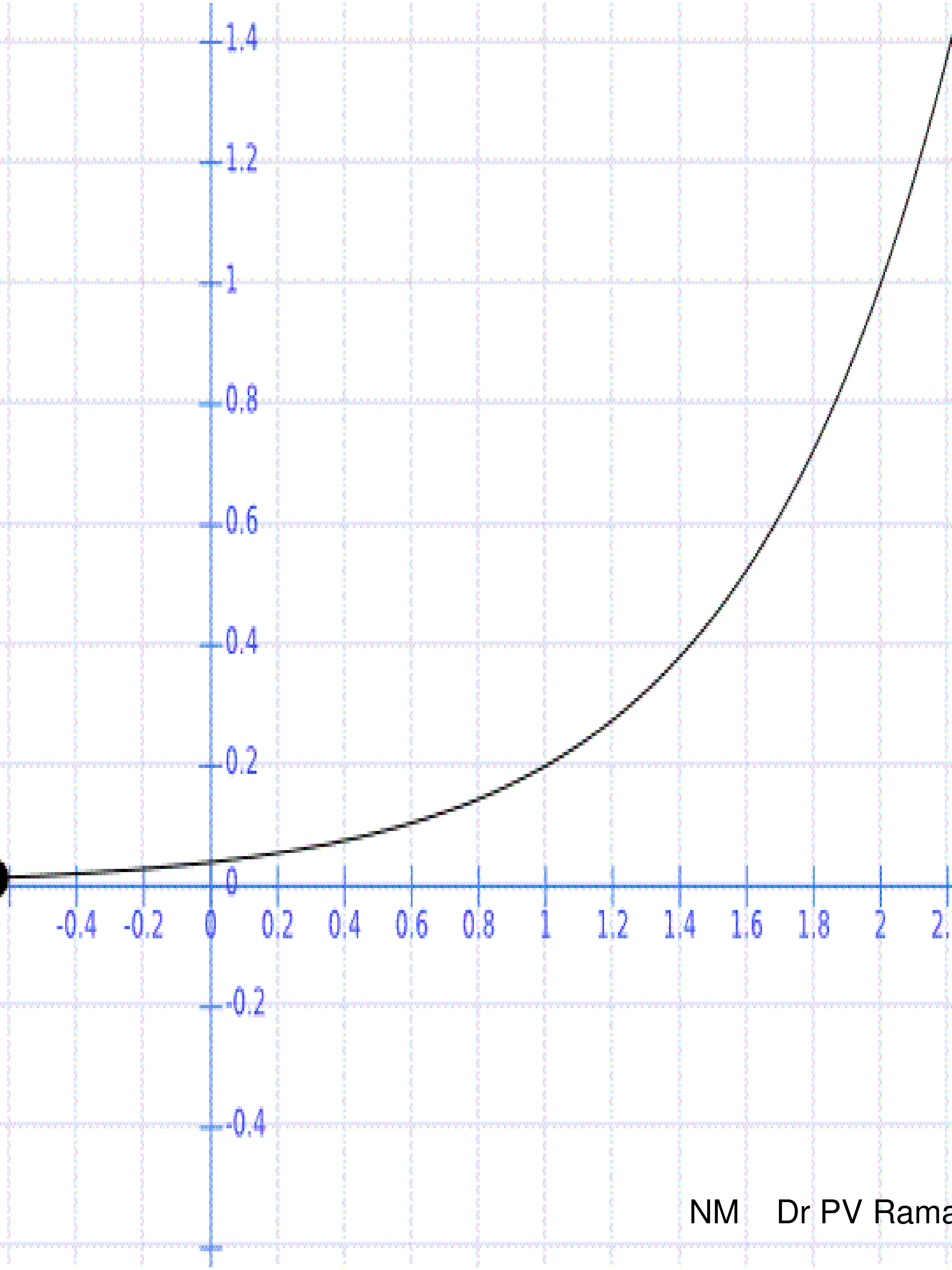
Lecture 10

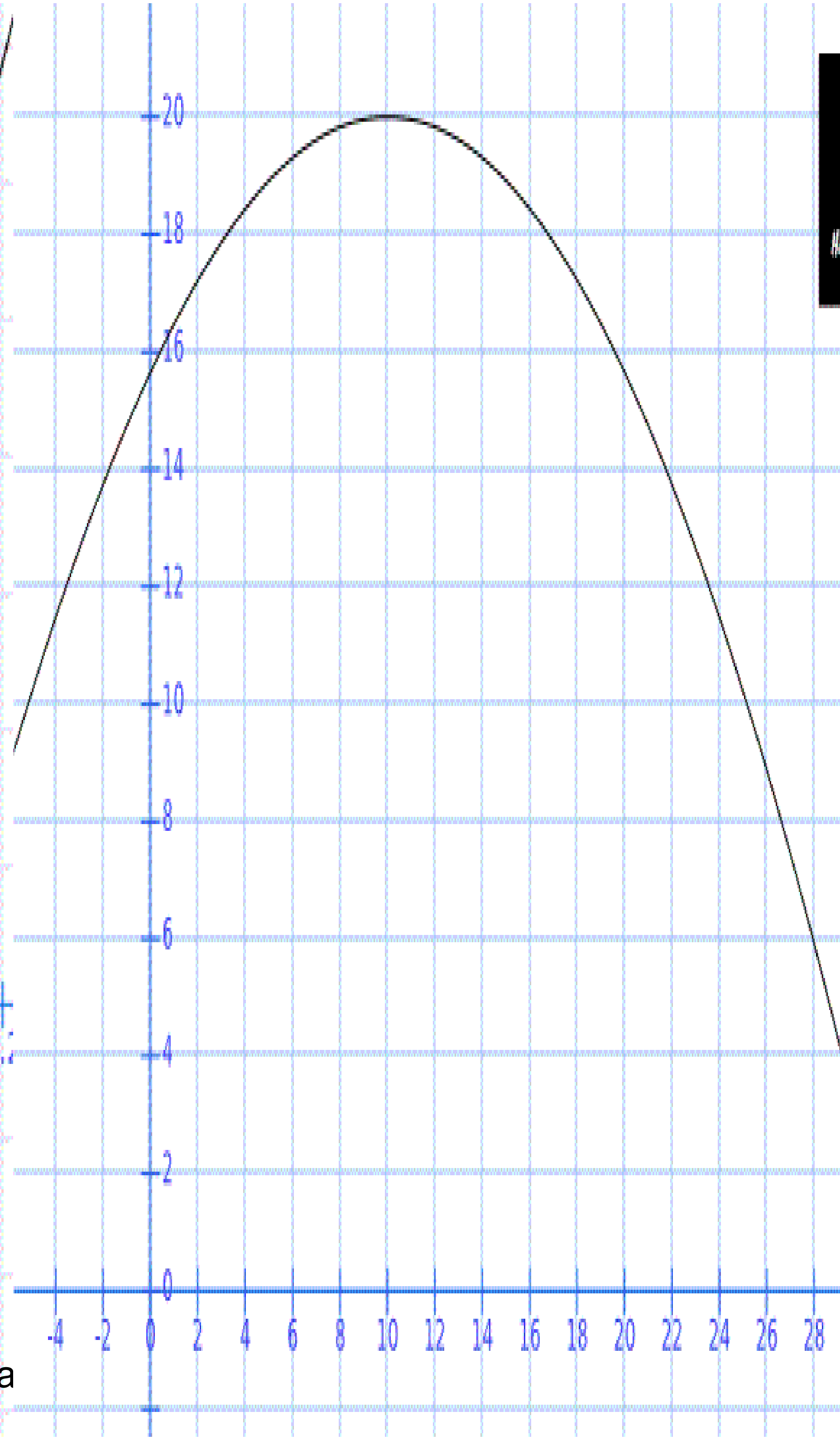
$$\rho\left(\frac{\partial u}{\partial t} + V \cdot \nabla u\right) = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + \rho f_x$$

$$\nabla^2 u = f$$

Dr. P V Ramana

Numerical Differentiation


1.4
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2


20
18
16
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12
10
8
6
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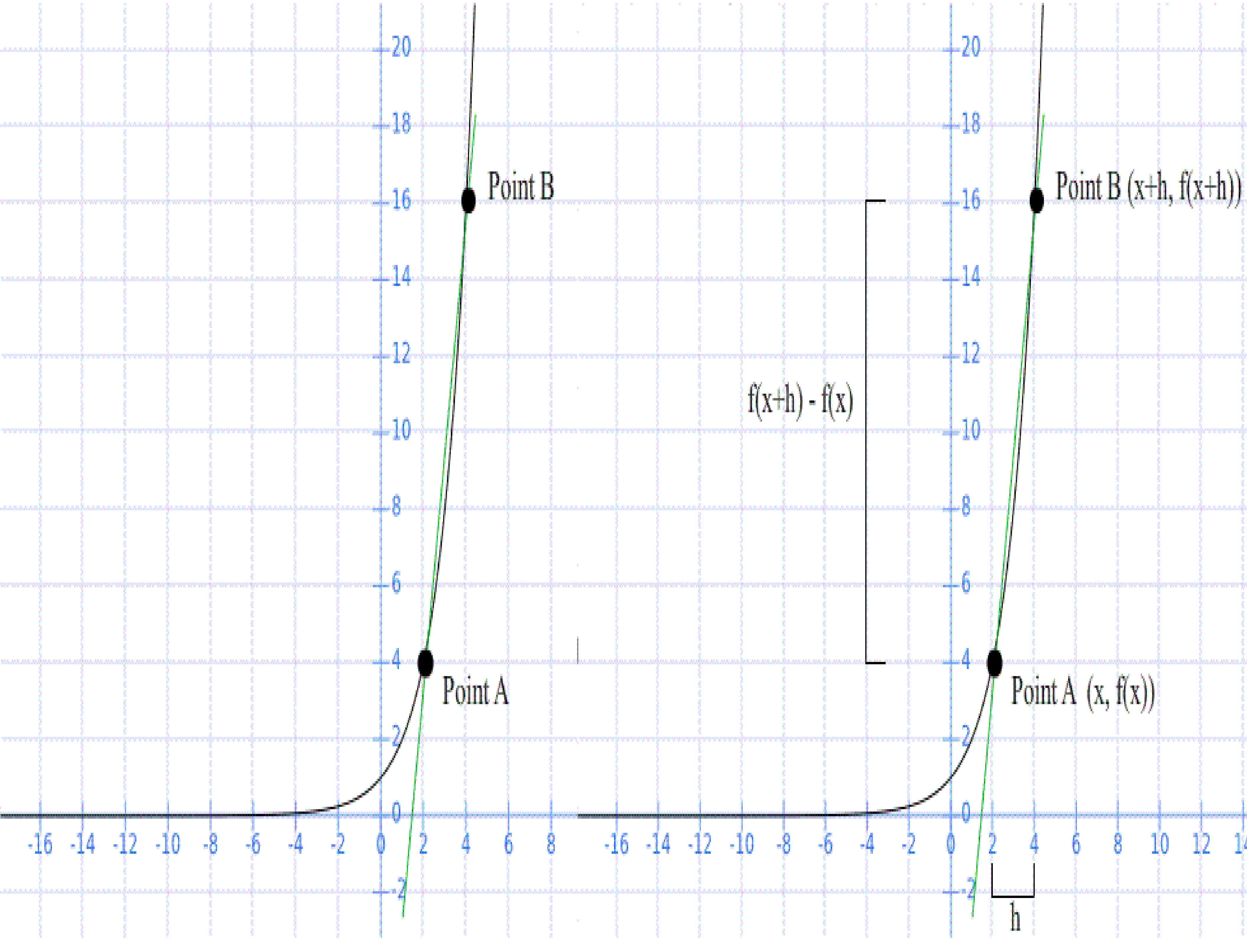
22
24
26
28



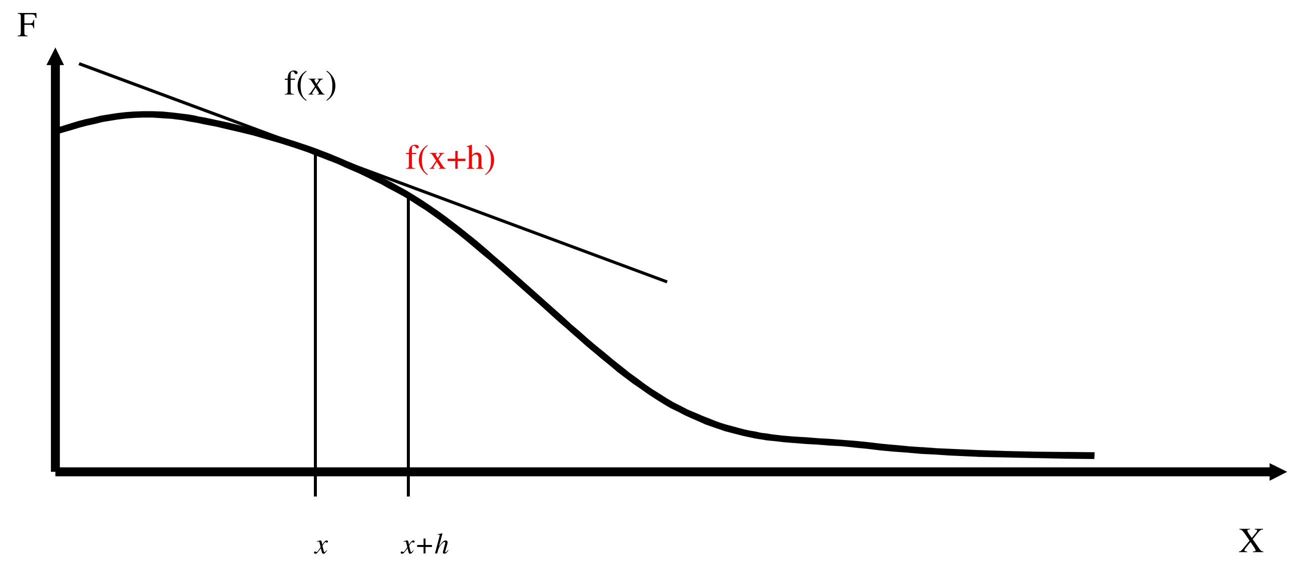
Point B
Point A
Point B (x+h, f(x+h))
f(x+h) - f(x)
Point A (x, f(x))
h

Numerical Differentiation

- The mathematical definition:

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

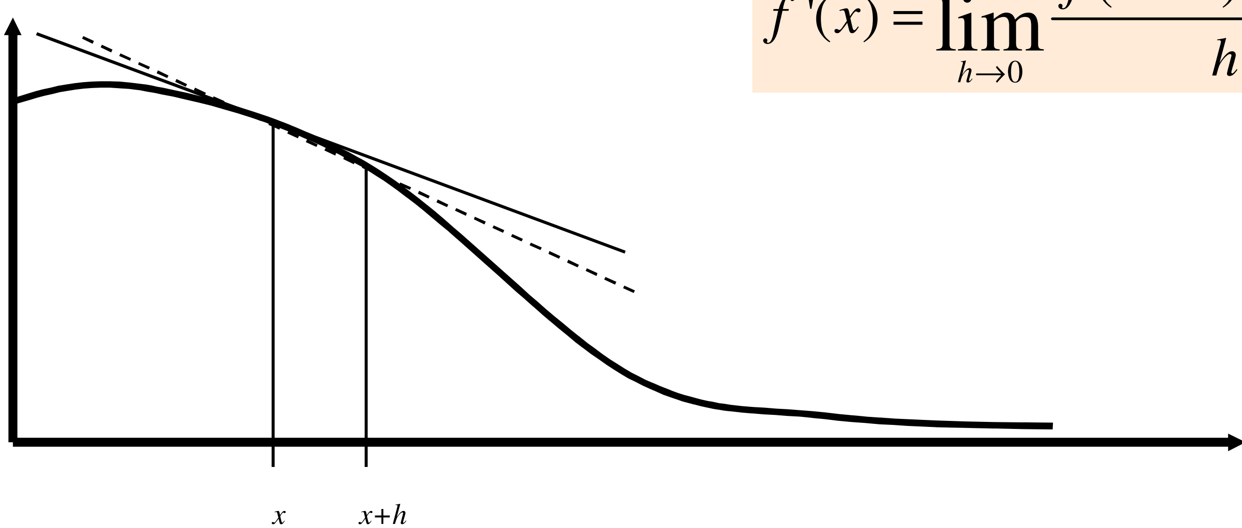
- Can also be thought of as the tangent line.



Numerical Differentiation

- One can not calculate the limit as h goes to zero, so one need to approximate it.
- Apply directly for a non-zero h leads to the slope of the secant curve.

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$



Numerical Differentiation

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \qquad error = O(h)$$

- This is called **Forward Differences** and can be derived using Taylor's Series:

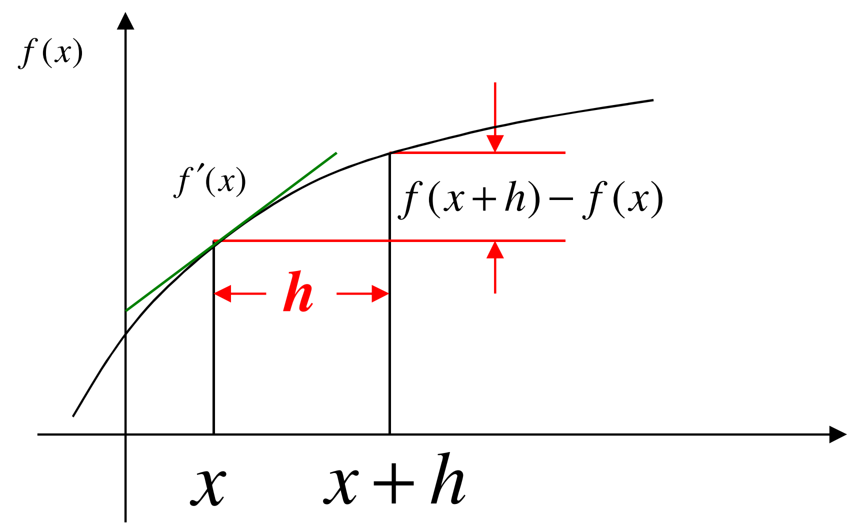
$$f(x+h) = f(x) + f'(x)h + f''(\xi)\frac{h^2}{2!}$$

$$\therefore f(x+h) - f(x) = f'(x)h + f''(\xi)\frac{h^2}{2!}$$

$$\therefore f'(x) = \frac{f(x+h) - f(x)}{h} - \cancel{f''(\xi)\frac{h}{2!}}$$

$$\therefore \frac{f(x+h) - f(x)}{h} \rightarrow f'(x) \;\; as \;\; h \rightarrow 0$$

Geometrically



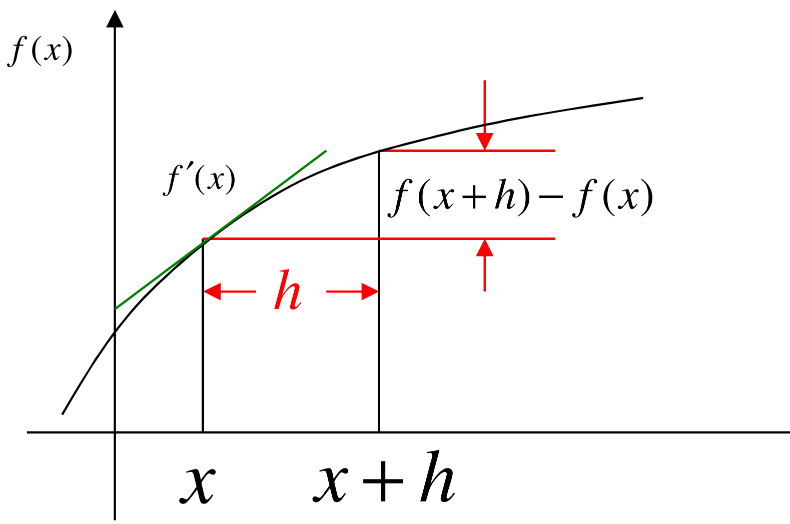
Theoretically speaking

Truncation Errors

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \qquad error = O(h)$$

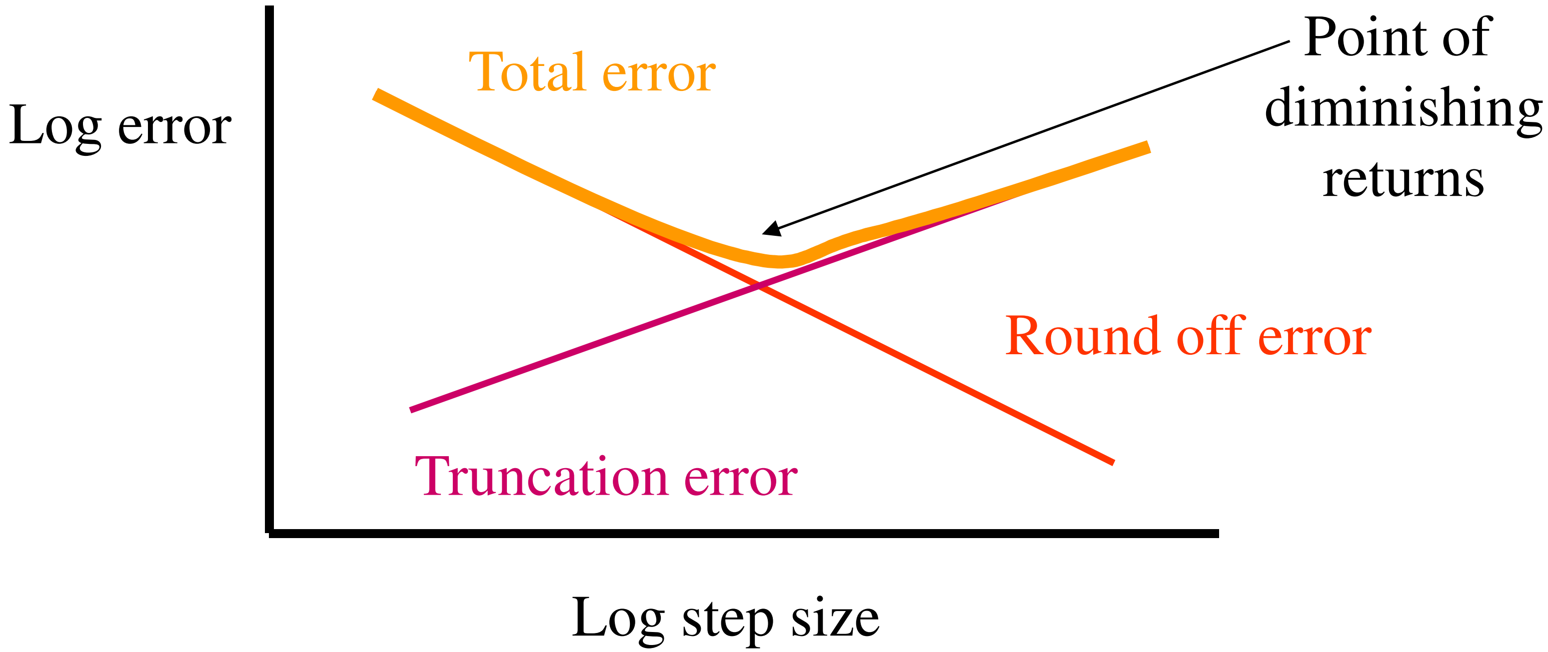
- Let $f(x)$ = a+e, and $f(x+h)$ = a+f.
- Then, as h approaches zero, e<<a and f<<a.
- With limited precision on our computer, our representation of $f(x) \approx a \approx f(x+h)$.
- One can easily get a random round-off bit as the most significant digit in the subtraction.
- Dividing by h, leads to a very wrong answer for $f'(x)$.

Geometrically



Error Tradeoff

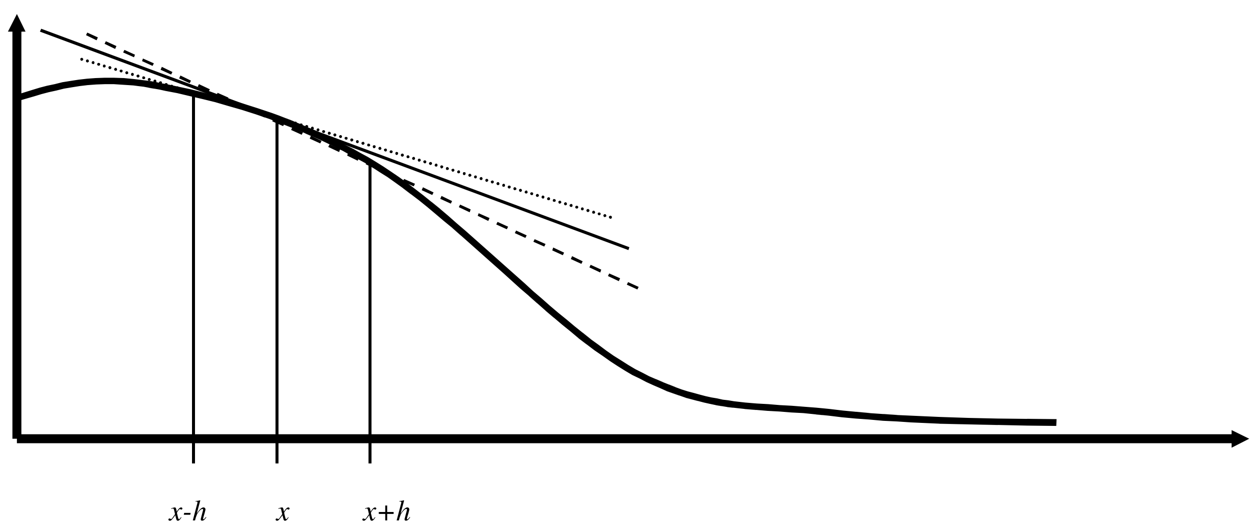
- Using a smaller step size reduces truncation error.
- However, it increases the round-off error.
- Trade off/diminishing returns occurs: Always think and test!



Numerical Differentiation

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \qquad error = O(h)$$

- This formula favors (or biases towards) the right-hand side of the curve.
- Why not use the left?



Numerical Differentiation

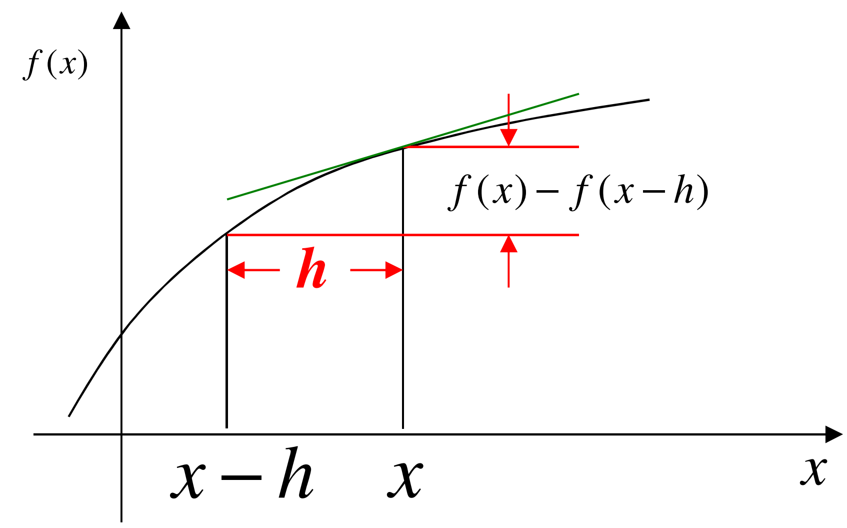
- This leads to the **Backward Differences** formula.

$$f(x-h) = f(x) - f'(x)h + f''(\xi)\frac{h^2}{2!}$$

$$\therefore f'(x) = \frac{f(x)-f(x-h)}{h} + f''(\xi)\frac{h}{2!}$$

$$\therefore \frac{f(x)-f(x-h)}{h} \to f'(x) \; as \; h \to 0$$

Geometrically



Numerical Differentiation

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \qquad error = O(h)$$

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$

$$error = O(h)$$

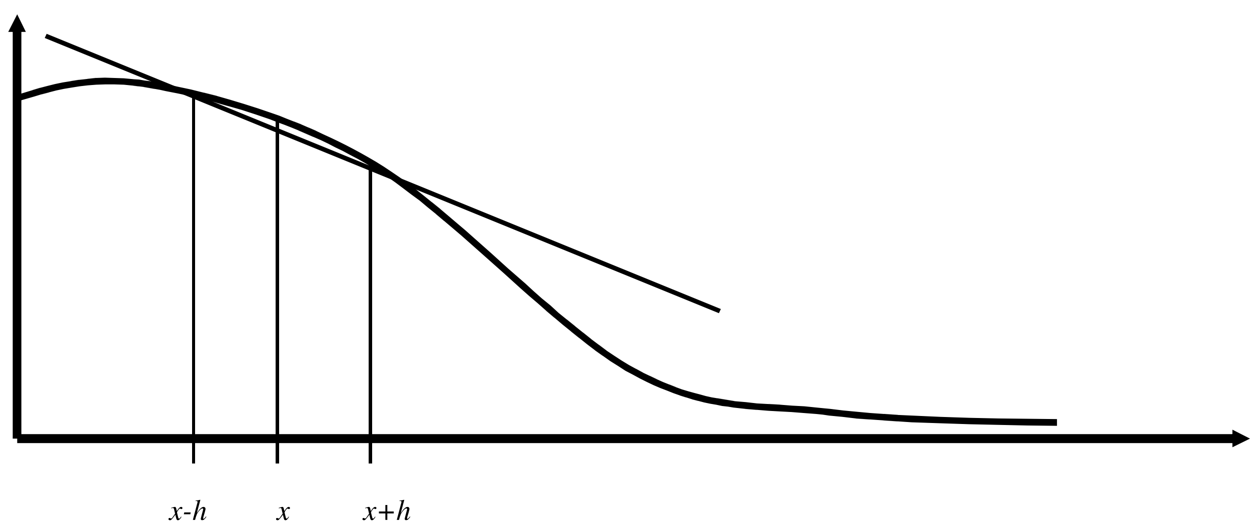
- Can do better?
- Let's average the two:

$$f'(x) \approx \frac{1}{2}\left(\underbrace{\frac{f(x+h) - f(x)}{h}}_{Forward\ difference} + \underbrace{\frac{f(x) - f(x-h)}{h}}_{Backward\ difference} \right) = \frac{f(x+h) - f(x-h)}{2h}$$

This is called the **Central Difference** formula.

Central Differences

- This formula does not *seem* very good.
  - It does not follow the calculus formula.
  - It takes the slope of the secant with width 2h.
  - The actual point interested in is not even evaluated.



Numerical Differentiation

- Is this any better?
- Let's use Taylor's Series to examine the error:

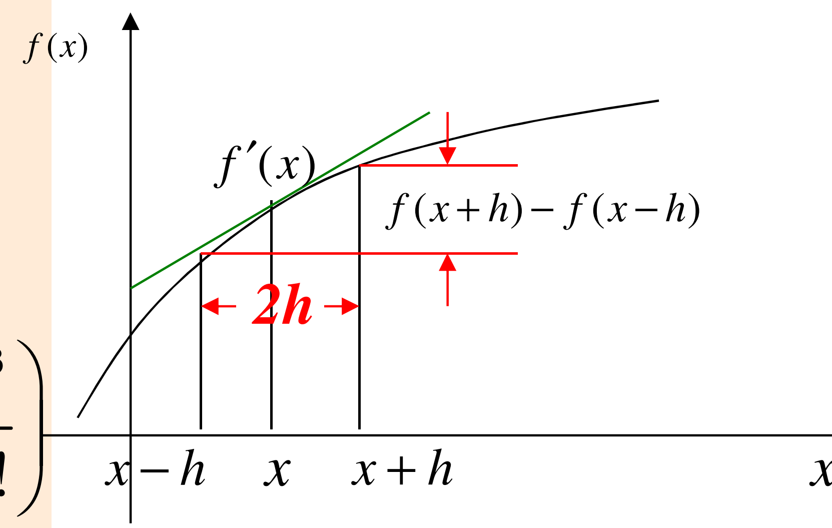
$$f(x+h)=f(x)+f'(x)h+f''(x)\frac{h^2}{2}+f'''(\xi)\frac{h^3}{3!}$$

$$f(x-h)=f(x)-f'(x)h+f''(x)\frac{h^2}{2}-f'''(\varsigma)\frac{h^3}{3!}$$

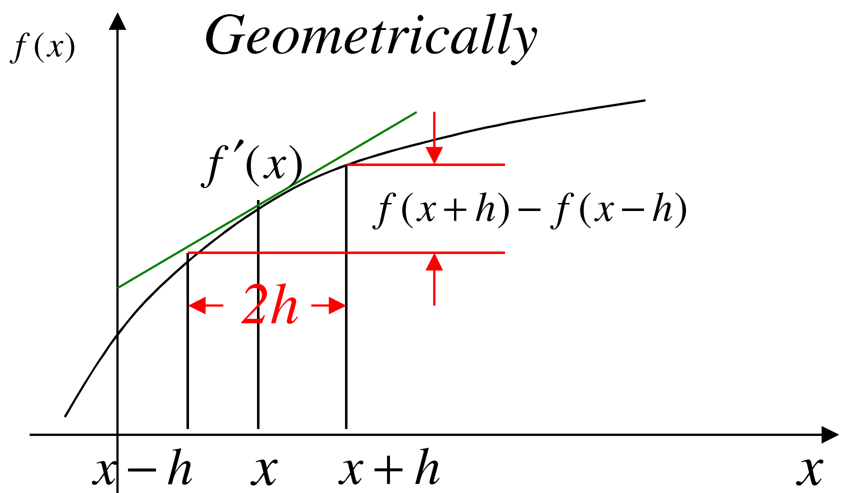
subtracting

$$f(x+h)-f(x-h)=2f'(x)h+\left(f'''(\xi)\frac{h^3}{3!}+f'''(\varsigma)\frac{h^3}{3!}\right)$$

Geometrically



Central Differences



- The central differences formula has much better convergence.

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{1}{6} f'''(\zeta) h^2, \zeta \in [x-h, x+h]$$

- Approaches the derivative as h^2 goes to zero!!

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O\left(h^2\right)$$

Recall

$$\frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Taylor Theorem:

$$f(x+h) = f(x) + f'(x)h + \frac{f^{(2)}(x)h^2}{2!} + \frac{f^{(3)}(x)h^3}{3!} + O(h^4)$$

$$E = O(h^n) \Rightarrow \exists\, real,\ finite\ C,\ \ such\ that: |E| \le C|h|^n$$

E is of order $h^n \Rightarrow E$ is approaching zero at rate similar to h^n

Three Formulas

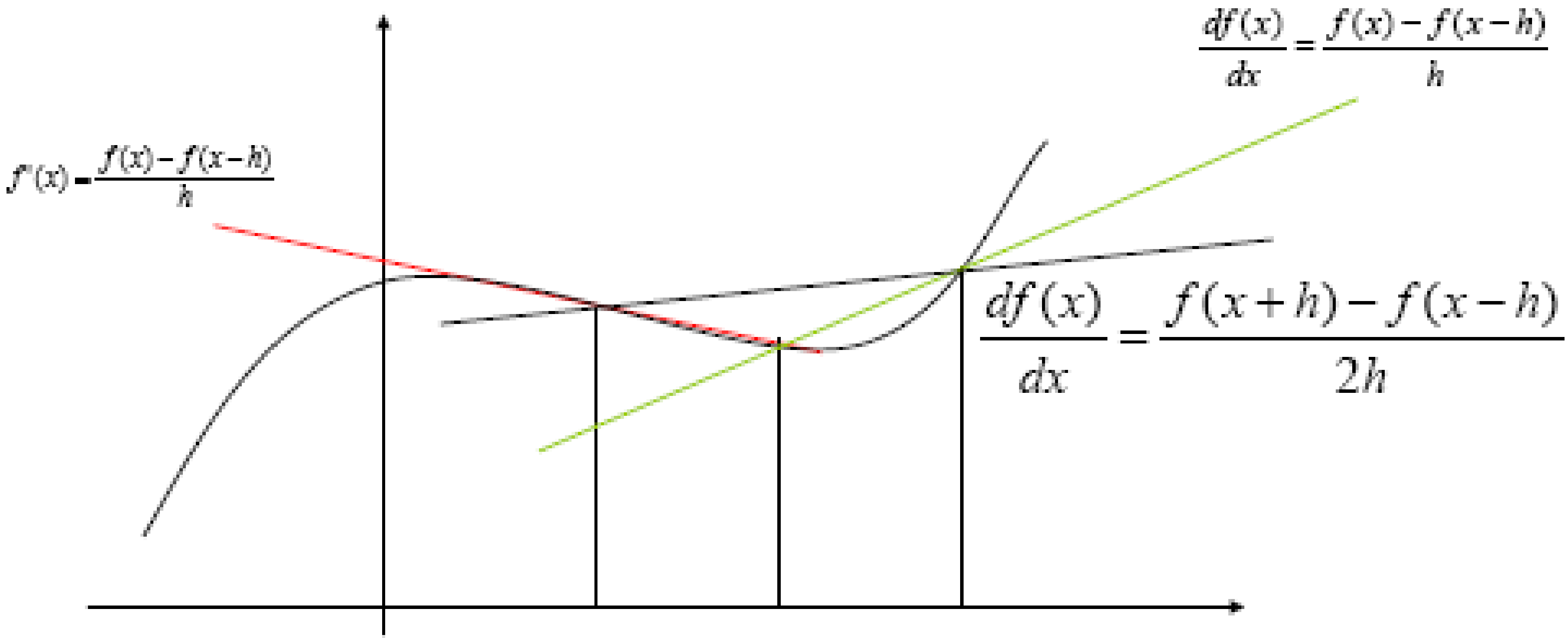
Forward Difference: $$\frac{df(x)}{dx} = \frac{f(x+h) - f(x)}{h}$$

Backward Difference: $$\frac{df(x)}{dx} = \frac{f(x) - f(x-h)}{h}$$

Central Difference: $$\frac{df(x)}{dx} = \frac{f(x+h) - f(x-h)}{2h}$$

Which method is better? How to judge?

The Three Formulas



Forward/Backward Difference Formula

Forward Difference:

$$f(x+h) = f(x) + f'(x)h + O(h^2)$$

$$\Rightarrow f'(x)h = f(x+h) - f(x) + O(h^2)$$

$$\Rightarrow f'(x) = \frac{f(x+h) - f(x)}{h} + O(h)$$

Backward Difference:

$$f(x-h) = f(x) - f'(x)h + O(h^2)$$

$$\Rightarrow f'(x)h = f(x) - f(x-h) + O(h^2)$$

$$\Rightarrow f'(x) = \frac{f(x) - f(x-h)}{h} + O(h)$$

Central Difference Formula

Central Difference:

$$f(x+h) = f(x) + f'(x)h + \frac{f^{(2)}(x)h^2}{2!} + \frac{f^{(3)}(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} + \dots$$

$$f(x-h) = f(x) - f'(x)h + \frac{f^{(2)}(x)h^2}{2!} - \frac{f^{(3)}(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} + \dots$$

$$f(x+h) - f(x-h) = 2f'(x)h + 2\frac{f^{(3)}(x)h^3}{3!} + \dots$$

$$\Rightarrow \quad f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

The Three Formulas (Revisited)

Forward Difference : $$\frac{df(x)}{dx} = \frac{f(x+h) - f(x)}{h} + O(h)$$

Backward Difference : $$\frac{df(x)}{dx} = \frac{f(x) - f(x-h)}{h} + O(h)$$

Central Difference : $$\frac{df(x)}{dx} = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

Forward and backward difference formulas are comparable in accuracy.
Central difference formula is expected to give a better answer.

Warning

- Still have truncation error problem.
- Consider the case of:
- Build a table with smaller values of *h*.
- What about large values of *h* for this function?

$$f(x) = \frac{x}{100}$$

$$f'(x) \approx \frac{\left\lfloor \frac{x+h}{100} \right\rfloor - \left\lfloor \frac{x-h}{100} \right\rfloor}{2h}$$

$at \;\; x = 1, h = 0.000333, with\; 6\; significant\; digit$

$$f'(x) \approx \frac{0.0100033 - 0.0099966}{0.000666666} = 0.010050$$

Relative error:

$$\frac{|0.01 - 0.010050|}{0.01} = 0.5\%$$

$$f(x) = \frac{x}{100}$$

$$f'(x) \approx \frac{\left\lfloor \frac{x+h}{100} \right\rfloor - \left\lfloor \frac{x-h}{100} \right\rfloor}{2h}$$

$at \;\; x = 1, h = 0.0003 \; with \; 4 \; significant\; digits$

$$f'(x) \approx \frac{0.010003 - 0.0099}{0.0006} = 0.0100$$

Relative error: 1%

Second Derivatives

- What if one need the second derivative?

$$f(x+h) = f(x) + f'(x)h + f''(x)\frac{h^2}{2} + f'''(x)\frac{h^3}{3!} + f^{(4)}(x)\frac{h^4}{4!} + f^{(5)}(x)\frac{h^5}{5!} + \cdots$$

$$f(x-h) = f(x) - f'(x)h + f''(x)\frac{h^2}{2} - f'''(\varsigma)\frac{h^3}{3!} + f^{(4)}(x)\frac{h^4}{4!} - f^{(5)}(x)\frac{h^5}{5!} + \cdots$$

- Any guesses?

Second Derivatives

- Let's cancel out the odd derivatives and double up the even ones:
  - Implies adding the terms together.

$$f(x+h)+f(x-h)=2f(x)+2f''(x)\frac{h^2}{2}+2f^{(4)}(x)\frac{h^4}{4!}+\cdots$$

Second Derivatives

$$f(x+h)+f(x-h)=2f(x)+2f''(x)\frac{h^2}{2}+\cancel{2f^{(4)}(x)\frac{h^4}{4!}}+\cdots$$

- Isolating the second derivative term yields:

$$f''(x)\approx\frac{f(x+h)-2f(x)+f(x-h)}{h^2}$$

- With an error term of:

$$E=-\frac{1}{12}h^2f^{(4)}(\xi)$$

Higher Order Formulas

$$f(x+h) = f(x) + f'(x)h + \frac{f^{(2)}(x)h^2}{2!} + \frac{f^{(3)}(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} + \ldots$$

$$f(x-h) = f(x) - f'(x)h + \frac{f^{(2)}(x)h^2}{2!} - \frac{f^{(3)}(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} + \ldots$$

$$f(x+h) + f(x-h) = 2f(x) + 2\frac{f^{(2)}(x)h^2}{2!} + 2\frac{f^{(4)}(x)h^4}{4!} + \ldots$$

$$\Rightarrow \quad f^{(2)}(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2)$$

$$\boxed{Error = -\frac{f^{(4)}(\xi)h^2}{12}}$$

Other Higher Order Formulas

$$f^{(2)}(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

$$f^{(3)}(x) = \frac{f(x+2h) - 2f(x+h) + 2f(x-h) - f(x-2h)}{2h^3}$$

$$f^{(4)}(x) = \frac{f(x+2h) - 4f(x+h) + 6f(x) - 4f(x-h) + f(x-2h)}{h^4}$$

Other formulas for $f^{(2)}(x), f^{(3)}(x)\ldots$ are also possible.

Use Taylor Theorem to prove them and obtain the error order.

2D or Partial Derivatives

- Remember: Nothing special about partial derivatives

$$\frac{\partial f}{\partial x}(x, y) \approx \frac{f(x+h, y) - f(x-h, y)}{2h}$$

$$\frac{\partial f}{\partial y}(x, y) \approx \frac{f(x, y+h) - f(x, y-h)}{2h}$$

3D or Partial Derivatives

$$\frac{\partial f}{\partial x}(x, y, z) \approx \frac{f(x+h, y, z) - f(x-h, y, z)}{2h}$$

$$\frac{\partial f}{\partial y}(x, y, z) \approx \frac{f(x, y+h, z) - f(x, y-h, z)}{2h}$$

$$\frac{\partial f}{\partial z}(x, y, z) \approx \frac{f(x, y, z+h) - f(x, y, z-h)}{2h}$$

Richardson Extrapolation

- Can do better?
- Is choice of *h*, a good one?
- Let's subtract the two Taylor Series expansions again:

$$f(x+h) = f(x) + f'(x)h + f''(x)\frac{h^2}{2} + f'''(x)\frac{h^3}{3!} + f^{(4)}(x)\frac{h^4}{4!} + f^{(5)}(x)\frac{h^5}{5!} + \cdots$$

$$f(x-h) = f(x) - f'(x)h + f''(x)\frac{h^2}{2} - f'''(\varsigma)\frac{h^3}{3!} + f^{(4)}(x)\frac{h^4}{4!} - f^{(5)}(x)\frac{h^5}{5!} + \cdots$$

subtracting

$$f(x+h) - f(x-h) = 2f'(x)h + 2\frac{f'''(x)}{3!}h^3 + 2\frac{f'''(x)}{3!}h^3 + 2f^{(5)}(x)\frac{h^5}{5!} + \cdots$$

Richardson Extrapolation

$$f(x+h)-f(x-h)=2f'(x)h+2\frac{f'''(x)}{3!}h^3+2\frac{f'''(x)}{3!}h^3+2f^{(5)}(x)\frac{h^5}{5!}+\cdots$$

- Assuming the higher derivatives exist, one can hold *x* fixed (which also fixes the values of *f(x)*), to obtain the following formula.

$$f'(x)=\frac{1}{2h}\left[f(x+h)-f(x-h)\right]+a_2h^2+a_4h^4+a_6h^6+\cdots$$

- Richardson Extrapolation examines the operator below as a function of *h*.

$$\varphi(h)=\frac{1}{2h}\left[f(x+h)-f(x-h)\right]$$

Richardson Extrapolation

$$f'(x) = \frac{1}{2h}\left[f(x+h) - f(x-h)\right] + a_2h^2 + a_4h^4 + a_6h^6 + \cdots$$

- This function approximates *f'(x)* to O(h^2) as saw earlier.
- Let's look at the operator as *h* goes to zero.

$$\varphi(h) = f'(x) - a_2h^2 - a_4h^4 - a_6h^6 - \cdots$$

$$\varphi(\frac{h}{2}) = f'(x) - a_2\left(\frac{h}{2}\right)^2 - a_4\left(\frac{h}{2}\right)^4 - a_6\left(\frac{h}{2}\right)^6 - \cdots$$

Same leading constants

Richardson Extrapolation

- Using these two formula's, one can come up with another estimate for the derivative that cancels out the h^2 terms.

$$\varphi(h) - 4\varphi(\frac{h}{2}) = -3f'(x) - \frac{3}{4}a_4 h^4 - \frac{15}{16}a_6 h^6 - \ldots$$

or

$$f'(x) = \varphi(\frac{h}{2}) + \frac{1}{3}\left[\varphi(\frac{h}{2}) - \varphi(h)\right] + O\left(h^4\right)$$

Extrapolates by assuming the new estimate undershot.

new estimate

difference between old and new estimates

Richardson Extrapolation

$$\varphi(h) - 4\varphi(\frac{h}{2}) = -3f'(x) - \frac{3}{4}a_4h^4 - \frac{15}{16}a_6h^6 - \cdots$$

or

$$f'(x) = \varphi(\frac{h}{2}) + \frac{1}{3}\left[\varphi(\frac{h}{2}) - \varphi(h)\right] + O\left(h^4\right)$$

- If h is small ($h<<1$), then h^4 goes to zero much faster than h^2.
- Cool!!!
- Can cancel out the h^6 term?
  - Yes, by using h/4 to estimate the derivative.

Richardson Extrapolation

- Consider the following *property*:

$$\varphi(h) = f'(x) - \sum_{k=1}^{\infty} a_{2k} h^{2k}$$
$$= L - \sum_{k=1}^{\infty} a_{2k} h^{2k}$$

- where L is unknown,

$$L = \lim_{h \to 0} \varphi(h) = f'(x)$$

as are the coefficients, a_{2k}.

Richardson Extrapolation

- Do not forget the formal definition is simply the central-differences formula:

$$\varphi(h) = \frac{1}{2h}\left[f(x+h) - f(x-h)\right]$$

- New symbology *(is this a word?)*:

$$D(n,0) \equiv \varphi\left(\frac{h}{2^n}\right)$$

$$= L + \sum_{k=1}^{\infty} A(k,0)\left(\frac{h}{2^n}\right)^{2k}$$

From previous slide

Richardson Extrapolation

- D(n,0) is just the central differences operator for different values of *h*.
- Proceed by computing D(n,0) for several values of n.
- Recalling our cancellation of the h^2 term.

$$
\begin{aligned}
f'(x) &= \varphi(\frac{h}{2}) + \frac{1}{3}\left[\varphi(\frac{h}{2}) - \varphi(h)\right] + O\left(h^4\right) \\
&= D(1,0) + \frac{1}{4-1}\left[D(1,0) - D(0,0)\right] + O\left(h^4\right)
\end{aligned}
$$

Richardson Extrapolation

- If let $h \rightarrow h/2$, then in general, one can write:

$$f'(x) = D(n,0) + \frac{1}{4-1}\left[D(n,0) - D(n-1,0)\right] + O\left(\left(\frac{h}{2^n}\right)^4\right)$$

- Let's denote this operator as:

$$D\left(n,1\right) = D(n,0) + \frac{1}{4^1 - 1}\left[D\left(n,0\right) - D\left(n-1,0\right)\right]$$

Richardson Extrapolation

- Now, one can formally define Richardson's extrapolation operator as:

$$D(n,m)=\frac{4^m}{4^m-1}D(n,m-1)-\frac{1}{4^m-1}D(n-1,m-1),\quad (1\le m\le n)$$

new estimate *old estimate*

- or

$$D(n,m)=D(n,m-1)+\frac{1}{4^m-1}\left[D(n,m-1)-D(n-1,m-1)\right]$$

Richardson Extrapolation

- Now, one can formally define Richardson's extrapolation operator as:

$$D(n,m) = D(n,m-1) + \frac{1}{4^m - 1}\left[D(n,m-1) - D(n-1,m-1)\right]$$

$$D(n,m) = \frac{1}{4^m - 1}\left[4^m D(n,m-1) - D(n-1,m-1)\right]$$

Memorize me!!!!

Richardson Extrapolation Theorem

- These terms approach *f'(x)* very quickly.

$$D(n,m) = L + \sum_{k=m+1}^{\infty} A(k,m)\left(\frac{h}{2^n}\right)^{2k}$$

Order starts much higher!!!!

Richardson Extrapolation

- Since $m \le n$, this leads to a two-dimensional triangular array of values as follows:

$$
\begin{array}{lllll}
D(0,0) & & & & \\
D(1,0) & D(1,1) & & & \\
D(2,0) & D(2,1) & D(2,2) & & \\
\quad \mathrm{M} & \quad \mathrm{M} & \quad \mathrm{M} & \mathrm{O} & \\
D(N,0) & D(N,1) & D(N,2) & \mathrm{L} & D(N,N)
\end{array}
$$

- One must pick an initial value of h and a max iteration value N.

Richardson Extrapolation

Central Difference: $f'(x)=\dfrac{f(x+h)-f(x-h)}{2h}+O(h^2)$

Can we get a better formula?

Hold $f(x)$ *and* x *fixed:*

$$\phi(h)=\frac{f(x+h)-f(x-h)}{2h}$$

$$\phi(h)=f'(x)-a_2h^2-a_4h^4-a_6h^6-\ldots$$

Richardson Extrapolation

$Hold\ \ f(x)\ and\ \ x\ \ fixed:$

$$\phi(h) = \frac{f(x+h) - f(x-h)}{2h}$$

$$\phi(h) = f'(x) - a_2 h^2 - a_4 h^4 - a_6 h^6 - \ldots$$

$$\phi(\frac{h}{2}) = f'(x) - a_2\left(\frac{h}{2}\right)^2 - a_4\left(\frac{h}{2}\right)^4 - a_6\left(\frac{h}{2}\right)^6 - \ldots$$

$$\phi(h) - 4\phi(\frac{h}{2}) = -3f'(x) - \frac{3}{4}a_4 h^4 - \frac{15}{16}a_6 h^6 - \ldots$$

$$\Rightarrow f'(x) = \frac{\phi(h) - 4\phi(\frac{h}{2})}{-3} + O\left(h^4\right)$$

Richardson Extrapolation Table

$D(0,0)=\Phi(h)$			
$D(1,0)=\Phi(h/2)$	$D(1,1)$		
$D(2,0)=\Phi(h/4)$	$D(2,1)$	$D(2,2)$	
$D(3,0)=\Phi(h/8)$	$D(3,1)$	$D(3,2)$	$D(3,3)$

Richardson Extrapolation Table

$$First\ Column:\quad D(n,0) = \phi\left(\frac{h}{2^n}\right)$$

$$Others:$$

$$D(n,m) = D(n,m-1) + \frac{1}{4^m - 1}\left[D(n,m-1) - D(n-1,m-1)\right]$$

$$D(n,m) = \frac{1}{4^m - 1}\left[4^m D(n,m-1) - D(n-1,m-1)\right]$$

Example 1

$$D(n,m)=\frac{4^m}{4^m-1}D(n,m-1)-\frac{1}{4^m-1}D(n-1,m-1),\quad (1\le m\le n)$$

$$f(x)=\frac{\left(\cos(100x^2)\right)^5}{x^3}$$

$$x=1.3,\ h=\frac{1}{128}$$

$$D(n,m)=\frac{1}{4^m-1}\left[4^m D(n,m-1)-D(n-1,m-1)\right]$$

f' = - (3cos(100x^2)^5)/x^4 - 1000cos(100x^2)^4sin(100x^2))/x^2

$$f(x)=\frac{\left(\cos(100x^2)\right)^5}{x^3}$$

$$x=1.3,\ h=\frac{1}{128}$$

$$D(0,0)=16.696386$$
$$D(1,0)=40.583393$$
$$D(2,0)=109.322528$$
$$D(3,0)=135.031747$$
$$D(4,0)=142.068615$$
$$D(5,0)=143.866937$$

Forward Difference $\frac{df(x)}{dx}=\frac{f(x+h)-f(x)}{h}+O(h)$

Backward Difference $\frac{df(x)}{dx}=\frac{f(x)-f(x-h)}{h}+O(h)$

Central Difference $\frac{df(x)}{dx}=\frac{f(x+h)-f(x-h)}{2h}+O(h^2)$

$$D(0,0),D(1,0)\longrightarrow D(1,1)$$

$$f(x)=\frac{\left(\cos(100x^2)\right)^5}{x^3}$$

$$x=1.3,\ h=\frac{1}{128}$$

Example 1

$$\Phi(h)=\frac{f(x+h)-f(x-h)}{2h}=D(0,0)=16.696386$$

$$\Phi(\frac{h}{2})=\frac{f(1.3039)-f(1.296)}{0.0078}=40.583393=D(1,0)$$

$$\Phi(\frac{h}{4})=\frac{f(1.3019)-f(1.2980)}{0.0039}=109.322528=D(2,0)$$

$$\Phi(\frac{h}{8})=\frac{f(1.3009)-f(1.2990)}{0.00195}=135.031747=D(3,0)$$

$$\Phi(\frac{h}{16})=\frac{f(1.30048)-f(1.29951)}{0.00095}=142.068615=D(4,0)$$

$$\Phi(\frac{h}{32})=\frac{f(1.30024)-f(1.29975)}{0.00048}=143.866937=D(5,0)$$

Example 1

$$D(n,m) = \frac{1}{4^m - 1}\left[4^m D(n,m-1) - D(n-1,m-1)\right]$$

$D(0,0) = 16.696386$, $\mathrm{D}(1,0) = 40.583393$, $\mathrm{D}(2,0) = 109.322528$

$$D(n,m) = D(n,m\text{-}1) + \frac{1}{4^m - 1}\left[D(n,m\text{-}1) - D(n-1,m\text{-}1)\right]$$

$$D(1,1) = D(1,0) + \frac{1}{4-1}\left[D(1,0) - D(0,0)\right] = 32.62105733$$

$$D(2,1) = D(2,0) + \frac{1}{4-1}\left[D(2,0) - D(1,0)\right] = 132.235574$$

$$D(3,1) = D(2,1) + \frac{1}{4^2-1}\left[D(2,1) - D(1,1)\right] = 143.601487$$

Example

$$D(n,m)=\frac{4^m}{4^m-1}D(n,m-1)-\frac{1}{4^m-1}D(n-1,m-1),\quad (1\le m\le n)$$

$$D(0,0)=16.696386$$

$$D(1,0)=40.583393 \qquad D(1,1)=48.583393$$

$$D(2,0)=109.322528 \qquad D(2,1)=132.235574$$

$$D(3,0)=135.031747 \qquad D(3,1)=143.601487$$

$$D(4,0)=142.068615 \qquad D(4,1)=144.414238$$

$$D(5,0)=143.866937 \qquad D(5,1)=144.466377$$

$$D(n,m)=\frac{1}{4^m-1}\left[4^m D(n,m-1)-D(n-1,m-1)\right]$$

$extrapolate\frac{1}{3}$

Example

$$D(0,0)=16.696386$$

$$D(1,0)=40.583393 \qquad D(1,1)=48.583393$$

$$D(2,0)=109.322528 \qquad D(2,1)=132.235574 \qquad D(2,2)=137.814897$$

$$D(3,0)=135.031747 \qquad D(3,1)=143.601487 \qquad D(3,2)=144.359214$$

$$D(4,0)=142.068615 \qquad D(4,1)=144.414238 \qquad D(4,2)=144.468421$$

$$D(5,0)=143.866937 \qquad D(5,1)=144.466377 \qquad D(5,2)=144.469853$$

$$extrapolate \frac{1}{15}$$

$$D(n,m)=\frac{1}{4^m-1}\left[4^m D(n,m-1)-D(n-1,m-1)\right]$$

Example

$$D(n,m)=\frac{4^m}{4^m-1}D(n,m-1)-\frac{1}{4^m-1}D(n-1,m-1),\quad (1\le m\le n)$$

16.696386					
40.583393	48.583393				
109.322528	132.235574	137.814897			
135.031747	143.601487	144.359214	144.463092		
142.068615	144.414238	144.468421	144.470154	144.470182	
143.866937	144.466377	144.469853	144.469876	144.469875	$D(5,5)=144.469875$

$extrapolate\,\frac{1}{3}$ $extrapolate\,\frac{1}{15}$ $extrapolate\,\frac{1}{63}$ $extrapolate\,\frac{1}{255}$ $extrapolate\,\frac{1}{1023}$

- **Which converges up to eight decimal places.**
- **Is it accurate?**

Example

- One can look at the (theoretical) error term on this example.

$$D(5,5) = L + \sum_{k=5+1}^{\infty} A(k,5)\left(\frac{h}{2^5}\right)^{2k}$$

$$= f'(1.3) + A(6,5)\left(\frac{1}{4096}\right)^{12} + \sum_{k=7}^{\infty} A(k,5)\left(\frac{h}{2^5}\right)^{2k}$$

2^{-144}

- Taking the derivative:

$$f'(1.3) = 144.469874253\mathrm{K}$$

Round-off error

Example 2

Evaluate numerically the derivative of :

$$f(x) = x^{\cos(x)} \qquad \text{at} \quad x = 0.6$$

Use Richardson Extrapolation with $h = 0.1$

Obtain D(2,2) as the estimate of the derivative.

f' = x^(cos(x) - 1)*cos(x) - x^cos(x)*log(x)*sin(x)

Example 2
First Column

$$f(x) = x^{\cos(x)} \text{ at } \quad x = 0.6 \text{ with } \quad h = 0.1$$

$$\Phi(h) = \frac{f(x+h) - f(x-h)}{2h}$$

$$\Phi(0.1) = \frac{f(0.7) - f(0.5)}{0.2} = 1.08483$$

$$\Phi(0.05) = \frac{f(0.65) - f(0.55)}{0.1} = 1.08988$$

$$\Phi(0.025) = \frac{f(0.625) - f(0.575)}{0.05} = 1.09115$$

Example 2
Richardson Table

$$D\left(n,m\right)=\frac{1}{4^m-1}\left[4^m D\left(n,m-1\right)-D\left(n-1,m-1\right)\right]$$

$$D(0,0)=1.08483\text{, D(1,0) = 1.08988, D(2,0)}=1.09115$$

$$D(n,m)=D(n,m\text{-}1)+\frac{1}{4^m-1}\left[D(n,m\text{-}1)-D(n-1,m\text{-}1)\right]$$

$$D(1,1)=D(1,0)+\frac{1}{4-1}\left[D(1,0)-D(0,0)\right]=1.09156$$

$$D(2,1)=D(2,0)+\frac{1}{4-1}\left[D(2,0)-D(1,0)\right]=1.09157$$

$$D(2,2)=D(2,1)+\frac{1}{4^2-1}\left[D(2,1)-D(1,1)\right]=1.09157$$

Example
Richardson Table

1.08483		
1.08988	1.09156	
1.09115	1.09157	1.09157

This is the best estimate of the derivative of the function.

All entries of the Richardson table are estimates of the derivative of the function.

The first column are estimates using the central difference formula with different h.

Richardson Extrapolation

- There are two ways to improve derivative estimates when employing finite divided differences:
  - Decrease the step size, or
  - Use a higher-order formula that employs more points.
- A third approach, based on **Richardson extrapolation**, uses two derivative estimates (with $O(h^2)$ error) to compute a third (with $O(h^4)$ error) , more accurate approximation. One can derive this formula following the same steps used in the case of the integrals:

$$h_2 = h_1 / 2 \quad \Rightarrow \quad \boxed{D \cong \frac{4}{3} D(h_2) - \frac{1}{3} D(h_1)}$$

High Accuracy Differentiation Formulas

- High-accuracy divided-difference formulas can be generated by including additional terms from the Taylor series expansion.

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

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

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

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

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

- Inclusion of the 2nd derivative term has improved the accuracy to $O(h^2)$.
- Similar improved versions can be developed for the *backward* and *centered* formulas

Forward finite-divided-difference formulas

First Derivative | **Error**

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

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

Second Derivative | **Error**

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

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

Backward finite-divided-difference formulas

First Derivative

Error

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

O(*h*)

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

O(*h*²)

Second Derivative

Error

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

O(*h*)

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

O(*h*²)

Centered finite-divided-difference formulas

First Derivative

Error

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

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

Second Derivative

Error

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

$$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}$$ **O(h^4)**

Derivation of the centered formula for $f''(x_i)$

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

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

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

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

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

Evaluate y = 1.2 -0 .25x - 0.5x^2 - 0.15x.^3 -0.1x^4 using MATLAB

Differentiation Using MATLAB

	x	*f(x)*
i-2	0	1.2
i-1	0.25	1.1035
i	0.50	0.925
i+1	0.75	0.6363
i+2	1	0.2

f(0) = 1.2
f(0.25) =1.1035
f(0.5) = 0.925
f(0.75) = 0.6363
f(1) = 0.2

First, create a file called **fx1.m** which contains y=f(x):

```
function y = fx1(x)
        y = 1.2 - .25*x - .5*x.^2 - .15*x.^3 -.1*x.^4 ;
```

Command window:

```
>> x=0:.25:1
     0     0.25     0.5     0.75     1
>> y = fx1(x)

   1.2    1.1035    0.925    0.6363    0.2

>> d = diff(y) ./ diff(x)    % diff() takes differences
   between consecutive vector elements

     d =   -0.3859   -0.7141   -1.1547   -1.7453
```

Forward: x = 0 0.25 0.5 0.75 1

Backward: x = 0.25 0.5 0.75 1

Example 3 :

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

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

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

At **x = 0.5** **True value** for First Derivative = **-0.9125**

Using finite divided differences and a step size of **h = 0.25** obtain:

	x	*f(x)*
i-2	0	1.2
i-1	0.25	1.1035
i	0.50	0.925
i+1	0.75	0.6363
i+2	1	0.2

	Forward *O(h)*	**Backward *O(h)***
Estimate	**-1.155**	**-0.714**
ε_t (%)	**26.5**	**21.7**

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

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

Forward difference of accuracy $O(h^2)$ is computed as:

$$f'(0.5) = \frac{-0.2 + 4(0.6363) - 3(0.925)}{2(0.25)} = -0.8593 \qquad \varepsilon_t = 5.82\%$$

Backward difference of accuracy $O(h^2)$ is computed as:

$$f'(0.5) = \frac{3(0.925) - 4(1.1035) + 1.2}{2(0.25)} = -0.8781 \qquad \varepsilon_t = 3.77\%$$

Derivatives of Unequally Spaced Data

- Derivation formulas studied so far (especially the ones with $O(h^2)$ error) require multiple points to be spaced evenly.

- Data from experiments or field studies are often collected at unequal intervals.

- Fit a ***Lagrange interpolating polynomial***, and then calculate the 1st derivative.

  As an example, second order *Lagrange interpolating polynomial* is used below*:*

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

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

Note that any three points, x_{i-1} x_i and x_{i+1} can be used to calculate the derivative.* ***The points do not need to be spaced equally.*