How to estimate error

Estimate errors

- Absolute error

$$|y_{ref} - y_{app}|$$

- Relative Error

$$\left|\frac{y_{ref} - y_{app}}{y_{ref}}\right|$$

Relative Error and Significant Digit

- The number of y_{app} is said to approximate y_{ref} to k significant digits if k is the largest non-negative integer for which

$$\frac{|y_{ref} - y_{app}|}{y_{ref}} < \frac{1}{0.1} \times 10^{-k} < 10 \times 10^{-k}$$

Example

- y_{ref} =0.123456789123456789

- 3 significant digit: $y_{app} = 0.123$

$$\left|\frac{y_{ref} - y_{app}}{y_{ref}}\right| = \left|\frac{0.000456789123456789}{0.123456789123456789}\right|$$

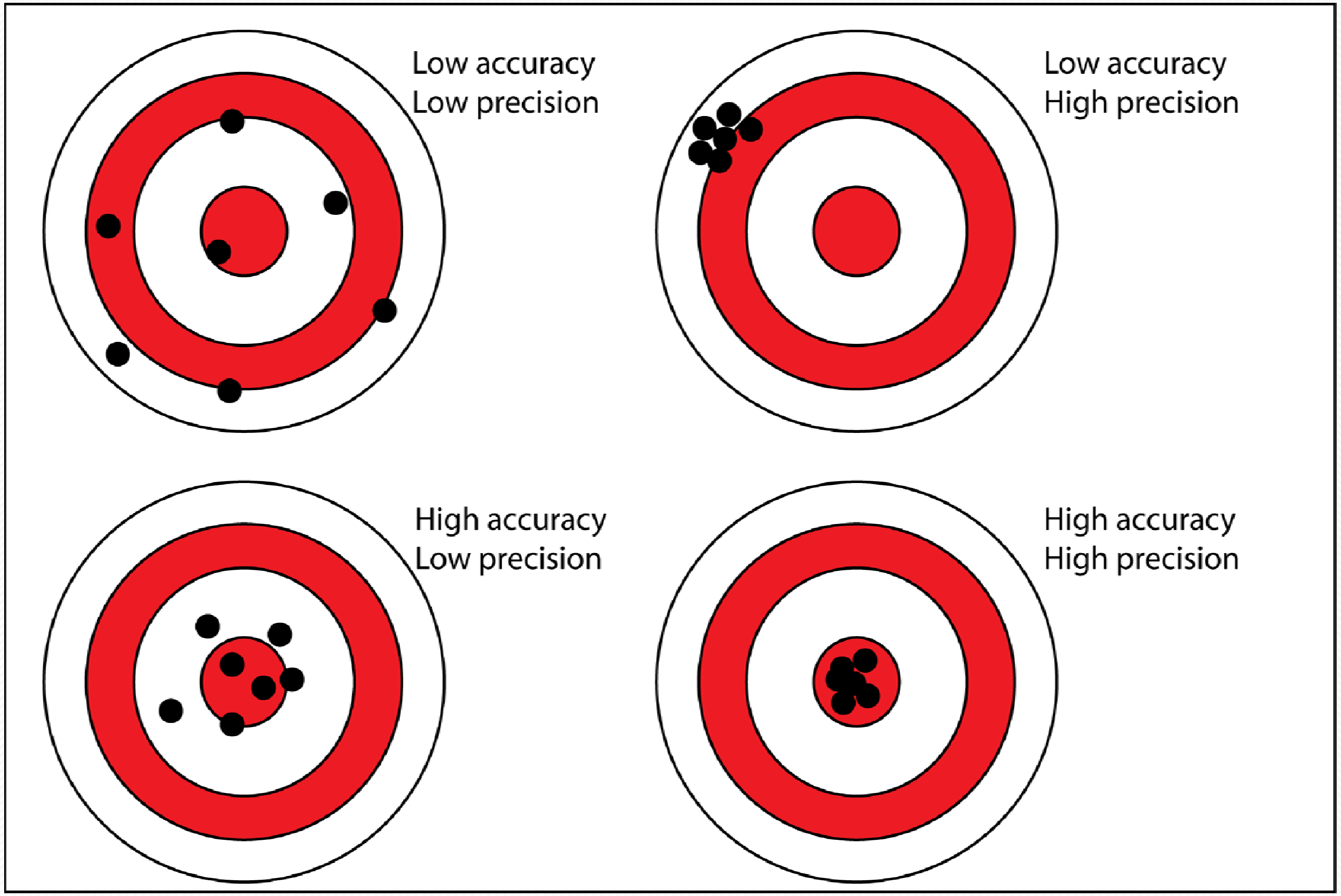
$$= 0.0037 < 10^{-2} = \ 10 \times 10^{-3}$$

- 6 significant digit $y_{app} = 0.123456$

$$\left|\frac{y_{ref} - y_{app}}{y_{ref}}\right| = \left|\frac{0.000000789123456789}{0.123456789123456789}\right|$$

$$= 6.4 \times 10^{-6} < \ 10 \times 10^{-6}$$

Accuracy(準確度) & Precision(精確度)



假如答案已知: My_exp() V.S. Exp()

```
N = 1, My_exp = 2.0000000000000000e+000, Exp = 2.7182818284590455e+000
N = 2, My_exp = 2.5000000000000000e+000, Exp = 2.7182818284590455e+000
N = 3, My_exp = 2.6666666666666665e+000, Exp = 2.7182818284590455e+000
N = 4, My_exp = 2.7083333333333330e+000, Exp = 2.7182818284590455e+000
N = 5, My_exp = 2.7166666666666663e+000, Exp = 2.7182818284590455e+000
N = 6, My_exp = 2.7180555555555554e+000, Exp = 2.7182818284590455e+000
N = 7, My_exp = 2.7182539682539684e+000, Exp = 2.7182818284590455e+000
N = 8, My_exp = 2.7182787698412700e+000, Exp = 2.7182818284590455e+000
N = 9, My_exp = 2.7182815255731922e+000, Exp = 2.7182818284590455e+000
N = 10, My_exp = 2.7182818011463845e+000, Exp = 2.7182818284590455e+000
N = 11, My_exp = 2.7182818261984929e+000, Exp = 2.7182818284590455e+000
N = 12, My_exp = 2.7182818282861687e+000, Exp = 2.7182818284590455e+000
N = 13, My_exp = 2.7182818284467594e+000, Exp = 2.7182818284590455e+000
N = 14, My_exp = 2.7182818284582302e+000, Exp = 2.7182818284590455e+000
N = 15, My_exp = 2.7182818284589949e+000, Exp = 2.7182818284590455e+000
```

假如答案未知: 只有近似值

- 假設運算次數越多，近似值會越一致。
- Set y_{ref}: 前一個近似值
  y_{app}: 目前的近似值

```
N = 1, My_exp = 2.0000000000000000e+000,
N = 2, My_exp = 2.5000000000000000e+000,
N = 3, My_exp = 2.6666666666666665e+000,
N = 4, My_exp = 2.7083333333333330e+000,
N = 5, My_exp = 2.7166666666666663e+000,
N = 6, My_exp = 2.7180555555555554e+000,
N = 7, My_exp = 2.7182539682539684e+000,
N = 8, My_exp = 2.7182787698412700e+000,
N = 9, My_exp = 2.7182815255731922e+000,
N = 10, My_exp = 2.7182818011463845e+000,
N = 11, My_exp = 2.7182818261984929e+000,
N = 12, My_exp = 2.7182818282861687e+000,
N = 13, My_exp = 2.7182818284467594e+000,
N = 14, My_exp = 2.7182818284582302e+000,
N = 15, My_exp = 2.7182818284589949e+000,
```

Numerical Differentiation

Goal:

Calculate Derivatives of all order at any point of any given function

BCCP: B.A. Stickler et al. Chap. 2

Computational Physics: R. Landau et. al. Chap. 6

Displacement, Velocity & Acceleration

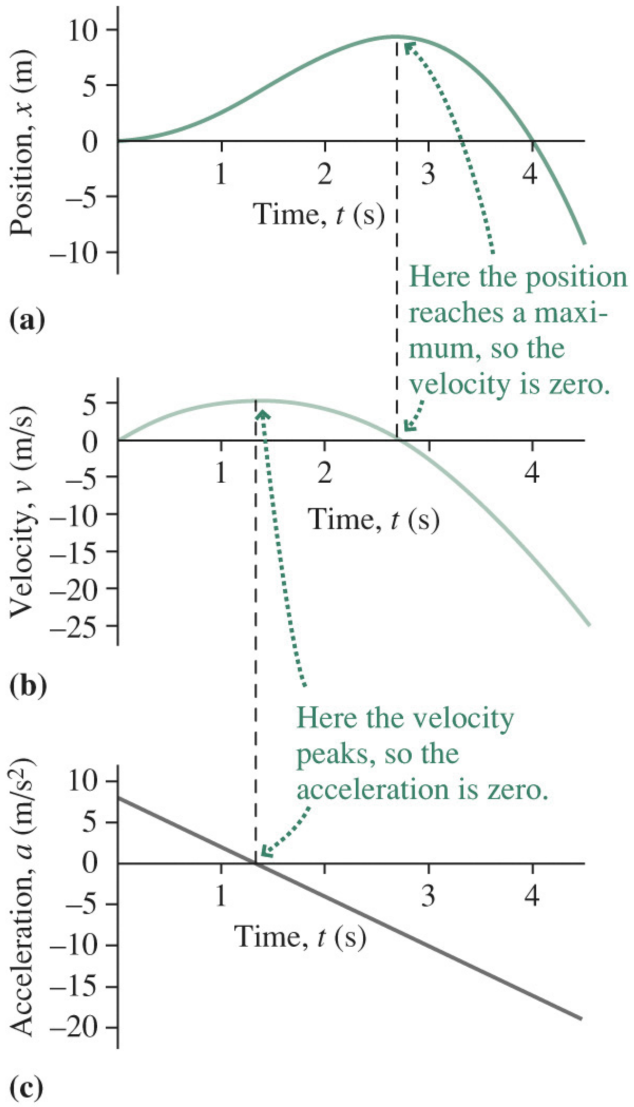
- **Displacement**
- $\Delta x = x_2 - x_1$
  $= x(t_i + \Delta t) - x(t_i)$

- **Instantaneous Velocity**

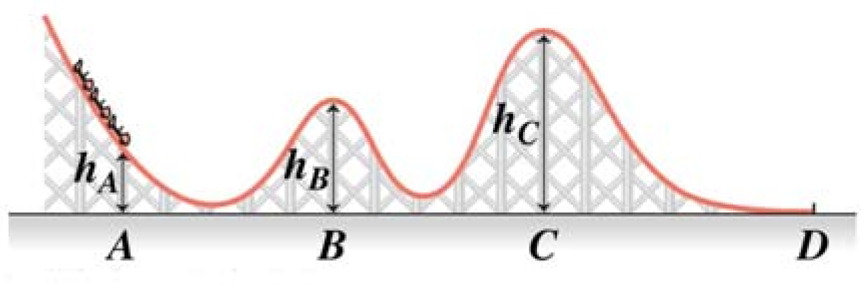
$$v = \lim_{\Delta t \to 0} \frac{\Delta x}{\Delta t} = \frac{dx}{dt}$$

- **Instantaneous Acceleration**

$$a = \lim_{\Delta t \to 0} \frac{\Delta v}{\Delta t} = \frac{dv}{dt}$$



7.4. Potential Energy Curves



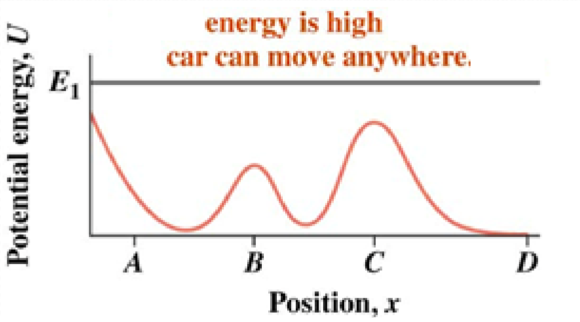
Frictionless roller-coaster track

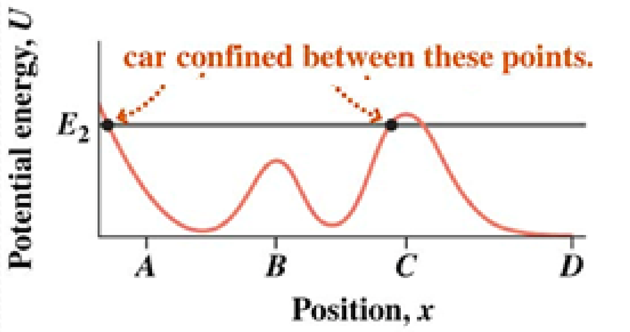
How fast must a car be coasting at point *A* if it's to reach point *D*?

Criterion: $E_A \ge U_C$

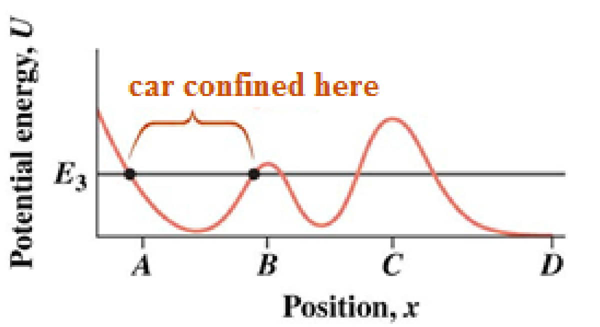
$$\frac{1}{2} m v_A^2 + m g h_A \ \ge \ m g h_C$$

$$v_A \ \ge \ \sqrt{2g\left(h_C - h_A \right)}$$





turning points



potential barrier

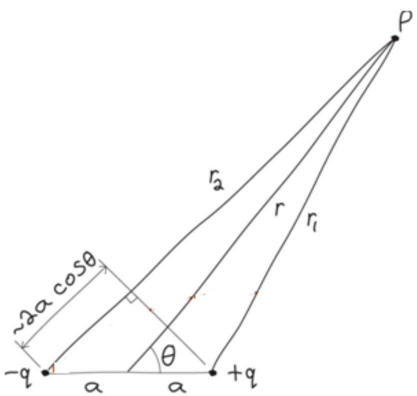
potential well

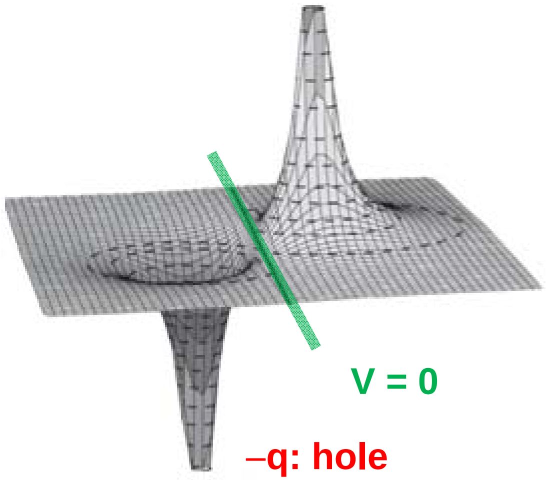
Dipole Potential

An electric dipole consists of point charges $\pm q$ a distance $2a$ apart.

Find the potential at an arbitrary point P, and approximate for the casewhere the distance to P is large compared with the charge separation.

$$V(P) = k\frac{q}{r_1} + k\frac{(-q)}{r_2} = kq\left(\frac{1}{r_1} - \frac{1}{r_2}\right) = kq\frac{r_2 - r_1}{r_2\, r_1}$$



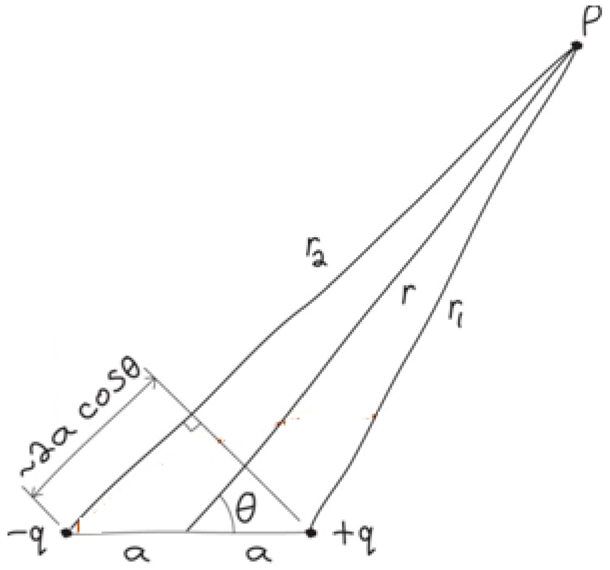


$p = 2qa$ = dipole moment

Dipole Field

An electric dipole consists of point charges $\pm q$ a distance $2a$ apart.

Find the potential at an arbitrary point P, and approximate for the casewhere the distance to P is large compared with the charge separation.



$$V(P) = k\frac{q}{r_1} + k\frac{(-q)}{r_2} \quad = kq\left(\frac{1}{r_1} - \frac{1}{r_2}\right) \quad = kq\,\frac{r_2 - r_1}{r_2\, r_1}$$

$$\vec{E}(\vec{r}) = -\frac{d}{d\vec{r}}V(\vec{r}) = -\nabla V(\vec{r})$$

$$E_x = -\frac{d}{dx}V(\vec{r})$$

$$E_z = -\frac{d}{dy}V(\vec{r})$$

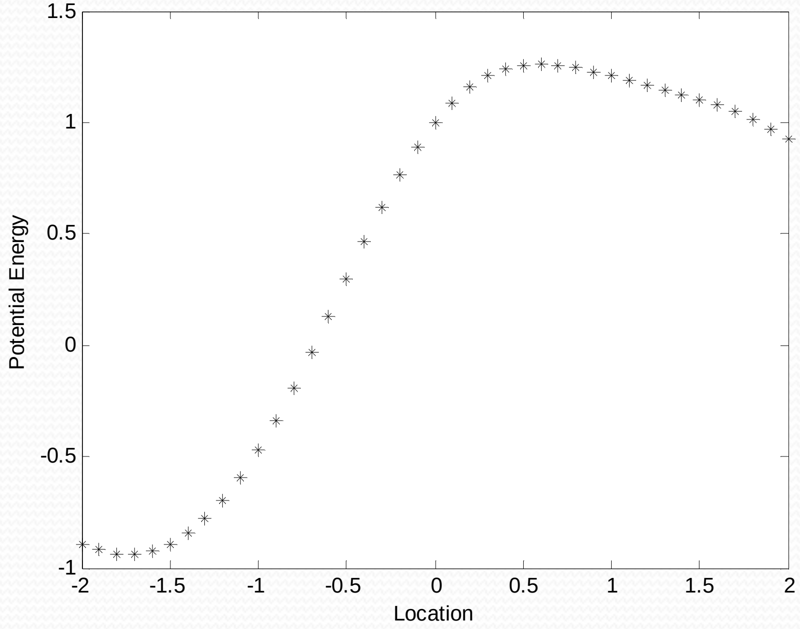
$$E_z = -\frac{d}{dz}V(\vec{r})$$

Problems to be solved

- Try to find the derivatives of a given function
  - Find f'(0.12345),

where f(x) = $Log(\sqrt{\sin\left(e^{-\left(x^2-2x+\frac{1}{e^x+e^{-x}}\right)}\right)}\ /(e^x + e^{-x^2})$

- Try to find the derivatives from a dataset



Numerical Differentiation

- Find the derivatives of any function @ any point
  - Forward / Backward Difference
  - Central Difference
- Optimize the solution
- Higher order derivative

Differentiation

- Definition of derivative

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

- Using Taylor Expansion on $f(x+h)$

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

Differentiation

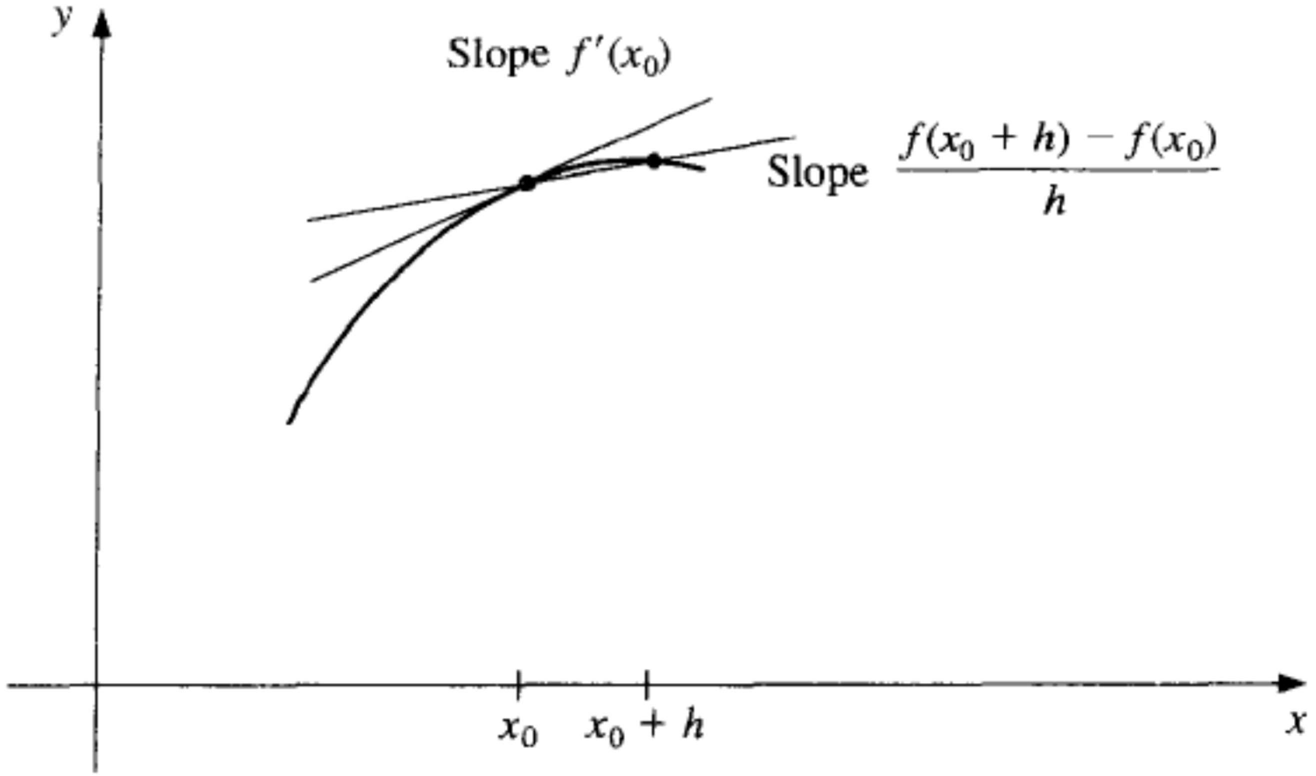
- Series of the derivative

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

- Approximation of a derivative

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

Differentiation



Forward Difference

- Use secant slope to approximate the slope of a tangent line.
- The error is of the order of h
- Smaller step MIGHT give better result.

Numerical Methods to calculate derivatives

- Forward Method/Backward Method/Central Difference
- N-pt Method
- Higher order Derivative
- Optimized Step Size

Backward Method

- Definition of derivative

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

- The Taylor series for $f(x-h)$

$$f(x-h) = f(x) - \frac{h}{1!} f'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f^{(3)}(x) + \ldots$$

Backward Method

- Series of the derivative

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

- Approximation of a derivative

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

Backward Difference

- Similar to Forward Difference, a secant slope is used to approximate the slope of a tangent line.

- Small step could lead to a better approximation

- The error is of the order of h

Example

- Find the numerical derivative of exp(x) at x = 1
- Take h = 0.1, 0.01 and 0.001

- exp(1)= 2.71828
- Derivative

$$f'(1) = \frac{d}{dx} e^x \Big|_{x=1} = e^1$$

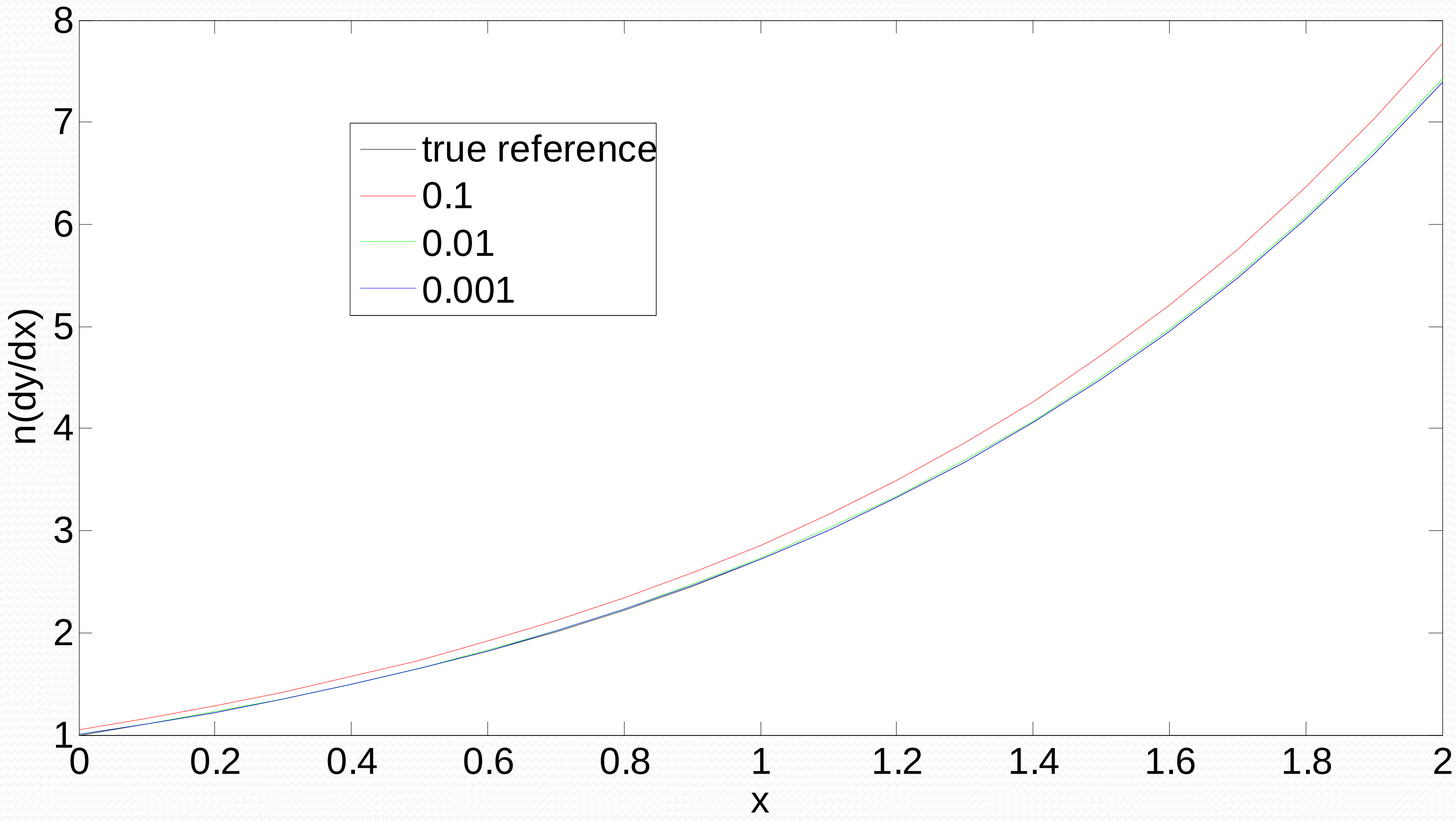
Example

h	exp(x-h)	exp(x)	exp(x+h)	Forward Difference	Error (Forward)	Backward Difference	Error (Backward)
0.1	2.45960	2.71828	3.00417	2.85884	0.14056	2.58679	0.13149
0.01	2.69123	2.71828	2.74560	2.73192	0.01364	2.70474	0.01355
0.001	2.71556	2.71828	2.72100	2.71964	0.00136	2.71692	0.00136

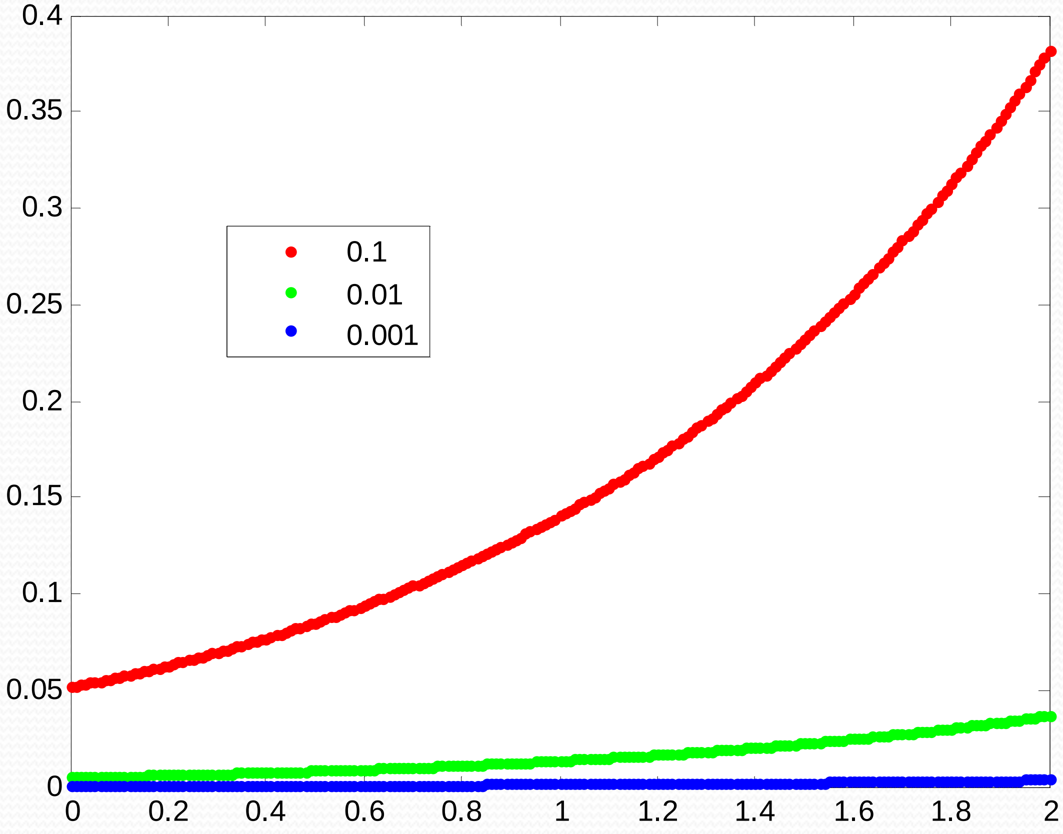
- Check the absolute error
  - The error is somewhat proportional to step size h

Example: Forward Difference

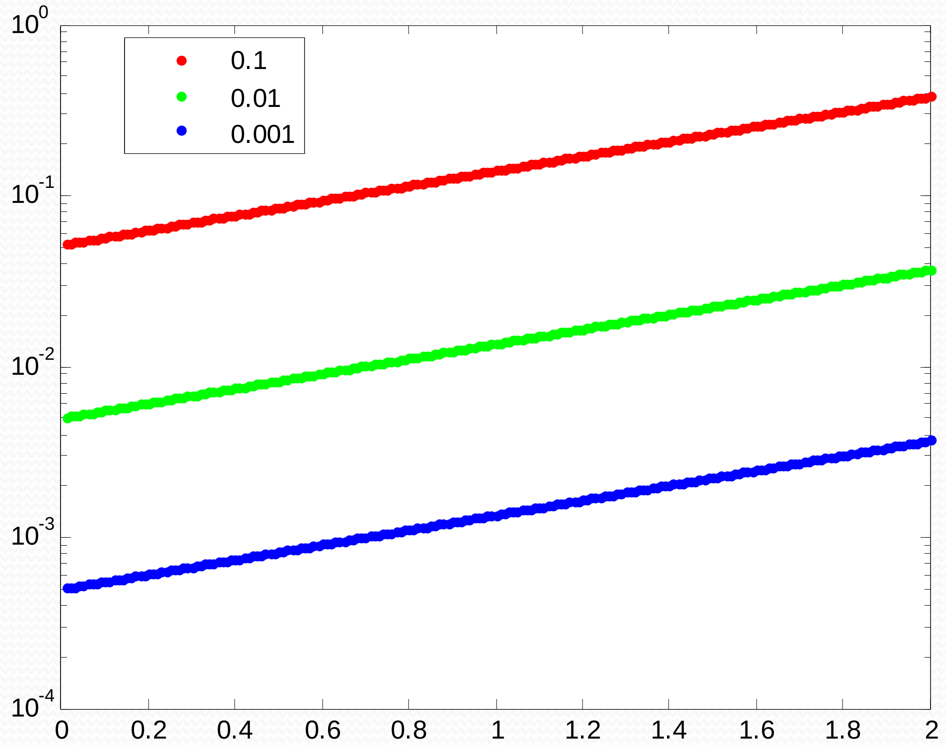
- How about the derivative at other values



Example: Absolute Error of Forward Difference



Example: Absolute Error of Forward Difference



Forward/backward Difference

- Forward Difference

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

- Backward Difference

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

Brief Review

- What we know about numerical differentiation

- A function is known and well defined on every point
  - E.g. f(x-2h), f(x-h), f(x), f(x+h), f(x+2h), …

- What we don't know are the derivatives
  - f'(x-2h), f'(x-h), f'(x), f'(x+h),…..

Goal of numerica differentiation

- Use the function value

  $f(x-2h)$, $f(x-h)$, $f(x)$, $f(x+h)$, $f(x+2h)$

- And their linear combination to approximate the derivatives
  - E.g. $f'(x) = a*f(x-h)+b*f(x)$;

    or $f'(x) = m*f(x-2h)+n*f(x-h)+k*f(x)+l*f(x-h)$…

Central Difference

- How about taking an average of the two differential form?

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

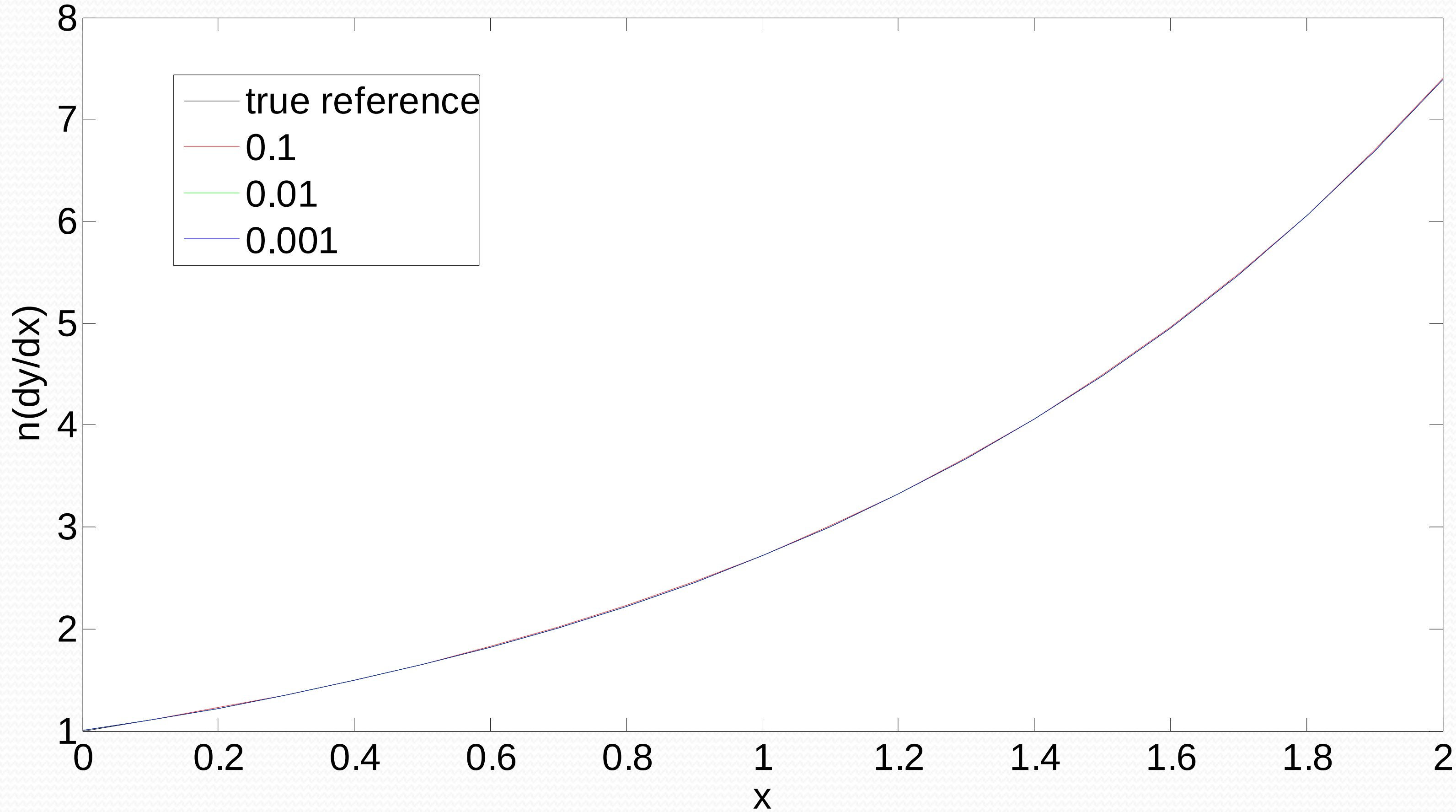
$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

Example

- Find the numerical derivative of exp(x) at x = 1
- Take h = 0.1, 0.01 and 0.001

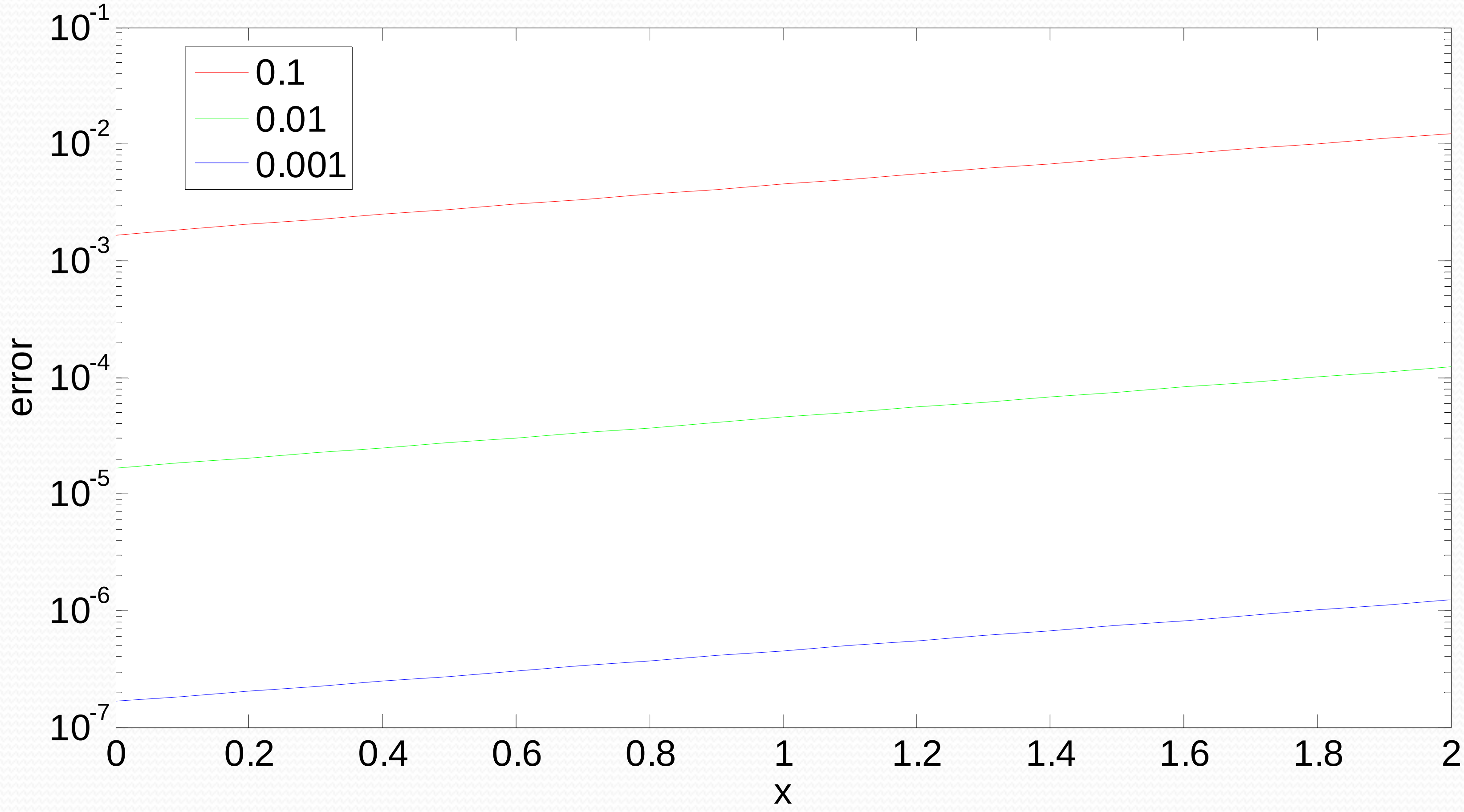
h	exp(x-h)	exp(x)	exp(x+h)	Forward Difference	Error (Forward) ~h	Central Difference	Error (Central) $\sim h^2$
0.1	2.459603	2.718282	3.004166	2.858842	0.140560	2.722815	0.004533
0.01	2.691234	2.718282	2.745601	2.731919	0.013637	2.718327	0.000045
0.001	2.715565	2.718282	2.721001	2.719641	0.001360	2.718282	0.000000

Example



true reference
0.1
0.01
0.001
n(dy/dx)
x
8
7
6
5
4
3
2
1
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2

Example



0.1
0.01
0.001
error
x
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2

Central Difference

- Increase precision by an order

- Can be used for estimation of derivative of every points not at the boundary

Optimize h for derivatives

To get a better derivative

- Forward Difference

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

- Central Difference

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

Small Step Size

- Small h could minimize error ?

- Estimate d/dx sin x at x = 0.9 with h = 1e-3, 1e-5, 1e-7, 1e-9

h	Cos(0.9)	Central Difference	Error
1.00E-03	0.621609968271	0.621609864669	1.03602E-07
1.00E-05	0.621609968271	0.621609968254	1.63314E-11
1.00E-07	0.621609968271	0.621609967943	3.27194E-10
1.00E-09	0.621609968271	0.621609985707	1.74364E-08

Effect of Round-Off error

- $\varepsilon(x)$ is the round off error of the machine number x from true x

- The two numbers for central difference

$$f(x+h) = \hat{f}(x+h) + \varepsilon(x+h)$$

$$f(x-h) = \hat{f}(x-h) + \varepsilon(x-h)$$

Error estimation

- For Central Difference

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi(x))$$

$$= \frac{\hat{f}(x+h) - \hat{f}(x-h)}{2h} + \frac{\varepsilon(x+h) - \varepsilon(x-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi(x))$$

$$= \hat{f}'(x+h) + ERROR$$

Error estimation

- The combination of approximation error and round-off error

$$f'(x) - \hat{f}'(x) = \frac{\varepsilon(x+h) - \varepsilon(x-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi(x))$$

- Typically $\varepsilon(x+h)$ & $\varepsilon(x-h)$

  will be bounded at a certain number E

- The final term is also bounded within x+h and x-h

Error estimation

- Error effect on Central Difference

$$\left| f'(x) - \frac{\hat{f}(x+h) - \hat{f}(x-h)}{2h} \right| \le \frac{E}{h} + \frac{h^2}{6} M$$

- Optimum h should minimize the error

$$\frac{\partial}{\partial h}\left(\frac{E}{h} + \frac{h^2}{6} M\right) = 0 \qquad \Rightarrow h = \sqrt[3]{\frac{3E}{M}}$$

Error estimation

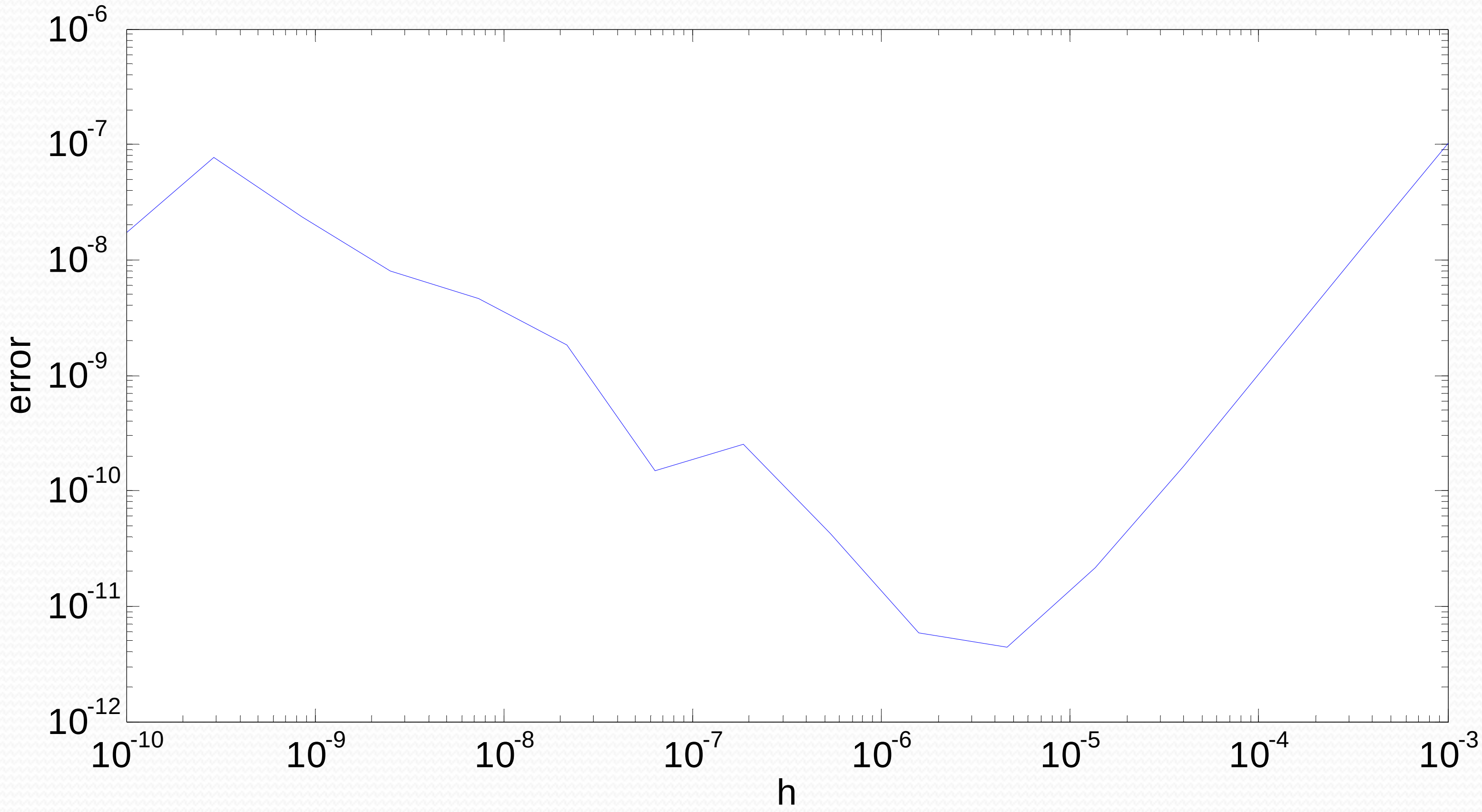
- Optimum h to estimate d/dx sin(x) around 0.9
- Upper bound of M

$$M = \max\left(\left|\frac{d^3}{dx^3}\sin x\right|\right) = \max(|-\cos x|)\big|_{around\,0.9}$$

- Estimate E: (64 bit)machine epsilon 10^{-16}

$$h \approx \sqrt[3]{\frac{3E}{M}} = \sqrt[3]{\frac{3\times 10^{-16}}{0.62}} = 7.85\times 10^{-6}$$

Error estimation



Higher Order Derivative

Intuitive Method

- 2^{nd} order Derivative is the derivative of 1^{st} order Derivative

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

- Find numerical result of f'(x), f'(x+h), f'(x-h), …
- Forward/Backward/Central/n+1 pt method…

A cleaver way

$$f(x+h) = f(x) + \frac{h^1}{1!} f'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f^{(3)}(x) + \ldots$$

$$f(x) = f(x)$$

$$f(x-h) = f(x) - \frac{h}{1!} f'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f^{(3)}(x) + \ldots$$

$$a * f(x+h) + b * f(x) + c * f(x-h) = Kh^2 f''(x) + O(h^m)$$

A cleaver way

$$f(x+h) = f(x) + \frac{h^1}{1!} f'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f^{(3)}(x) + \ldots$$

$$f(x) = f(x)$$

$$f(x-h) = f(x) - \frac{h}{1!} f'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f^{(3)}(x) + \ldots$$

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

2^{nd} Order Derivative

- The 2^{nd} Order Derivative Formula

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

- The error is proportional to h^2

Example

h	exp(x-2h)	exp(x-h)	exp(x)	exp(x+h)	exp(x+2h)
0.1	2.225541	2.459603	2.718282	3.004166	3.320117
0.01	2.664456	2.691234	2.718282	2.745601	2.773195
0.001	2.712851	2.715565	2.718282	2.721001	2.723724

Forward Difference

exp'(x):FD	exp'(x+h):FD	exp''(x):FD	exp''(x)
2.858842	3.159509	3.006670	2.720548
2.731919	2.759375	2.745624	2.718304
2.719641	2.722362	2.721002	2.718282

Central Difference

exp'(x-h):CD	exp'(x+h):CD	exp''(x):CD	exp''(x)
2.463704	3.009175	2.727355	2.720548
2.691279	2.745647	2.718372	2.718304
2.715565	2.721002	2.718283	2.718282

Higher Order Derivative

- You may keep differentiating a lower order derivative for a higher order one
  - Error would accumulate

- Using analytical formula to estimate the differential form
  - 2^{nd} order : 3 points
  - 3^{rd} order : 5 points

3rd Order: 4 points or 5 points?