Numerical Differentiation

- *Math = Language of Science (easiest way)*
- *Differentiation = Basic Math*
- *Science on Computers $\Rightarrow$ Math on Computers*
- *Topic on its own, or prelim for ODEs*

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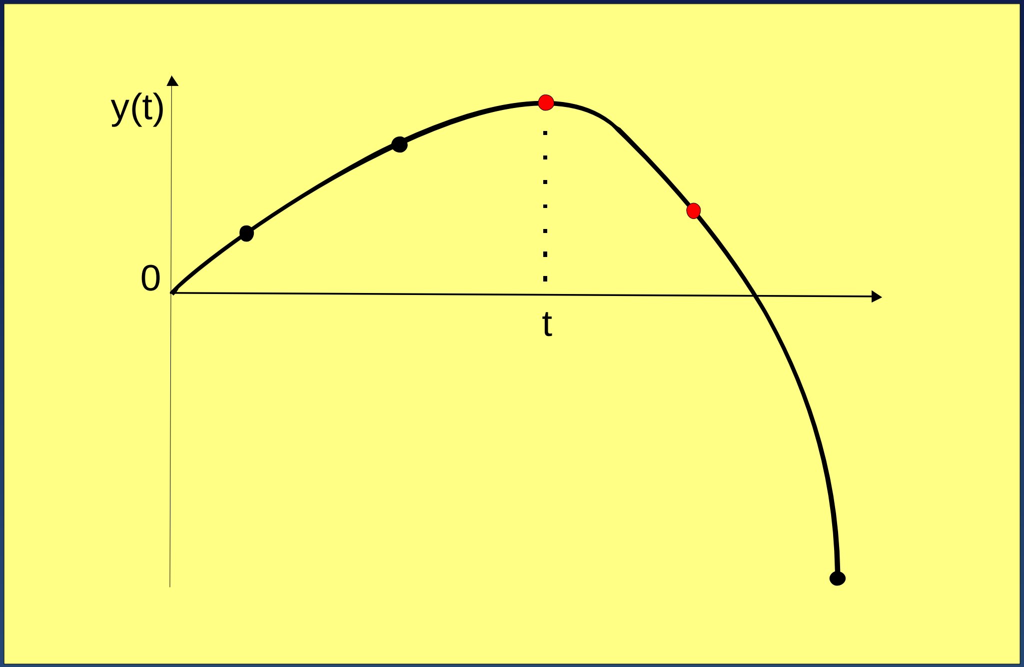
Problem: Velocity from Position



- **Measured *y(t)* @ fixed t's**
- **Determine *dy(t)/dt***
- **No analytic *y(t)*, just table**
- ***y(0), y(h), y(2h), …***
- ***h* = "step size"**

Math: **Derivative = difference = slope**

$$\frac{dy(t)}{dt} \stackrel{\text{def}}{=} \lim_{h\to 0} \frac{f(t+h) - f(t)}{h}. \quad (1)$$

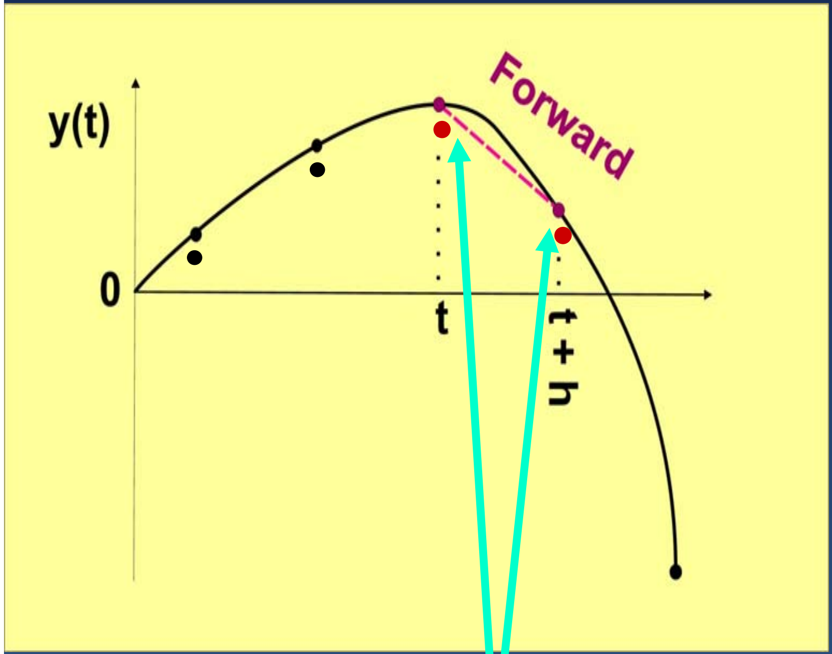
Applied Math (CS):

$$0 \le dy/dt \le \epsilon_m$$

Algorithm: Forward Difference

Taylor Series Expansion (moves function one step *h* forward):

$$y(t+h) \;=\; y(t) + hy'(t) + \frac{h^2}{2} y''(t) + \ldots \qquad (2)$$



Solve for *y′(t)*

$$y'_c(t) \quad \simeq \quad \frac{y(t+h) - y(t)}{h} \qquad (3)$$

$$\simeq \quad y'(t) - \frac{h}{2} y''(x) + \ldots \qquad (4)$$

Geometric: 2 points straight line forward

(computed)

Error ∝ h

Forward Difference: Example

$$y'_c(t) \simeq \frac{y(t+h) - y(t)}{h} \qquad (5)$$

(***h*** = step size)

Function*:* ***y(t) = a + b t²*** *(6)*

Exact Derivative: ***y'(t) = 2bt*** *(7)*

Forward Diff Approximation: y'c ≅ y(t+h) − y(t)

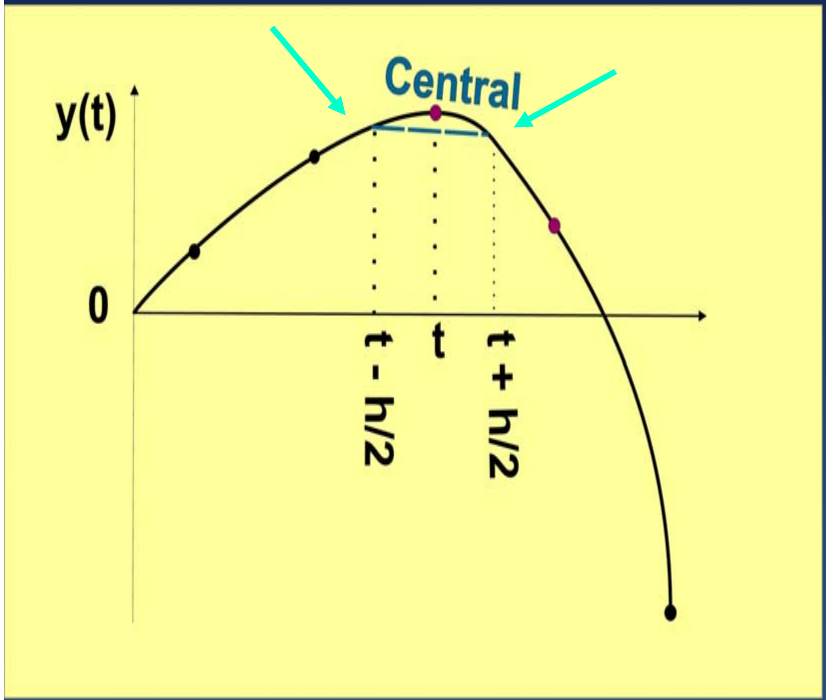
= 2bt + bh *(8)*

⇒ **Need very small h to work!**

[not a good algorithm, but useful at the start; y(0), y(h)]

Improved Algorithm: Central Difference

$$y'_c(t) \approx \frac{y(t+h/2) - y(t-h/2)}{h} \qquad (9)$$



Taylor series ***y(t ± h/2)***

$$y'_c(t) \simeq y'(t) + \frac{1}{24}h^2 y^{(3)}(t) + \cdots \qquad (10)$$

- **h² error**
- **(9): all even derivatives cancel**
- **1 order better than forward diff**
- **Exact for** ***y(t) = a + b t²***
- **Better rule** $\Rightarrow$ **larger** ***h***

Geometric: *h/2* on either side
still 2 pts *h* apart

Assessment: Differentiation Errors

- See text for details (set approx error = Round Off error)

Round-off error $$\epsilon_{RO} \approx \frac{\Delta y}{\Delta t} \approx \frac{\epsilon_m}{h} \quad (11)$$

Best h values $$h_{\mathbf{fd}} \approx 5 \times 10^{-8}, \qquad h_{\mathbf{cd}} \approx 3 \times 10^{-5}. \quad (12)$$

1. Differentiate cos x and exp(x) at x=0.1, 1., & 100
2. Use forward-, central-& extrapolated-difference rules
3. Print out the derivative and its relative error as functions of h
4. Reduce the step size *h* until it equals ε_m
5. Plot $\log_{10}(\mathcal{E})$ *vs* $\log_{10}(h)$. Compare to estimates above.
6. Where does approximation error or round off error dominate?

Extension: Second Derivatives

E.G.: Force = m y"(t)

Central Difference Derivative: $$f'(x) \simeq \frac{f(x+h/2) - f(x-h/2)}{h} \qquad (13)$$

of first derivative

$$f^{(2)}(x) \simeq \frac{f'(x+h/2) - f'(x-h/2)}{h} \qquad (14)$$

$$f^{(2)}(x) \simeq \frac{[f(x+h) - f(x)] - [f(x) - f(x-h)]}{h^2} \qquad (15)$$

$$= \frac{f(x+h) + f(x-h) - 2f(x)}{h^2} \qquad (16)$$

Exercise

1. ***Calculate the second derivative of cos x.***
2. ***Test it over four cycles.***
3. ***Start with h ≈ π /10, let h $\Rightarrow$ machine precision.***