Numerical differentiation

- Goal: We have gathered experimental measurements and want to obtain a derivative
  - If we have a physical reason to believe that the data will follow a straight line or a parabola, it is best to use a best fit approach
  - If not, need to take the derivative directly
- 2-point differentiation:

$$\left.\frac{\partial y}{\partial x}\right|_{x_i} \approx \frac{y_{i+1}-y_i}{x_{i+1}-x_i}$$

Intuitive but inaccurate

- Consider Taylor series expansion

$$y_{i+1} \approx y_i + \left.\frac{\partial y}{\partial x}\right|_{x_i}(x_{i+1}-x_i) + \frac{1}{2}\left.\frac{\partial^2 y}{\partial x^2}\right|_{x_i}(x_{i+1}-x_i)^2 + \ldots.$$

2-point differentiation neglects all terms of 2nd and higher order!

Numerical differentiation

- How about 3 point differentiation?

$$y_{i+1} \approx y_i + \left.\frac{\partial y}{\partial x}\right|_{x_i}(x_{i+1}-x_i) + \frac{1}{2}\left.\frac{\partial^2 y}{\partial x^2}\right|_{x_i}(x_{i+1}-x_i)^2 + \frac{1}{3!}\left.\frac{\partial^3 y}{\partial x^3}\right|_{x_i}(x_{i+1}-x_i)^3 + \ldots.$$

$$y_{i-1} \approx y_i + \left.\frac{\partial y}{\partial x}\right|_{x_i}(x_{i-1}-x_i) + \frac{1}{2}\left.\frac{\partial^2 y}{\partial x^2}\right|_{x_i}(x_{i-1}-x_i)^2 + \frac{1}{3!}\left.\frac{\partial^3 y}{\partial x^3}\right|_{x_i}(x_{i-1}-x_i)^3 + \ldots.$$

$$y_{i+1} - y_{i-1} \approx \left.\frac{\partial y}{\partial x}\right|_{x_i}(x_{i+1}-x_{i-1}) + \theta\left(\Delta x^3\right)$$

if $\Delta x = x_{i-1}-x_i = x_{i+1}-x_i$ constant!

- Thus:

$$\left.\frac{\partial y}{\partial x}\right|_{x_i} = \frac{y_{i+1}-y_{i-1}}{x_{i+1}-x_{i-1}} = \frac{y_{i+1}-y_{i-1}}{2\Delta x}$$

- Five point differentiation is even better

$$\left.\frac{\partial y}{\partial x}\right|_{x_i} = \frac{2y_{i+2} + y_{i+1} - y_{i-1} - 2y_{i-2}}{10\Delta x}$$

Example

- Consider a sphere falling into a fluid: calculate velocity at $t = 10s$

i	t_i *(s)*	x_i *(mm)*
0	0	0
1	2	25
2	4	67
3	6	172
4	8	288
5	10	387
6	12	575
7	14	756
8	16	961
9	18	1188

2 points differentiation

$$\left.\frac{\partial x}{\partial t}\right|_{t=10s} = \frac{y_{i+1} - y_i}{\Delta x} = \frac{575 - 387}{2} = 94 \ \ cm/s$$

3 points differentiation

$$\left.\frac{\partial x}{\partial t}\right|_{t=10s} = \frac{y_{i+1} - y_{i-1}}{2\Delta x} = \frac{575 - 288}{2 \times 2} = 71.8 \ \ cm/s$$

5 points differentiation

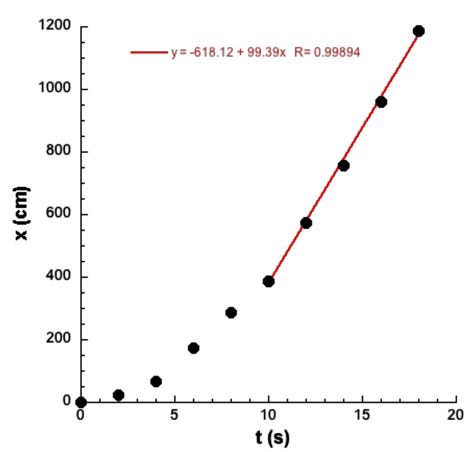
$$\left.\frac{\partial x}{\partial t}\right|_{t=10s} = \frac{2y_{i+2} + y_{i+1} - y_{i-1} - 2y_{i-2}}{10\Delta x} =$$

$$\left.\frac{\partial x}{\partial t}\right|_{t=10s} = \frac{2(756) + 575 - 288 - 2(172)}{10 \times 2} = 72.8 \ \ cm/s$$

Example

t_i *(s)*	2 pt dif	3 pt dif	5 pt dif
0	12.5	X	X
2	21.5	17.0	X
4	52.0	36.8	36.2
6	58.0	55.0	47.2
8	49.5	53.8	61.5
10	94.0	71.8	72.8
12	90.5	92.3	85.8
14	102.5	96.5	99.4
16	113.4	108	X
18	x	X	X

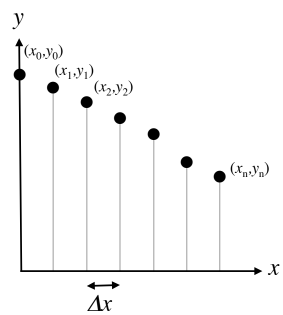
Chaotic *v.* smooth



At t ≥ 10s, dx/dt = 99.4 cm/s

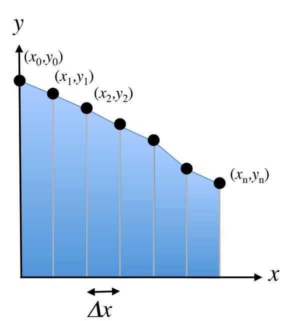
Numerical integration

- Goal: We have gathered experimental measurements and want to obtain a the area under the curve or integrate the function
  - Trapezoidal rule
  - Simpson's rule
  - Both require constant Δx



Numerical integration

- Trapezoidal rule
  - Discretize by assuming a straight line between 2 consecutive points and sum the area of the resulting trapezoids
  - Low accuracy (as little as 1st order)

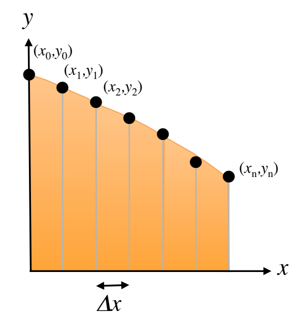


$$\int_{x_0}^{x_n} y(x)\,dx \approx \Delta x\left[\frac{1}{2}y_0 + y_1 + y_2 + \ldots + \frac{1}{2}y_n\right]$$

Better with more points

Numerical integration

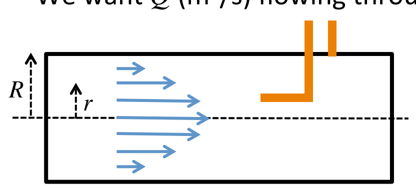
- Simpson's rule
  - Assume a parabola between 3 consecutive points and sum the area under each paraboloid
  - Requires odd number of points
  - Higher accuracy (as much as 3rd order)



$$\int_{x_0}^{x_n} y(x)\,dx \approx \Delta x\left[\frac{1}{3}y_0 + \frac{4}{3}y_1 + \frac{2}{3}y_2 + \frac{4}{3}y_3 + \frac{2}{3}y_4 + \ldots + \frac{4}{3}y_{n-1} + \frac{1}{3}y_n\right]$$

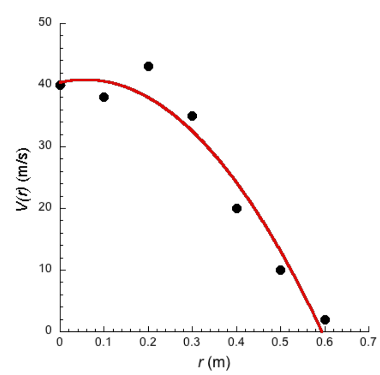
Example: Pitot traverse

- We want Q (m^3/s) flowing through a pipe from discrete $V(r)$ measurements



$$Q = \int_0^{2\pi}\int_0^R r.V(r)\,dr\,d\theta = 2\pi\int_0^R r.V(r)\,dr$$

Index	r (m)	V (m/s)
0	0	40
1	0.1	38
2	0.2	46
3	0.3	35
4	0.4	20
5	0.5	10
6	0.6	2

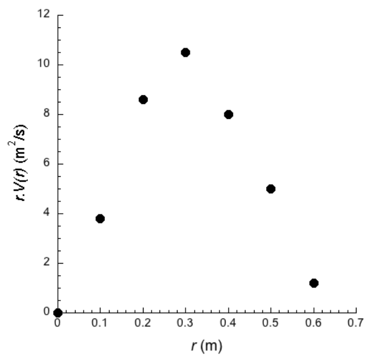


Need to integrate $r.V(r)$ not $V(r)$

Example: Pitot traverse

- We want Q (m^3/s) flowing through a pipe from discrete $V(r)$ measurements

Index	r (m)	V (m/s)	$r.V(r)$ (m^2/s)
0	0	40	0
1	0.1	38	3.8
2	0.2	46	8.6
3	0.3	35	10.5
4	0.4	20	8.0
5	0.5	10	5.0
6	0.6	2	1.2



$$Q = 2\pi \int_0^{0.6} r.V(r)\,dr \approx 2\pi.\Delta r\left[\frac{1}{3}(r_0V_0)+\frac{4}{3}(r_1V_1)+\frac{2}{3}(r_2V_2)+\ldots+\frac{1}{3}(r_6V_6)\right]$$

$$Q \approx 2\pi(0.1)\left[\frac{1}{3}(0)+\frac{4}{3}(3.8)+\frac{2}{3}(8.6)+\frac{4}{3}(10.5)+\frac{2}{3}(8.0)+\frac{4}{3}(10.5)+\frac{1}{3}(1.2)\right] = \boxed{23\ m^3/s}$$

Example: Pitot traverse

- What if we average velocities

Index	r (m)	V (m/s)	$r.V(r)$ (m^2/s)
0	0	40	0
1	0.1	38	3.8
2	0.2	46	8.6
3	0.3	35	10.5
4	0.4	20	8.0
5	0.5	10	5.0
6	0.6	2	1.2

$$\overline{V} = \sum_i \frac{V_i}{n} = \frac{(40+38+46+35+20+10+2)}{7} = 26.9\ m/s$$

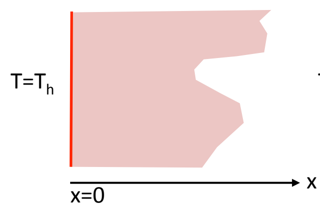
$$\overline{Q} = \overline{V}.A = 26.9 \times \pi(0.6)^2 = \boxed{30.4\ m^3/s}$$

This approach overestimates Q by 30%!

Alternative: if we are in the laminar range, we know that the velocity profile should be parabolic => do a parabolic fit or linearize by taking the logarithm and do a best fit

Order of magnitude estimates

- Engineers often need to estimate quantities
  - How long to reach steady state?
  - How long, wide, thick… should something be?
- Always look for quick ways to estimate quantities
- Consider the transient heating of a semi-infinite slab



T = T(x,t) and 1D conduction

At time t = 0, change the temperature of the x = 0 face from T_o to T_h

$$\frac{1}{\alpha}\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}$$

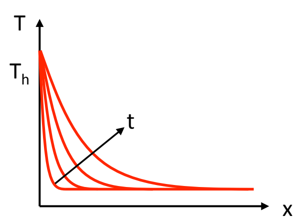
$$T(x,0) = T_o$$
$$T(0,t) = T_h$$
$$T(\infty,t) = T_o$$

Order of magnitude estimates

- The solution is:

$$\frac{T(x,t) - T_h}{T_o - T_h} = erf\left(\frac{x}{2\sqrt{\alpha t}}\right)$$

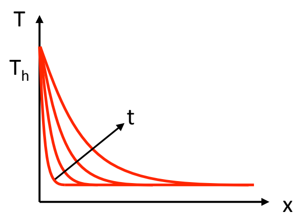
$$erf(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-u^2}du$$



- How long will the heat front take to reach a particular position (e.g., x = 5 cm)?

Order of magnitude estimates

- Make linear assumption and assume that when the heat front reaches x the temperature at this point is:



$$T(x,t) = \frac{T_o + T_h}{2}$$

$$T(x,t) = T_o + \frac{T_h - T_o}{2}$$

$$\frac{T(x,t) - T_o}{T_h - T_o} = \frac{1}{2}$$

From PDE solution:

$$\frac{T(x,t) - T_h}{T_o - T_h} = erf\left(\frac{x}{2\sqrt{\alpha t}}\right) = \frac{1}{2}$$

$$\frac{x}{2\sqrt{\alpha t}} = 0.48 \quad \Rightarrow \quad \frac{x^2}{4\alpha t} = 0.23 \quad \Rightarrow \quad \frac{x^2}{\alpha t} = 0.92$$

$$\frac{x^2}{\alpha t} \approx 1$$

Order of magnitude estimates

- Now, look at how long it will take to reach x = 5 cm with rods made up of different materials

For a glass rod: α = 0.0034 cm^2/s

$$t \approx \frac{x^2}{\alpha} = \frac{5^2}{0.0034} = 7353 \ s \approx 2h$$

For a copper rod: α = 1.17 cm^2/s

$$t \approx \frac{x^2}{\alpha} = \frac{5^2}{1.17} = 21.4 \ s$$

We can use the same approximation to determine how far a heat front will move over a given period of time (e.g., t = 100s)

$$x_{glass} \approx \sqrt{\alpha t} = \sqrt{0.0034 \times 100} = 0.6 \ cm$$

$$x_{copper} \approx \sqrt{\alpha t} = \sqrt{1.17 \times 100} = 10.8 \ cm$$

Order of magnitude estimates

Thus, the time required to reach steady state in a rod of length L can be estimated using:

$$F_o = \frac{\alpha t}{x^2} \approx 1$$

So, for a brass rod that is 10” (25 cm) in length and using α_{brass} = 0.314 cm^2/s

$$t_{SS} \approx \frac{L^2}{\alpha} = \frac{25^2}{0.341} = 1833\ s \approx 0.5h$$