NUMERICAL DIFFERENTIATION:

recall Taylor Series:

$$f(x+\delta x) = f(x) + f'(x)\,\delta x + \tfrac{1}{2} f''(x)\,\delta x^2 + \ldots$$

"The Big O"

$$\Rightarrow \quad f(x+\delta x) - f(x) = f'(x)\,\delta x + O(\delta x^2)$$

$$\Rightarrow \quad f'(x) = \frac{f(x+\delta x) - f(x)}{\delta x} + O(\delta x^{\text{[illegible]}})$$ Forward Difference.

Similarly,

$$f'(x) = \frac{f(x) - f(x-\delta x)}{\delta x} + O(\delta x^{\text{[illegible]}})$$

Can we do better? Consider

$$f(x+\delta x) - f(x-\delta x) = 0 + 2f'(x)\,\delta x + 0 + O(\delta x^3)$$

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

What about 2nd Derivatives?

$$f(x+\delta x) + f(x-\delta x) = 2f(x) + 0 + \tfrac{2}{2} f''(x)\,\delta x^2 + 0 + O(\delta x^4)$$

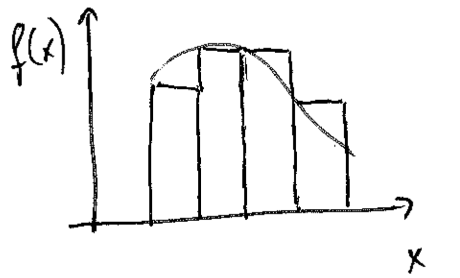
$$\Rightarrow \quad f''(x) = \frac{f(x+\delta x) + f(x-\delta x) - 2f(x)}{\delta x^2} + O(\delta x^2)$$

Numerical Integration:

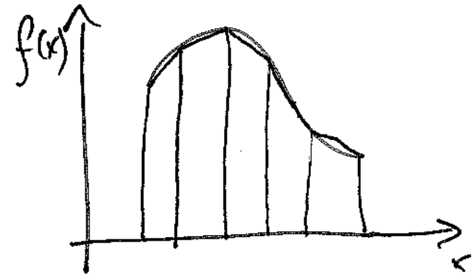
Suppose we want to evaluate $\int_a^b f(x)\,dx$

The basic numerical approach is simple: divide the interval $[a, b]$ into n subintervals, ~~& the~~ of width $\delta x = \frac{b-a}{n}$ and then add up $\sum_{i=0}^{n} f(x_i)\,\delta x$; graphically,

$(x_i = a + i\delta x)$



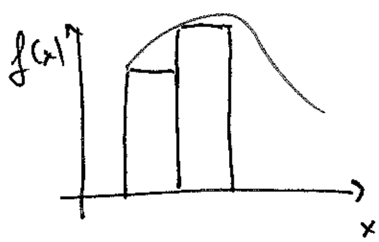
We see we can easily improve our estimate by making trapezoids



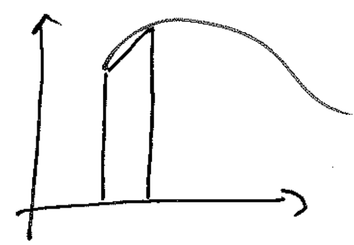
Trapezodal Rule: How do we get the trapezoids?

Consider the following piece of integral $\frac{1}{2}\left(f(x_i)\,\delta x + f(x_{i+1})\,\delta x\right)$

graphically:



sum $\longrightarrow$



so $$\int_a^b f(x)\,dx \approx \frac{\delta x}{2}\left[\left(f(x_0)+f(x_1)\right)+\left(f(x_1)+f(x_2)\right)+\dots\left(f(x_{n-1})+f(x_n)\right)\right]$$

so every number appears twice except the endpoints.

$$\Rightarrow \boxed{\int_a^b f(x)\,dx \approx \frac{\delta x}{\cancel{2}} \sum_{i=1}^{n-1} f(x_i) + \frac{\delta x}{2}\left(f(x_0)+f(x_n)\right)}$$

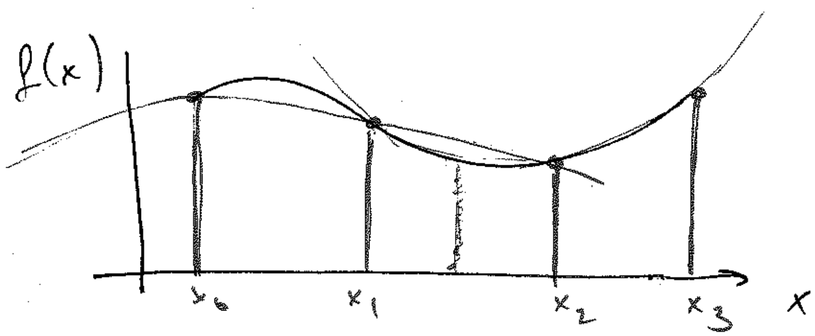
What is the error in ~~f~~ the trapezoidal rule? This is more complicated ... w/o derivation

$$\text{error} \le \frac{M(b-a)^3}{12n^2} \quad \text{where} \quad M = \max\left(f''(x)\right) \text{ on } [a,b]$$

$$\le O(\delta x^2)$$

SIMPSON'S RULE:

A simple way to improve on the trap rule is to use curved segments instead of straight lines. Simpson's rule uses parabolas to make a better estimate.



We use three points to make a parabola

$$p(x) = Ax^2 + Bx + C$$

$$\int_{-\delta x}^{\delta x} p(x)\,dx = \frac{\delta x}{3}\left(2A\,\delta x^2 + 6C\right)$$

To simplify, let's first consider just 3 points, $x_0 = -\delta x,\ x_1 = 0,\ x_2 = \delta x$

The parabola through these points has eqn

$$p(x) = Ax^2 + Bx + C$$

$$p(x_0) = f(x_0) = A\delta x^2 - B\delta x + C$$

$$p(x_1) = f(0) = C$$

$$p(x_2) = f(x_2) = A\delta x^2 + B\delta x + C$$

$$p_0 + p_1 + p_2 = \int_{-\delta x}^{\delta x} p(x)\,dx$$

$$\Rightarrow \quad 2A\delta x^2 + 2f(0) = f(x_0) + f(x_2)$$

$$\cancel{A = \frac{f(x_0) + f(x_2) - 2f(x_1)}{2\delta x^2}}$$ not important

$$\Rightarrow \int_{-\delta x}^{\delta x} p(x)\,dx = \frac{\delta x}{3}\left(2A\,\delta x^2 + 6C\right)$$

$$= \frac{\delta x}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]$$

notice that shifting along the x-axis cause no change!!

$$\Rightarrow \int_a^b f(x)\,dx \approx \frac{\delta x}{3}\Big\{ \left[f(x_0) + 4f(x_1) + f(x_2) \right] + \left[f(x_2) + 4f(x_3) + f(x_4) \right] + \dots$$

$$\dots + \left[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n) \right] \Big\}$$

$$= \frac{\delta x}{3} \Big[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \dots$$

$$+ 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n) \Big]$$

where n even & $\delta x = \frac{b-a}{n}$

The error $\leq \dfrac{M(b-a)^5}{180 n^4}$ where $M = \max\left[f^{(4)}(x)\right]$ on $[a,b]$

$\propto$
$O(\delta x^4)$

RADIOACTIVE DECAY:

Physically, we know the rate of decay of radioactive material $\propto$ to the amount of material. Should be obvious, since if there is more stuff, it can emit more ~~radioactive~~ high energy particles. Mathematically,

$$\frac{dN}{dt} = -\lambda N \qquad \lambda = \text{rate} = \frac{1}{\tau}$$

$N =$ amount of stuff

This of course has solution

$$N(t) = N_0 e^{-\lambda t}.$$

Suppose we did not know this ... could we solve with a computer given N at some arbitrary t?

Forward diff $\quad \dfrac{dN}{dt} = \dfrac{N(t+\Delta t) - N(t)}{\Delta t}$

or $\quad N(t+\Delta t) = N(t) + \dfrac{dN}{dt}\Delta t \qquad$ "Euler Method"

For radioactive decay, $N(t+\Delta t) = N(t)(1-\lambda \Delta t) + O(\delta t^2)$

We can use this repeatedly to estimate N at any arbitrary time in the future.