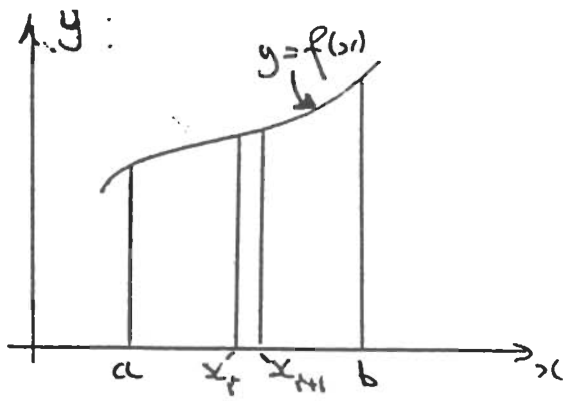
6. *Numerical Integration*

Wish to evaluate $I = \int_a^b f(x)dx$ where $f(x)$ cannot be integrated analytically.



6.1 *Trapezium Rule (linear interpolation)*

Divide range into N equal strips of width

$$h = \frac{b-a}{N}$$

Let $a = x_0 < x_1 < x_2 \cdots < x_N = b$.

Neglect curvature of the N arcs by replacing them by chords (*i.e.* linear interpolation).

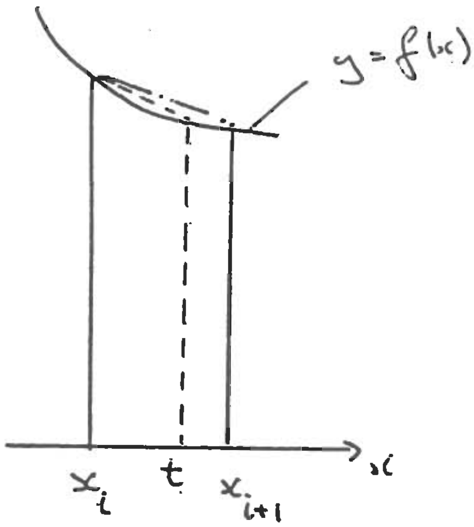
Area of r^{th} strip

$$= \frac{h}{2}(f(x_r) + f(x_{r+1}))$$

$$= \frac{h}{2}(y_r + y_{r+1})$$ say.

$$\therefore \text{ Total area } \cong \sum_{r=0}^{N-1} \frac{h}{2}(y_r + y_{r+1})$$

$$A_{trap} = \frac{h}{2}(y_0 + 2y_1 + \ldots + 2y_{N-1} + Y_N)$$



Error. Define error to be

$$\in_N = I_N - I$$

Wait to see how $\in_N$ varies with N. Consider one strip, and introduce

$$\in(t) = \left(\frac{t-x_i}{2}\right)\left[f(x_i) + f(t)\right] - \int_{x_i}^{t} f(t')dt'$$

Then, $\in'(t) = \frac{1}{2}[f(x_i) + f(t)] + \left(\frac{t - x_i}{2}\right) f'(t) - f(t).$

Note that $\in'(x_i) = 0.$

Also, $\in''(t) = \left(\frac{t - x_i}{2}\right) f''(t).$

Let m and M denote min and max values of $|f''(x)|$ for $x \in [a,b]$.

Then

$$\tfrac{1}{2}(t - x_i)m \le |\in''(t)| \le \tfrac{1}{2}(t - x_i)M.$$

Integrate from x_i to t, using fact that $\in'(x_i) = 0$; then

$$\tfrac{1}{4}(t - x_i)^2 m \le |\in'(t)| \le \tfrac{1}{4}(t - x_i)M$$

Integrate again from x_i to x_{i+1}, using fact that $\in(x_i) = 0$; then

$$\tfrac{1}{12}h^3 m \le |\in(x_{i+1})| \le \tfrac{1}{12}h^3 M.$$

Now sum over all strips

$$\Rightarrow \quad \tfrac{1}{12}m(b-a)h^2 \le \in \le \tfrac{1}{12}M(b-a)h^2$$

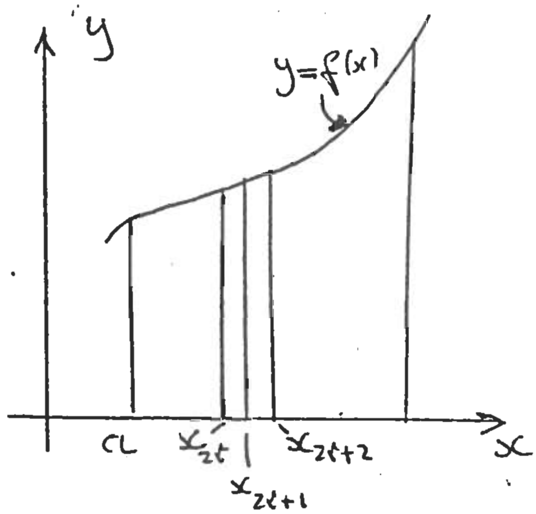
i.e. $\quad \in \propto h^2.$

6.2 *Simpson's Rule (quadratic interpolation)*

Improves linear interpolation by replacing *chord with* parabola's.

Divide range into *even* number N of equal strips.

Consider strips in pairs.



Area of r^{th} and $(r+1)^{th}$ pair $\int_{x_{2r}}^{x_{2r+2}} f(x)dx.$

Let $c = x_{2r+1}$ = centre of pair of strips.

Introduce new integration variable

$$t = x - c, \quad dt = dx$$

$$x\Big|_{x_{2r}}^{x_{2r+2}} \sim t\Big|_{-h}^{h}$$

where $$h = \frac{b-a}{N}$$ as before.

Area of pair of strips $= \int_{-h}^{h} f(c+t)dt$.

Taylor expansion: $$\int_{-h}^{h} (f(x) + tf'(c) + \frac{t^2}{2} f''(c) + \ldots)dt$$

$$\cong 2h(f(c) + 0 + \frac{f''(c)}{3!} h^2).$$

Wish to eliminate $f''(c)$ by writing it in terms of $f(c+h), f(c-h)$

$$f(c+h) = f(c) + hf'(c) + \frac{h^2}{2!} f''(c) + \ldots$$

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

or, $$f''(c) = \frac{f(c+h) + f(c-h) - 2f(c)}{h^2}$$

$\therefore$ Area of pair of strips $$= 2h\left\{ f(c) + \frac{f(c+h) + f(c-h) - 2f(c)}{3!} \right\}$$

$$= \frac{h}{3}(f(c-h) + 4f(c) + f(c+h))$$

or, writing
$$f(c) \equiv f(x_{r+1}) = y_{r+1}$$
$$f(c-h) \equiv f(x_r) = y_r$$
$$f(c+h) \equiv f(x_{r+2}) = y_{r+2}$$

Area of pair of strips $= \frac{h}{3}(y_r + 4y_{r+1} + y_{r+2})$

Hence, total area

$$= \frac{h}{3}((y_0 + 4y_1 + y_2) + (y_2 + 4y_3 + y_4) + \ldots + (y_{N-2} + 4y_{N-1} + y_n))$$

$$= \frac{h}{3}(y_0 + 4y_1 + 2y_2 + 4y_3 + \ldots + 4y_{N-1} + y_N)$$

$$= \frac{h}{3}(y_0 + 4\sum_{ordinates}^{odd} + 2\sum_{ordinates}^{even} + y_N)$$

Error $= A - A_{Simpson} \propto h^4, A =$ actual size

Error now scales like h^4.

Increase accuracy by Richardson extrapolation:

Have $A - A_{Simpson} \propto h^4$

h known, $A_{Simpson}$ obtained from above formula, wish to find A, the unknown.

$A = A_{Simpson}(h) + \alpha h^4 = A_N + \alpha h^4$, say , A, α unknown

For $2N$ strips, $h \to h/2$

$$A = A_{Simpson}\left(\frac{h}{2}\right) + \alpha\left(\frac{h}{2}\right)^4 = A_{2N} + \frac{\alpha}{16}h^4, \text{ say}$$

Solve for A, find $A = \frac{16A_{2N} - A_N}{15} + O(h^6)$.

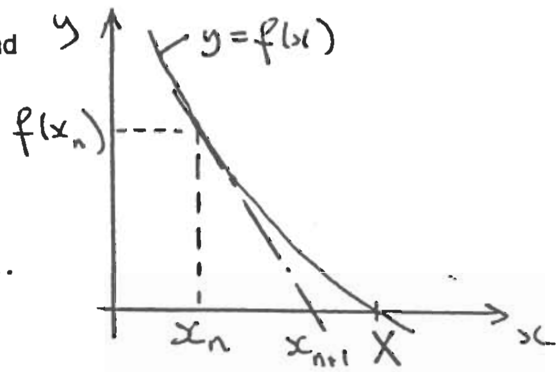
Error $\propto h^6$

6.3 ***Solution of Equations by an Iterative Process***

Wish to solve the equation $f(x)=0$ for which an analytic solution is not (readily) attainable

$$e.g. \quad x=\tan x \quad \text{or} \quad x-\tan x \equiv f(x)=0$$

Graphically, have $f(x)$ as shown, wish to find $x=X$ s.t. $f(X)=0$.



Take initial guess $=x_1$, and find better approximations $x_2, x_3 \ldots$ according to the following iterative scheme:

If the n^{th} estimate is x_n, construct a tangent to the curve $y=f(x)$ at $x=x_n$.

Where the tangent crosses the x-axis is the next estimate x_{n+1}. Then

$$f'(x_n)=\frac{0-f(x_n)}{x_{n+1}-x_n}$$

or $\qquad x_{n+1}=x_n-f(x_n)/f'(x_n)$. Newton-Raphson algorithm.

What is rate of convergence?

Let X be the required solution *i.e.* $f(X)=0$.

Let e_n be error at n^{th} approximation, so that

$$e_n=X-x_n$$

Then, $x_{n+1}=x_n-\dfrac{f(x_n)}{f'(x_n)}$ becomes

$$X-e_{n+1}=X-e_n-\frac{f(X-e_n)}{f'(X-e_n)}$$

Taylor exp: $=X-e_n-\dfrac{(f(X)-e_nf'(X)+\frac{e_n^2}{2}f''(X)\ldots}{(f'(X)-e_nf''(X)+\ldots}$

Use of

$$f(X) = 0 \Rightarrow X - e_{n+1} = X - \frac{e_n(f'(X) - e_n f''(X) - e_n(f'(X) - \frac{e_n^2}{2} f'')}{f'(X) - e_n f''(X)}$$

$$= X + \frac{\frac{1}{2} e_n^2 f''(X)}{f'(X) - e_n f''(X)}$$

or, $e_{n+1} = -\frac{1}{2} e_n^2 \frac{f''(X)}{f'(X)} + O(e_n^3).$

$\therefore$ very fast convergence (*i.e.* if $e_n \sim 0.1, e_{n+1} \sim 0.01, e_{n+2} \sim 0.0001$, etc.).

Second order process.

Example, solve $x^2 = 12$ (*i.e.* find $x = \sqrt{12}$).

Here $f(x) = x^2 - 12.$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n = \frac{x_n^2 - 12}{2x_n}$$

$$= \tfrac{1}{2}(x_n + 12/x_n).$$

Try $x_1 = 3$, find

n	x_n
1	3
2	3.5
3	3.4643
4	3.46410

Correct answer: = 3.4641016...

$\therefore$ excellent agreement after only four iterations.

6.4 *Solution of first order ode's by integration*

The Runge-Kutt method (Modified Euler)

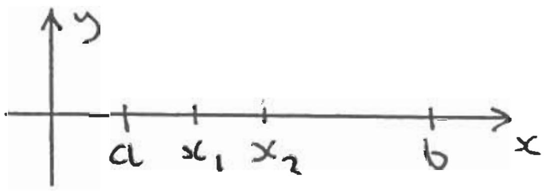
Given $\dfrac{dy}{dx} = f(x,y)$ (1)

wish to find $y(b)$ given $y(a)$.

Several variations of RK method; here we consider only the simplest (based on trapezium rule).

Divide range (a,b) into N intervals, width $h = \dfrac{b-a}{N}$

$a = x_0 < x_1 < x_2 \ldots < x_N = b$



Step 1: Integrate from x_0 to x_1 using trapezium rule to estimate integral

$$\begin{aligned} y_1 - y_0 &= \int_{x_0}^{x_1} f(x,y))dx \\ &\cong \frac{h}{2}\{f(x_0,y_0) + f(x_1,y_1)\} \end{aligned} \quad (2)$$

where we write $y_n \equiv y(x_n)$.

Note that the unknown y_1 appears in $f(x_1,y_1)$ on right hand side. Approximate

y_1 by a Taylor expansion; $\begin{aligned} y_1 &\cong y_0 + hy_0' \\ &= y_0 + hf(x_0,y_0). \end{aligned}$ from (1)

$\therefore f(x_1,y_1) \cong f(x_1, y_0 + hf(x_0,y_0))$

and so (2) gives

$$y_1 = y_0 + \frac{h}{2}(k_1 + k_2)$$

where $k_1 = f(x_0,y_0), k_2 = f(x_1, y_0 + hk_1)$.

Step 2: Integrate from x_1 to x_2 using the above procedure. Then,

$$y_2 = y_1 + \frac{h}{2}(k_1 + k_2)$$

where k_1, k_2 are now given by

$$k_1 = f(x_1, y_1), k_2 = f(x_2, y_1 + hk_1).$$

Step 3: Repeat as required, so that for the $(n+1)^{th}$ step, have

$$y_{n+1} = y_n + \frac{h}{2}(k_1 + k_2)$$

where $k_1 = f(x_n, y_n), k_2 = f(x_{n+1}, y_n + hk_1)$.

Can show that error αh^2.

6.6 *Gaussian Elimination*

Wish to solve the linear system

$$A\mathbf{x} = \mathbf{b}, \qquad A = \text{matrix} .$$

Basic idea: take linear combinations of the equations to eliminate some of the variables. Illustrate general technique with an example.

Ex. solve

$$\begin{aligned} 2x_1 - x_2 + 3x_3 &= 3 \\ x_1 + 2x_3 &= 3 \\ x_1 + x_2 + 2x_3 &= 4. \end{aligned}$$

Here

$$A = \begin{pmatrix} 2 & -1 & 3 \\ 1 & 0 & 2 \\ 1 & 1 & 2 \end{pmatrix}, \qquad \mathbf{b} = \begin{pmatrix} 3 \\ 3 \\ 4 \end{pmatrix}$$

Step 1: Write in an extended matrix notation

$$\begin{array}{llll|l} (1)- & 2 & -1 & 3 & 3 \\ (2)- & 1 & 0 & 2 & 3 \\ (3)- & 1 & 1 & 2 & 4 \end{array}$$

Method: make zeroes in 1st column below diagonal of A by subtracting multiples of (1):

$$\begin{array}{llll|l} (1)' & 2 & -1 & 3 & 3 \\ (2)' = (2) - \frac{1}{2}(1) & 0 & \frac{1}{2} & \frac{1}{2} & \frac{3}{2} \\ (3)' = (3) - \frac{1}{2}(1) & 0 & \frac{3}{2} & \frac{1}{2} & \frac{5}{2} \end{array}$$

Now make zeroes on 2nd column below diagonal by suitable multiples of (2):

$$\begin{array}{llll|l} (1)'' & 2 & -1 & 3 & 3 \\ (2)'' & 0 & \frac{1}{2} & \frac{1}{2} & \frac{3}{2} \\ (3)'' = (3)' - (2)' & 0 & 0 & -1 & -2 \end{array}$$

Now have an upper triangular matrix (xero below diagonal of A). Easily solve by back subn. working from bottom to top; *i.e.*

$(3)'' \Rightarrow -x_3 = -2$ or $x_3 = 2$

$(2)'' \Rightarrow \frac{1}{2}x_2 + x_3 = \frac{3}{2}$ or $x_3 = 1$

$(3)'' \Rightarrow 2x_1 - x_2 + 3x_3 = 3$ or $x_1 = -1.$

Method much faster than other methods, such as Cramer's Rule.

Note: if pivot (*i.e.* diagonal element 2 in equation (1) or $\frac{1}{2}$ in equation (2)') is zero, simply interchange rows.

6.7 *Gauss-Jordan Elimination*

Useful method for finding the ***Inverse*** of a matrix. Suppose we wish to find A^{-1}, where

$$A = \begin{bmatrix} 2 & -1 & 3 \\ 1 & 0 & 2 \\ 1 & 1 & 2 \end{bmatrix}$$

as before.

Step 1: Write in the extended (or *augmented*) matrix notation

$$\begin{array}{l} (1)- \\ (2)- \\ (3)- \end{array} \quad \left[\begin{array}{ccc|ccc} 2 & -1 & 3 & 1 & 0 & 0 \\ 1 & 0 & 2 & 0 & 1 & 0 \\ 1 & 1 & 2 & 0 & 0 & 1 \end{array}\right]$$

Method: make zeroes in 1st column below diagonal of A by subtracting suitable multiples of (1)

$$\begin{array}{l} (1)' \\ (2')=(2)-\frac{1}{2}(1) \\ (3')=(3)'-\frac{1}{2}(1) \end{array} \quad \left[\begin{array}{ccc|ccc} 2 & -1 & 3 & 1 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 1 & 0 \\ 0 & \frac{3}{2} & \frac{1}{2} & -\frac{1}{2} & 0 & 1 \end{array}\right]$$

Now make zeroes on 2nd column below diagonal by subtracting suitable multiples of $(2)'$

$$\begin{array}{l} (1)'' \\ (2)'' \\ (3)''=(3)'-3(2') \end{array} \quad \left[\begin{array}{ccc|ccc} 2 & -1 & 3 & 1 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 1 & 0 \\ 0 & 0 & -1 & 1 & -3 & 1 \end{array}\right]$$

Now make zeroes on last column *above* diagonal: by subtracting multiples of $(3)''$

$$\begin{array}{l} (1)'''=(1)''+3(3)'' \\ (2)'''=(2)''+\frac{1}{2}(3)'' \\ (3)''' \end{array} \quad \left[\begin{array}{ccc|ccc} 2 & -1 & 0 & 4 & -9 & 3 \\ 0 & \frac{1}{2} & 0 & 0 & -\frac{1}{2} & \frac{1}{2} \\ 0 & 0 & -1 & 1 & -3 & 1 \end{array}\right]$$

Finally, make zeroes on second column above diagonal by subtracting multiples of

$(2)'''$

$$\begin{array}{ll} (1)^{IV} = (1)''' + 2(2)''' & \left(\begin{array}{ccc|ccc} 2 & 0 & 0 & 4 & -10 & 4 \\ 0 & \tfrac{1}{2} & 0 & 0 & -\tfrac{1}{2} & \tfrac{1}{2} \\ 0 & 0 & -1 & 1 & -3 & 1 \end{array}\right) \\ (2)^{IV} & \\ (3)^{IV} & \end{array}$$

Now make remaining diagonal elements unity

$$\begin{array}{ll} (1)^{V} = \tfrac{1}{2}(1)^{IV} & \left(\begin{array}{ccc|ccc} 1 & 0 & 0 & 2 & -5 & 2 \\ 0 & 1 & 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & -1 & 3 & -1 \end{array}\right) \\ (2)^{V} = 2(2)^{IV} & \\ (3)^{s} = -1(3)^{IV} & \end{array}$$

Then, matrix on right hand side is A^{-1}.