CMM notes week 3

$$x^2 + xy = 10$$
$$y + 3xy^2 = 57$$

$$x_{i+1} = \frac{10 - x_i^2}{y}$$

$$y_{i+1} = 57 - 3x_i y_i^2$$

initial guess $x_0 = 1.5$
$y_0 = 3.5$

instead we do

$$\left.\begin{array}{l} x_{i+1} = \sqrt{10 - x_i y_i} \\ y_{i+1} = \sqrt{\dfrac{57 - y_i}{3x_i}} \end{array}\right\rangle$$ so values do not diverge

use x_{i+1} (which is the estimated root) into the y_{i+1} equation (as $x_i = x_{i+1}$)

Conditions for fixed point iteration

$$\left|\frac{du}{dx}\right| + \left|\frac{du}{dy}\right| < 1 \qquad \left|\frac{dv}{dx}\right| + \left|\frac{dv}{dy}\right| < 1$$ for 2 equations u & v.

difficult to implement if 2 conditions are not respected.

Newton-Raphson

$$u_{i+1} = u_i + (x_{i+1} - x_i)\frac{du_i}{dx} + (y_{i+1} - y_i)\frac{du_i}{dv}$$

$$v_{i+1} = v_i + (x_{i+1} - x_i)\frac{dv_i}{dx} + (y_{i+1} - y_i)\frac{dv_i}{dy}$$

$$x_{i+1} = x_i - \frac{u_i \frac{dv_i}{dy} - v_i \frac{du_i}{dy}}{\frac{du_i}{dx}\frac{dv_i}{dy} - \frac{du_i}{dy}\frac{dv_i}{dx}} \qquad y_{i+1} = y_i - \frac{v_i \frac{du_i}{dx} - u_i \frac{dv_i}{dx}}{\frac{du_i}{dx}\frac{dv_i}{dy} - \frac{du_i}{dy}\frac{dv_i}{dx}}$$

determinant

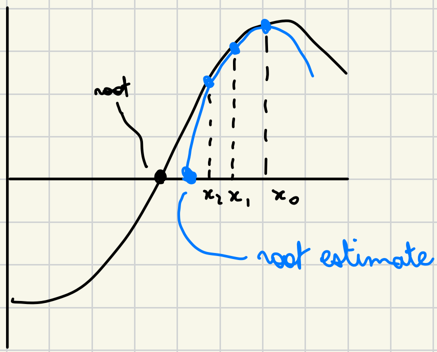
- write polynomials in this form:

$f_n(x)$ $\quad f_3(x) = ((a_3 x + a_2)x + a_1)x + a_0$

- we get rid of the roots we already know

e.g $(x-1)(x+5)(x+3)$ $\quad$ if we know $x=1$, we can divide everything by $(x-1)$

Muller's technique - variant of secant



projects a parabola instead

we take 3 points x_0, x_1, x_2 and express our function (in this case quadratic), about one point x_2:

$$f(x_0) = a(x_0 - x_2)^2 + b(x_0 - x_2) + c$$
$$f(x_1) = a(x_1 - x_2)^2 + b(x_1 - x_2) + c$$
$$f(x_2) = a(\cancel{x_2 - x_2})^2 + b(\cancel{x_2 - x_2}) + c \quad \text{we get } c$$

$h_0 = x_1 - x_0 \qquad h_1 = x_2 - x_1$

$$\delta_0 = \frac{f(x_1) - f(x_0)}{x_1 - x_0} \qquad \delta_1 = \frac{f(x_2) - f(x_1)}{x_2 - x_1}$$

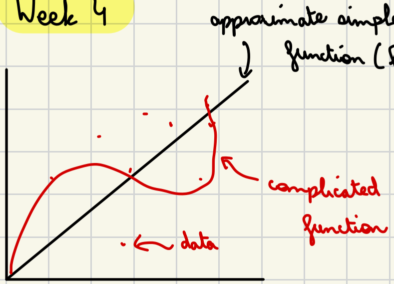
$$\left.\begin{aligned} a &= \frac{\delta_1 - \delta_0}{h_1 + h_0} \\ b &= a h_1 + \delta_1 \\ c &= f(x_2) \end{aligned}\right\} \text{coefficients of a new test polynomial}$$

$$x_3 - x_2 = \frac{-2c}{b \pm \sqrt{b^2 - 4ac}}$$

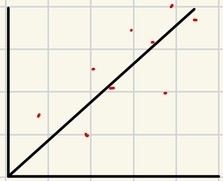
next approximation of the root

$$\varepsilon_a = \left| \frac{x_3 - x_2}{x_3} \right| \times 100$$

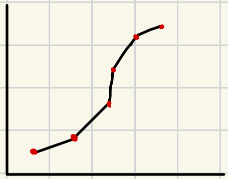
Week 4



Regression:



linear regression

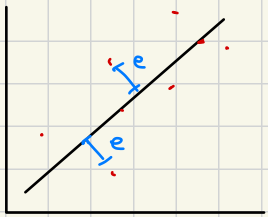


linear interpolation

Least-squares regression

$$y = a_0 + a_1 x + e$$

$$e = y - a_0 - a_1 x$$



$$\sum_{i=1}^{n} e_i = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i)$$

$$S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i)^2$$

minimize sum of squares of residuals

Least-square for straight line

$$y = a_0 + a_1 x$$

$$\left.\begin{aligned} \frac{dS_r}{a_0} &= -2\sum_{i=1}^{n} (y_i - a_0 - a_1 x_i) = 0 \\ \frac{dS_r}{a_1} &= -2\sum_{i=1}^{n} [(y_i - a_0 - a_1 x_i) x_i] = 0 \end{aligned}\right\} \text{minimize } S_r$$

$$a_1 = \frac{n\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

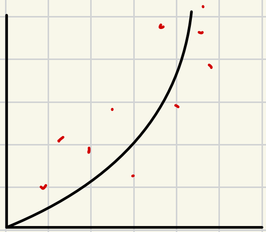
$$a_0 = \bar{y} - a_1 \bar{x}$$

$$\bar{y} = \frac{\sum_{i=1}^{n} y_i}{n} \qquad \bar{x} = \frac{\sum_{i=1}^{n} x_i}{n}$$

Polynomial regression

$$y = a_0 + a_1 x + a_2 x^2 + e$$

$$y = a_0 + a_1 x + a_2 x^2 + \ldots + a_m x^m + e$$



Quadratic regression

$$S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i - a_2 x_i^2 \right)^2$$

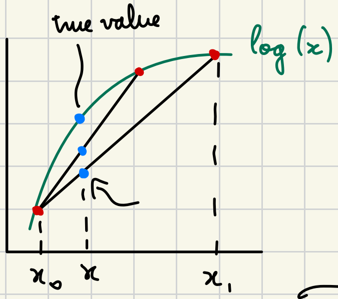
$$\frac{dS_r}{da_0} = 0$$

$$\frac{dS_r}{da_1} = 0$$

$$\frac{dS_r}{a_2} = 0$$

Interpolation

To approximate a function:



linear interpolation:

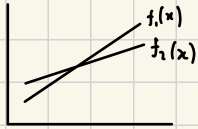
- choose 2 points (x_0, x_1) and apply this function:

$$f(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0)$$

the smaller the range, the better

Second order interpolation needs 3 point estimates

Week 5 - Linear Algebra



- solution of systems of linear equations

Cramer's rule

$[A]\{X\} = \{B\}$

$$[A] = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$x_1 = \frac{\begin{vmatrix} b_1 & a_{12} & a_{13} \\ b_2 & a_{22} & a_{23} \\ b_3 & a_{32} & a_{33} \end{vmatrix}}{D}$$

Only for systems of 3 equations

$D = \left[\, \overline{|X} \,\right]$

cannot be computerised, not iterative process

Gauss Elimination

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n &= b_1 \\ a'_{22}x_2 + a_{23}x_3 + \ldots + a'_{2n}x_n &= b_2 \\ a_{2n}x_n &= b_n \end{aligned}$$

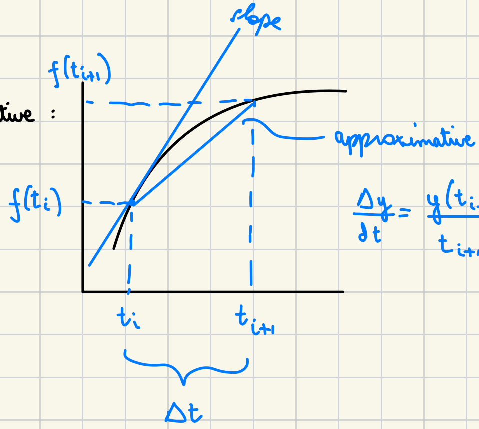
an then back substitution

- cannot handle division by 0.
- accumulate inaccuracies due to round-off error.
- ill-conditioned systems.

use partial pivoting -> change order of equations if one of them has a near-zero coefficient

Week 6 - ODE 1

· Approximation of a derivative :



$$\frac{\Delta y}{dt} = \frac{y(t_{i+1}) - y(t_i)}{t_{i+1} - t_i}$$

Taylor's series

$$f(x_{i+1}) = f(x_i) + \frac{f'(x_i)}{1!}h + \ldots + \frac{f^{(n)}(x_i)}{n!}h^n + R_n$$

$$h = x_{i+1} - x_i \qquad R_n = \frac{f^{(n+1)}(\xi)\,h^{n+1}}{(n+1)!}$$

truncation error

One-step methods

Solve equations in the form $\frac{dy}{dx} = f(x,y)$ with a given initial condition $y_0 = y(x_0)$

extrapolate from y_i to y_{i+1} over a step h

$$y_{i+1} = y_i + \phi h$$

ϕ: estimate of an appropriate slope of the function y over the step h

We then use this to compute over a large interval

Euler method

$$y_{i+1} = y_i + \underbrace{f(x_i + y_i)}\, h$$

from differential equation as 1st derivative of y at point x_i

Runge-Kutta - smaller error than Euler

$$y_{i+1} = y_i + \underbrace{\phi(x_i, y_i, h)}_{\text{increment function}} h$$

$\phi = a_1 k_1 + a_1 k_1 + \dots + a_n k_n$

$k_1 = f(x_i, y_i)$

$k_2 = f(x_i + p_1 h, y_i + q_{11} k_1 h)$

Week 7: System of ODEs and stiff equations

$$\frac{dy_1}{dx} = f_1(x, y_1, \dots, y_n) \qquad y_1^0 = y_1(x_0)$$

$$\frac{dy_n}{dx} = f_n(x, y_1, y_2, \dots, y_n) \qquad y_n^0 = y_n(x_0)$$

example: airplane motion

If we apply Euler:

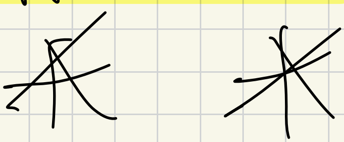
$$y_j^{i+1} = y_j^i + \phi_j h$$

n values

ϕ_j — estimate of slope

use solve_ivp

Stability of the ODE solution methods



Stiff ODEs

- with a fast component (low h range) & slow component (high h range)
- need small step for whole solution

Unconditionally stable methods - Implicit Euler – for stiff ODE

- uses information at locations that have not yet been computed

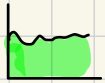
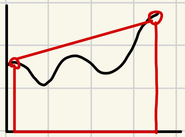
$$y_{i+1} = y_i + f(x_{i+1}, y_{i+1})h$$

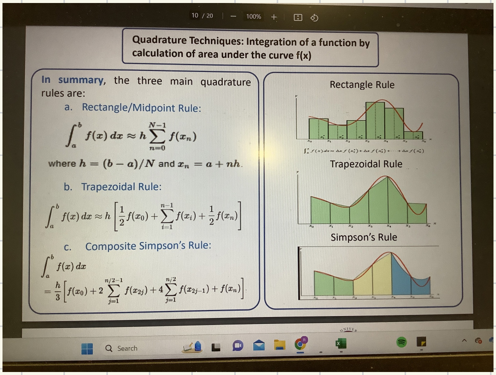
use x_{i+1} to compute slope (derivative)

$$F(y_{i+1}) = y_i + f(x_{i+1}, y_{i+1})h - y_{i+1} = 0$$

find root of $F(y_{i+1})$

Week 8: Numerical integration

- Quadrature techniques =>  area under curve, approximation
- Adaptive techniques =>  calculation of area under $f(x)$



Composite Simpson's rule

3/8 Simpson's rule

- interpolate using a cubic

Adaptive algorithms

Week 10: Optimisation of functions

- $\frac{\Delta y}{\Delta x} = 0$

- 1D dimensional
- 2D optimisation

$\Big\}$ with constraints $\quad d_i(x) \leq a_i$
$\quad e_i(x) = b_i$

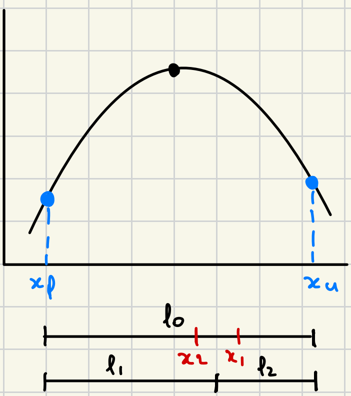
- linear function + linear constraints => linear programming
- quadratic $f(x)$ + linear constraints => quadratic programming
- non-linear $f(x)$ + non-linear constraints => non-linear programming

- degrees of freedom: n: number of dimensions in x vector
  p: number of equality constraints
  m: number of inequality constraints

$m + p < n$ to obtain a solution, a optimisation is overconstrained.

1D - Golden search technique => follow bisection but we target max or min.

- select 2 points either side of maxima/minima



$$l_0 = l_1 + l_2$$
$$\frac{l_1}{l_0} = \frac{l_2}{l_1}$$

$$\Bigg\rangle \quad \underbrace{\frac{l_1}{l_1 + l_2} = \frac{l_2}{l_1}}_{1 + R = \frac{1}{R}} \qquad R = \frac{l_2}{l_1}$$

$$1 + R = \frac{1}{R} \implies R^2 + R - 1 = 0$$

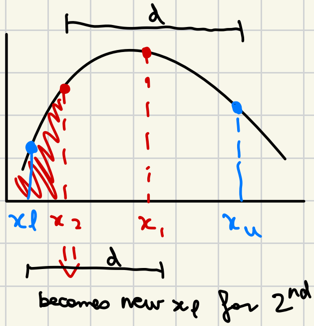
$R = \frac{\sqrt{5}-1}{2} = 0.61803 \Leftarrow$ golden ratio

$d = \frac{\sqrt{5}-1}{2}(x_u - x_\ell)$

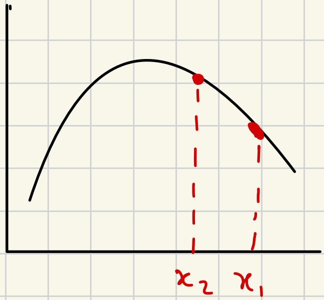
$x_1 = x_\ell + d$

$x_2 = x_u - d$

· $f(x_1) > f(x_2)$: all points left to x_2 can be eliminated as no max occurs



· $f(x_1) < f(x_2)$: all points right of x_1 can be eliminated



does that mean x_1 & x_2 are on one side of maxima or not?

$\varepsilon_a = (1-R)\left|\frac{x_u - x_\ell}{x_{opt}}\right| \times 100$

Newton's method – used when derivative can be easily found., only if initial guess is sufficiently close.

$x_{i+1} = x_i - \frac{f'(x_i)}{f''(x_i)}$ ~ max/min ← whether it is max or min

find root of $f'(x)$ basically

Newton's method 2 variable

- we need 2^{nd} derivative with relation to x & y
- Hessian: $|H| = \frac{\partial^2 f}{\partial x^2} \frac{\partial^2 f}{\partial y^2} - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2$ is a test point for either a max or min

$$|H| = \frac{\partial^2 f}{\partial x^2}\frac{\partial^2 f}{\partial y^2} - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2$$

If $|H| > 0$ and $\partial^2 f/\partial x^2 > 0$, then $f(x, y)$ has a local minimum.
If $|H| > 0$ and $\partial^2 f/\partial x^2 < 0$, then $f(x, y)$ has a local maximum.
If $|H| < 0$, then $f(x, y)$ has a saddle point.

$$x_{i+1} = x_i - J . H^{-1}$$

jacobian matrix $J = \begin{bmatrix} \frac{\partial F_1}{\partial x_1} & \cdots & \frac{\partial F_1}{\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial F_m}{\partial x_1} & \cdots & \frac{\partial F_m}{\partial x_n} \end{bmatrix}$

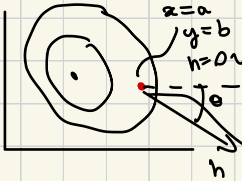
$$H = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix}$$

only if $H \neq 0$

if determinant $= 0$, no solution

Week 11: Optimisation 2

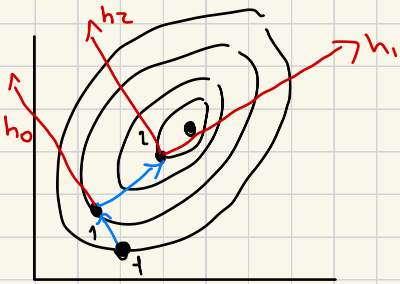
- Gradient methods => finding shortest route to the top of a mountain



$x=a$
$y=b$
$h=0$ variety of local heights, ridges, etc.

1) find where we are

$g(h)$ is optimisation path where $g'(h)=0$ at the top.



$$g'(h) = \frac{\partial f}{\partial x}\cos\theta + \frac{\partial f}{\partial y}\sin\theta = 0$$

$$x = x_0 + \frac{\partial f}{\partial x} h$$

$$y = y_0 + \frac{\partial f}{\partial y} h$$

Lagrange multiplier technique

$$L(y) = f(x) + \gamma g(x)$$

objective function

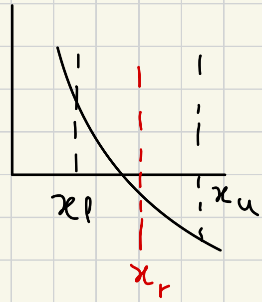
equality constraint

Bisection method (closed)

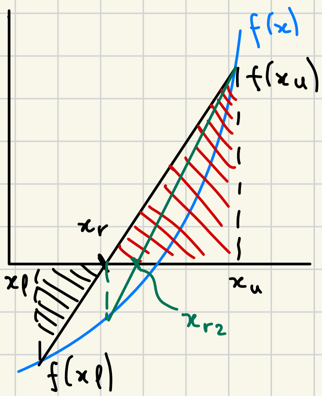
- upper & lower boundary - guess the mid-point as root $x_r = \frac{x_l + x_u}{2}$
- keep iterating until within tolerance

$f(x_l) \times f(x_u) \; > < = 0$

evaluates this



False position method



- x_r is the initial guess

$$\frac{f(x_l)}{x_r - x_l} = \frac{f(x_u)}{x_r - x_u}$$

· iterates until satisfactory estimate is achieved

· if FPM does not converge change it to: $x_r = x_u - \frac{0.5\, f(x_u)(x_l - x_u)}{f(x_l) - 0.5\, f(x_u)}$

Single fixed point iteration (closed)

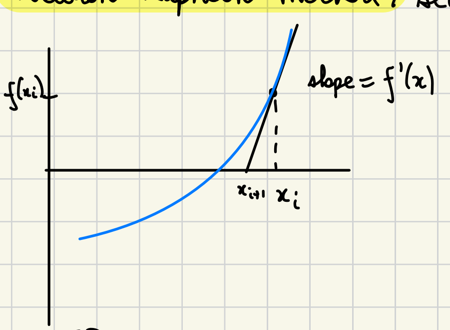
· express the equation in terms of x. E.g. $x^2 - 2x + 3 = 0 \Rightarrow x = \frac{x^2+3}{2}$

· predict a new value of x using an old one.

$$x_{i+1} = g(x) = \frac{x_i^2 + 3}{2}$$

Newton Raphson method / secant (closed)

secant calculates an approximation to the point derivative (for unknown derivative)



$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

you need to know derivative of $f(x)$ to use.

Not solvable if:

- asymptotic function
- multiple minima
- cyclic/periodic functions
- no real root domain.

FP guaranteed to find the root, secant not.

Modified secant technique (closed)

- derivative is calculated by retaining one old point and taking a small increment of value

Inverse quadratic interpolation

- for imaginary roots

Ralston for multiple roots