Root finding

given some function $\vec{f}(\vec{x})$, find $\vec{x}^*$

such that $\underline{\vec{f}(\vec{x}^*) = 0}$

generally, root finders are <u>iterative</u>: we start from an initial guess and then successively improve it

→ do not know in advance how much work is necessary

xamples of root-finding problems

magnetization m of a ferromagnet

$$m = \tanh(\alpha m) \quad , \alpha \text{ parameter}$$

iemann ζ function

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}$$ (analytically continued in the complex plane)

Collect \$1 mil if all non-integer s have $\mathrm{Re}(s) = \frac{1}{2}$

Eigenvalue problem

$$A\vec{x} = \lambda\vec{x}$$

both $\vec{x}, \lambda$ unknown $\longrightarrow$ non-linear problem for $\begin{pmatrix} \vec{x} \\ \lambda \end{pmatrix}$

(linear eigenvalue problem. Typically solved using specialized methods)

Sometimes $A(\lambda)\vec{x} = \lambda\vec{x}$

structural mechanics: $(A_2\lambda^2 + A_1\lambda + A_0)\vec{x} = 0$, $\vec{x}$: eigenmode

-> iterative method

Nonlinear BVP

$$\frac{d^2x}{dt^2} = -\frac{GM}{x^2}, \quad x(t_a) = x(t_b) = 0 \qquad \text{(1D gravity)}$$

$\downarrow$

finite difference matrix A

$$\rightarrow \quad A\vec{x} = \vec{f}(\vec{x}), \quad \vec{f}(\vec{x}) = GM\begin{pmatrix} \frac{1}{x_1} \\ \frac{1}{x_2} \\ \vdots \\ \frac{1}{x_N} \end{pmatrix} \quad \text{depends on } x_i!$$

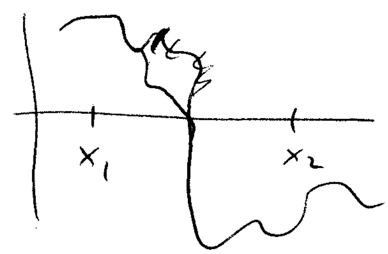
Root finding in 1D

Bisection search

Bracket a zero: pick x_1, x_2 such that

$$\mathrm{sign}\, f(x_1) \neq \mathrm{sign}\, f(x_2)$$

$\rightarrow$ $f(x)$ must have a zero in between



halve the interval and compute $f\left(\frac{x_1+x_2}{2}\right)$

if $\mathrm{sign}\left(f\left(\frac{x_1+x_2}{2}\right)\right) \neq \mathrm{sign}\, f(x_1)$, repeat the algorithm on $\left[x_1, \frac{x_1+x_2}{2}\right]$,

otherwise repeat on $\left[\frac{x_1+x_2}{2}, x_2\right]$

each step shrinks the interval containing the zero by a factor of 2.

Error analysis / Convergence rate

- saw: # of correct digits <u>linear</u> in

  # of iterations

subinterval in which the root is ~~des~~ <u>halved</u> at each iteration

Suppose initial interval is $\Delta_0 = |[a, b]|$

then $\Delta_1 = \frac{1}{2}\Delta_0$ <u>always</u>

So:

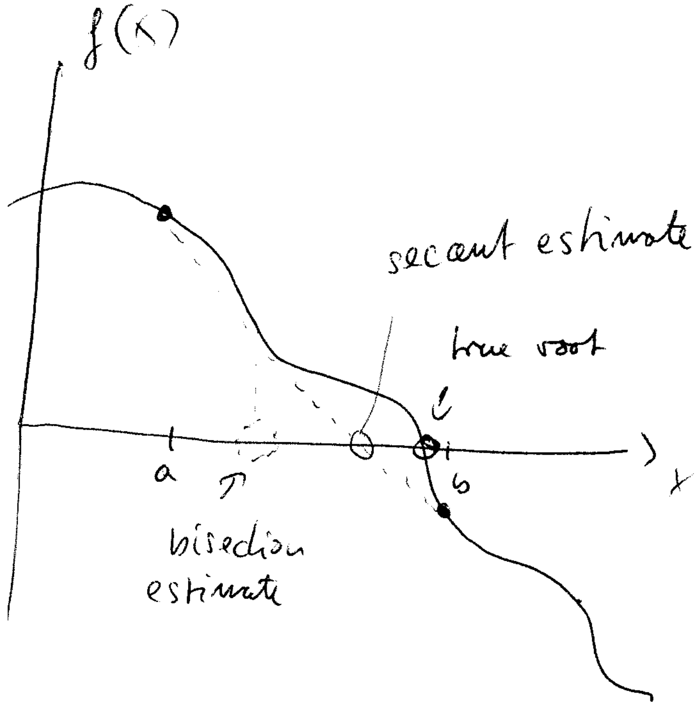
$$\Delta_n = \frac{1}{2}\Delta_{n-1} = \frac{1}{2}\cdot\frac{1}{2}\Delta_{n-2} = \dots = \frac{1}{2^n}\Delta_0$$

Convergence <u>exponentially fast</u> (faster than anything we have seen, N-C, finite-diff, ODE were all algebraic $\sim N^p$)

Nomenclature: bisection has <u>linear</u> convergence (because $\left(\frac{1}{2}\right)^n$ has exponent <u>linear</u> in n.

(compare to <u>first-order</u> $\sim \frac{1}{N}$)

Secant method



like bisection, bracket root on $[a, b]$, $\mathrm{sign}(f(a)) \neq \mathrm{sign}(f(b))$

estimate root as $x^* = b - \dfrac{b-a}{f(b)-f(a)} f(b)$

$$\rightarrow \qquad x_{n+1} = x_n - \frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})} f(x_n)$$

can jump out of bracket $\rightsquigarrow$ less robust than bisection

convergence like ϵ^p, $p = \frac{1+\sqrt{5}}{2} \sim 1.6$

$e_{n+1} = O(e_n^p)$

Newton-Raphson (or often just Newton's method)

. Consider secant step

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

f diff'able

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

second derivation

$$f(x) = f(x_n) + (x - x_n) f'(x_n) + \mathcal{O}((x-x_n)^2)$$

+ $f(x^*) = 0$ we find

$$0 = f(x_n) + (x^* - x_n) f'(x_n)$$

$$\Rightarrow \quad x^* = x_n - \frac{f(x_n)}{f'(x_n)}$$

=> approximate $f(x)$ by a linear function, then jump to that function's zero.

Convergence analysis

Let x_0 be the true root $f(x_0) = 0$

Then close to the root,

$$f(x_0) = 0 = f(x_n) + f'(x_n)(x_0 - x_n) + \frac{1}{2} f''(x_n)(x_0 - x_n)^2 + O((x_0 - x_n)^3)$$

$$\Rightarrow \underbrace{\left(x_0 - x_n + \frac{f(x_n)}{f'(x_n)}\right)}_{= x_0 - x_{n+1} = e_{n+1}} = -\frac{1}{2} \frac{f''(x_n)}{f'(x_n)} \underbrace{(x_0 - x_n)^2}_{= e_n^2} + O((x_0 - x_n)^3)$$

error

$$\Rightarrow \quad e_{n+1} = C\, e_n^2 \quad \text{(quadratic convergence)}$$

$$e_{n+1} \sim e_n^2 \sim (e_{n-1}^2)^2 = e_{n-1}^{2\cdot 2} = e_{n-2}^{2\cdot 2\cdot 2} = \dots = e_0^{2^{n+1}}$$

number of correct digits <u>doubles</u> at each step ouble roots

double root a x = a

Ex: $f(x) = (x-a)^2$

-> error analysis breaks down — $f'(x_0) = 0$ -> linear convergence

'ewton's method in n-d

$$\vec{f}(\vec{x}) = \vec{0} \qquad \vec{f} : \mathbb{R}^n \longrightarrow \mathbb{R}^n$$

Newton requires these to be the same

inear case: $A\vec{x} = 0$ (special methods)

onlinear case:

$$\vec{f}(\vec{x}+\vec{\Delta}) = \vec{f}(\vec{x}) + J\vec{\Delta} + O(\vec{\Delta}^2)$$

$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & & \\ \frac{\partial f_n}{\partial x_1} & \cdots & \frac{\partial f_n}{\partial x_n} \end{pmatrix} \quad \text{(Jacobian)}$$

at a zero:

$$\vec{0} \approx f(\vec{x}) + J\vec{\Delta}$$

$$\longrightarrow \quad \vec{\Delta} = -J^{-1} f(\vec{x})$$ (numerically: solve system of eqns)

$$\longrightarrow \quad \vec{x}_{n+1} = \vec{x}_n - J^{-1}(\vec{x}_n)\, \vec{f}(\vec{x}_n)$$