Basic Numerical Methods

Iterations

$$X_{n+1} = X_n - f(X_n) / f'(X_n)$$

Std. Newton's method

Variant:

Steffensen's method (No derivative is required)

$$f'(X_n) \longrightarrow \frac{f(X_n + f(X_n)) - f(X_n)}{f(X_n)}$$

Fun: $f(X_n)$ is used as ΔX for its smallness

Secant method

$$f'(X_n) \longrightarrow \frac{f(X_n) - f(X_{n-1})}{X_n - X_{n-1}}$$

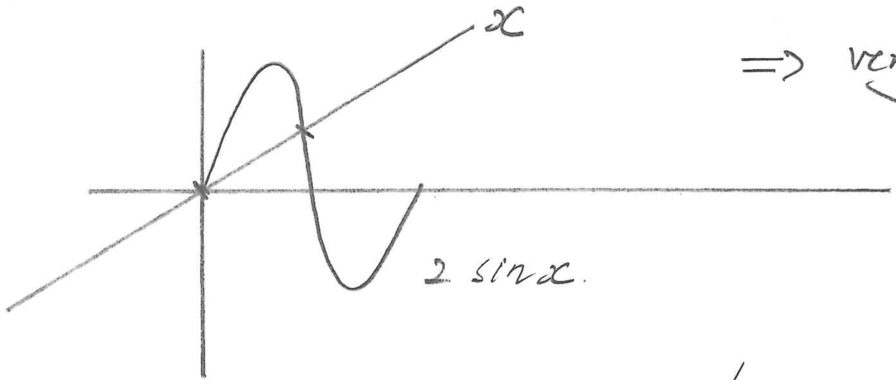
$\longrightarrow$ need 2 previous steps to get the next for finding roots

e.g. $f(x) = x - 2\sin(x)$

$$f(x) = x - r\,x(1-x)$$

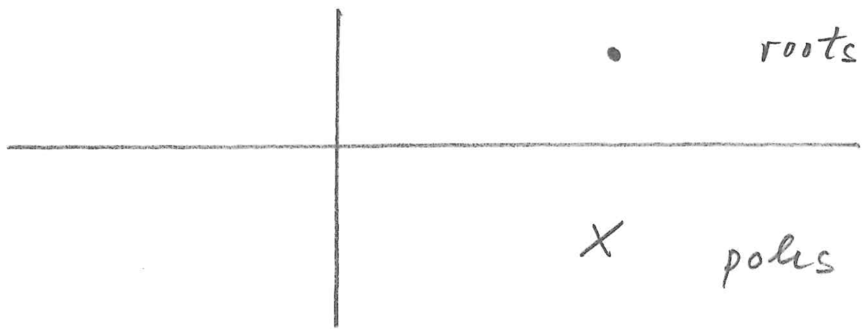
↳ appears logistic map

Note that a good method for finding roots is "just plot it"



⇒ very powerful

especially on a complex plane



or

studying Energy surfaces.

Deriving Newton's law

if x_0 is the root

$$f(x_0) = 0 \approx f(x) + (x_0 - x) f'(x)$$
$$+ \frac{1}{2} (x_0 - x) f''(x) (x_0 - x)$$
$$+ \cdots$$

1st order

$$x_0 = x - f(x) / f'(x) \Rightarrow$$ Newton's method

2nd order

$$(x_0 - x) \left[f'(x) + \frac{1}{2} f''(x) (x_0 - x) \right] = - f(x)$$

$$x_0 = x - \frac{f(x)}{f'(x) + \frac{1}{2} f''(x) \underline{(x_0 - x)}}$$

replace with $-f/f'$

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

$$= x_n - \frac{f(x_n) f'(x_n)}{f'(x_n)^2 - \frac{1}{2} f''(x_n) f(x_n)}.$$

$\longrightarrow$ Halley's method
(a cubic method)

<u>Nevertheless</u>

Simplicity is gold

higher order method $\neq$ better

$\longrightarrow$ more costly

$\longrightarrow$ stability issues in derivatives

Demo

e.g 1 finding inverse

$$f(x) = \frac{1}{x} - a$$

$$f'(x) = -1/x^2$$

$$f''(x) = 2/x^3$$

Newton's method:

$$x_{n+1} = x_n + x_n(1 - a x_n) \quad //$$

Halley's method

$$x_{n+1} = x_n - \frac{\left(\frac{1}{x_n} - a\right)\frac{-1}{x_n^2}}{\left(\frac{-1}{x_n^2}\right)^2 - \frac{1}{2}\frac{2}{x_n^3}\left(\frac{1}{x_n} - a\right)}$$

$$= x_n + \frac{x_n(1 - a x_n)}{1 - (1 - a x_n)}$$

//

see $(1 - a x_n)$ appears naturally ?

$\Delta \to 0 \quad x_n \to 1/a$ our solution

make sense !

e.g. 2 finding sqrt

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

$$x_{n+1} = x_n - \frac{x_n^2 - a}{2x_n} \quad \text{for Newton's method}$$

$$= x_n - \frac{1}{2}\left(x_n - \frac{a}{x_n}\right) = \frac{1}{2}\left(x_n + \frac{a}{x_n}\right)$$

$$x_{n+1} = x_n - \frac{2x_n(x_n^2 - a)}{3x_n^2 + a} \quad \text{for Halley's method}$$

$$= \frac{x_n^3 + 3x_n a}{3x_n^2 + a}$$

$\Rightarrow$ Julia Implementation

Newton's Vs Steffensen Vs Halley's

Root finding of eigenvalue solver

$\det(M - \lambda I) \leftrightarrow f(\lambda)$. characteristic polynomial

find all roots by eigenvalue solver!

$$f(x) = c_0 + c_1 x + \cdots + c_{N-1} x^{N-1} + x^N$$

set to 1.

$$\vec{c} = (c_0, c_1, \cdots, c_{N-1})$$

allows us to form the companion matrix

Eric p. 71

$$C = \begin{bmatrix} 0 & 0 & \cdots & 0 & -c_0 \\ 1 & 0 & \cdots & 0 & -c_1 \\ 0 & 1 & \cdots & 0 & \vdots \\ \vdots & \vdots & & 1 & -c_{N-1} \end{bmatrix}$$

related to Vandemonde Matrix.

$\vec{\lambda}_C \leftrightarrow$ roots of $f(x)$.

Improving convergence by Shanks' transformation

$$S(N) = \sum_{i=1}^{N} a_i \quad \text{sum up to } N \text{ terms.}$$

Eric p. 97.

$$\tilde{S} \longrightarrow \frac{S_{N-1} S_{N+1} - S_N^2}{S_{N-1} + S_{N+1} - 2S_N}$$

4 study how S_∞ is reached

$N \quad S_N \quad \tilde{S} \quad \tilde{S}(\tilde{S}) \quad \cdots$

$\vdots$

see Julia Implementation.

$$\sum_{n=1}^{\infty} \frac{1}{n^2} \longrightarrow \frac{\pi^2}{6} \quad \text{but very slowly}$$

Shanks transform is very good!