Convergence Order

Numerical Integration methods we've seen converge as follows — under appropriate assumptions —

$$|\epsilon_{i+1}| \cong \alpha |\epsilon|_i$$

(not the mathematically rigorous defn. — see Ralston 78, e.g.)

this leads to $|\epsilon_i| \cong C^i$

Let's look at another very important numerical method.

Example

Square-Root Algorithm, given N

$x_0 = 1$;

$x_{i+1} = \frac{1}{2}(x_i + N/x_i)$ until $|x_{i+1} - x_i| < \varepsilon$.

Intuition: at convergence $x = \frac{1}{2}(x + N/x)$

… if convergence takes place

$\Rightarrow \quad x = N/x \Rightarrow \quad x^2 = N$

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iteration	N = 2, Error	N = 100 Error
1	0.08578	40.50
2	0.00245	16.24
3	0.00000 2112	5.025
4	*	0.8404
5		0.03258
6		0.000052
7		*

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* Thanks to Prof. David Dobkin

Empirically, we observe that

# of places <u>doubles</u> (approximately)
every iteration — eventually

Note that this is <u>ultimate</u> behavior.
Eg. if N is very small

$$x_{i+1} \approx x_i/2$$ ... until we get close

# of places doubling is example of

$$\varepsilon_{i+1} \approx \alpha|\varepsilon_i|^2 \longrightarrow$$ called <u>quadratic convergence</u>

$$\varepsilon_{i+1} \approx \alpha|\varepsilon_i| \longrightarrow$$ called <u>linear convergence</u>

Linear $\varepsilon_{i+1} \approx c^i$

quadratic $\varepsilon_{i+1} \approx c^{2^i}$

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this is an example of a root-finding, or zero-finding problem in one real variable —

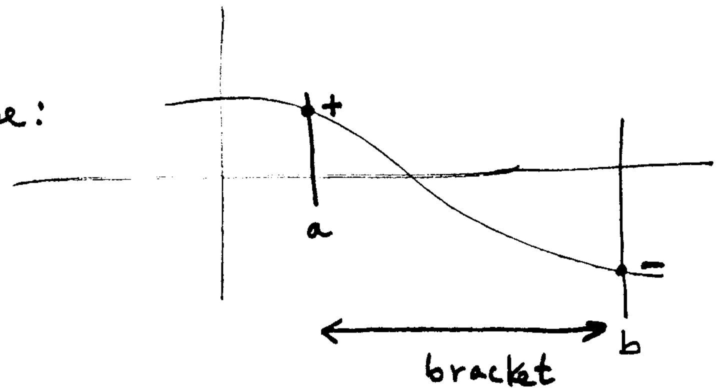
$$x^2 - N = 0$$

Root Finding in one-D:

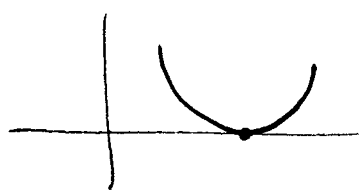
Issues:
- choosing starting point, interval(?)
- convergence?
- rate of convergence?

Dangers lurk! → insight & knowledge is crucial

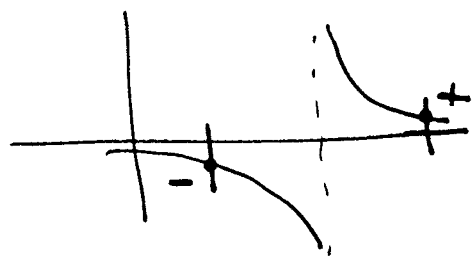
Good case:



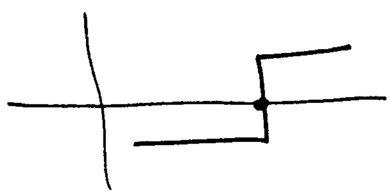
tangent:
(double root)



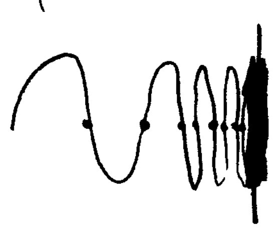
singularity:



discontinuity:

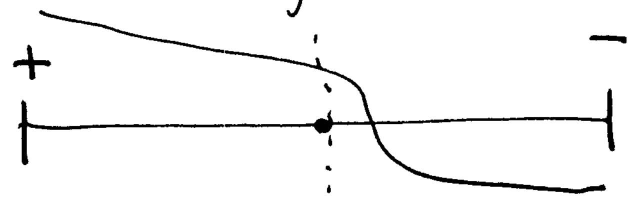


pathology:



$\sin(1/x)$ e.g.

Bisection Simple, linear convergence, very reliable



$$\boxed{\begin{array}{l}\text{bracket}\\ \text{evaluate at midpoint}\\ \text{halve bracket}\end{array}}$$

$$\varepsilon_{n+1} = \frac{1}{2}\varepsilon_n$$ linear convergence

must succeed.

tolerance for termination – requires thought, use relative size

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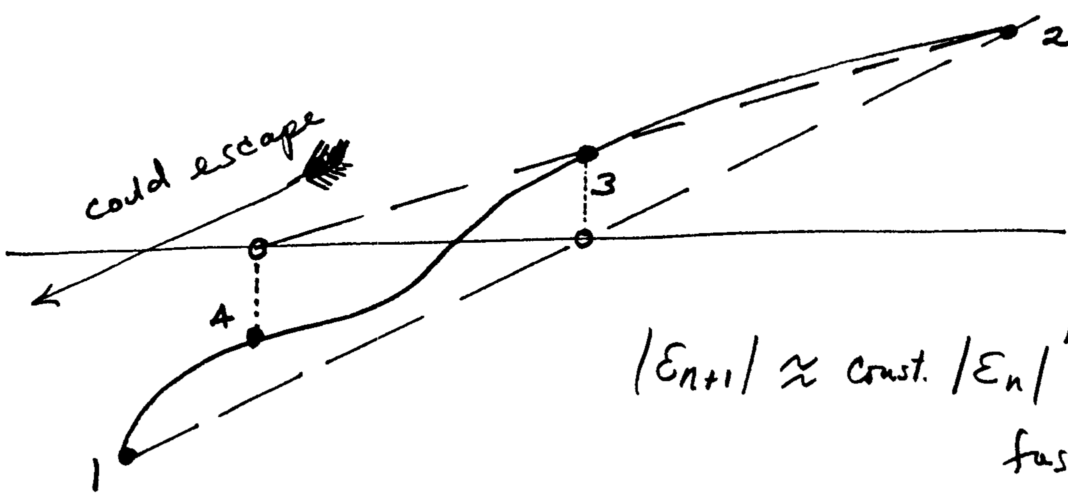
→ Other Classical Methods: sometimes faster, more dangerous

See [Press et al. NR] [Ralston78] [Acton70]

Secant Method Extrapolate or Interpolate linearly through two most recent points.



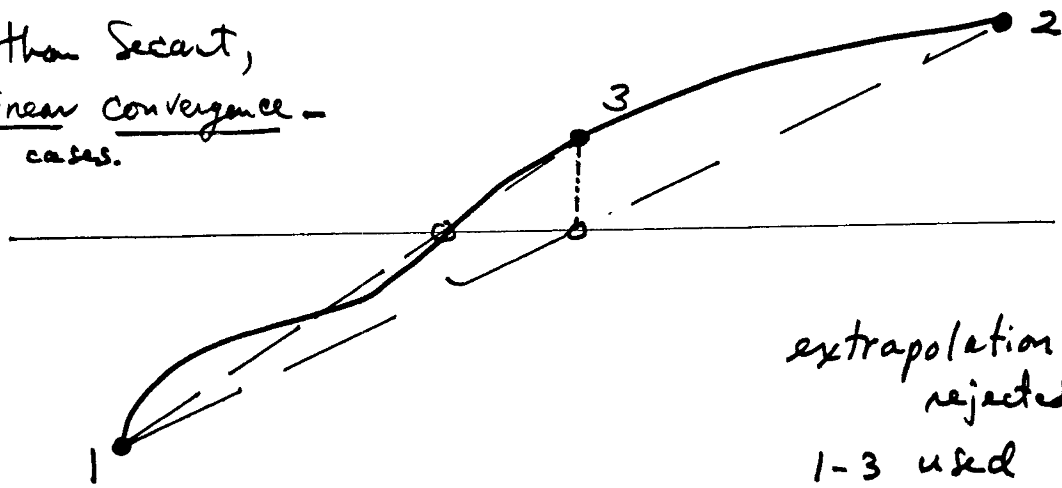
$$|\varepsilon_{n+1}| \approx \text{const.}\,|\varepsilon_n|^{1.618}$$

faster, but more dangerous

False Position (Regula falsi)

Interpolate between most recent points that bracket root.

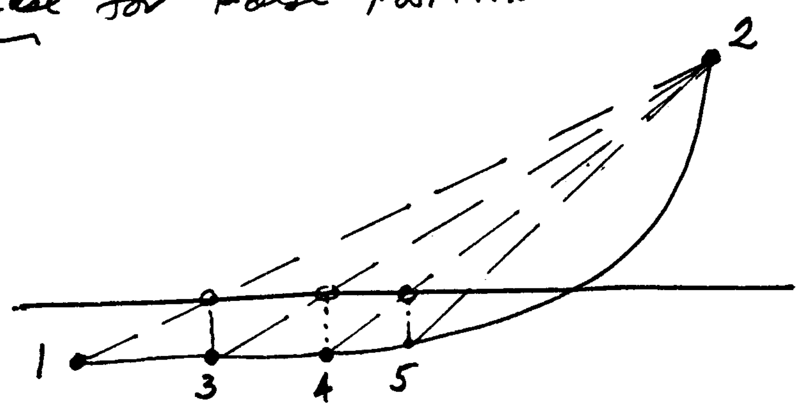
Safer than Secant, but linear convergence in bad cases.



extrapolation 2-3 rejected

1-3 used

Bad Case for False Position:

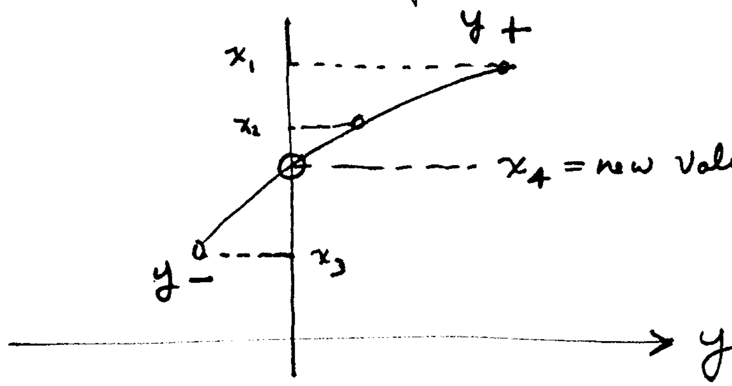


[Press et al.] Numerical Recipes recommends state-of-the-art

Brent's Method [Brent 73 Algorithms for Minimization Without Derivatives Prentice-Hall]

Combines
- root bracketing
- bisection (if interpolation outside current bracket)
- inverse quadratic interpolation

Inverse quadratic interpolation



x_4 = new value (set $y = 0$ in x = quadratic in y)

Claim is superlinear (at least in smooth cases)
but safe (because of bisection backup)

All these methods avoid using derivatives.

back to Sir Isaac...

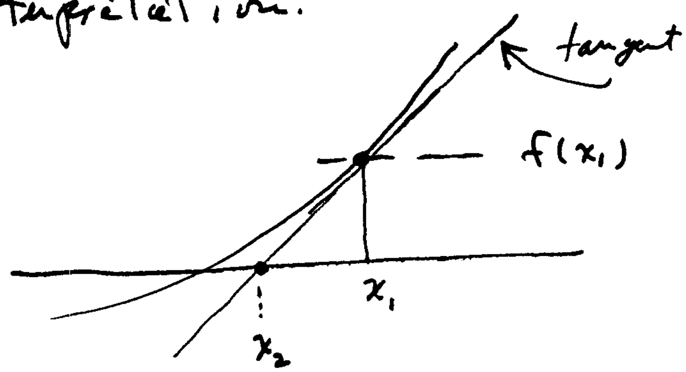
Newton-Raphson Method:

Taylor series

$$f(x+\delta) \approx f(x) + f'(x)\,\delta + \cdots = 0$$

use $\boxed{\delta = -\frac{f(x)}{f'(x)}}$

Geometric interpretation:



$$\frac{f(x_1)}{x_1 - x_2} = f'(x_1) \Rightarrow \quad x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$$

Can be extended to n-dimensions, and is very useful — when <u>close</u>.

BTW, back to square-root algorithm:

Solve $f(x) = x^2 - N = 0$

$f'(x) = 2x$

$$x_{i+1} = x_i - \frac{x_i^2 - N}{(2x_i)} = \frac{1}{2}\left(x_i + \frac{N}{x_i}\right)$$

which we started with today.

In the bad old days, division was done in software

$$\frac{a}{b} = a*\left(\frac{1}{b}\right) \quad \text{So we need inverse}$$

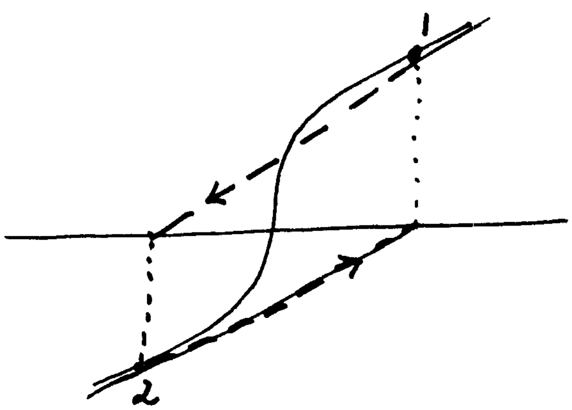
Solve
$$f(x) = b - \frac{1}{x} = 0$$
$$f'(x) = \frac{1}{x^2}$$

iteration
$$x_{i+1} = x_i - \frac{b - \frac{1}{x_i}}{\frac{1}{x_i^2}} = x_i*(2 - b*x_i)$$

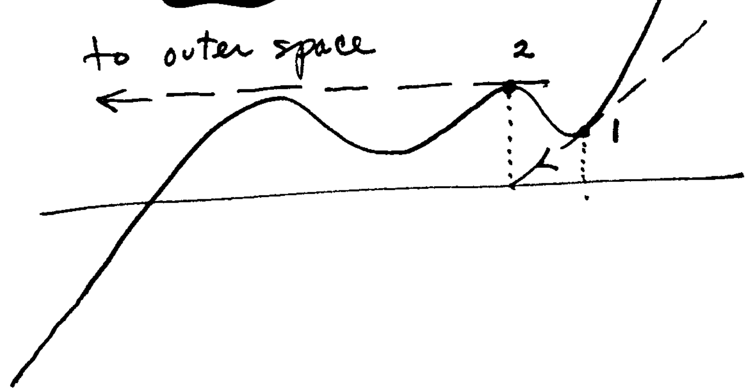
Uses multiplication & subtraction.

Requires initial estimate $0 < x_0 < 2/b$ [Atkinson85]

Bad Cases for Newton-Raphson



infinte loop



worse

Proof of Quadratic Convergence:

[Press et al., Atkinson, etc.]

$$f(\alpha) = f(x_n) + (\alpha - x_n) f'(x_n) + \frac{1}{2}(\alpha - x_n)^2 f''(c_n)$$

where $c_n \in [\alpha, x_n]$

and α is the desired root, $f(\alpha) = 0$

divide by $f'(x_n)$ (which can't be zero!)

$$0 = \underbrace{\frac{f(x_n)}{f'(x_n)}}_{x_n - x_{n+1}} + (\alpha - x_n) + (\alpha - x_n)^2 \frac{f''(c_n)}{2f'(x_n)}$$

$$0 = \cancel{x_n} - x_{n+1} + \alpha - \cancel{x_n} + (\alpha - x_n)^2 \frac{f''(c_n)}{2f'(x_n)}$$

$$\Rightarrow \quad (\alpha - x_{n+1}) = \left[-\frac{f''(c_n)}{2f'(x_n)}\right](\alpha - x_n)^2$$

$$\epsilon_{n+1} \cong \text{const.}\ \epsilon_n^2$$

Good Starting Point all important

Common Strategy
- Start with bisection
- polish off with Newton-Raphson

Polynomial root finding is a specialized art —
try to use highly evolved package, test answers

Zero-Finding: 2.2.10

In higher dimensions, we are in a jungle.

Insight, estimates, physical arguments — all help.

Newton-Raphson is the only general tool that's practical, but must be nursed to work on problems that are at all difficult.

There's a "Basin of Convergence":

Suppose, e.g., we want to use N-R to solve cubic

$$z^3 - 1 = 0$$

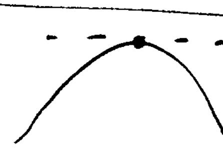
$$z_{i+1} = z_i - \frac{(z_i^3 - 1)}{3 z_i^2}$$

in complex z-plane.

Mark all starting points that converge to $z = 1$.

... Julia sets, fantastic pictures ...

Next topic: Optimization



Easier in general, especially in higher dimensions.