

Review: pros and cons of different methods

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① For root finding + fixed points $f(x)=0$, or $x=g(x)$

Univariate case

BISECTION

problem it solves: root finding

requirements: f , a continuous function

bracket $[a,b]$, $f(a) \cdot f(b) < 0$

convergence: linear, with rate $\frac{1}{2}$

$$\text{i.e. error } e_k = \left(\frac{1}{2}\right)^k \cdot e_0$$

pros:

+ simple

+ if requirements met, it's guaranteed to work

cons:

- needs more than a starting guess, needs a bracket

- kind of slow convergence

FIXED PT. ITERATION

problem it solves: finds a fixed pt., $x=g(x)$

requirements: g , a continuous function

x_0 , a starting point

convergence:

Converges if you can establish a domain D

for which ① $x \in D \Rightarrow g(x) \in D$

② g is contractive on D

If P is the fixed pt., and g is differentiable,

convergence is $\begin{cases} \text{linear, w/ rate } |g'(P)| & \text{if } 0 < |g'(P)| < 1 \\ \text{Superlinear} & \text{if } g'(P) = 0 \end{cases}$

(and won't converge if $|g'(P)| \geq 1$)

pros:

+ no derivative g' nor bracket $[a,b]$ needed

+ it's a "meta" algorithm: Newton is a special case

cons:

- need not converge...

- can be slow

p. 2, pros and cons

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NEWTON'S METHOD

problem it solves: rootfinding, $f(x) = 0$ } recasts as fixed pt. problem,
 $g(x) = x - f(x)/f'(x)$

requirements: f and f'

x_0 , initial guess

convergence: ① if f, f' and f'' are continuous, and x_0 is sufficiently close to a simple root P , it will converge to P
i.e. $f'(P) \neq 0$

② if additionally $|g''(x)|$ is bounded on some interval around P ,
 $g(x) = x - f(x)/f'(x)$

then convergence is quadratic (very fast!)

pros:

- + No bracket needed
- + Quadratic convergence is super fast

cons:

- need derivative f'
- fails if $f'(x_k) = 0$ at any iteration
- needs x_0 to be "close enough" to the root
- doesn't have quadratic convergence in all cases
(ex: $f(x) = x^2$, root is $P = 0$, $f'(P) = 0$
so not a simple root)
- can diverge
- practical (robust) implementations are more likely to converge but also more complicated.

SECANT METHOD

Similar to Newton but...

- not quadratic convergence ($\alpha=2$) but still superlinear
w/ order of convergence $\alpha = \frac{1+\sqrt{5}}{2} \approx 1.62$

- supply two initial points, x_0 and x_1 ,
+ don't need to use f'

p. 3, pros and cons

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Multivariate Case

BISECTION - not applicable

FIXED PT. ITERATION

- Similar to univariate case. $\vec{x} \leftarrow G(\vec{x})$

pro⁺ + no matrix inversion / solving linear equations needed

NEWTON'S METHOD

- Same pros/cons as univariate case. $\vec{x} \leftarrow \vec{x} - J_F(\vec{x})^{-1} \cdot F(\vec{x})$

con⁻ - matrix inversion costs $O(n^3)$, bad in high dimension

QUASI-NEWTON METHODS (ex. Broyden's)

- generalizes secant method, similar pros/cons

pro⁺ + avoids matrix inverse via tricks like Sherman-Morrison, so much cheaper than Newton in high dimension

Multivariate Optimization

STEEPEST DESCENT / GRADIENT DESCENT

* problem it solves: $\min_{\vec{x} \in \mathbb{R}^n} g(\vec{x})$, $g: \mathbb{R}^n \rightarrow \mathbb{R}$

requirements: \vec{x}_0 starting point
 g and ∇g
learning rate / stepsize η

convergence: think of as fixed-point iteration on

$$G(\vec{x}) = \vec{x} - \eta \cdot \nabla g(\vec{x}), \text{ so similar}$$

* it really solves

find \vec{x} st.

$$\nabla g(\vec{x}) = \vec{0}$$

which gives the stationary points / critical points

to the optimization problem

can diverge

if it converges, does so linearly or sublinearly

More likely (but not guaranteed) to converge to a "good" critical point

pros: + simple
+ scales well to large dimension
+ avoids local max, somewhat avoids saddle pts.

cons:

- may diverge
- may not return a global minimum
- convergence can be slow
- must choose a stepsize, or use a linesearch

no method can without further assumptions

p. 4, pros and cons

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NEWTON'S METHOD FOR OPTIMIZATION

→ * problem it solves: $\min_{\vec{x} \in \mathbb{R}^n} g(\vec{x}) : \mathbb{R}^n \rightarrow \mathbb{R}$

same
caveat
as
before

requirements: Starting point \vec{x}_0 ,
 ∇g and $\nabla^2 g$

convergence: think of as Newton's method (for root-finding)
applied to ∇g , so $\vec{x} \leftarrow \vec{x} - J_{\nabla g}^{-1}(\vec{x}) \cdot \nabla g(\vec{x})$
i.e. $\vec{x} \leftarrow \vec{x} - \nabla^2 g(\vec{x})^{-1} \cdot \nabla g(\vec{x})$

need not converge, but when it does, usually fast

pros: + usually fast convergence

cons: - unless you add a linesearch, it can easily converge to a local max or saddle pt..
- need not converge
- fails if $\nabla^2 g(\vec{x}_k)$ becomes singular
- needs $\nabla^2 g$ (Autodiff is partially helpful)
- needs to invert/solve $n \times n$ system, so $O(n^3)$

GAUSS-NEWTON

problem it solves: nonlinear least squares, $\min_{\vec{x} \in \mathbb{R}^n} g(\vec{x})$ where $g(\vec{x}) = \sum_{i=1}^m \frac{1}{2} f_i(\vec{x})^2$

requirements: Starting pt. \vec{x}_0

F , and Jacobian J_F ($F(\vec{x}) = \begin{bmatrix} f_1(\vec{x}) \\ \vdots \\ f_m(\vec{x}) \end{bmatrix}$), i.e. $J_F = \begin{bmatrix} -\nabla f_1^T \\ \vdots \\ -\nabla f_m^T \end{bmatrix}$

convergence: we didn't discuss,

but it need not work. When it does,
usually faster than gradient descent
but slower than Newton

$$\vec{x} \leftarrow \vec{x} - (J^T J)^{-1} J^T F$$

pros:

- + allows $m \neq n$
- + fast
- + unlike Newton applied to g , it doesn't need $\nabla^2 g$

cons:

- must invert/solve $n \times n$ system, so $O(n^3)$

- may not converge (robust version Levenberg-Maquardt is better)