Root Finding

COS 323

Reminder

- Sign up for Piazza
- Assignment 0 is posted, due Tue 9/25

Last time..

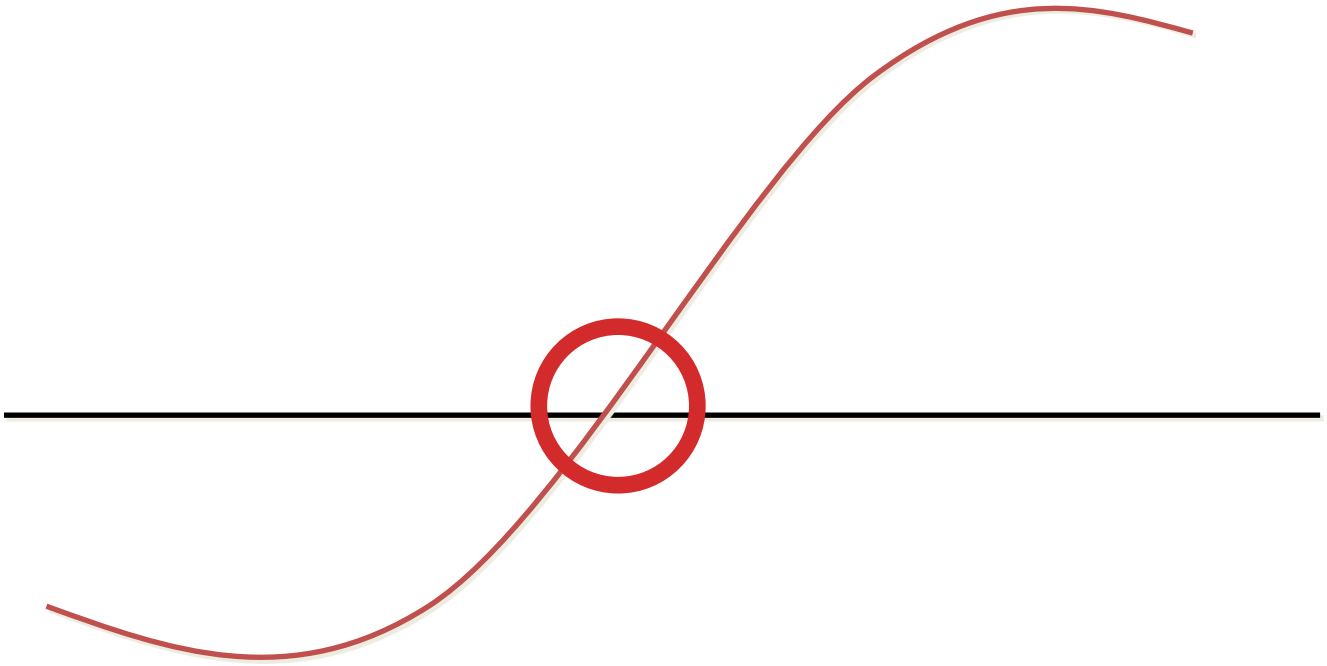
- Floating point numbers and precision
- Machine epsilon
- Sources of error
- Sensitivity and conditioning
- Stability and accuracy
- Asymptotic analysis and convergence order

Today

- Root finding definition & motivation
- Standard techniques for root finding
  - Algorithms, convergence, tradeoffs
- Example applications of Newton's Method
- Root finding in > 1 dimension

1-D Root Finding

- Given some function, find location where $f(x)=0$



Why Root Finding?

- Solve for x in any equation: $f(x) = b$ where $x = ?$

  $\rightarrow$ find root of $g(x) = f(x) - b = 0$

  - Might not be able to solve for x directly

    e.g., $f(x) = e^{-0.2x}\sin(3x-0.5)$

  - Evaluating f(x) might itself require solving a differential equation, running a simulation, etc.

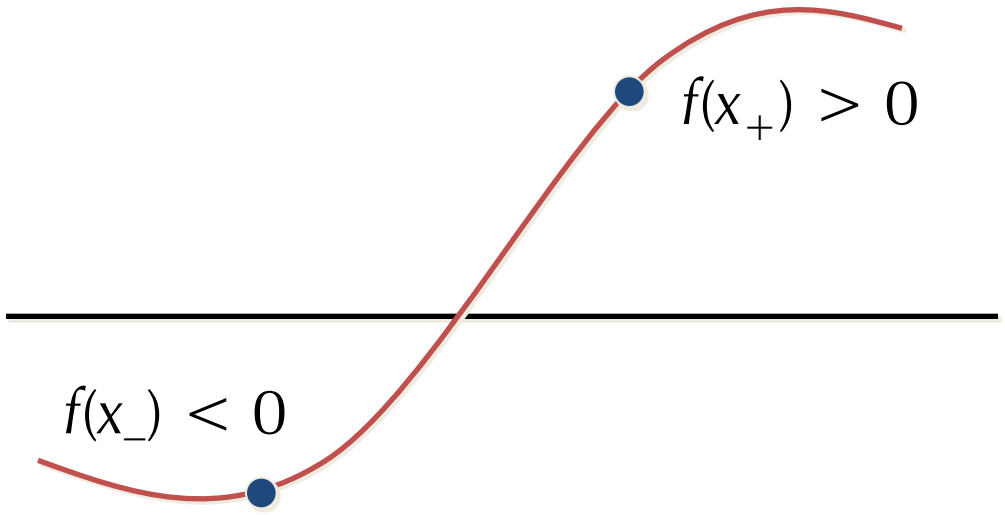
Why Root Finding?

- Engineering applications: Predict dependent variable (e.g., temperature, force, voltage) given independent variables (e.g., time, position)

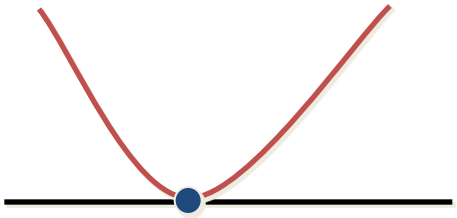
- Focus on finding ***real*** roots

Bracket-Based Methods

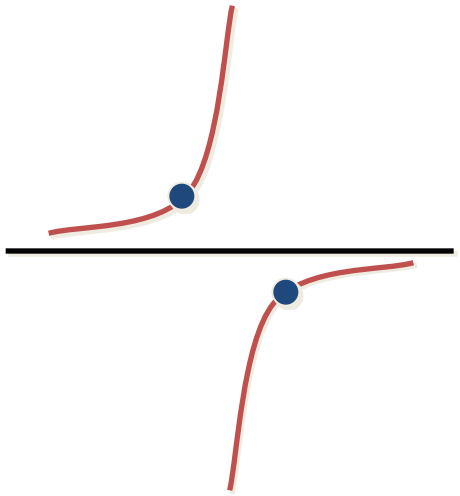
- Given:
  - Points that ***bracket*** the root
  - A ***well-behaved*** function
- Can always find ***some*** root



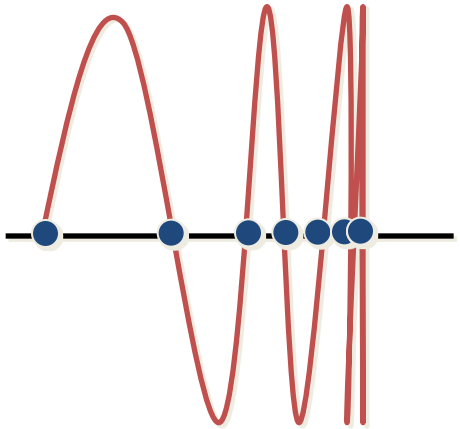
What Goes Wrong?



Tangent point: very difficult to find



Singularity: brackets don't surround root



Pathological case: infinite number of roots – e.g. sin(1/x)

Bisection Method

- Given points x_+ and x_- that bracket a root, find
$$x_{half} = \tfrac{1}{2}\,(x_+ + x_-)$$
and evaluate $f(x_{half})$
- If positive, $x_+ \leftarrow x_{half}$ else $x_- \leftarrow x_{half}$
- Stop when x_+ and x_- close enough
- If function is continuous, this ***will*** succeed in finding ***some*** root

Error Convergence of Iterative Methods

- **(Absolute) error bound** ε_n at step n:

  ε_n bounds $|x_{estimated\ at\ step\ n} - x_{true}|$

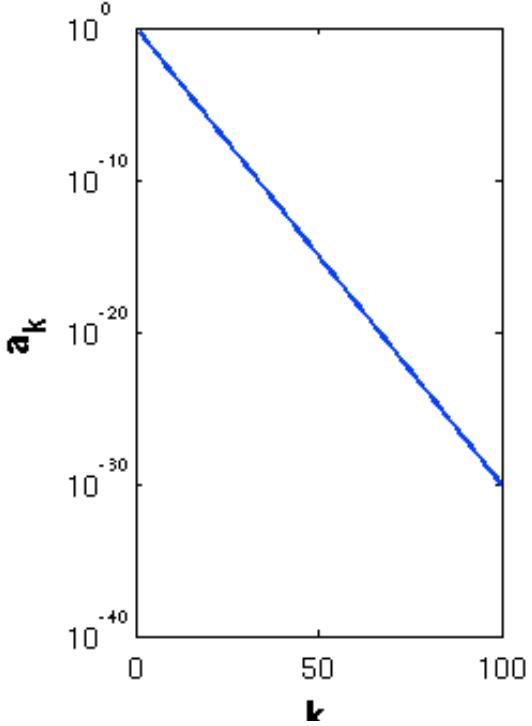
- **Convergence**: describes how ε_{n+1} relates to ε_n
- **Linear** convergence**:**

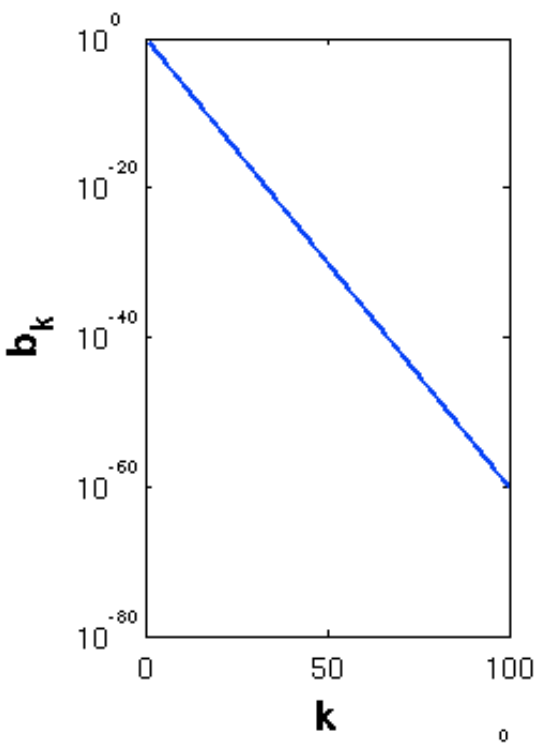
  $|\varepsilon_{n+1}| = c\,|\varepsilon_n|$ for some $c \in (0,1)$

- **Superlinear** convergence:

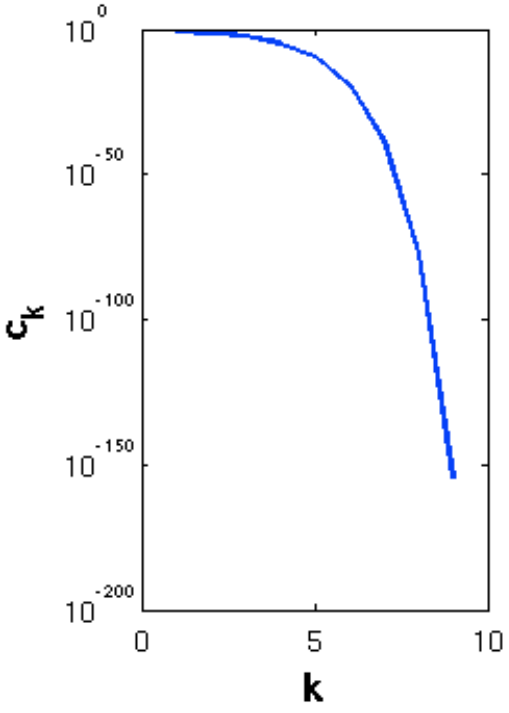
  $|\varepsilon_{n+1}| = c\,|\varepsilon_n|^q$ for some $c \in (0,1)$, $q > 1$

Linear:

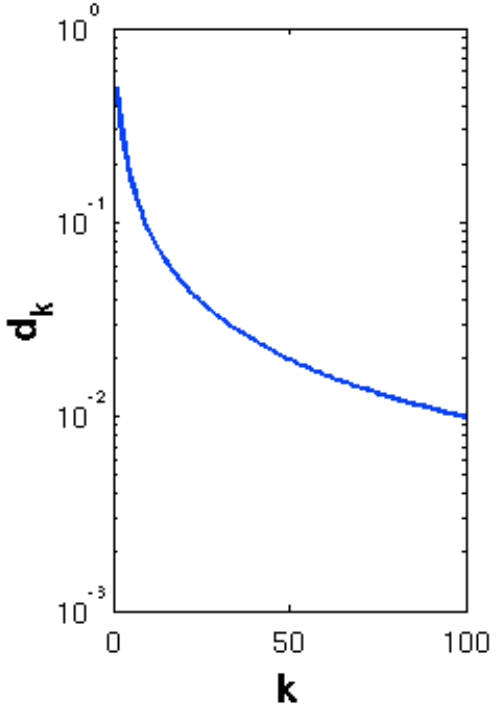




Superlinear:



Sublinear:



Bisection Error Convergence

- Very robust method: guaranteed to find root!
- Convergence rate:
  - Error bounded by size of [x_+… $x\_$] interval
  - Interval shrinks in half at each iteration
  - So, error bound cut in half at each iteration:

$$|\varepsilon_{n+1}| = \tfrac{1}{2} |\varepsilon_n|$$

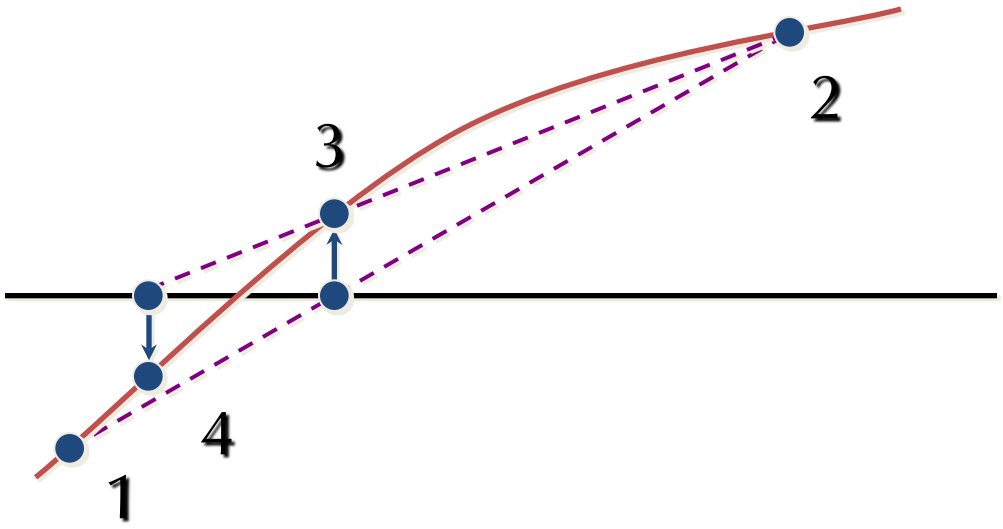
  - Linear convergence!
  - One extra bit of accuracy in x at each iteration

Faster Root-Finding

- Fancier methods get super-linear convergence
  - Typical approach: model function locally by something whose root you can find exactly
  - Model didn't match function exactly, so iterate
  - In many cases, these are less safe than bisection

Secant Method

- Interpolate or extrapolate through two most recent points



Secant Method Convergence

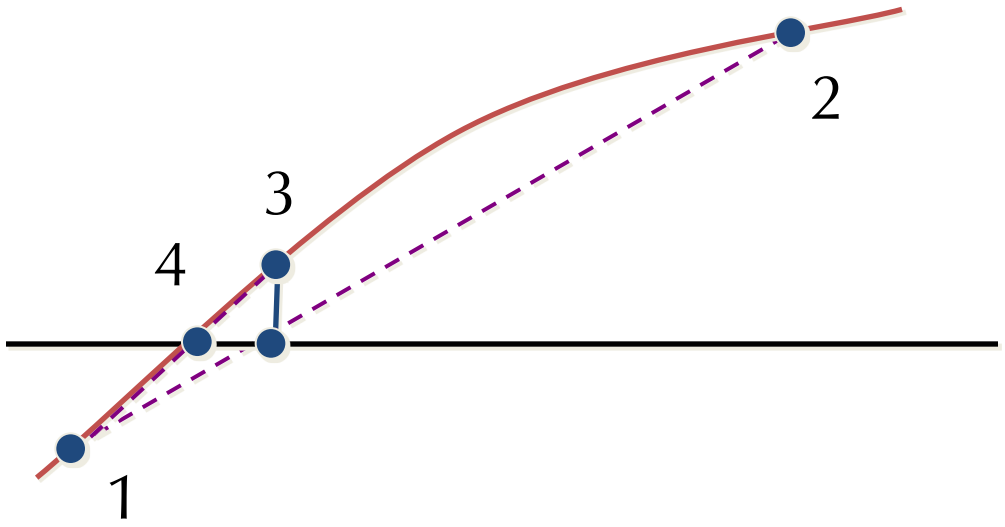
- Faster than bisection:

$$|\varepsilon_{n+1}| = c\,|\varepsilon_n|^{1.6}$$

- Faster than linear: number of correct bits multiplied by 1.6
- Drawback: only true if ***sufficiently close*** to a root of a ***sufficiently smooth*** function
  - Does not guarantee that root remains bracketed

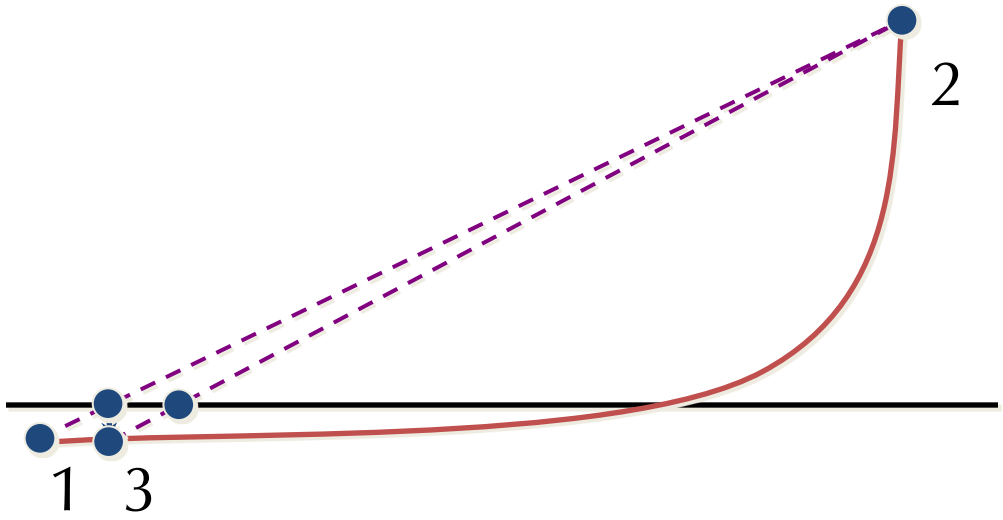
False Position Method

- Similar to secant, but guarantees bracketing



- Stable, but linear in bad cases

False Position Failure



Other Interpolation Strategies

- Ridders' method: fit exponential to $f(x_+)$, $f(x_-)$, and $f(x_{half})$
- Van Wijngaarden-Dekker-Brent method: inverse quadratic fit to 3 most recent points if within bracket, else bisection
- Both of these ***safe*** if function is nasty, but ***fast*** (super-linear) if function is nice

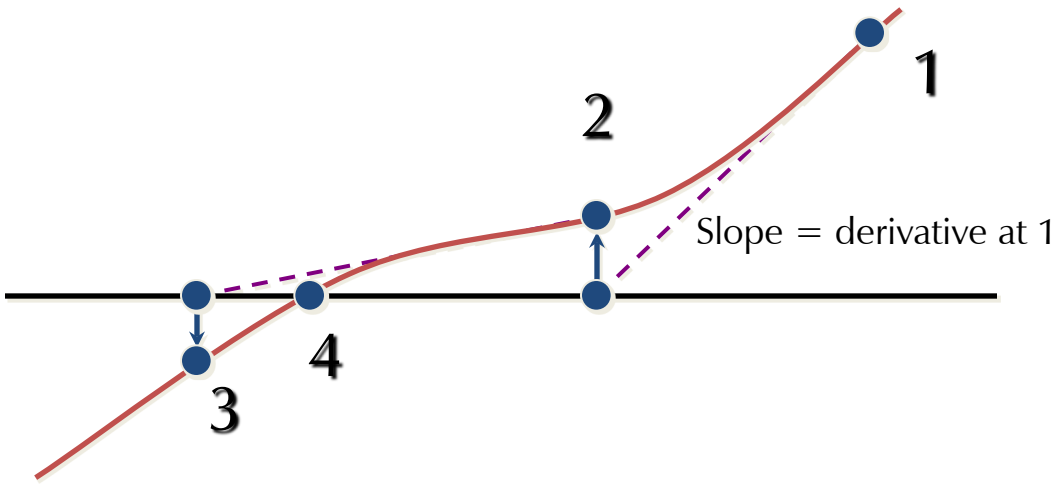
Demo

Newton-Raphson

- Best-known algorithm for getting ***quadratic*** convergence when derivative is easy to evaluate
- Quadratic: # correct bits doubles each iteration!

$$|\varepsilon_{n+1}| = c\,|\varepsilon_n|^2$$

- Another variant on the extrapolation theme



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

Newton-Raphson convergence

- Begin with Taylor series

$$f(x_n+\delta) = f(x_n) + \delta f'(x_n) + \delta^2 \frac{f''(x_n)}{2} + \ldots \overset{want}{=} 0$$

- Divide by derivative (can't be zero!)

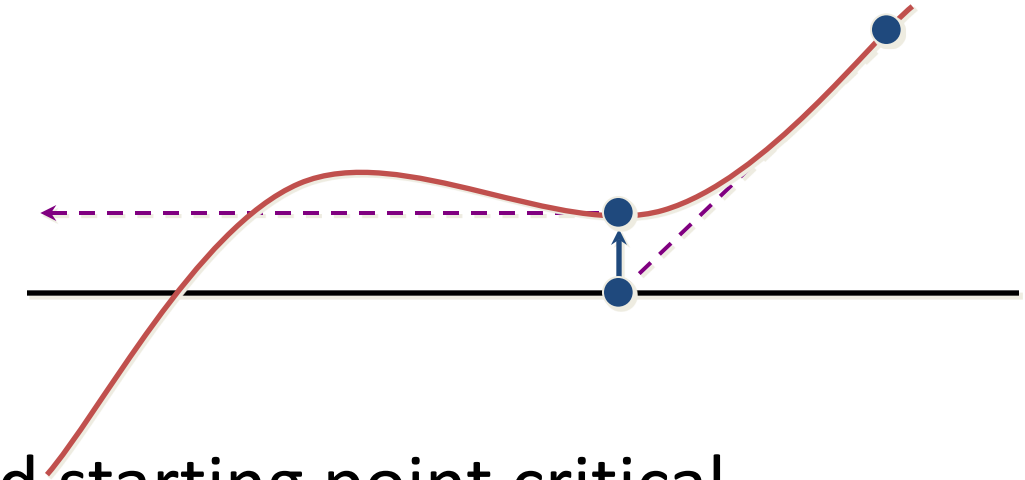
$$\frac{f(x_n)}{f'(x_n)} + \delta + \delta^2 \frac{f''(x_n)}{2f'(x_n)} = 0$$

$$-\delta_{Newton} + \delta + \delta^2 \frac{f''(x_n)}{2f'(x_n)} = 0$$

$$\delta_{Newton} - \delta = \frac{f''(x_n)}{2f'(x_n)}\delta^2 \qquad \Rightarrow \boxed{\varepsilon_{n+1} \sim \varepsilon_n^{\,2}}$$

Newton-Raphson

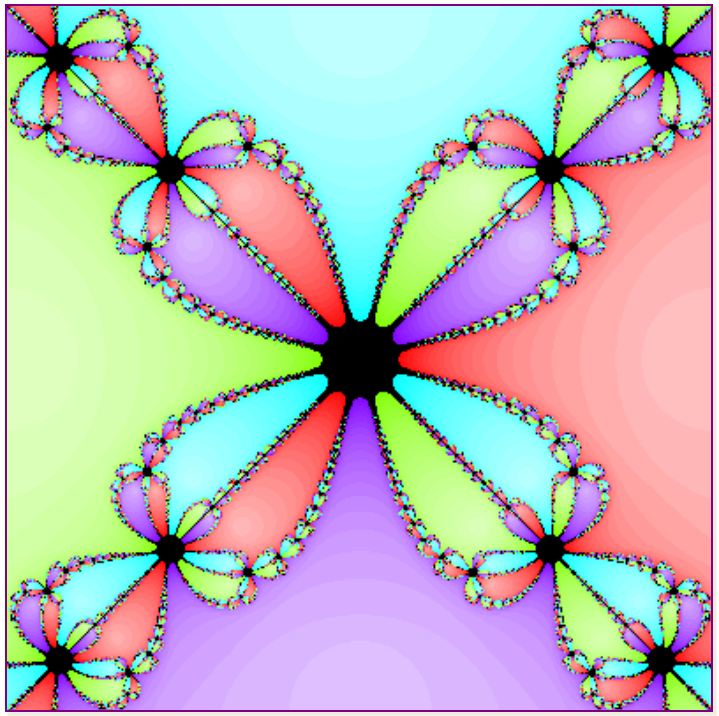
- Method fragile: can easily get confused



- Good starting point critical
  - Newton popular for “polishing off” a root found approximately using a more robust method
- Quadratic only for simple root

Newton-Raphson Convergence

- Can talk about "basin of convergence": range of x_0 for which method finds a root
- Can be extremely complex: here's an example in 2-D with 4 roots



Common Example of Newton: Square Root

- Let $f(x) = x^2 - a$: zero of this is square root of a
- $f'(x) = 2x$, so Newton iteration is

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

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

- "Divide and average" method (~2000 B.C.)

Reciprocal via Newton

- Division is slowest of basic operations
- On some computers, hardware divide not available (!): simulate in software

$$\frac{a}{b} = a * \frac{1}{b}$$

$$f(x) = \frac{1}{x} - b = 0$$

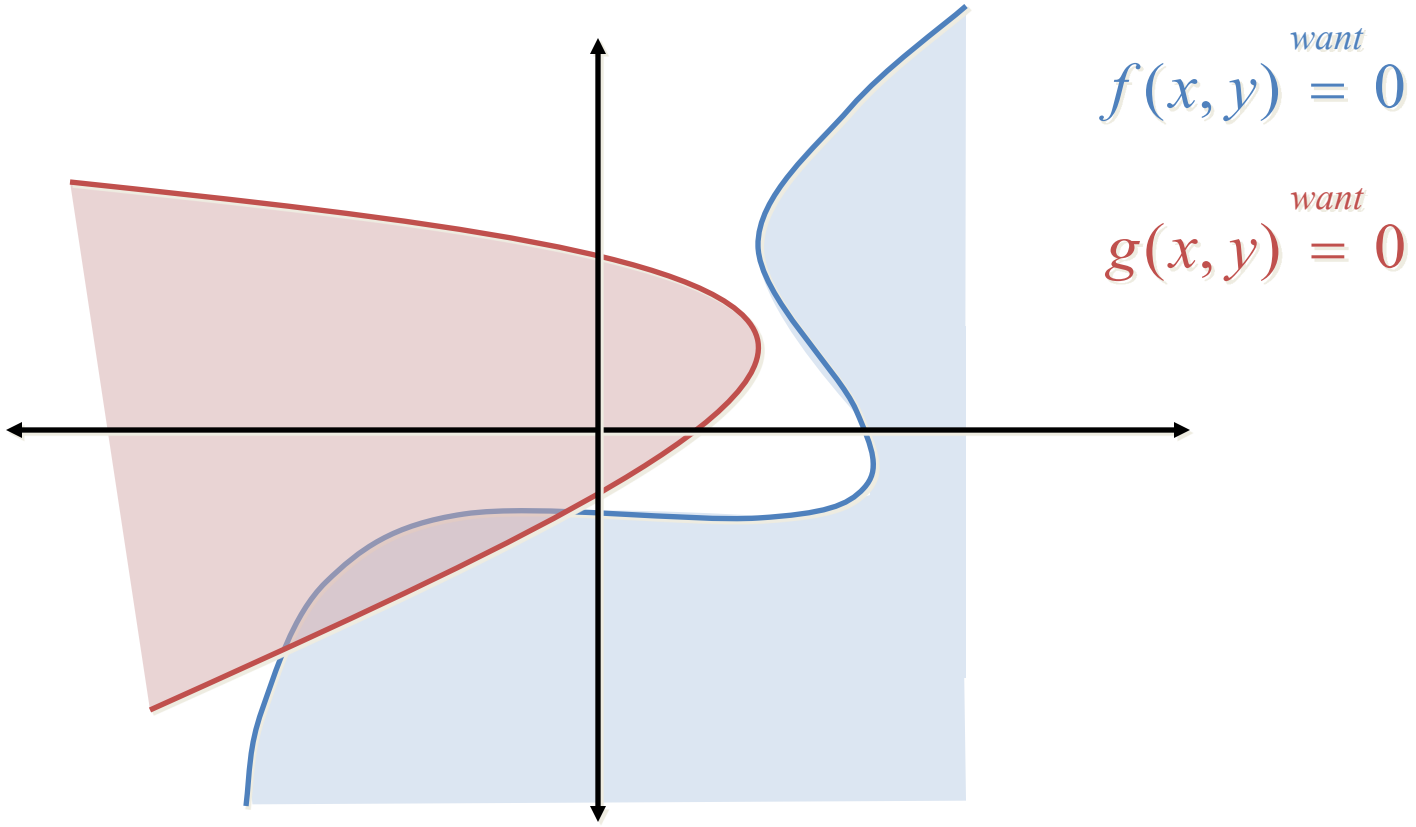
$$f'(x) = -\frac{1}{x^2}$$

$$x_{n+1} = x_n - \frac{\frac{1}{x} - b}{-\frac{1}{x^2}} = x_n\left(2 - bx_n\right)$$

- Need only subtract and multiply

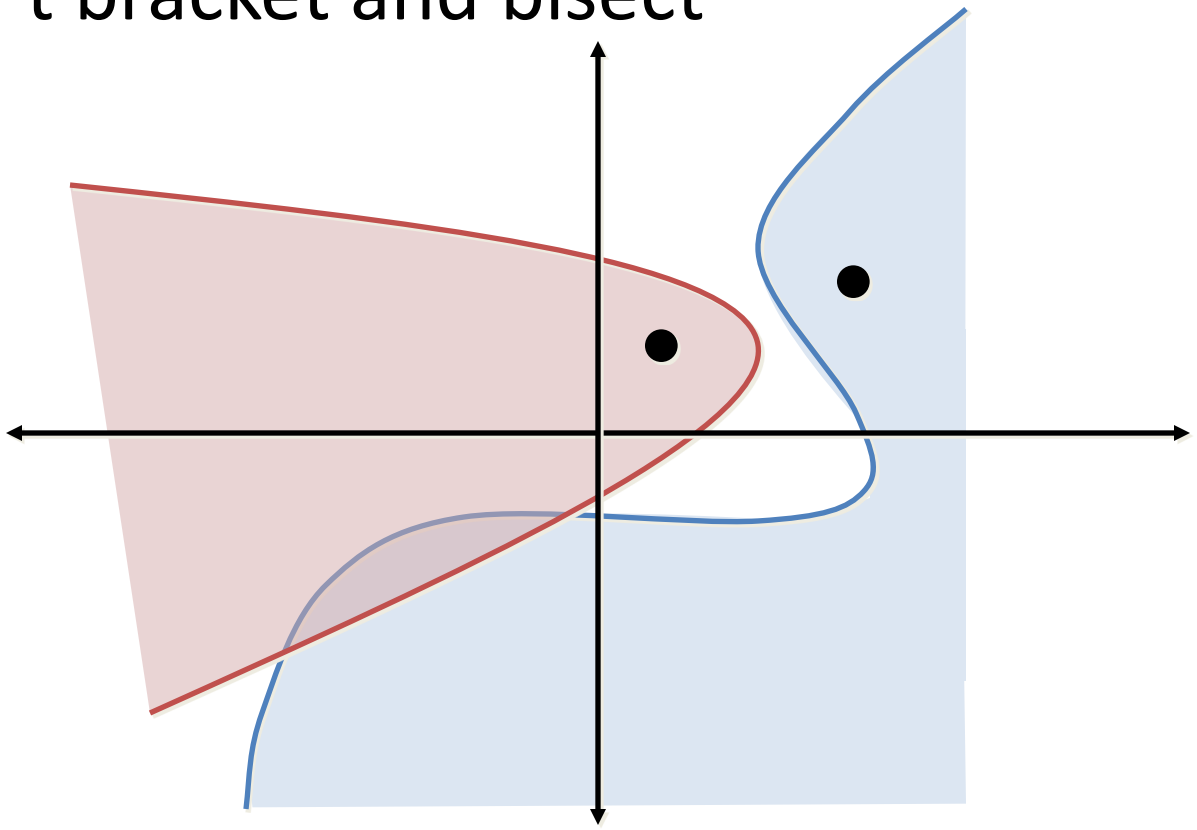
Rootfinding in >1D

- Behavior can be complex: e.g. in 2D



Rootfinding in >1D

- Can’t bracket and bisect



- Result: few general methods

Newton in Higher Dimensions

- Start with

$$f(x,y) \overset{want}{=} 0$$

$$g(x,y) \overset{want}{=} 0$$

- Write as vector-valued function

$$\mathbf{f}(\mathbf{x}_n) = \begin{pmatrix} f(x,y) \\ g(x,y) \end{pmatrix}$$

Newton in Higher Dimensions

- Expand in terms of Taylor series

$$\mathbf{f}(\mathbf{x}_n + \boldsymbol{\delta}) = \mathbf{f}(\mathbf{x}_n) + \mathbf{f}'(\mathbf{x}_n)\,\boldsymbol{\delta} + \ldots \overset{want}{=} 0$$

- **f**′ is a Jacobian

$$\mathbf{f}'(\mathbf{x}_n) = \mathbf{J} = \begin{pmatrix} \frac{\partial \mathbf{f}}{\partial x} & \frac{\partial \mathbf{f}}{\partial y} \end{pmatrix}$$

Newton in Higher Dimensions

- 1-dimensional case: $\delta = f(x_n) / f'(x_n)$
- N-dimensional: Solve for $\boldsymbol{\delta}$

$$\boldsymbol{\delta} = -\mathbf{J}^{-1}(\mathbf{x}_n)\,\mathbf{f}(\mathbf{x}_n)$$

- Requires matrix inversion (we'll see this later)
- Often fragile – must be careful
  - Keep track of whether error decreases
  - If not, try a smaller step in direction $\boldsymbol{\delta}$

Recap: Tradeoffs

- Bracketing methods (Bisection, False-position)
  - Stable, slow
- Open methods (Secant, Newton)
  - Possibly divergent, fast
  - Newton requires derivative
- Hybrid methods (Brent)
  - Combine bracketing & open methods in a principled way

Practical notes

- Root-finding in Matlab:
  - fzero: For finding root of a single function
    Combines “safe” and “fast” methods
  - roots: For finding polynomial roots
- Excel:
  - Goal Seek: Drive an equation to 0 by adjusting 1 parameter
  - Solver: Can vary multiple parameters simultaneously, also minimize & maximize
- Tip: Plot your function first!!!