Class 8. Root Finding in 1-D

Nonlinear Equations

- Often (most of the time??) the relevant system of equations is nonlinear in the unknowns.
- Then, cannot decompose as $\mathbf{A}\mathbf{x} = \mathbf{b}$. Oh well.
- Instead write as:
  1. $f(x) = 0$ (for functions of one variable, i.e., 1-D);
  2. $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ (for $\mathbf{x} = (x_1, x_2, ..., x_n)$, $\mathbf{f} = (f_1, f_2, ..., f_n)$, i.e., n-D).
- Not guaranteed to have any real solutions, but generally do for astrophysical problems.

Solutions in 1-D

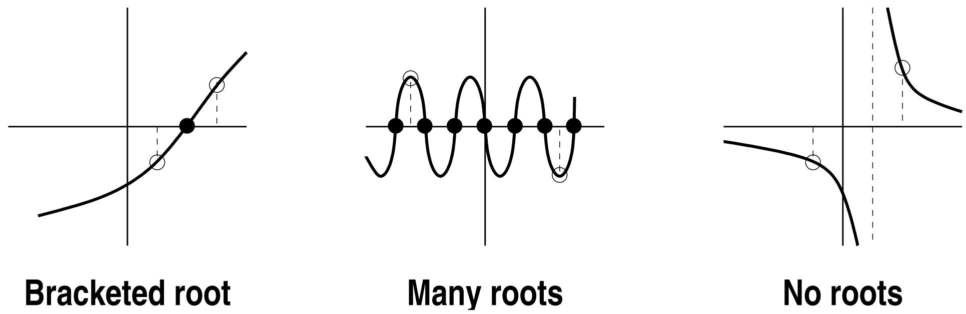
- Generally, solving multi-D equations is much harder, so we'll start with the 1-D case first...
- By writing $f(x) = 0$ we have reduced the problem to solving for the roots of f.
- In 1-D it is usually possible to trap or bracket the desired roots and hunt them down.
- Typically all root-finding methods proceed by iteration, improving a trial solution until some convergence criterion is satisfied.

Function Pathologies

- Before blindly applying a root-finding algorithm to a problem, it is essential that the form of the equation in question be understood: graph it!
- For smooth functions, good algorithms will always converge, provided the initial guess is good enough.
- Pathologies include discontinuities, singularities, multiple or very close roots, or no roots at all!

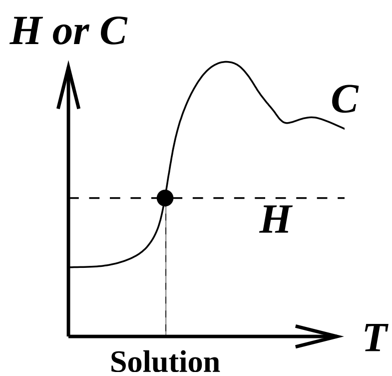
Numerical Root Finding

- Suppose $f(a)$ and $f(b)$ have opposite sign.
- Then, if f is continuous on the interval (a, b), there must be at least one root between a and b (this is the Intermediate Value Theorem).
- Such roots are said to be bracketed.



Example Application

- Use root finding to calculate the equilibrium temperature of the ISM.
- The ISM is a very diffuse plasma.
  - Heated by nearby stars and cosmic rays.
  - Cooled by a variety of processes:
    * Bremsstrahlung: collisions between electrons and ions.
    * Atom-electron collisions followed by radiative decay.
    * Thermal radiation from dust grains.
- Equilibrium temperature given when rate of heating H = rate of cooling C.
  - Often H is not a function of temperature T.
  - Usually C is a complex, nonlinear function of T.



- To solve, find T such that $H - C(T) = 0$.

Bracketing and Bisection

- *NRiC* §9.1 lists some simple bracketing routines that search for sign changes of f:
  - `zbrac()`: expand search range geometrically;
  - `zbrak()`: look for roots in subintervals.
- Once bracketed, root is easy to find by bisection:

– Evaluate f at interval midpoint $(a+b)/2$.
– Root must be bracketed by midpoint and whichever a or b gives f of opposite sign.
– Bracketing interval decreases by 2 each iteration:

$$\varepsilon_{n+1} = \varepsilon_n/2.$$

– Hence to achieve error tolerance of ε starting from interval of size ε_0 ($\varepsilon \leq \varepsilon_0$) requires $n = \log_2(\varepsilon_0/\varepsilon)$ step(s).

Convergence

- Bisection converges linearly (first power of ε).
- Methods for which

$$\varepsilon_{n+1} = \text{constant} \times (\varepsilon_n)^m,\ m > 1,$$

  are said to converge superlinearly.
- Note error actually decreases exponentially for bisection. It converges "linearly" because successive significant figures are won linearly with computational effort (i.e., $\underline{1} \to 0.\underline{5} \to 0.2\underline{5} \to 0.12\underline{5} \to \cdots$).

Tolerance

- What is a practical tolerance ε for convergence?
- Best you can do is machine precision (e_m, about 10^{-7} in single precision); more practically, absolute convergence within $e_m(|a|+|b|)/2$ is used.
- Sometimes consider fractional accuracy,

$$\frac{|x_{i+1} - x_i|}{|x_i|} \sim e_m,$$

  but this can fail for x_i near zero.

Newton-Raphson Method

- Can we do better than linear convergence? Duh!
- Expand $f(x)$ in a Taylor series:

$$f(x+\delta) = f(x) + f'(x)\delta + \frac{f''(x)}{2}\delta^2 + ...$$

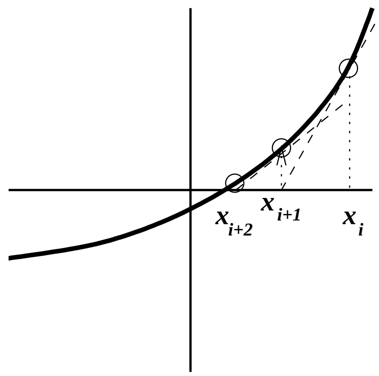
- For small $|\delta|$, drop higher-order terms, so:

$$f(x+\delta) = 0 \text{ implies } \delta = -\frac{f(x)}{f'(x)}.$$

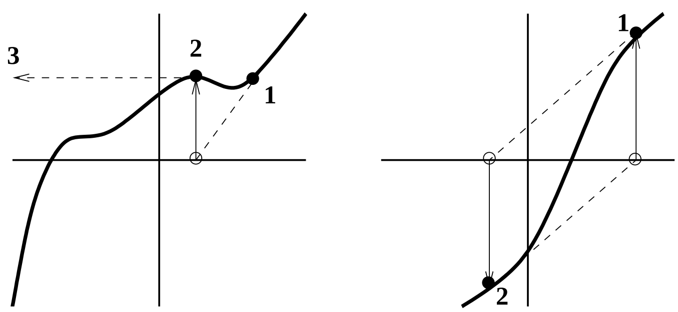
- δ is correction added to current guess of root, i.e.,

$$x_{i+1} = x_i + \delta.$$

- Graphically, Newton-Raphson (NR) uses tangent line at x_i to find zero crossing, then uses x at zero crossing as next guess:



- Note: only works near root...
  - When higher order terms important, NR fails spectacularly. Other pathologies exist too:



Shoots to infinity **Never converges**

- Why use NR if it fails so badly?
- Can show that

$$\varepsilon_{i+1} = -\varepsilon_i^2 \frac{f''(x)}{2f'(x)},$$

i.e., *quadratic* convergence!

- Note both $f(x)$ and $f'(x)$ must be evaluated each iteration, plus both must be continuous near root.
- Popular use of NR is to "polish up" bisection root.