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 $Ax = b$. Oh well.
- Instead write as:
  1. $f(x) = 0$ (for functions of one variable, i.e., 1-D);
  2. $f(x) = 0$ (for $x = (x_1, x_2, ..., x_n)$, $f = (f_1, f_2, ..., f_n)$, 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 $H = \text{rate of cooling} \ C$.
  - 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 $\varepsilon$ starting from interval of size $\varepsilon_0$ ($\varepsilon \leq \varepsilon_0$) requires $n = \log_2(\varepsilon_0/\varepsilon)$ step(s).

**Convergence**
- Bisection converges **linearly** (first power of $\varepsilon$).
- 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., $1 \rightarrow 0.5 \rightarrow 0.25 \rightarrow 0.125 \rightarrow \cdots$).

**Tolerance**
- What is a practical tolerance $\varepsilon$ 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:
  \[ f(x + \delta) = f(x) + f'(x)\delta + \frac{f''(x)}{2}\delta^2 + \ldots \]
- For small $|\delta|$, drop higher-order terms, so:
  \[ f(x + \delta) = 0 \text{ implies } \delta = -\frac{f(x)}{f'(x)}. \]
• $\delta$ 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:

  1. Shoots to infinity
  2. 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.