Nonlinear Equations

- Often (most of the time??) the relevant system of equations is <u>not linear in the unknowns</u>.
- Then, cannot decompose as $A\mathbf{x} = \mathbf{b}$. Oh well.
- Instead write as:

(1) $f(x) = 0$ function of one variable (1-D)

(2) $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ $\mathbf{x} = (x_1, x_2, \ldots, x_n)$, $\mathbf{f} = (f_1, f_2, \ldots, f_n)$ (n-D)

- Not guaranteed to have <u>any</u> real solutions, but generally do for astrophysical problems.

Solutions in 1-D

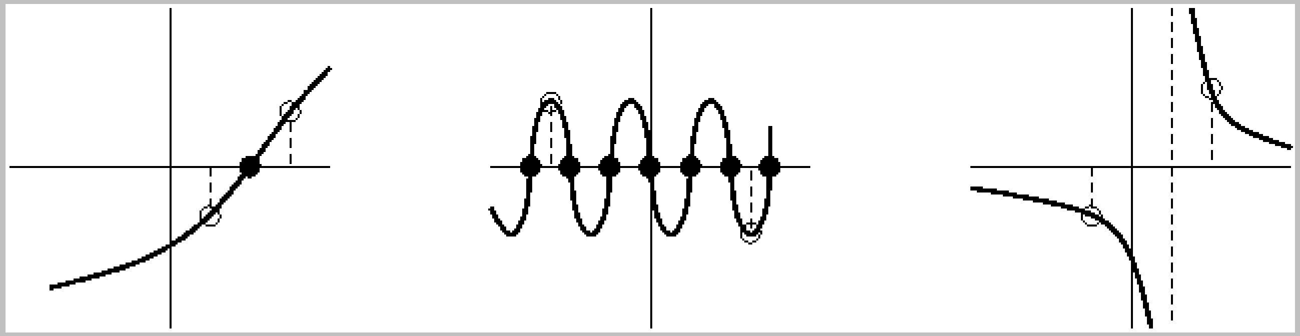
- Generally, solving multi-D equations is <u>much</u> harder, so we'll start with the 1-D case first...
- By writing $f(x) = 0$ we have reduced the problem to solving for the <u>roots</u> of f.
- In 1-D it is usually possible to trap or <u>bracket</u> the desired roots and hunt them down.
- Typically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



Bracketed root Many roots No roots

Example Application

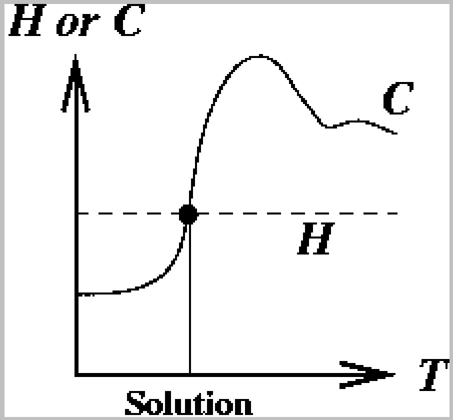
- Use root finding to calculate the equilibrium temperature of the ISM.
- The ISM is a very diffuse plasma.
  - Heated by nearby stars and cosmic rays.
  - Cooled by a variety of processes:
    - Bremsstrahlung: collisions between electrons and ions
    - Atom-electron collisions followed by radiative decay
    - Thermal radiation from dust grains

Example, Cont'd

- 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.
- 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 requires $n = \log_2(\varepsilon_0/\varepsilon)$ steps.

Convergence

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

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

are said to converge superlinearly.

- Note error actually decreases exponentially for bisection. It converges "linearly" because successive figures are won linearly with computational effort.

Tolerance

- What is a practical tolerance ε for convergence?
- Cannot be less than round-off error.
- For single-precision (`float`) accuracy, typically take $\varepsilon = 10^{-6}$ in <u>fractional</u> error.

  i.e. $$\frac{f(x) - f(x_r)}{f(x_r)} \sim 10^{-6}$$

  where x = numerical solution, x_r = actual root.
- When $f(x_r) = 0$ this fails, so use $\varepsilon = 10^{-6}$ as <u>absolute</u> error (or perhaps use ε(|a| + |b|)/2).

Newton-Raphson Method

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

$$f(x + \delta) = f(x) + f\,'(x)\,\delta + f\,''(x)\,\delta^2/2 + \ldots$$

- For $\delta \ll x$, drop higher order terms, so:

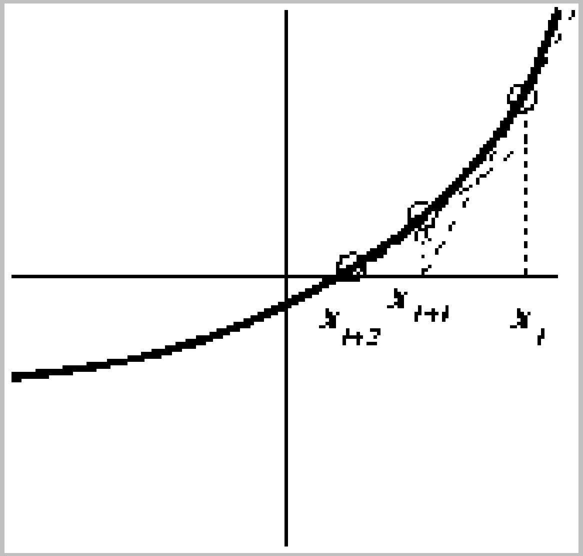
$$f(x + \delta) = 0 \Rightarrow \delta = -\,f(x)\,/\,f\,'(x)$$

- δ is correction added to current guess of root:

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

Newton-Raphson, Cont'd

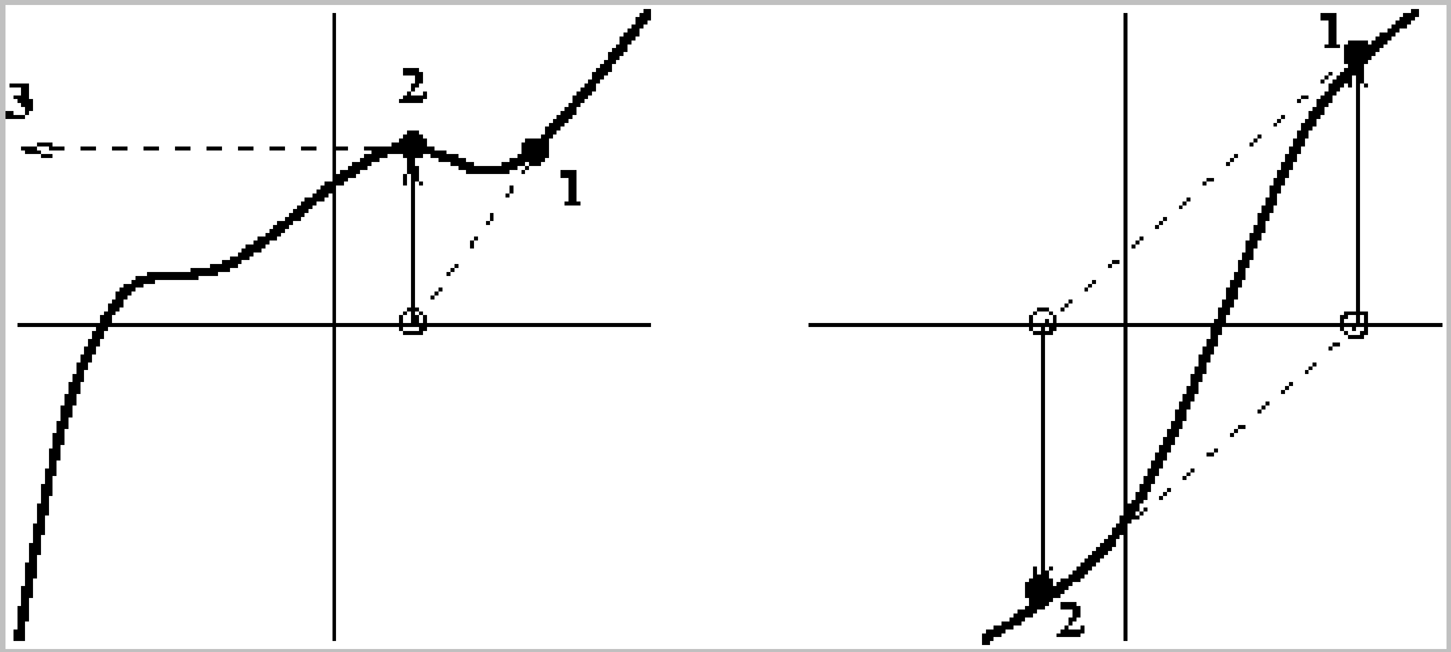
- Graphically, Newton-Raphson (NR) uses tangent line at x_i to find zero crossing, then uses x at zero crossing as next guess:



- Note: only works near root ($\delta << x$)...

Newton-Raphson, Cont'd

- When higher order terms important, NR fails spectacularly. Other pathologies exist too:



Shoots to infinity

Never converges

Newton-Raphson, Cont'd

- Why use NR if it fails so badly?
- Rate of convergence:

$$\varepsilon_{i+1} = \varepsilon_i - f(x_i) \,/\, f\,'(x_i)$$

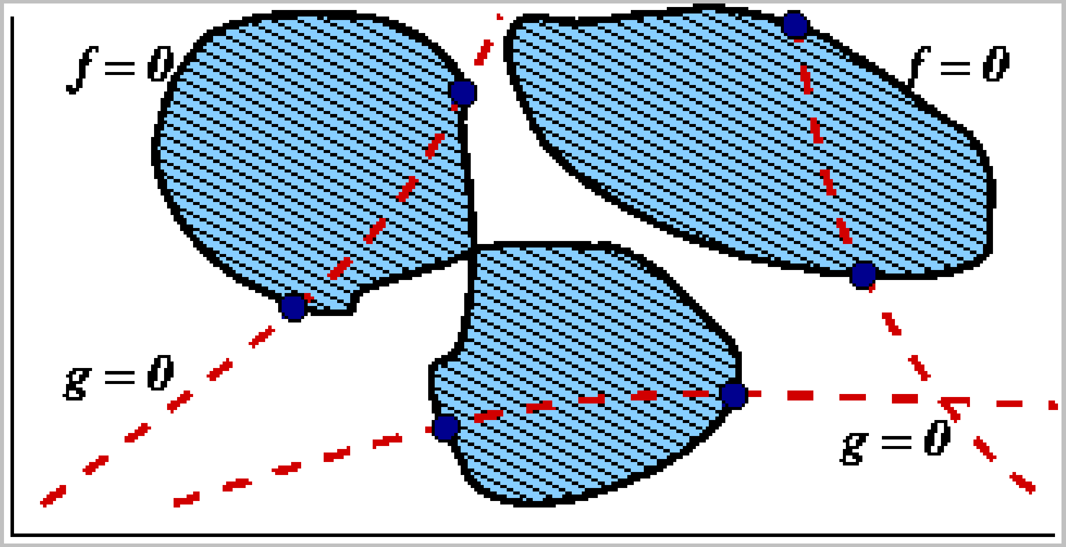
- Taylor expand $f(x_i)$ & $f\,'(x_i)$ to get:

$$\varepsilon_{i+1} = -\,\varepsilon_i^{\,2}\, f\,''(x_i) \,/\, f\,'(x_i) \qquad \text{[quadratic!]}$$

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

Nonlinear Systems of Equations

- Consider the system $f(x,y) = 0$, $g(x,y) = 0$. Plot zero contours of f & g:



- No information in f about g, and vice versa.
  - In general, no good method for finding roots.

Nonlinear Systems, Cont'd

- If you are near root, best bet is NR.

  e.g. For $\mathbf{F}(\mathbf{x}) = \mathbf{0}$, choose $\mathbf{x}_{i+1} = \mathbf{x}_i + \delta$, where

  $$\mathbf{F}'(\mathbf{x})\,\delta = -\,\mathbf{F}(\mathbf{x})$$

  - This is a matrix equation: $\mathbf{F}'(\mathbf{x})$ is a matrix with elements $\partial F_i / \partial x_j$. The matrix is called the Jacobian.

- Written out:

$$\frac{\partial f}{\partial x}\delta_x + \frac{\partial f}{\partial y}\delta_y = -f(x,y)$$

$$\frac{\partial g}{\partial x}\delta_x + \frac{\partial g}{\partial y}\delta_y = -g(x,y)$$

Nonlinear Systems, Cont'd

- Given initial guess, must evaluate matrix elements and RHS, solve system for δ, and compute next iteration $\mathbf{x}_{i+1}$. Then repeat (must solve 2×2 linear system each time).
- Essentially the non-linear system has been linearized to make it easier to work with.
- NriC 9.7 discusses a global convergence strategy that combines multi-D NR with "backtracking" to improve chances of finding solutions.

Example: Interstellar Chemistry

- ISM is multiphase plasma consisting of electrons, ions, atoms, and molecules.
- Originally, the ISM was thought to be too hostile for molecules.
- But in 1968-69, radio observations discovered absorption/emission lines of NH_3, H_2CO, H_2O, ...
- Lots of organic molecules, e.g. CH_3CH_2OH (ethanol).

Example, Cont'd

- In some places, all atoms have been incorporated into molecules.
- For example, molecular clouds: dense, cold clouds of gas composed primarily of molecules.

  (T ~30 K, n ~10^6 cm^{-3}, M ~10^{5-6} $M_\odot$, R ~ 10 -100 pc).

- How do you predict what abudances of different molecules should be, given *n* and *T*?
- Need to solve a <u>chemical reaction network</u>.

Example, Cont'd

- Consider reaction between two species A and B:

  $A + B \rightarrow AB$ reaction rate = $n_A n_B R_{AB}$

- Reverse also possible:

  $AB \rightarrow A + B$ reaction rate = $n_{AB} R'_{AB}$

- In equilibrium:

(1) $n_A n_B R_{AB} = n_{AB} R'_{AB}$

(2) $n_A + n_{AB} = n_A^0$

(3) $n_B + n_{AB} = n_B^0$

\ Normalizations: #
/ A & B conserved

Example, Cont'd

- Substitute normalization equations into reaction equations to get quadratic in n_{AB}, easily solved.
- However, many more possible reactions:
  - AC + B ↔ AB + C (exchange reaction)
  - ABC ↔ AB + C (dissociation reaction)
- Wind up with large nonlinear system describing all forward/reverse reactions, involving known reaction rates R. Must solve given fixed n^0 & T.

Numerical Derivatives

- For NR and function minimization, often need derivatives of functions. It's always better to use an analytical derivative if it's available.
- If you're stuck, could try:

$$f \;\; (x) \approx \frac{f(x+h) - f(x)}{h}$$

- However, this is very susceptible to RE. Better:

$$f \;\; (x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

- Read NriC 5.7 before trying this!