Root Finding in 1-D

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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

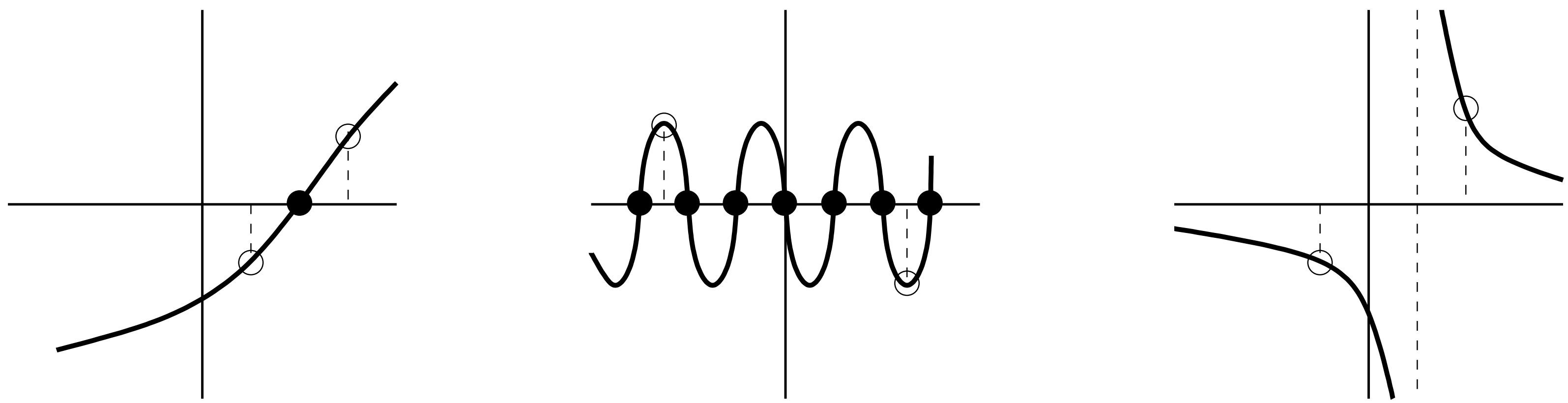
- Generally, solving multi-D equations is <u>much</u> harder, so we'll start with the 1-D case first...
- By writing $f(x) = 0$ we have reduced the problem to solving for the <u>roots</u> of f.
- In 1-D it is usually possible to trap or <u>bracket</u> the desired roots and hunt them down.
- Typically 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 <u>bracketed</u>.

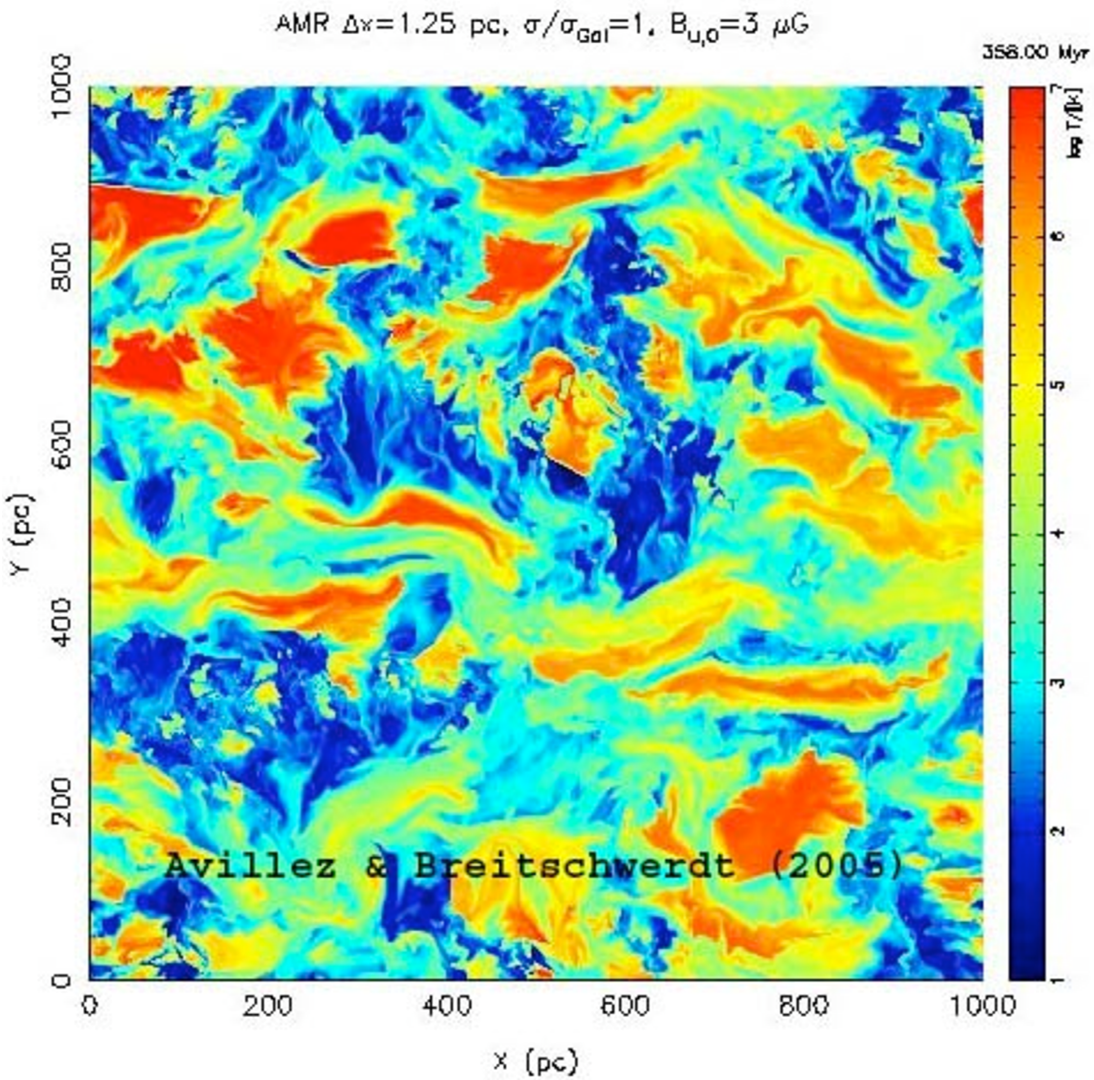


Bracketed root **Many roots** **No roots**

Example Application

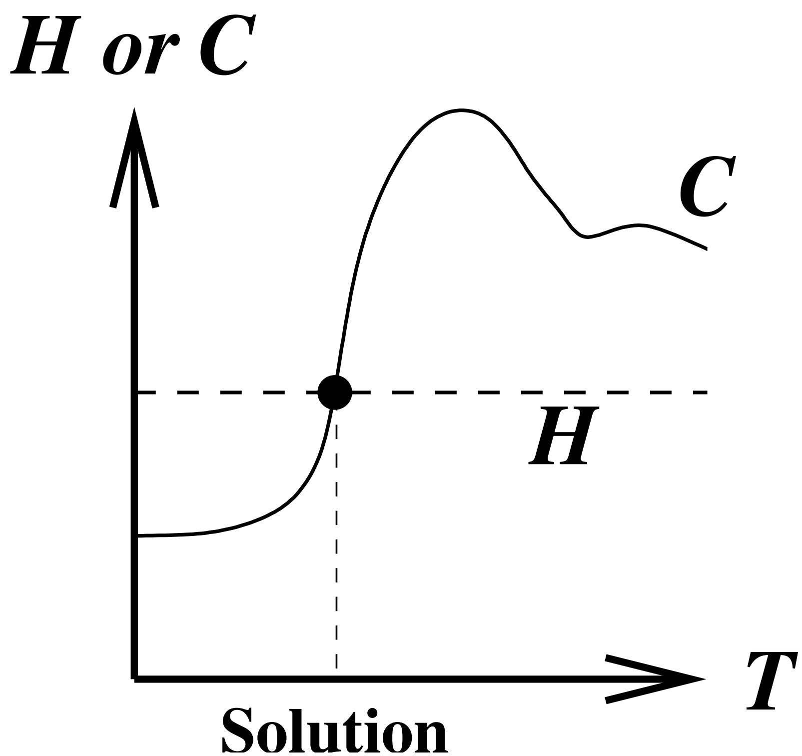
- Use root finding to calculate the equilibrium temperature of the ISM.
- The ISM is a very diffuse plasma.
  - Heated by nearby stars and cosmic rays.
  - Cooled by a variety of processes:
    - Bremsstrahlung: collisions between electrons and ions.
    - Atom-electron collisions followed by radiative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

Simulations of Multi-phase ISM



Example Application (cont..)

- 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 <u>bisection</u>:
  - 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:

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

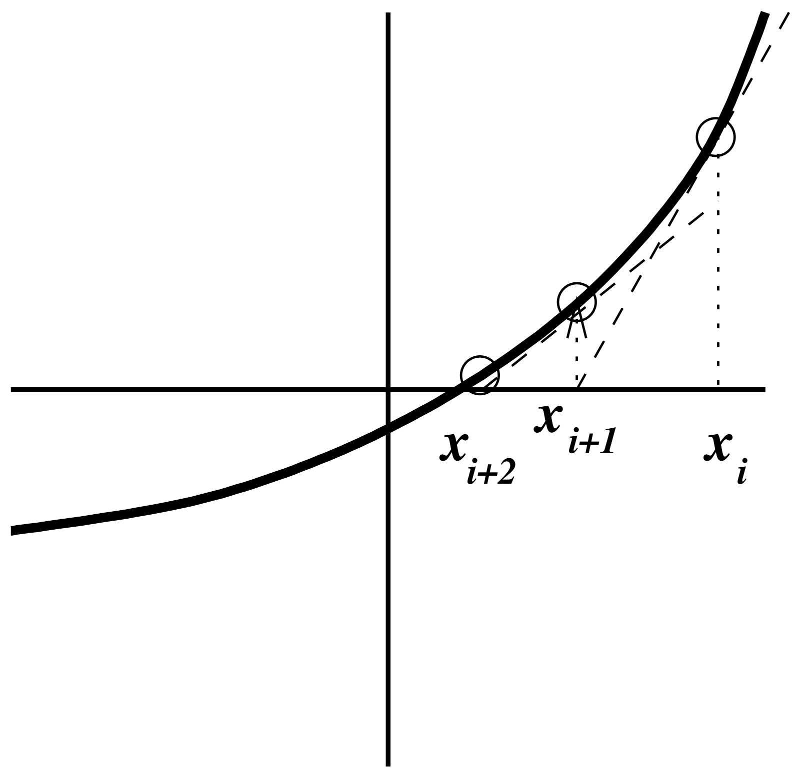
- For small $|\delta|$, drop higher-order terms, so:

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

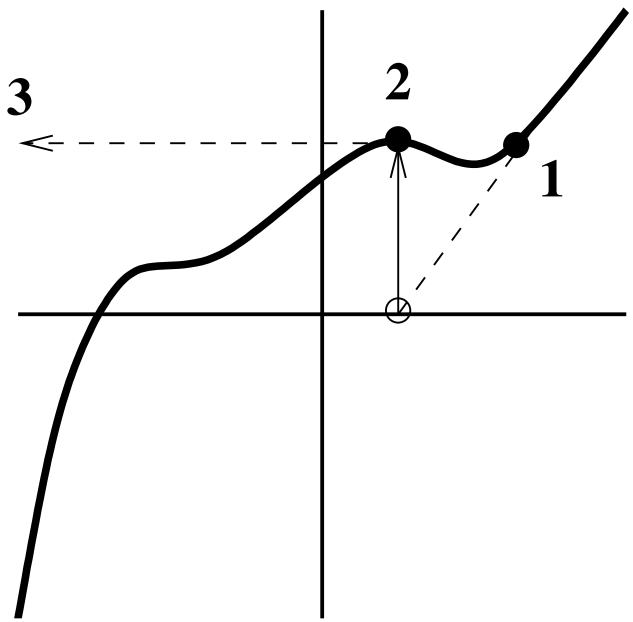
- δ is correction added to current guess of root, i.e.,

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

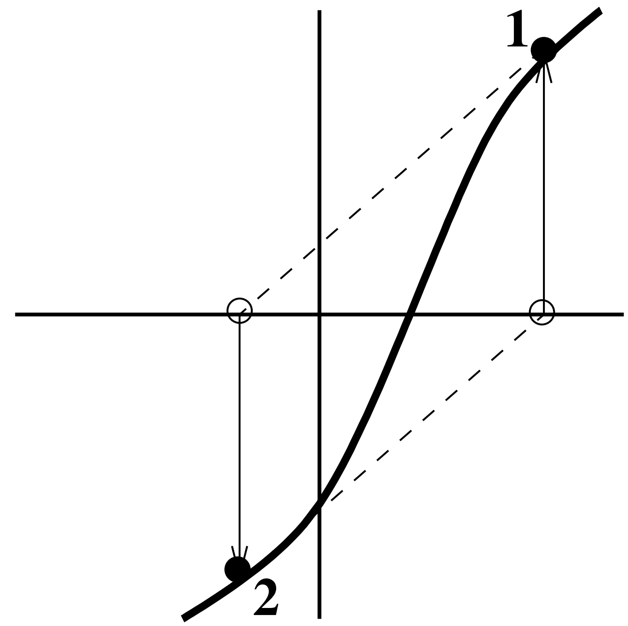
- Graphically, Newton-Raphson (NR) uses tangent line at x_i to find zero crossing, then uses x at zero crossing as next guess:



- 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.

Quadratic convergence

- Suppose α is the root. According to Taylor's theorem,

$$0 = f(\alpha) = f(x_n) + f'(x_n)(\alpha - x_n) + \frac{f''(\xi_n)}{2}(\alpha - x_n)^2$$

where ξ_n is between x_n and α. Since $x_{n+1} \equiv x_n - f(x_n)/f'(x_n)$,

$$\alpha - x_{n+1} = -\frac{f''(\xi_n)}{2f'(x_n)}(\alpha - x_n)^2$$

that is

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

or

$$|\varepsilon_{i+1}| \leq M\varepsilon_i^2,$$

where M is a constant

Square root of a number (from Wiki)

Consider the problem of finding the square root of a number. There are many methods of computing square roots, and Newton's method is one. For example, if one wishes to find the square root of 612, this is equivalent to finding the solution to

$$x^2 = 612$$

The function to use in Newton's method is then,

$$f(x) = x^2 - 612$$

with derivative,

$$f'(x) = 2x$$

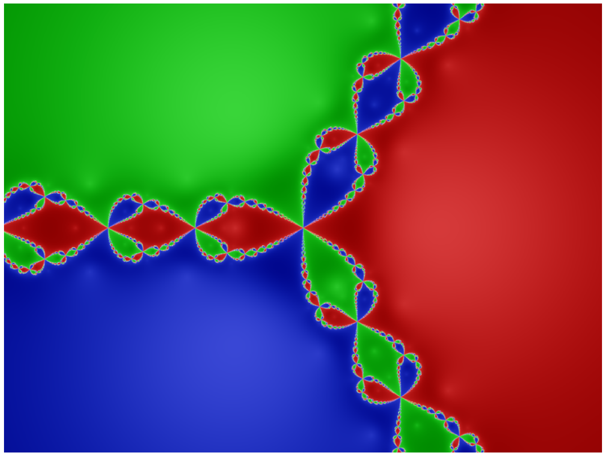
With an initial guess of 10, the sequence given by Newton's method is

$$\begin{array}{lllll}
x_1 & = & x_0 - \frac{f(x_0)}{f'(x_0)} & = & 10 - \frac{10^2-612}{2\times 10} & = & 35.6 \\
x_2 & = & x_1 - \frac{f(x_1)}{f'(x_1)} & = & 35.6 - \frac{35.6^2-612}{2\times 35.6} & = & \underline{2}6.3955 \\
x_3 & = & \vdots & = & \vdots & = & \underline{24.7}90635492455 \\
x_3 & = & \vdots & = & \vdots & = & \underline{24.738}688290475 \\
x_5 & = & \vdots & = & \vdots & = & \underline{24.73863375736}7
\end{array}$$

Where the correct digits are underlined. With only a few iterations one can obtain a solution accurate to many decimal places.

Newton's method and fractals

- The Newton's method works also for complex numbers
  - For instance, $z^3 = 1$ has 1 real and two complex roots $[\exp(\pm 2\pi i/3)]$.
  - The method does not always converge to the real root. The colors in the image below show the root reached (similarly one can show the number of iterations to convergence) for starting points in the complex plane .... this is a fractal!



- Newton's formula for the set above: $z_{j+1} = z_j - \frac{z_j^3 - 1}{2z_j^2}$