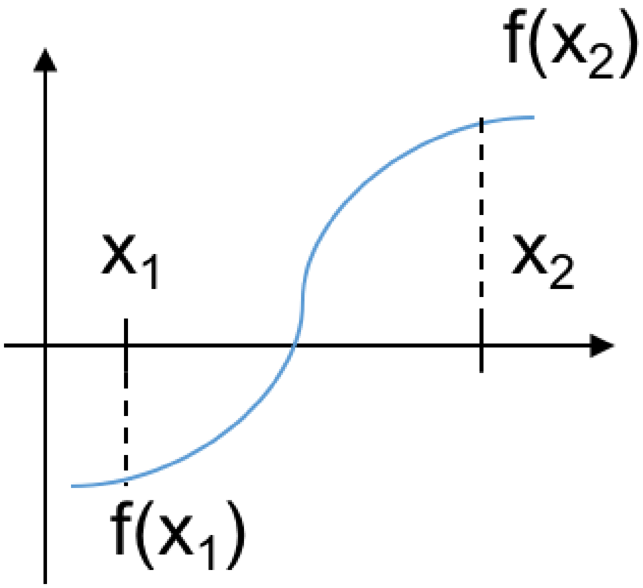
Nonlinear Equations

- Find roots of f(x). That is, find the value of x so that f(x)=0.
- All nonlinear algebraic problems can be written in the form f(x)=0. Just move all terms to one side of the equation.
- Numerical methods for nonlinear problems proceed by setting an initial guess for the solution, and iterating to improve the guess until some desired error tolerance is achieved.
- Open and Closed domain methods.
- Here:
  - discuss closed domain methods
  - one equation in one unknown

Bound the Solution

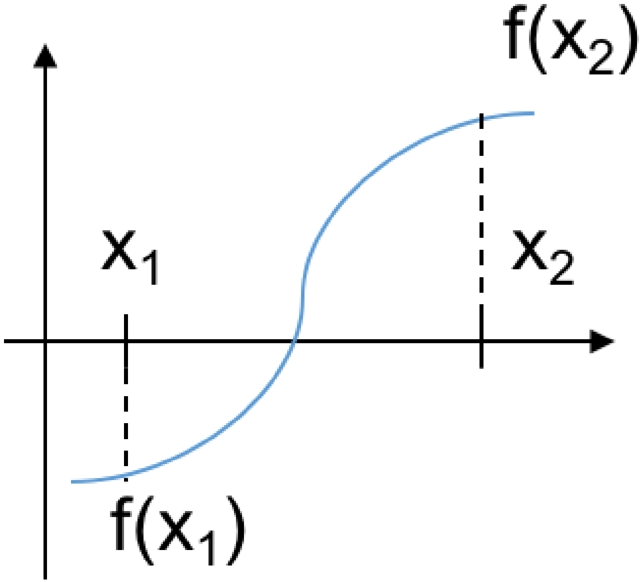
- Bracket the root: Choose two guesses for the solution: x1 and x_2.
- If $f(x_1) \cdot f(x_2) < 0$ then the two guesses bracket the root.
- This implies that the root is between the two guesses.



Procedures

Question: How to get good guesses or bracket the root?

- **Graph it.**
  - Visual picture can be very helpful.
  - Provides an intial guess of the root.
  - Indicates the function behavior, and possible problem areas.
  - May not be practical, however.
    - Cost of function evaluation may be excessive.



Procedures

- **Do a simple incremental search.**
  - Simply set a small Δx and search the domain for $f(x)=0$.
  - Obviously not very practical.
- **Past experience**
  - Output of one problem may be a good guess for the input of another problem.
    - This especially true in cases where we do multiple solves, which is quite common.
  - Use intuition:
    - species mass fractions should be between 0 and 1.
    - most temperatures in K should be in reasonable ranges.

Procedures

- **Solve a simpler problem** to get a guess for the harder problem.
  - For example, if solving for a nonideal gas, get an initial guess using an ideal gas.
  - Another example, if solving for temperature with a variable heat capacity, find a temperature guess using a constant heat capacity, which results in an easy linear solve for the guess.
  - In combustion, we might solve using a simple 1-step reaction mechanism, instead of a more complex 400 step mechanism.

$$h = \int_{T_r}^{\mathbf{T}} c_p(T)dT$$

↓

$$h = c_p \cdot (\mathbf{T} - T_r)$$

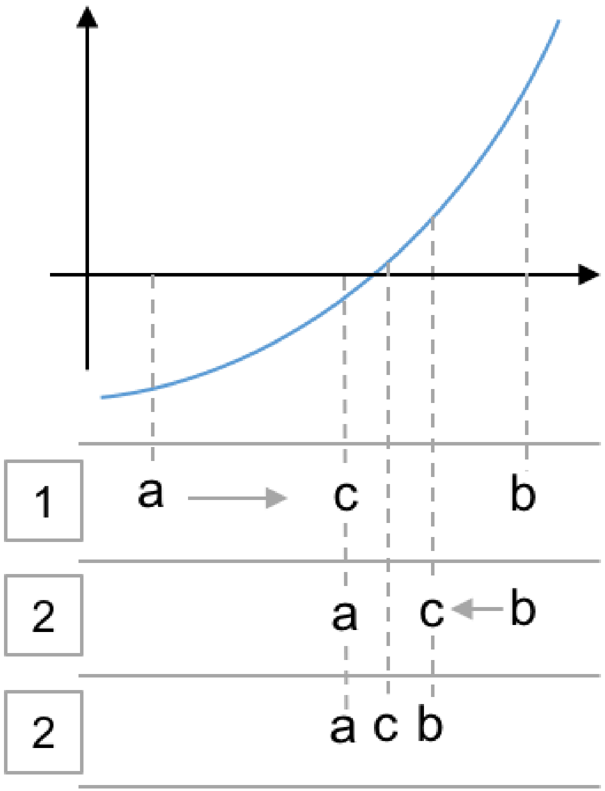
Refine

Once you have a bracket refine the root

- Reduce the size of the interval, while maintaining the bracket.
- Two methods:
  - **bisection**,
  - **regula falsi (false position)**
  - These are robust (they work!), but they are not overly fast.

Bisection

- Guess two points that bracket the root: a, b
- Check for f(a)=0 or f(b)=0
- Bracket tests:
  - f(a) f(b) < 0
  - (f(a)>0 and f(b)<0) or
    (f(a)<0 and f(b)>0)
- Refine: c = (a+b)/2
- Select new bracket:
  - if f(a) f(c) < 0 → b=c
  - else a = c

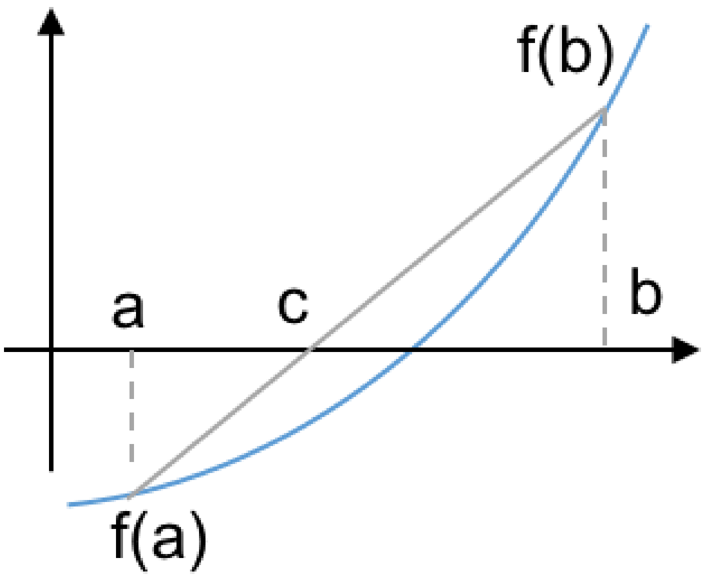


Bisection Error

- The error is always bounded by $\epsilon n \leq |b-a|$
- $\epsilon_{n+1}=\epsilon_n/2 \rightarrow$ **linear convergence**
- ϵ_0,
- $\epsilon_1=\epsilon_0/2$,
- $\epsilon_2=\epsilon_1/2 = \epsilon_0/4 = \epsilon_0/2^2 \rightarrow \quad \epsilon_n=\epsilon_0/2^n$.
- Hence:$n=\log_2 (\epsilon_0 / \epsilon_n)$
- **That is, to reduce the error from $\epsilon_0 \leq |a-b|$ to some desired ϵ_n requires $n = \log_2 (\epsilon 0/\epsilon n)$ iterations.**

Regula Falsi

Rather than bisect the interval to find c, draw an intersecting line between f(a) and f(b) as an approximation to the function.



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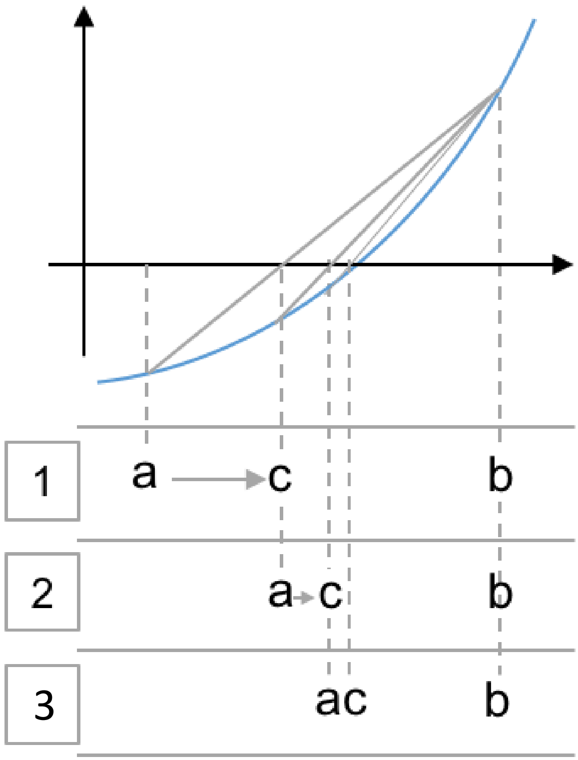


- Solve the root of this linear approximation:
  - that is, where the line intersects the x-axis where y=f(x) is zero.
  - Equation for the line:

$$f_l(x) = f(a) + \frac{f(b) - f(a)}{b - a}(x - a).$$

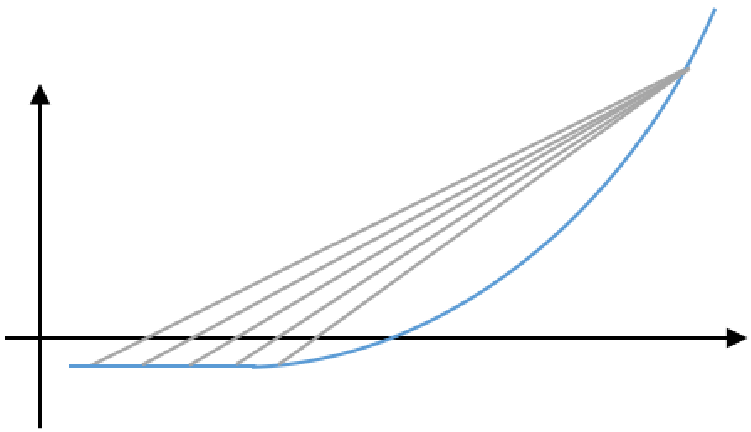
  - Then let $f_l(c)=0$ and solve for c to get:

$$c = a - f(a)\frac{b - a}{f(b) - f(a)}.$$

- To retain the bracket, replace a or b with c as for bisection.

Regula Falsi

- Robust
- Usually faster than bisection
- No error bound though.
- May get superlinear convergence
  - Keeping the old versus new function evaluation...
- Consider the following case though (slow):



Convergence

When to stop?

- $|b-a|<\epsilon$
  - absolute error
  - works for x=1
  - not so good for x=1020
- $|b-a|/|c|<\epsilon$
  - relative error
- $|f(c)|<\epsilon$
  - error in function versus error in root.

- On the left, the bracket is narrow, but the function is not zero.
- On the right, the function is near zero, but the bracket is not narrow.
- Do both: $|b-a|/|c|<\epsilon 1$ and $|f(c)|<\epsilon 2$.