

Trial-and-Error Searching

(almost science)

Rubin H Landau

With

Sally Haerer and Scott Clark

Computational Physics for Undergraduates
BS Degree Program: Oregon State University

“Engaging People in Cyber Infrastructure”
Support by EPICS/NSF & OSU

Root Finding by “Trial and Error”

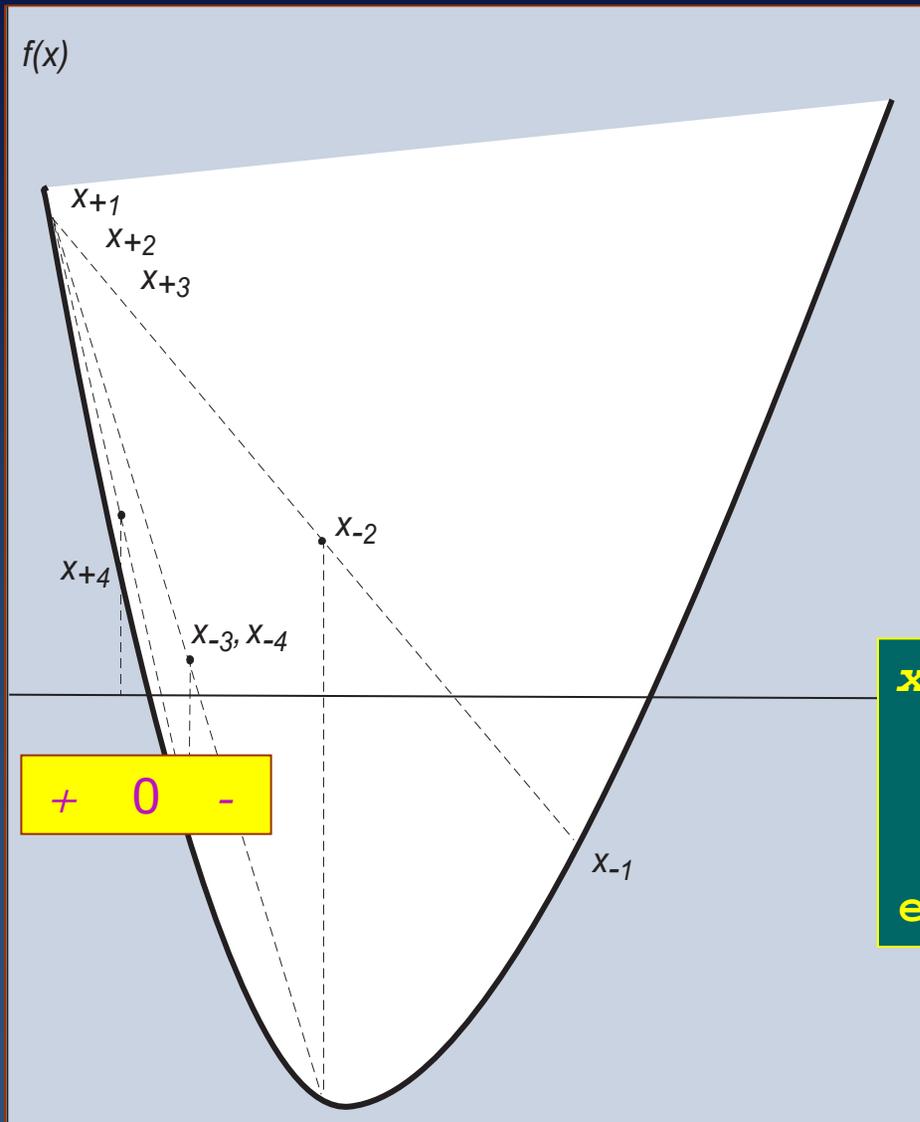
- “Root” = solution of standard equation

$$f(x) = 0, \quad (1)$$

$$\text{if } g(x) = h(x)? \Rightarrow f(x) = g(x) - h(x) \quad (2)$$

- Search for solutions by guessing (intelligent)
- Guess = “trial” → error → improved guess
- End: $f(x) \approx 0$ ($< \varepsilon$), or exhaustion (JFK)
- “Trial and error” \neq fixed number of steps
- Artificial intelligence (makes decisions)

Bisection Algorithm: $f(x)=0$



Assume sign change occurs:

$$f(x_-) < 0$$

$$f(x_+) > 0$$

Algorithm:

$$x = (x_- + x_+)/2$$

$$\text{if } (f(x) f(x_+) > 0) \text{ } x_+ = x$$

$$\text{else } x_- = x$$

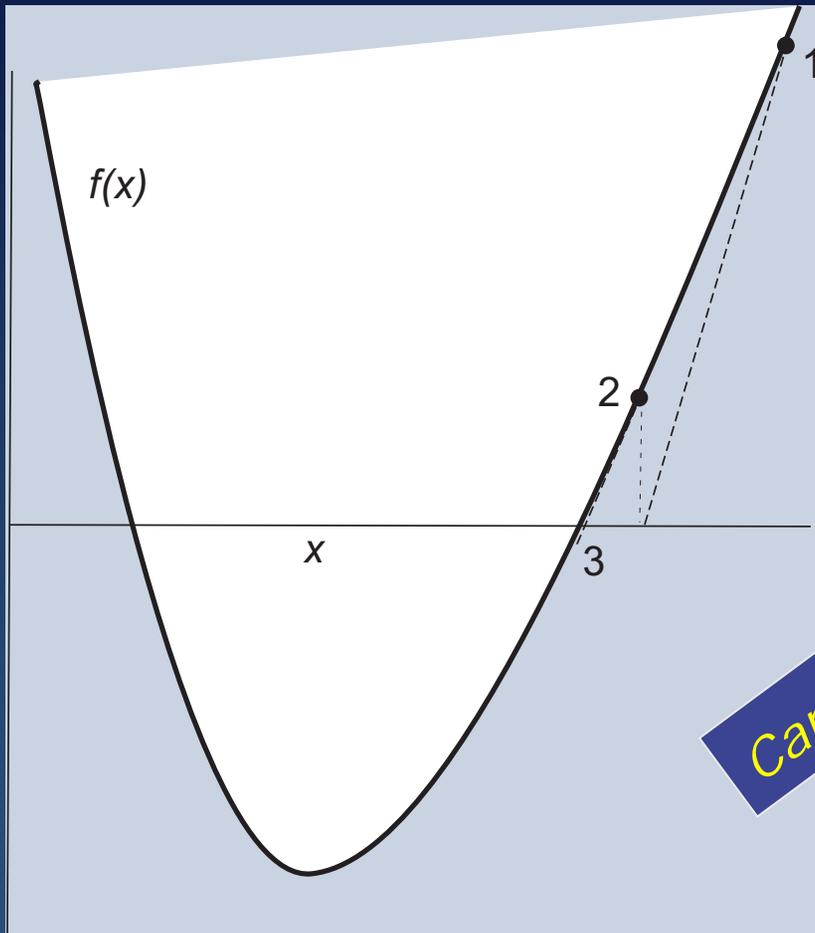
- *Slow*
- *Can't fail*

Newton-Raphson Algorithm: $f(x) = 0$

- Quicker, less robust than bisection
- Approximate $f(x) \approx$ linear function

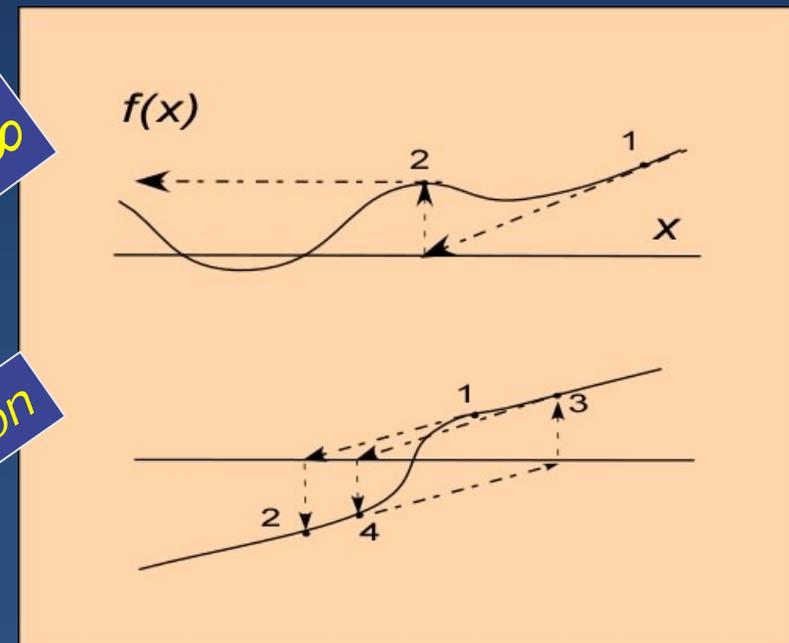
$$f(x) \approx ax + b \simeq 0 \quad (3)$$

$$\Rightarrow x = -b/a \quad (4)$$



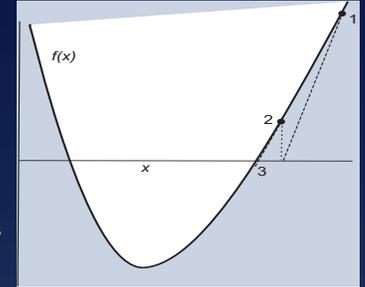
Can go to ∞

Can just go on



Analytic Newton Raphson

- Want to solve $f(x) = 0$
- Old guess \rightarrow correction \rightarrow new guess \rightarrow correction ...



$$x_0 \quad \Delta x \quad (?) \quad x_1 = x_0 + \Delta x \quad (5)$$

- 2 term Taylor expansion of f (straight line tangent)

$$f(x_0 + \Delta x) \simeq f(x_0) + \frac{df}{dx}(x_0) \Delta x + \dots \quad (6)$$

$$f(x_0 + \Delta x) = 0 \Rightarrow \Delta x = -\frac{f(x_0)}{df(x_0)/dx} \quad (7)$$

- Evaluate df/dx numerically

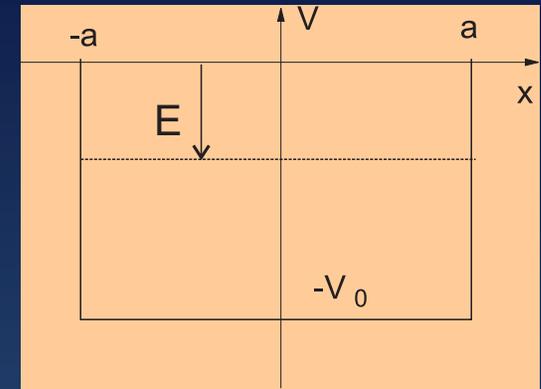
$$\frac{df}{dx} \simeq \frac{f(x + \Delta x) - f(x)}{\Delta x} \quad (8)$$

Time for Exercises **in Lab**

Exercise 1: Quantum Bound State

1. Write or modify `Bisection.java` to solve E :

$$\sqrt{10 - E} \tan(\sqrt{10 - E}) = \sqrt{E}$$



- Plot to see approximate roots
- Warning*: $\tan(x)$ singularities get in the way
- Equivalent equation + moved singularities (show)

$$\sqrt{E} \cot(\sqrt{10 - E}) = \sqrt{10 - E} \quad (2)$$

- Plot, solve, compare with *Maple* or *Mathematica*

Exercise 2: Newton-Raphson Roots

a. Use *Newton-Raphson method*

$$\sqrt{E} \cot(\sqrt{10 - E}) = \sqrt{10 - E}$$

b. Compare with bisection results

c. "10" $\propto V_0$ (potential depth)

20, 30 \Rightarrow deeper state (E)?

