Trial-and-Error Searching

(almost science)

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Computational Physics for Undergraduates

BS Degree Program: Oregon State University

"Engaging People in Cyber Infrastructure"

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Root Finding by “Trial and Error”

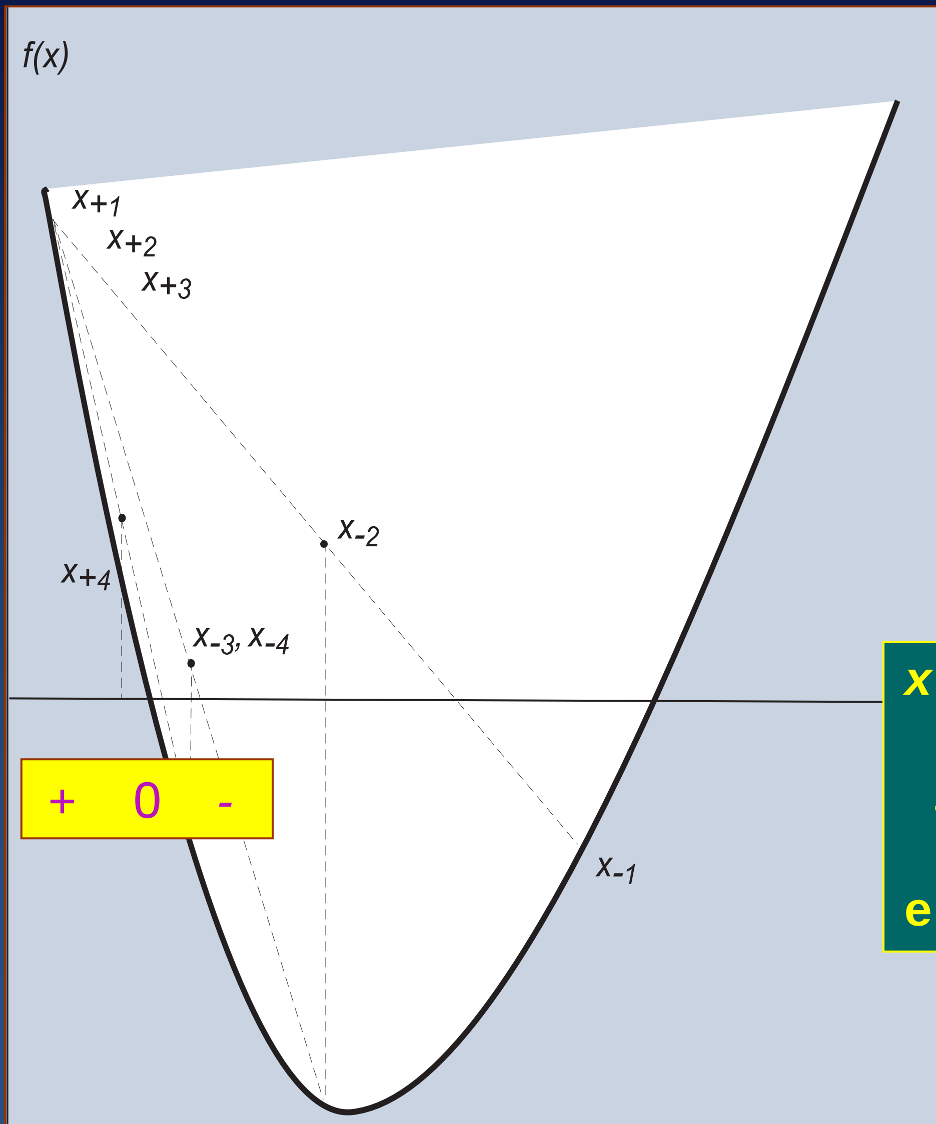
- “Root” = solution of standard equation

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

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

- Search for solutions by guessing (intelligent)
- Guess = “trial” $\rightarrow$ error $\rightarrow$ 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:

$$f(x_-) \quad < \quad 0$$

$$f(x_+) \quad > \quad 0$$

Algorithm:

```
x = (x- +  x+)/2

 if ( f (x) f (x+) > 0 ) x+ = x

else x- = x
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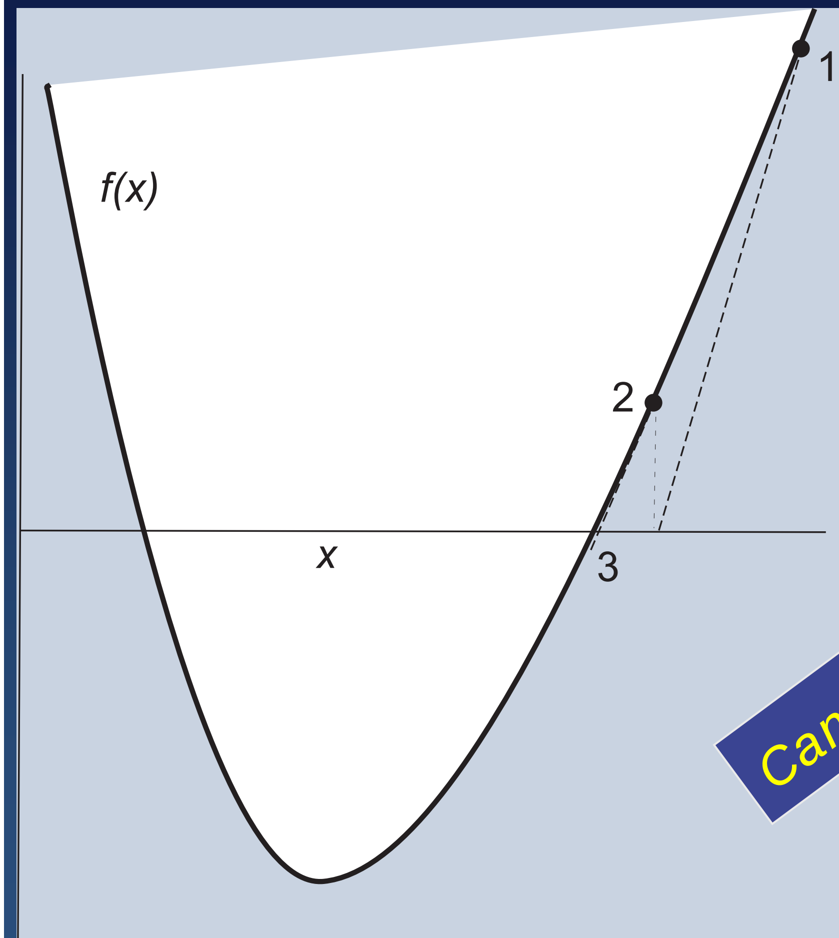
- ***Slow***
- ***Can't fail***

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



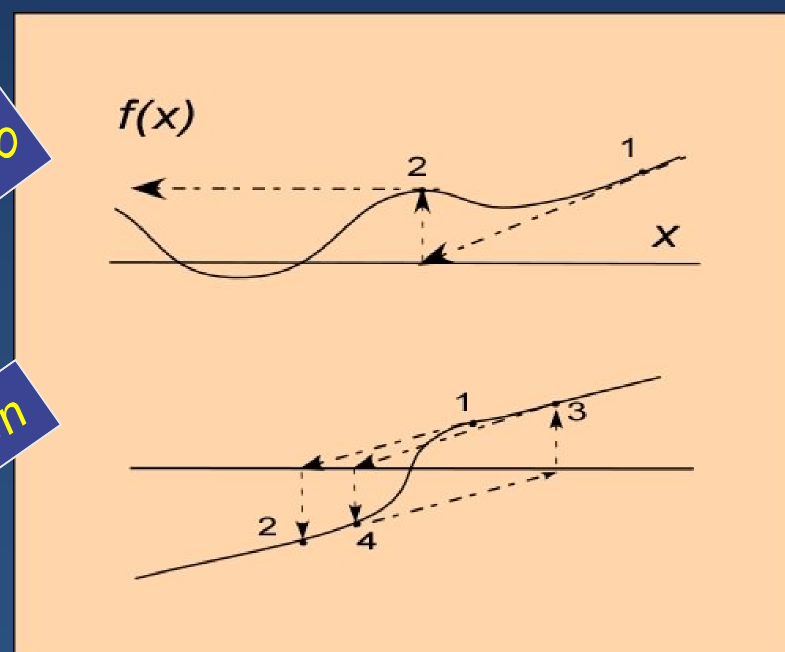
- Quicker, less robust than bisection
- Approximate $f(x) \approx$ linear function

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

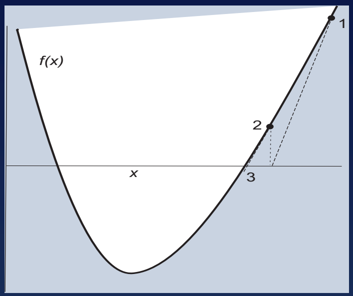
$$\Rightarrow \quad x = -b/a \qquad (4)$$

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 …

$$x_o \qquad \Delta x \ \ (?) \qquad x_1 = x_o + \Delta x \tag{5}$$

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

$$f(x_0 + \Delta x) \simeq f(x_0) + \frac{df}{dx}(x_0)\,\Delta x + \cdots \tag{6}$$

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

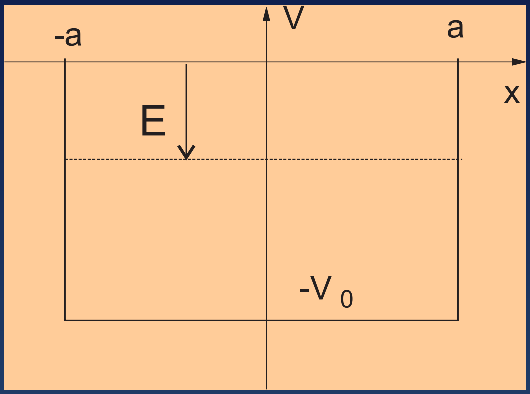
- Evaluate df/dx numerically

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

Time for Exercises in Lab

Exercise 1: Quantum Bound State

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



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

   a. Plot to see approximate roots

   b. *Warning*: $\tan(x)$ singularities get in the way

   c. Equivalent equation + moved singularities (show)

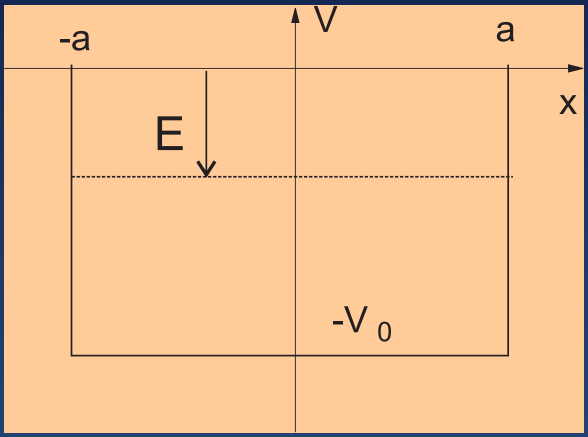
$$\sqrt{E}\,\cot(\sqrt{10-E}) = \sqrt{10-E} \qquad (2)$$

   d. 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" α V_0 (potential depth)

20, 30 $\Rightarrow$ deeper state (E)?

