MCEN 3030

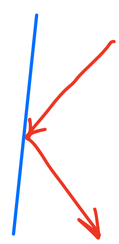
7 Mar 2024

HW + Quiz #6 Due Monday

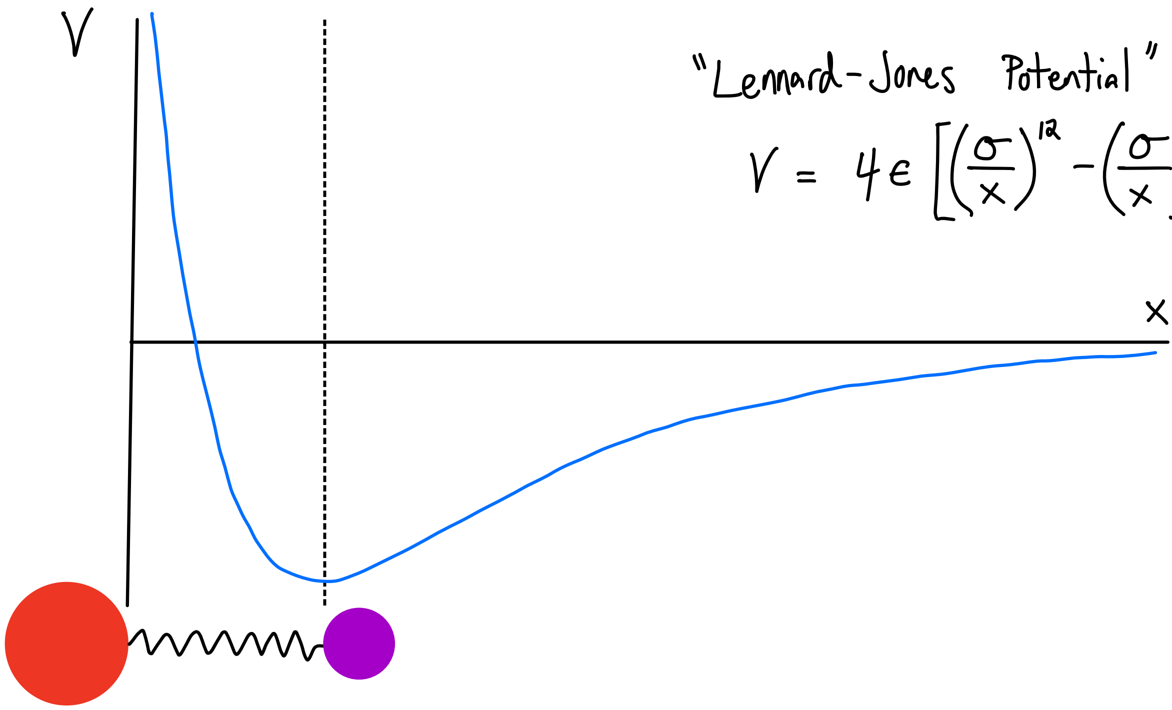
Last time: QR ← be on lookout for additional doc

today: Optimization
(1D, unconstrained)

Interesting thing I was just reading: Fast Inverse Square Root, used in Quake engine. Not exactly relevant to today(?), other than a similar goal to make efficient calculations.



Motivation



"Lennard-Jones Potential"

$$V = 4\epsilon\left[\left(\frac{\sigma}{x}\right)^{12} - \left(\frac{\sigma}{x}\right)^{6}\right]$$

What is the equilibrium separation distance of the atoms?

Analytically: $\frac{dV}{dx} = 0$ where?

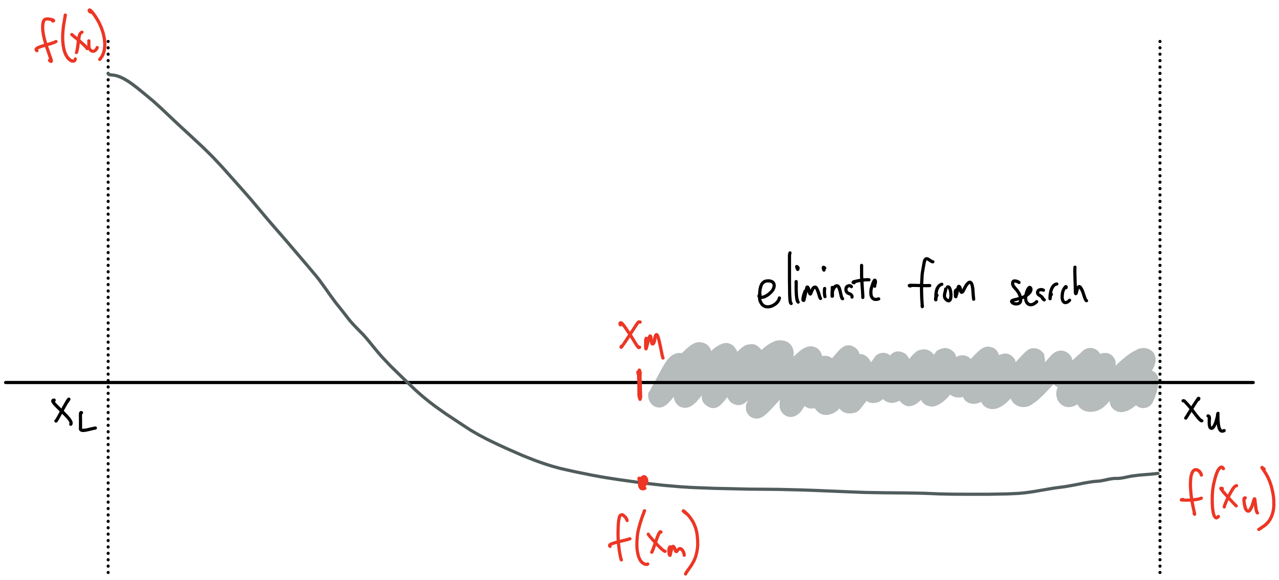
* Requires an ability to analytically evaluate derivative
  - Could follow-up with root-finding methods, e.g. Bisection or Newton-Raphson

This is an example of a 1D unconstrained optimization problem

1D: only have one independent variable

unconstrained: no second equation we also must consider

Recall: Bisection Method



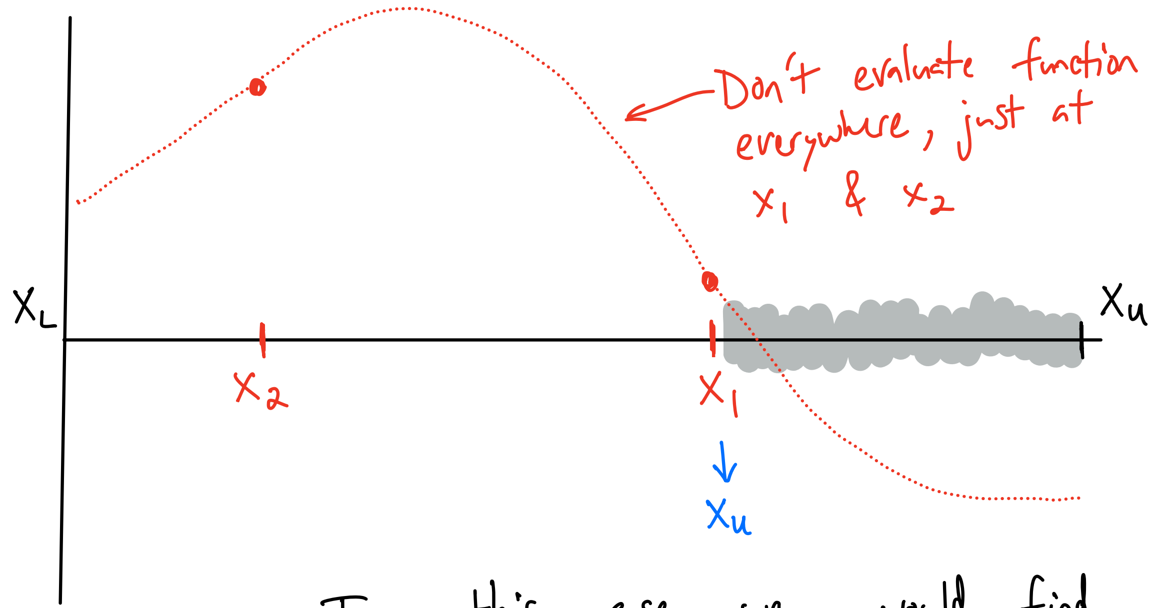
- We toss out half the remaining search region each iteration based on evaluation of the function at lower, middle, and upper points, until we feel we are sufficiently close to the root.

Golden Search Method

Idea: If we are seeking the location of a max of $f(x)$ on an interval $[x_L, x_u]$...

could be modified to min

Evaluate $f(x_1)$ & $f(x_2)$ for two interior points:



In this case we would find

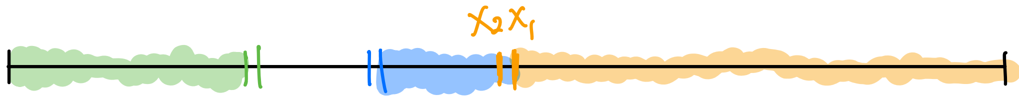
$$f(x_2) > f(x_1)$$

$\Longrightarrow$ We can say the maximum is not located on the interval $x_1 \longrightarrow x_u$

(assuming only one maximum)

How to be strategic about choice of x_1 & x_2?

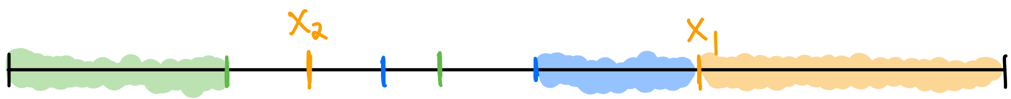
One idea: 49.999% & 50.000%



After 3 iterations: 6 function calls

& about 12.5% left

Another: thirds



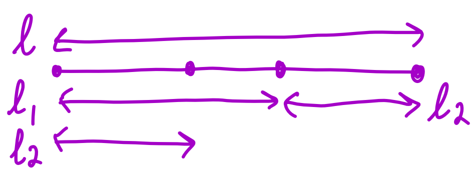
After 3 iterations: 6 function calls

& $\left(\frac{2}{3}\right)^3 = \frac{8}{27} \approx 29.6\%$

Here is the dream: Above, with each iteration we had to recalculate $x_1, x_2, f(x_1), \& \ f(x_2)$.

Can we systematically identify the right fraction such that we only need to calculate, say, x_1 & $f(x_1)$ (or x_2 & $f(x_2)$) with each iteration.

→ The answer is essentially the Golden Ratio.



$\ell_1 + \ell_2 = \ell$ & want $\frac{\ell_1}{\ell} = \frac{\ell_2}{\ell_1}$

(then $\ell_{1,new} = \ell_{2,old}$)

$\frac{\ell_1 + \ell_2}{\ell_1} = \frac{\ell_1}{\ell_2} \Rightarrow 1 + R = \frac{1}{R}$. Solution: $R = \frac{\ell_2}{\ell_1} = \frac{-1 \pm \sqrt{5}}{2}$

Algorithm

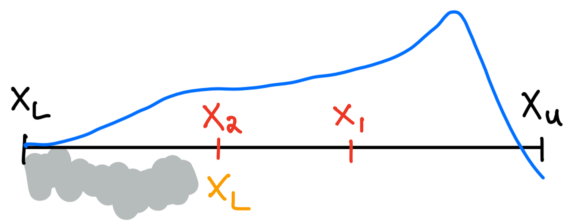
0) Define an interval $x_L \rightarrow x_u$ on which there is one max (or min)

1) Choose interior points based on the Golden Ratio

$$x_1 = x_L + d(x_u - x_L) \qquad x_2 = x_u - d(x_u - x_L) \qquad d = \frac{\sqrt{5}-1}{2} = 0.618\ldots$$

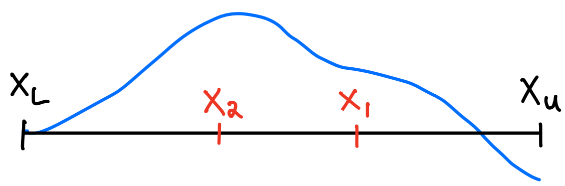
2) Evaluate $f(x_1)$ & $f(x_2)$

3) If $f(x_1) > f(x_2)$



- Throw away interval from $x_L \rightarrow x_2$
- Redefine $x_L = x_2$
- Redefine $x_2 = x_1$
- Locate $x_1 = x_L + d(x_u - x_L)$ & evaluate $f(x_1)$
- Iterate until happy

If $f(x_1) < f(x_2)$



- Throw away interval from $x_1 \rightarrow x_u$
- Redefine $x_u = x_1$
- Redefine $x_1 = x_2$
- Locate $x_2 = x_u - d(x_u - x_L)$ & evaluate $f(x_2)$
- Iterate