2023 전산물리 과제

1. Given a = -1 and b = 2 interval bracket in a minimum search, find the first x1 and x2 values using the Golden Section Search where f1 and f2 are evaluated.

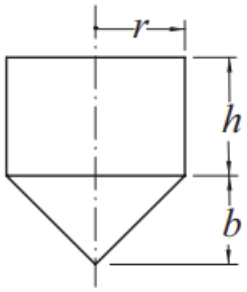
2. The Lennard-Jones potential between two molecules is

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

where ε and σ are constants, and r is the distance between the molecules. Find σ/r that minimizes the potential.

3. Determine the smallest distance from the point (1, 2) to the parabola $y = x^2$

4.



The cylindrical container has a conical bottom and an open top. If the volume V of the container is to be $1.0\,m^3$, find the dimensions r, h, and b that minimize the surface area S. Note that

$$V = \pi r^2\left(\frac{b}{3} + h\right)$$

$$S = \pi r\left(2h + \sqrt{b^2 + r^2}\right)$$