Supplemental material – PHYS 6260
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Newman Chapter 6: Solution of Linear and Non-linear Equations

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6.4: Maxima and Minima of Functions

Finding the maxima and minima of functions is closely related to root finding. Minimization problems have several physical meanings, such as finding equilibrium points from potential energy and variational methods for solving quantum mechanics problems. These problems are both one- and multi-dimensional, plus there exists *local* and *global* minima and maxima. The methods inspected here will find them but cannot distinguish between the two. They exist when

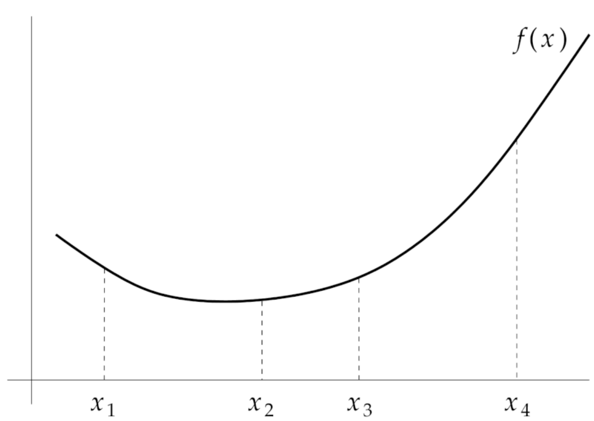
$$\frac{\partial f}{\partial x_i} = 0 \qquad \text{for all } i \tag{1}$$

is true, so we can use the root finding methods but applied to their derivatives. In addition to these methods, there are two additional methods that are useful for numerical data that don't have functional forms. In these two methods, we will be looking at minimization specifically. For maximization, we would just find the minimum of $-f(x)$.

Golden ratio search

The *golden ratio search* is similar to the binary search but it uses four points ($x_1 \ldots x_4$) instead of three. First, we need an initial guess at the bounds. If at least one of the interior values $f(x_2)$ and $f(x_3)$ is less than the exterior points $f(x_1)$ and $f(x_4)$, then we know that there must be at least one minimum between x_1 and x_4. This is illustrated in the Figure below.

If the function is smaller at x_2, the minima must exist between x_1 and x_3. If the function is smaller at x_3, the minima must exist between x_2 and x_4. Using this information, we can



narrow our search in the next iteration. However to put this procedure into practice, we must choose where the interior points are located. We don't want to favor either side, so we pick them symmetrical around the midpoint,

$$x_2 - x_1 = x_4 - x_3. \tag{2}$$

We also want to pick the points that makes the search as efficient as possible, taking the fewest iterations. Define z as the ratio between the width of the bracketing interval before and after each step. In the case where the minimum lays between x_1 and x_3,

$$z = \frac{x_4 - x_1}{x_3 - x_1} = \frac{x_2 - x_1 + x_3 - x_1}{x_3 - x_1} = \frac{x_2 - x_1}{x_3 - x_1} + 1, \tag{3}$$

eliminating x_4. In the case of the minimum existing in the right-hand side of the search interval, we would start with $z = (x_4 - x_1)/(x_4 - x_2)$ but end with the same result. For the next step, we also notice (see the Figure) that the ratio

$$z = \frac{x_3 - x_1}{x_2 - x_1} \tag{4}$$

We can equate these two expressions and find that $z^2 - z - 1 = 0$, which has a solution,

$$z = \frac{1 + \sqrt{5}}{2} = 1.618... \tag{5}$$

which is the *golden ratio*. It pops up in many, many physics and mathematics problems, along with art, music, and architecture. Now knowing the position of the interior points, we can summarize the complete golden ratio search procedure:

1. Choose two initial outside points x_1 and x_4, then calculate the interior points x_2 and x_3 with the golden ratio. Evaluate $f(x)$ at these four points and check whether one of the interior points is the minimum of our the four. Also choose a target accuracy at this time.
2. If $f(x_2) < f(x_3)$, then the minimum lies between x_1 and x_3. In this case, x_3 becomes the new x_4, and there will be a new value for x_2, chosen with the golden ratio rule. Evaluate $f(x)$ at this new point.
3. Otherwise, the minimum lies between x_2 and x_4. Then x_2 becomes the new x_1, x_3 becomes the new x_2, and we calculate a new value for x_3 and $f(x_3)$.
4. If $x_4 - x_1$ is greater than the tolerance, repeat from step #2. Otherwise, calculate $(x_2 + x_3)/2$ and this is the final estimate of the position of the minimum.

Note that the golden ratio search suffers the same shortcomings as the binary search, in that it only works for one variable and needs an initial search interval.

Example 6.5: The Buckingham Potential

The Buckingham potential is an approximation representation of the potential energy of interaction between atoms in a solid or gas as a function of distance r between them:

$$V(r) = V_0 \left[\left(\frac{\sigma}{r} \right)^6 - e^{-r/\sigma} \right] \tag{6}$$

that has a sharp barrier just outside $r/\sigma = 1$ has a minimum shortly outside of this barrier and exponentially approaches zero as r increases.

This potential contains a short-range repulsive (Pauli exclusion) force between the atoms and a longer-range attractive (Van der Waals) force. We want to find where these two forces balance, forming a stable equilibrium point where the potential is at a minimum. Here's a program that will perform a golden ratio search with $\sigma = 1$ nm. The normalization constant V_0 is not needed for a minimum search.

```
from math import exp,sqrt

# Constants
sigma = 1.0              # Value of sigma in nm
accuracy = 1e-6          # Required accuracy in nm
z = 0.5*(1+sqrt(5))      # Golden ratio

# Function to calculate the Buckingham potential
def f(r):
    return (sigma/r)**6 - exp(-r/sigma)

# Initial positions of the four points
x1 = sigma/10
x4 = sigma*10
x2 = x4 - (x4-x1)/z
x3 = x1 + (x4-x1)/z

# Initial values of the function at the four points
f1 = f(x1)
f2 = f(x2)
f3 = f(x3)
f4 = f(x4)

# Main loop of the search process
while x4-x1 > accuracy:
#
#  To be completed in class
#
```

```
# Print the result
print("The minimum falls at %.6f nm % (0.5*(x1+x4)))
```

It returns the answer `1.630516 nm`.

The Gauss-Newton method and gradient descent

The Gauss-Newton and gradient descent methods are extensions of the Newton method, which can be used for two or more variables. First, the Gauss-Newton method finds the roots of the derivative, $f'(x) = 0$, using the Newton method. To find the updated solution, we replace $f(x)$ by $f'(x)$ in the original formulation, obtaining

$$x' = x - \frac{f'(x)}{f''(x)} \tag{7}$$

This method will converge very quickly, but we need to know the closed-form 1st and 2nd order derivative, which is not always the case. If we still have the first-order derivative $f'(x)$ we can use an approximation to the Gauss-Newton method, called *gradient descent*, where we take

$$x' = x - \gamma f'(x), \tag{8}$$

where γ is a constant that represents a rough guess at $1/f''(x)$. One nice property of this method is that γ doesn't need to accurate and can be negative or positive, depending on whether we are searching for a minimum or maximum, respectively.

Even if we can't calculate $f'(x)$ analytically, we can use something similar to the secant method to estimate the derivative

$$f'(x_2) \simeq \frac{f(x_2) - f(x_1)}{x_2 - x_1}, \tag{9}$$

where x_1 and x_2 are two points near x. We then can use this estimate in the next update in the search,

$$x_3 = x_2 - \gamma \frac{f(x_2) - f(x_1)}{x_2 - x_1}. \tag{10}$$

Minimization problems are widespread in the sciences, computer science, and engineering, thus there has been much work on making more accurate and efficient minimization techniques. There are many other methods to find maxima and minima, such as Powell's method, the conjugate gradient methods, and the BFGS method, and we have just covered the basics.