

1. (a) The probability P of an individual having genotypes AA, BB, or OO (in other words having two genotypes that are the same) is p^2 , q^2 , and r^2 , respectively, for each of the genotypes aforementioned. Therefore, the probabilities of an individual having two different genes correspond to the complements of these original probabilities. That is, $1 - p^2$ for any genotype with A, $1 - q^2$ for any genotype with B, and $1 - r^2$ for any genotype with O.
- (b) i. In order to directly maximize a function of two variables, we can derive a function of three variables such that $f(p, q, r) = 1 - p^2 - q^2 - r^2$. Then we can substitute our equation from the Hardy-Weinberg Principle to arrive at an equation of two variables $f(p, q) = 1 - p^2 - q^2 - (1 - p - q)^2$. Solving for the maximum, we conclude that the maximum is $\frac{2}{3}$ at the point $(p, q) = (\frac{1}{3}, \frac{1}{3})$.
- ii. Now by using the method of Lagrange multipliers we still want to maximize our original function $f(p, q, r) = 1 - p^2 - q^2 - r^2$; however, we have the constraint g , which says $p + q + r = 1$.

$$\begin{cases} \frac{\partial f}{\partial p} - \lambda \frac{\partial g}{\partial p} = -2p - \lambda = 0 \\ \frac{\partial f}{\partial q} - \lambda \frac{\partial g}{\partial q} = -2q - \lambda = 0 \\ \frac{\partial f}{\partial r} - \lambda \frac{\partial g}{\partial r} = -2r - \lambda = 0 \\ g(p, q) - c = 1 - p - q - r = 0 \end{cases}$$

By solving the system of linear equations, we find the following:

$$\begin{pmatrix} -2 & 0 & 0 & -1 \\ 0 & -2 & 0 & -1 \\ 0 & 0 & -2 & -1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} p \\ q \\ r \\ \lambda \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Once again, we find that the maximum is $\frac{2}{3}$ at the point $(p, q, r) = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$.

- (c) In this context, the Lagrange Multiplier represents the increase in the percentage (or likelihood) that two genes can be put together differently under the Hardy-Weinberg Principle with respect to the percentage of each A, B, and O bloodtype in the population. That is, the value of λ represents the rate of change of this highest percentage of different genes possible (given the constraint from the Principle) as the proportion of gene A, gene B, and gene O increase in a sample population. It can also be thought of as the marginal difference of these percentages.
2. (a) Setting the function $f(x) = 0$, the root(s) of the function are revealed:

$$\begin{aligned} f(x) = 0 &= e^x - xe^x \\ &= e^x - xe^x \\ &= e^x(1 - x) \end{aligned}$$

Given this equation, the following equations are true:

$$e^x = 0$$

$$1 - x = 0$$

From the first equation, $x = \ln(0) \rightarrow \infty$, and there are therefore no real roots from this. Therefore, $x = 1$ is the only real root.

- (b) The following tables give a representation of the Newton, Secant, and Bisection methods as mentioned in the problem set:

x_0	iters	x_*
1/2	7	1.0
2	7	1.0
10	17	1.0
-1/2	738	-745.744
-5	1473	-745.918

Table 1: Newton's Method

(x_0, x_1)	iters	x_*
(0, 2)	13	1.0
(0, 10)	•	$< -190,000$
(-1, 2)	1067	-745.742
(-5, 5)	1064	-743.968
(-10, 2)	1059	-744.891

Table 2: Secant Method

Note that the at the point (0,10), the numerical result of x is too extreme and out of range. The program listed NaN (not a number) as the output.

$[x_L, x_R]$	iters	x_*
[0, 2]	1	1.0
[-5, 5]	43	1.0000000000002274
[-10, 2]	41	0.9999999999995453
[-1, 2]	43	1.0000000000002274
[0, 1]	43	0.9999999999995453

Table 3: Bisection Method

- (c) The initial parameters for each method directly impact the success in finding the roots for a function:
- Newton's Method takes in only one value of the function x_0 , a function $f(x)$, and its derivative $f'(x)$, but it may not converge if x_0 is too far away from the root. Furthermore, if the given function is not continuous or differentiable near the root, Newton's Method will diverge.
 - The Secant Method takes in two initial parameters, x_0 and x_1 , and can be more useful if dealing with a non-differentiable, non-continuous function as mentioned

above. However, if $f(x_L)f(x_R) \geq 0$ at any point in the iteration, then the Secant Method fails.

- iii. Finally, the Bisection Method takes in three initial parameters: a function, f , the starting point of an interval over f , a , and the ending point on that interval, b . Like the Secant Method, there is no need for differentiation in this method, allowing for a non-continuous or non-differentiable function. However, because we are finding the midpoint in this method (or bisecting the function over a given interval), the Bisection Method fails if there is a double root. That is, it fails when $f(a)$ and $f(b)$ have the same sign at each step over the interval. In this case, it is not clear which half of the interval to take at each step.
- (d) Some initial parameters are not successful for the Secant Method because there exists a horizontal asymptote at $x = 0$. As such, the function approaches zero as $x \rightarrow -\infty$. The value of x is too small relative to the value of x at that point, i.e. the point $x = 10$.

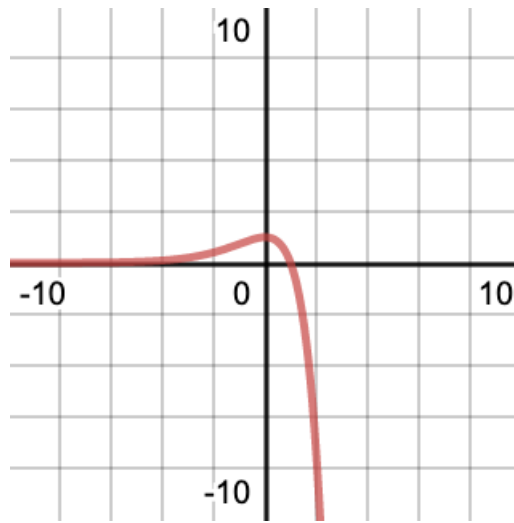


Figure 1: $f(x) = e^x - xe^x$

Therefore, the following limit is true:

$$\lim_{x \rightarrow -\infty} f(x) = 0$$

- (e) The Secant Method algorithm will continue to iterate until it reaches that value of $f(x_k) = 0$, yet we know from the definition of an asymptote that this will never happen. Thus, a better termination condition to determine convergence would be to incorporate some convergence limiting test into our algorithm. For example, we could include a function value convergence test, which would terminate the iteration when all function values f_j are small enough in some sense. You could also use an absolute error criterion, which would terminate the amount of iterations after the difference between successive iterations reaches a specific, pre-determined amount. This is somewhat more reasonable because you do not really know how large or small your margin to error is, and normalizing your iterations this way makes your stopping condition independent of scale.
3. (a) Setting the function $f(x) = 0$, the root(s) of the function are revealed:

$$f(x) = 0 = x^3 - 5x$$

$$= x(x^2 - 5)$$

Given this equation, the following equations are true:

$$x = 0$$

$$x^2 - 5 = 0$$

From the first equation, $x = 0$. From the second equation, $x^2 = 5 \Rightarrow x = \pm \sqrt{5}$.

(b) Using Newton's Method,

x_0	iters	x_*
1	•	•
-1	•	•
2	5	2.236
10	9	2.236
-10	9	-2.236

Table 4: Newton's Method (pt. 2)

- (c) If $f(x) = x^3 - 5x$, then $f'(x) = 3x^2 - 5$. By calculating the first two iterations of Newton's method:

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 1 - \frac{f(1)}{f'(1)} = 1 - \frac{4}{f'(2)} = -1$$

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = 1 - \frac{f(-1)}{f'(-1)} = 1 - \frac{4}{f'(-2)} = 1$$

Because our approximations for x oscillate back and forth right at the beginning, Newton's Method fails to provide an approximation for the function.

4. Because there are some instances where a discontinuity can exist (i.e. a zero in the second derivative for Newton's Method), continuity can impact which method is used in root-finding.
 - (a) For the function $f_1(x) = x^2 - a$, **Newton's Method** would be best because this function is easily differential and continuous regardless of the real value of a . Newton's Method assumes the function f to have a continuous derivative, which it does.
 - (b) For the function $f_2(x) = x^{1/5}$, we have to be careful not to approximate with any negative valued x . The derivative of f is not differentiable at any negative value of x and for any negative values of x . Therefore, Newton's Method would not work. The **Secant Method**, however, would be a better choice because it does not rely on the differentiability of f , as it replaces the derivative in Newton's Method with a finite difference of values.

5. As mentioned in question four, continuity is one important component in determining which method of root-finding to use. If a function is not continuous at certain points, has a derivative that is not continuous, or is simply not differentiable, then Newton's Method has some serious flaws when it comes to root-finding. The Secant Method replaces the derivative in Newton's Method with a finite difference, as mentioned above. Although the method does not require the computation (nor the existence) of a derivative, it comes at the cost of slower convergence. The Bisection Method is one of the simplest algorithms for root finding, but it also requires a continuous function. Although the bisection method is sound, it gains one and only one bit of accuracy with each iteration, as it involves finding the midpoint (or bisection) of a given interval.