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MAT 397— Fall 2020

Applied Problems:

Maxima & Minima

“I believe that new mathematical schemata, new systems of axioms, certainly new systems of mathematical structures will be suggested by the study of the living world.”

—Stan Ulam

Biological Diversity

A common misconception about the theory of evolution is that it is a theory of randomness—which cannot be further from the truth. The theory of evolution is vastly complicated, but at its core it roughly works as follows: some individuals in the population will experience genetic mutation. Of course, given a large population and an ‘easy to occur’ mutation, this will probably happen for many individuals in the population. If the mutation can be passed on and helps the individual survive in the environment, then these genes will come to dominate in the population, and the process repeats. Even if the mutation only increases the survivability of the individual by 0.001%, given enough individuals and a large enough period of time, these individuals will dominate in the long run. Consider an analogy with income: if a group of workers only make \$0.001 more per hour than another group, assuming the first group doesn’t dissolve (i.e., die out) then in the span of tens of thousands of hours, these individuals will have much more money than the second group.

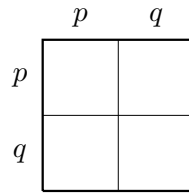
However, the predictability of genetics rests on Statistics and Probability. It may not be possible to say which individuals will have mutations or will survive in the long term. Instead of attempting to make predictions about individuals in a population, we can apply the laws of Statistics and Probability to allow us to make accurate predictions about the population(s) as a whole. For instance, I cannot say much about the height of a random male individual in the United States with certainty, but I can say with certainty that 90% of such males will have height between 64 inches and 73.7 inches (based on current data).

We can use these statistical and probabilistic principles, along with some Calculus, to create predictions about populations as a whole, especially with regards to their genetics. In fact, farmers use this when inbreeding cattle to maintain genetically stable herds—the so-called coefficient of inbreeding. We will examine such laws in two special cases.

Hardy-Weinberg Law:¹ In the absence of other evolutionary influences, the Hardy-Weinberg Law states that allele and genotype frequencies remain constant from generation to generation. In a simple case, there are only two alleles, say A and B , which occur with probability p and q , respectively. Then if the individuals in the population mate randomly, you can expect a probability of p^2 for individuals having genetic type AA and q^2 for genetic type BB (the homozygotes, or ‘same genes’), and $2pq$ for genetic type AB (the heterozygotes, or ‘different genes’). This follows from the simple application of laws of probability for a sequence of independent events. [Can you see

¹Hardy was a very famous mathematician who wrote a book called, *A Mathematician’s Apology*, where he said, “I have never done anything useful. No discovery of mine has made, or is likely to make, directly or indirectly, for good or ill, the least difference to the amenity of the world.” Reading the book, or about his life, especially his collaboration and ‘discovery’ of the Indian mathematician Srinivasa Ramanujan—who is arguably one of the greatest mathematicians having made major contributions to many fields of Mathematics despite having died young and having taught himself nearly everything he knew without any help. You might watch *The Man Who Knew Infinity* about his life, or the book by the same name.

why these are the probabilities drawing a simple Punnett square like the one below?]



Of course, the Hardy-Weinberg Law requires many assumptions about the population, which we will not discuss here. Now think about a gene with three alleles. As an example, we can consider blood type, which has three alleles: A , B , and O . In this case, the homozygous individuals have blood ‘type’ AA , BB , and OO , while those with blood ‘type’ AB , AO , or BO , are heterozygous. The Hardy-Weinberg Law states that the proportion of individuals in the population with heterozygous type is given by

$$P(p, q, r) := 2pq + 2pr + 2qr$$

where p, q, r represent the percent of alleles of type A , B , and O in the population, respectively. Because one ultimately, after this genetic combination at birth, has type A , B , or O , we know that $p + q + r = 1$.

Problem:

- (a) Show that the maximum proportion of heterozygous individuals in the population is at most $2/3$.

Of course, we can make predictions for more than just the genetic diversity for a single population. Instead, we can examine ecological diversity more broadly. There are many measures of biodiversity. However, a common measure because of its understandability is the Shannon Diversity Index (or Shannon-Wiener Index)—though there are others. The concept was originally used by Claude Shannon in Information Theory. [You might be familiar with him from his mathematical work in Computer Science, especially if you learn Cryptology.] For an environment with three populations, A, B, C , the index is

$$H(x, y, z) := -x \ln x - y \ln y - z \ln z$$

where x, y, z are the proportion of the species A, B, C in the environment, respectively. [Observe by definition, $x + y + z = 1$.]

- (b) What happens if there is only one population, e.g. $x = 1$ and $y = z = 0$?
- (c) What is the index if all the populations are equally abundant?
- (d) What happens if all the populations are ‘very different’ in size? [It may be easier just to try it in a few examples.]
- (e) What happens if one population is very dominant?
- (f) Given (c) and (d), discuss how this index measures ‘diversity.’
- (g) Show that the maximum value of H occurs when $x = y = z = \frac{1}{3}$, with maximum value $\ln 3$.

Solution.

- (a) Strictly speaking, we want to maximize $P(p, q, r) := 2pq + 2pr + 2qr$ with respect to the restriction $p + q + r = 1$ —making this a Lagrange Multiplier problem. However, observe we can solve $p + q + r = 1$ for any of p, q, r , and use this in $P(p, q, r) := 2pq + 2pr + 2qr$. This avoids Lagrange Multipliers. Because each of the equations is ‘symmetric’ in p, q, r , we can do this for any of the variables. We choose r . So we have $r = 1 - p - q$. Then

$$P(p, q, r) = P(p, q, 1 - p - q) = -2p^2 - 2q^2 + 2p + 2q - 2pq$$

Define $f(p, q) = -2p^2 - 2q^2 + 2p + 2q - 2pq$. We want to maximize $f(p, q)$.

$$\begin{aligned}\frac{\partial f}{\partial p} &= 2 - 4p - 2q \\ \frac{\partial f}{\partial q} &= 2 - 2p - 4q\end{aligned}$$

Setting these partials to zero, we have the following system of equations:

$$\begin{aligned}4p + 2q &= 2 \\ 2p + 4q &= 2\end{aligned}$$

Taking twice the second equation and subtracting it from the first, we find $-6q = -2$, so that $q = 1/3$. Then using the first equation, we find that $4p + 2/3 = 2$ so that $p = 1/3$. Then $r = 1 - p - q = 1 - 1/3 - 1/3 = 1/3$. However, we need show that this is indeed a maximum. We can just examine the Hessian for $f(p, q)$:

$$\begin{pmatrix} f_{pp} & f_{pq} \\ f_{qp} & f_{qq} \end{pmatrix} = \begin{pmatrix} -4 & -2 \\ -2 & -4 \end{pmatrix}$$

We find a sequence of principal minors $d_1 = -4 < 0$ and $d_2 = (-4)(-4) - (-2)(-2) = 16 - 4 = 12 > 0$. Therefore, $(p, q) = (1/3, 1/3)$ is indeed a maxima, so that $(p, q, r) = (1/3, 1/3, 1/3)$ is a maxima.

- (b) First, observe that

$$\lim_{w \rightarrow 0^+} -w \ln w = \lim_{w \rightarrow 0^+} \frac{\ln(1/w)}{1/w} \stackrel{\text{L.H.}}{=} \lim_{w \rightarrow 0^+} \frac{\frac{1}{1/w} \cdot -\frac{1}{w^2}}{-1/w^2} = \lim_{w \rightarrow 0^+} w = 0$$

So we can ‘define’ $f(w) = -w \ln w$ to be 0 at 0. Because everything is ‘symmetric’ in x, y, z , we can assume $x = 1.00$ and $y = z = 0$. Then we have

$$\lim_{(x,y,z) \rightarrow (1,0,0)} H(x, y, z) := -\ln 1 - 0 - 0 = \ln 1 = 0$$

Therefore, the diversity index is 0 if there is only one population. This makes sense, because then there is no diversity.

- (c) Let $x = y = z = p$, for some proportion p . Then we find

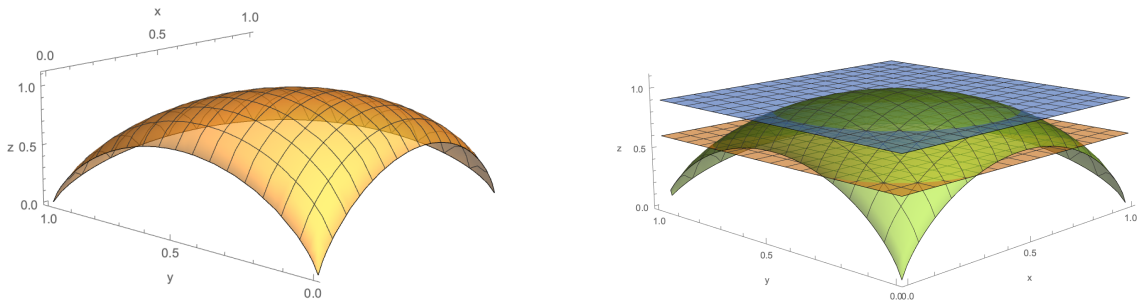
$$H(x, y, z) = H(p, p, p) = -p \ln p - p \ln p - p \ln p = -3p \ln p = \ln(p^{-3p})$$

But because $x + y + z = 1$, we are forced to have $3p = 1$ so that $p = 1/3$. Then $H(p, p, p) = H(1/3, 1/3, 1/3) = \ln((1/3)^{-1}) = \ln(3) \approx 1.09861$.

(d) We simply create a table to see the values of H when x, y, z are ‘very different’.

x	y	z	$H(x, y, z)$
0.01	0.24	0.75	0.604321
0.10	0.50	0.40	0.943348
0.45	0.45	0.10	0.948915
0.70	0.10	0.20	0.801819
0.90	0.05	0.05	0.394398

Observe that all the values for $H(x, y, z)$ are between 0 and 1, mostly staying between 0.60 and 0.95. In fact, using the fact that $z = 1 - x - y$, we can plot the function $H(x, y, z)$ for $0 < x < 1$, $0 < y < 1$.



From the plots above, we can see that ‘most’ of the values lie in this range. Notice also that if the populations are all very similar, i.e. $x \approx y \approx z$, then we are on the ‘top’ of the surface where it seems $H > 0.90$. So perhaps, we expect H to be ‘small’ when the populations are very different in size, and expect H to be ‘large’ when the populations are roughly equally diverse.

(e) Say that one population is dominant. Without loss of generality, let’s assume that population A is dominant, with proportion x . Then assume B, C are equally likely with proportion $y = z = (1 - x)/2$; that is, take ‘what is left over’ from x , split it in half, and divide it equally among B and C . Then we have

$$H(x, y, z) = H\left(x, \frac{1-x}{2}, \frac{1-x}{2}\right) = -x \ln x + (x-1) \ln\left(\frac{1-x}{2}\right)$$

Now we can take x to be ‘dominate’, i.e. close to 100%, and see what the values of H are: Observe these values are much smaller than those observed in (c). So if one population is very

x	H
0.90	0.394398
0.92	0.334221
0.94	0.268556
0.96	0.19567
0.98	0.111902
0.99	0.062933

dominant, we might expect values of H (‘much’) less than 0.60.

- (f) Observe that H is attempting to measure how the total population in an environment is distributed among the various populations. The more ‘equitable’ the distribution, the larger the value of H .
- (g) We want to maximize $H(x, y, z) := -x \ln x - y \ln y - z \ln z$ with respect to the condition that $x + y + z = 1$. Again, this would call for Lagrange Multipliers, except we can solve for one of x, y, z in $x + y + z = 1$, and use this in $H(x, y, z)$. Because the equations are ‘symmetric’ in x, y, z , we choose to solve for z . Using $z = 1 - x - y$, we have

$$H(x, y, z) = H(x, y, 1 - x - y) = -x \ln x - y \ln y + (x + y - 1) \ln(1 - x - y)$$

Define $g(x, y) := -x \ln x - y \ln y + (x + y - 1) \ln(1 - x - y)$. Then we want to maximize $g(x, y)$. Taking partials, we find

$$\begin{aligned} \frac{\partial g}{\partial x} &= -1 - \frac{x + y - 1}{1 - x - y} - \ln x + \ln(1 - x - y) = -\ln(x) + \ln(1 - x - y) \\ \frac{\partial g}{\partial y} &= -1 - \frac{x + y - 1}{1 - x - y} + \ln(1 - x - y) - \ln y = -\ln y + \ln(1 - x - y) \end{aligned}$$

Setting these to zero, we have a system of equations

$$\begin{aligned} \ln(x) &= \ln(1 - x - y) \\ \ln(y) &= \ln(1 - x - y) \end{aligned}$$

Exponentiating, this implies $x = 1 - x - y$ and $y = 1 - x - y$. But then we immediately see that $x = y$. But then $x = 1 - x - y = 1 - x - x = 1 - 2x$ so that $x = 1/3$. Therefore, $y = 1/3$ and then $z = 1 - 1/3 - 1/3 = 1/3$. We must show this is a maximum, which we can do by examining the Hessian:

$$\begin{pmatrix} g_{xx} & g_{xy} \\ g_{yx} & g_{yy} \end{pmatrix} = \begin{pmatrix} -\frac{1}{x} + \frac{1}{x + y - 1} & \frac{1}{x + y - 1} \\ \frac{1}{x + y - 1} & -\frac{1}{y} + \frac{1}{x + y - 1} \end{pmatrix} \Big|_{(x,y)=(1/3,1/3)} = \begin{pmatrix} -6 & -3 \\ -3 & -6 \end{pmatrix}$$

Then we have principal minors $d_1 = -6 < 0$ and $d_2 = (-6)(-6) - (-3)(-3) = 36 - 9 = 27 > 0$. Therefore, $x = y = z = 1/3$ is a maximum for $g(x, y)$, and therefore for $H(x, y, z)$. Then we have maximum value

$$H(1/3, 1/3, 1/3) = -(1/3) \ln(1/3) - (1/3) \ln(1/3) - (1/3) \ln(1/3) = -\ln(1/3) = \ln(3) \approx 1.09861$$