PPS

This document provides our solutions to the 11 exercises included in the nice and concise brochure "A Primer of Probability & Statistics" (PPS) written by Ziheng Yang. We hope that the solutions included in this document could serve as a supplemental material accompanying our tentative solutions for Ziheng Yang's influential books Computational Molecular Evolution (CME2006) and Molecular Evolution: A Statistical Approach (MESA2014). Scripts associated with some exercises are provided on the online repository https://github.com/sishuowang/Solutions_Manual_CME2006_MESA2014/. The difficulty of the exercises of PPS is much lower compared with those from the above two, so beginners are suggested to start with PPS. Note as indicated on the first page of PPS, "Permission is granted to copy those notes provided that no fee is charged and that this copyright notice is not removed".

© Sishuo Wang 2024 • Exercise 1. (Summing up large numbers). Use the above procedure to calculate the logarithm of the sum $e^{1000} + e^{1200} + e^{1215} + e^{1216}$. [The answer is 1216.31326.]

$(1) x_i$	10^{-10}	10^{-15}	10^{-20}	10^{-25}	
(2) $y_i =$	-23.02585	-34.53878	-46.05170	-57.56463	Largest $y^* =$
$log\{x_i\}$					-23.02585
$(3) z_i = y_i - y^*$	0	-11.51283	-23.02575	-34.53868	
(4) $\exp\{z_i\}$	1	10^{-5}	10^{-10}	10^{-15}	Sum $s = 1.000010$

Solution.

We provide the following R script.

```
R
exponents <- c(1000, 1200, 1215, 1216)
yi <- exponents
y_star <- max(yi)
zi <- yi - y_star
s <- sum(exp(zi))
final_result <- y_star + log(s)

cat("Exponents:", exponents, "\n")
cat("yi values:", yi, "\n")
cat("Ju values:", yi, "\n")
cat("Largest y*:", y_star, "\n")
cat("zi values:", zi, "\n")
cat("zi values:", exp(zi), "\n")
cat("Sum s:", s, "\n")
cat("Final result:", final_result, "\n")</pre>
```

• Exercise 2 (matrix addition and multiplication). Suppose $A = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$, $I = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$, $D = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

$$\begin{bmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{bmatrix}$$
. Confirm that $IA = AI = A$. Calculate DA and AD . What pattern did you see?

Calculate A^2 , and D^n , for any natural number n.

Solution.

a)

$$IA = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$$

$$= \begin{bmatrix} 1 \times a + 0 \times b + 0 \times c & 1 \times b + 0 \times e + 0 \times h & 1 \times c + 0 \times f + 0 \times i \\ 0 \times a + 1 \times d + 0 \times g & 0 \times b + 1 \times e + 0 \times h & 0 \times c + 1 \times f + 0 \times i \\ 0 \times a + 0 \times d + 1 \times g & 0 \times b + 0 \times e + 1 \times h & 0 \times c + 0 \times f + 1 \times i \end{bmatrix}$$

$$= \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$$

$$= AI$$

$$= A.$$

b)

$$\begin{split} AD &= \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} \times \begin{bmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{bmatrix} = \begin{bmatrix} ad_1 & bd_2 & cd_3 \\ dd_1 & ed_2 & fd_3 \\ gd_1 & hd_2 & id_3 \end{bmatrix}, \\ DA &= \begin{bmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{bmatrix} \times \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} = \begin{bmatrix} d_1a & d_1b & d_1c \\ d_2d & d_2e & d_2f \\ d_3g & d_3h & d_3i \end{bmatrix}. \end{split}$$

c)

$$A^{2} = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} \times \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} = \begin{bmatrix} a^{2} + bd + cg & ab + be + ch & ac + bf + ci \\ da + ed + fg & db + e^{2} + fh & dc + ef + fi \\ ga + hd + ig & gb + he + ih & gc + hf + i^{2} \end{bmatrix}.$$

$$D^{n} = \begin{bmatrix} d_{1}^{n} & 0 & 0 \\ 0 & d_{2}^{n} & 0 \\ 0 & 0 & d_{3}^{n} \end{bmatrix}.$$

• **Exercise 3** (matrix inversion). Find A^{-1} where $A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$. [Hint. Let $A^{-1} = \begin{bmatrix} r & s \\ t & u \end{bmatrix}$. Find r, s, t, u by solving the equations $AA^{-1} = I$]

Solution.

We suppose that the matrix A is not singular. In other words, the determinant of A is not zero ($|A| \neq 0$). According to the hint, we have

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} r & s \\ t & u \end{bmatrix} = \begin{bmatrix} ar+bt & as+bu \\ cr+dt & cs+du \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Hence,

$$\begin{cases} ar + bt = 1\\ as + bu = 0\\ cr + dt = 0\\ cs + du = 1 \end{cases}$$

By solving this system of equations, we get

$$r = -\frac{d}{bc - ad}$$
, $t = \frac{c}{bc - ad}$, $s = -\frac{b}{(ad - bc)}$, $u = \frac{a}{ad - bc}$.

Alternatively, we can use Cramer's Principle:

$$A^{-1} = \frac{1}{|A|} \operatorname{adj}(A)$$

where

$$|A| = ad - bc$$

$$adj(A) = \begin{bmatrix} d & -c \\ -h & a \end{bmatrix}.$$

Hence,

$$A^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -c \\ -b & a \end{bmatrix}.$$

This is exactly the same as obtained by using the hint.

• Exercise 4 (eigensolution for the Jukes & Cantor model). Find the eigensolution of

$$Q = \begin{bmatrix} -3\lambda & \lambda & \lambda & \lambda \\ \lambda & -3\lambda & \lambda & \lambda \\ \lambda & \lambda & -3\lambda & \lambda \\ \lambda & \lambda & \lambda & -3\lambda \end{bmatrix}$$

Solution.

This is basically part of Problem 1.2 in CME2006. Hence, we directly provide the solution as follows.

Eigen values:
$$\mu = (0, -4\lambda, -4\lambda, -4\lambda)$$
. Eigen vectors: $v_1 = (1,1,1,1), v_2 = (1,-1,0,0), v_3 = (0,1,-1,0), v_4 = (0,0,1,-1)$.

• Exercise 5* (Transition probability matrix under Kimura's 2-parameter model). Use the result of the Example (equation 1.13) to calculate e^{Qt} , where t is a scalar.

Solution.

According to the problem statement, the instantaneous rate matrix of the model is

$$Q = \begin{bmatrix} -\alpha - 2\beta & \beta & \alpha & \beta \\ \beta & -\alpha - 2\beta & \beta & \alpha \\ \alpha & \beta & -\alpha - 2\beta & \beta \\ \beta & \alpha & \beta & -\alpha - 2\beta \end{bmatrix}.$$

According to equation (1.13) of PPS, the eigen decomposition of Q is given by

$$Q = \begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & -1 \\ 1 & -1 & 1 & 0 \\ 1 & -1 & -1 & 0 \end{bmatrix} \times \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & -4\beta & 0 & 0 & 0 \\ 0 & 0 & -2(\alpha+\beta) & 0 \\ 0 & 0 & 0 & -2(\alpha+\beta) \end{bmatrix} \times \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} \\ 0 & 0 & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & 0 & 0 \end{bmatrix}$$

Hence, the transition probability matrix can be calculated as

$$P(t) = e^{Qt}$$

$$= \begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & -1 \\ 1 & -1 & 1 & 0 \\ 1 & -1 & -1 & 0 \end{bmatrix} \times e^{\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & -4\beta & 0 & 0 & 0 \\ 0 & 0 & -2(\alpha+\beta) & 0 \\ 0 & 0 & 0 & -2(\alpha+\beta) \end{bmatrix}} \times \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} \\ 0 & 0 & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & -1 \\ 1 & -1 & 1 & 0 \\ 1 & -1 & -1 & 0 \end{bmatrix} \times \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & e^{-4\beta} & 0 & 0 & 0 \\ 0 & 0 & e^{-2(\alpha+\beta)} & 0 & 0 \\ 0 & 0 & e^{-2(\alpha+\beta)} & 0 & 0 \\ 0 & 0 & e^{-2(\alpha+\beta)} \end{bmatrix} \times \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} \\ 0 & 0 & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & 0 & 0 \end{bmatrix}$$

$$= \frac{1}{4} \begin{bmatrix} (1 + e^{-4t\beta} + 2e^{-2t(\alpha+\beta)}) & (1 + e^{-4t\beta} - 2e^{-2t(\alpha+\beta)}) & 1 - e^{-4t\beta} & 1 - e^{-4t\beta} \\ 1 - e^{-4t\beta} & 1 - 1e^{-4t\beta} & 1 - 1e^{-4t\beta} & 1 + e^{-4t\beta} + 2e^{-2t(\alpha+\beta)} & 1 + e^{-4t\beta} - 2e^{-2t(\alpha+\beta)} \\ 1 - e^{-4t\beta} & 1 - 1e^{-4t\beta} & 1 + e^{-4t\beta} - 2e^{-2t(\alpha+\beta)} & 1 + e^{-4t\beta} - 2e^{-2t(\alpha+\beta)} \\ 1 - e^{-4t\beta} & 1 - 1e^{-4t\beta} & 1 + e^{-4t\beta} - 2e^{-2t(\alpha+\beta)} & 1 + e^{-4t\beta} + 2e^{-2t(\alpha+\beta)} \end{bmatrix}$$

The above is exactly the same as Eq. 1.9 of CME2006.

• Exercise 6 The Monty Hall problem is a probability puzzle based on the US television game show Let's Make a Deal, originally hosted by Monty Hall. It is also called the Monty Hall paradox. Suppose you are given the choice of three doors: Behind one door is a car; behind the other two, goats. You pick a door, say No. 1, and the host, who knows what's behind the doors, opens another door, say No. 3, which has a goat. He then says to you, "Do you want to pick door No. 2?" Calculate the probability of winning if you do not switch and if you switch. Hint: Define A1: behind door 1 is a car; A2: behind door 1 is a goat. Define B: winning. Then apply the law of total probability (eq. 2.9) for each of the two options (switching and no switching).

Solution.

Define the following events

- o W_i : winning car is begind door i.
- o H_i : Host's choice is door i.

Apparently,

$$P(W_1) = P(W_2) = P(W_3) = \frac{1}{3}$$

Now calculate the following conditional probabilities. If you choose door 1, then that the host chooses door 2 or door 3 is equally likely, which means that $P(H_3|W_1) = \frac{1}{2}$. If you choose door 2, the host has to choose door 3, i.e., $P(H_3|W_2) = 1$. If you choose door 3, the host can choose any door but not door 3, which in other words, implies $P(H_3|W_3) = 0$. Hence, based the law of total probability, we have

$$P(H_3) = \sum_{i=1}^3 P(W_i) P(H_3 | W_i) = \frac{1}{3} \times (\frac{1}{2} + 1) = \frac{1}{2}.$$

According to Bayes' theorem, we have

$$P(W_1|H_3) = \frac{P(H_3|W_1)P(W_1)}{P(H_3)} = \frac{1}{2} \times \frac{1}{3} / (\frac{1}{2}) = \frac{1}{3},$$

$$P(W_2|H_3) = \frac{P(H_3|W_2)P(W_2)}{P(H_3)} = 1 \times \frac{1}{3}/(\frac{1}{2}) = \frac{2}{3}.$$

The above indicates that the chance of winning if you switch to door 2 is $\frac{2}{3}$ while if you decide to stick with door 1 it is $\frac{1}{3}$.

• Exercise 7 (inverse gamma distribution). Suppose $f(x) = \frac{\beta^{\alpha}}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x}$. Let $y = \frac{1}{x}$. Derive the density of y.

Solution.

$$f_Y(y) = \left| \frac{dx}{dy} \right| \times f_X\left(\frac{1}{y}\right)$$
$$= \frac{1}{y^2} \times \frac{\beta^{\alpha}}{\Gamma(\alpha)} y^{-(\alpha-1)} e^{-\frac{\beta}{y}}$$
$$= \frac{\beta^{\alpha}}{\Gamma(\alpha)} y^{-\alpha-1} e^{-\frac{\beta}{y}}.$$

• Exercise 8. Suppose $f(x) = \frac{1}{\mu} e^{-\frac{x}{\mu}}$, $0 < x < \infty$. Let $y = 1 - e^{-\frac{x}{\mu}}$. Show that y has the uniform distribution by deriving the density of y. [Hint. $F(x) = 1 - e^{-\frac{x}{\mu}}$ is the C.D.F. of x. First determine the range of y.]

Solution.

We can establish a more general proof that y = F(x) has a uniform distribution on [0,1] for any distribution where F(x) is the CDF of a distribution with PDF f(x).

$$f_Y(y) = \left| \frac{dx}{dy} \right| \times f_X(F^{-1}(y))$$
$$= \frac{1}{f_X(F^{-1}(y))} \times f_X(F^{-1}(y))$$
$$= 1.$$

Apparently, the range of Y is [0,1]. So we have

$$f_Y(y) = \begin{cases} 1, 0 \le y \le 1 \\ 0, \text{ otherwise.} \end{cases}$$

• Exercise 9. Calculate P^2 using equation (4.1)

$$P = \{p_{ij}\} = \begin{bmatrix} 0.7 & 0.2 & 0.1 \\ 0.1 & 0.8 & 0.1 \\ 0.3 & 0.3 & 0.4 \end{bmatrix}.$$

Solution.

$$\begin{split} P^2 &= \begin{bmatrix} 0.7 & 0.2 & 0.1 \\ 0.1 & 0.8 & 0.1 \\ 0.3 & 0.3 & 0.4 \end{bmatrix} \times \begin{bmatrix} 0.7 & 0.2 & 0.1 \\ 0.1 & 0.8 & 0.1 \\ 0.3 & 0.3 & 0.4 \end{bmatrix} \\ &= \begin{bmatrix} .7 \times .7 + .2 \times .1 + .1 \times .3 & .7 \times .2 + .2 \times .8 + .1 \times .3 & .7 \times .1 + .2 \times .1 + .1 \times .4 \\ .1 \times .7 + .8 \times .1 + .1 \times .3 & .1 \times .2 + .8 \times .8 + .1 \times .3 & .1 \times .1 + .8 \times .1 + .1 \times .4 \\ .3 \times .7 + .3 \times .1 + .4 \times .3 & .3 \times .2 + .3 \times .8 + .4 \times .3 & .3 \times .1 + .3 \times .1 + .4 \times .4 \end{bmatrix} \\ &= \begin{bmatrix} 0.54 & 0.33 & 0.13 \\ 0.18 & 0.69 & 0.13 \\ 0.36 & 0.42 & 0.22 \end{bmatrix}. \end{split}$$

• Exercise 10* (Jukes & Cantor model of DNA sequence evolution). The evolution of a nucleotide site in a DNA sequence is described by a Markov chain. The four states are the nucleotides T, C, A, G. In every generation the nucleotide changes to one of the three other nucleotides with probability λ. The transition matrix is thus

$$P = \begin{bmatrix} 1 - 3\lambda & \lambda & \lambda & \lambda & \lambda \\ \lambda & 1 - 3\lambda & \lambda & \lambda \\ \lambda & \lambda & 1 - 3\lambda & \lambda \\ \lambda & \lambda & \lambda & 1 - 3\lambda \end{bmatrix}.$$

The nucleotides are ordered T, C, A, and G. Calculate P^n . To be specific, consider the evolution of a site in a DNA sequence in the human-chimpanzee ancestor down to the modern human. Let $\lambda =$

 $\frac{1}{3} \times 10^{-8}$ per generation, with 500,000 generations from the common ancestor to the present (assuming 10 years in one generation).

Solution.

According to the problem statement, we first fine the eigen decomposition of P as follows

$$P = V\Lambda V^{-1}$$

$$= \begin{bmatrix} 1 & -1 & -1 & -1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 - 4\lambda & 0 & 0 \\ 0 & 0 & 1 - 4\lambda & 0 \\ 0 & 0 & 1 - 4\lambda & 0 \end{bmatrix} \times \frac{1}{4} \begin{bmatrix} 1 & 1 & 1 & 1 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 3 & -1 \end{bmatrix}.$$

Accordingly, we have

$$\begin{split} P^n &= \underbrace{V\Lambda V^{-1} \times V\Lambda V^{-1} \times ... \times V\Lambda V^{-1}}_{n} \\ &= V \times \underbrace{\Lambda \times ... \times \Lambda}_{n} \times V^{-1} \\ &= \begin{bmatrix} 1 & -1 & -1 & -1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & (1 - 4\lambda)^n & 0 & 0 & 0 \\ 0 & 0 & (1 - 4\lambda)^n & 0 & 1 \\ 0 & 0 & 0 & (1 - 4\lambda)^n \end{bmatrix} \times \frac{1}{4} \begin{bmatrix} 1 & 1 & 1 & 1 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 3 & -1 \\ -1 & -1 & -1 & 3 \end{bmatrix} \\ &= \begin{bmatrix} \frac{1}{4}(1 + 3(1 - 4\lambda)^n) & \frac{1}{4}(1 - (1 - 4\lambda)^n) & \frac{1}{4}(1 - (1 - 4\lambda)^n) & \frac{1}{4}(1 - (1 - 4\lambda)^n) \\ \frac{1}{4}(1 - (1 - 4\lambda)^n) & \frac{1}{4}(1 - (1 - 4\lambda)^n) & \frac{1}{4}(1 - (1 - 4\lambda)^n) & \frac{1}{4}(1 - (1 - 4\lambda)^n) \\ \frac{1}{4}(1 - (1 - 4\lambda)^n) & \frac{1}{4}(1 - (1 - 4\lambda)^n) & \frac{1}{4}(1 - (1 - 4\lambda)^n) & \frac{1}{4}(1 - (1 - 4\lambda)^n) \\ \frac{1}{4}(1 - (1 - 4\lambda)^n) & \frac{1}{4}(1 - (1 - 4\lambda)^n) & \frac{1}{4}(1 - (1 - 4\lambda)^n) & \frac{1}{4}(1 - (1 - 4\lambda)^n) \end{bmatrix} \end{split}$$

An associated Mathematica script ("Exercise 10.m") is available at the online repository.

Exercise 11: Calculate the stationary distribution of the Markov chain specified by equation (4.1). Use equation (4.11) to form two linear equations. Use them together with $\pi_1 + \pi_2 + \pi_3 = 1$ to solve the three unknowns π_1 , π_2 , π_3 . The stationary distribution gives us the proportions of sunny, cloudy and raining days.

Solution.

Eq. (4.11) is given in Exercise 9 as

$$P = \begin{bmatrix} 0.7 & 0.2 & 0.1 \\ 0.1 & 0.8 & 0.1 \\ 0.3 & 0.3 & 0.4 \end{bmatrix}.$$

Define $\pi = [\pi_1 \quad \pi_2 \quad \pi_3]$. According to $\pi P = \pi$, we have

$$\begin{cases} \pi_1 + \pi_2 + \pi_3 = 1 \\ 0.7\pi_1 + 0.1\pi_2 + 0.3\pi_3 = \pi_1 \\ 0.2\pi_1 + 0.8\pi_2 + 0.3\pi_3 = \pi_2 \\ 0.1\pi_1 + 0.1\pi_2 + 0.4\pi_3 = \pi_3 \end{cases}$$

By solving the system of equations, we obtain

$$\pi_1=0.3214, \pi_2=0.5357, \pi_3=0.1429.$$

An associated Mathematica script ("Exercise 11.m") is available at the online repository.