ISyE 6420 Spring 2025

## Homework 5

## Q1

The data in the file enzyme.csv gives the initial rate of reaction of an enzyme (y) and the substrate concentration (x). Consider the following nonlinear regression model:

$$y = \frac{\theta_1 x}{\theta_2 + x} + \epsilon$$

where  $\epsilon_i \stackrel{\text{iid}}{\sim} N\left(0, \sigma^2\right)$ ,  $\theta_1 > 0$ , and  $\theta_2 > 0$ . Assume noninformative priors for  $\theta_1$ ,  $\theta_2$ , and  $\sigma^2$ . You can choose appropriate prior distributions.

- (a) Plot the marginal posterior densities of  $\theta_1$ ,  $\theta_2$ , and  $\sigma^2$ . Use  $\theta_1 = 200$ ,  $\theta_2 = 0.1$ , and  $\sigma^2 = 100$  (equivalently,  $\tau = 0.01$ ) for initializing the MCMC chain.
- (b) Provide evidence that your model has converged, whether it is a trace plot, lack of divergences, the Gelman-Rubin statistic (Rhat), or something else.
- (c) Compute 95% credible intervals, the mean, and the standard deviation for each of the three parameters. (From now on, we will rarely specify which type of credible interval—you may use the default for your chosen software.)
- (d) Plot the posterior predictive distribution of y when x = 0.75 and provide the 95% credible intervals.

## $\mathbf{Q2}$

Walpole et al.  $(2007)^1$  provide data from a study on the effect of magnesium ammonium phosphate on the height of chrysanthemums, which was conducted at George Mason University in order to determine a possible optimum level of fertilization, based on the enhanced vertical growth response of the chrysanthemums. Forty chrysanthemum seedlings were assigned to 4 groups, each containing 10 plants. Each was planted in a similar pot containing a uniform growth medium. An increasing concentration of MgNH<sub>4</sub>PO<sub>4</sub>, measured in grams per bushel, was added to each plant. The 4 groups of plants were grown under uniform conditions in a greenhouse for a period of 4 weeks. The treatments and the respective changes in heights, measured in centimeters, are given in the following table:

<sup>&</sup>lt;sup>1</sup>Walpole, W. A., Myers, R. H., Myers, S. L., and Ye (2007). *Probability and Statistics for Engineers and Scientists* (9th ed.). Pearson.

Treatment			
$50~\mathrm{g/bu}$	$100 \mathrm{\ g/bu}$	$200~\mathrm{g/bu}$	400 g/bu
13.2	16.0	7.8	21.0
12.4	12.6	14.4	14.8
12.8	14.8	20.0	19.1
17.2	13.0	15.8	15.8
13.0	14.0	17.0	18.0
14.0	23.6	27.0	26.0
14.2	14.0	19.6	21.1
21.6	17.0	18.0	22.0
15.0	22.2	20.2	25.0
20.0	24.4	23.2	18.2

Solve the problem as a one-way ANOVA. Use STZ constraints on treatment effects.

- (a) Do different concentrations of MgNH<sub>4</sub>PO<sub>4</sub> affect the average attained height of chrysanthemums? Look at the 95% credible sets for the differences between treatment effects.
- (b) Find the 95% credible set for the contrast  $\mu_1 \mu_2 \mu_3 + \mu_4$ .
- (c) In a standard one-way ANOVA, we assume constant variance  $\sigma^2$  for each group. If you relax that assumption and put a prior on each group's standard deviation ( $\sigma_i$  for i = 1, ..., 4), do the results from (a) and (b) change? Do the contrasts between the posterior distributions of each  $\sigma_i$  show that they were significantly different?

## Q3

The data set (available as wolves.csv) described below provides skull morphometric measurements on wolves ( $Canis\ lupus\ L$ .) coming from two geographic locations: Rocky Mountain (0) and Arctic (1). The original source of the data is from Jolicoeur (1959)<sup>2</sup>, and many authors have subsequently used this data to illustrate various multivariate statistical procedures.

The goal of Jolicoeur's study was to determine how location and gender affect skull shape among wolf populations. There were 9 predictor variables measured (see Table 1).

 $<sup>^2</sup>$ Jolicoeur, P. (1959). Multivariate geographical variation in the wolf *Canis lupus L. Evolution*, **13**(3), 283–299. Data here are given in inches.

Table 1: Wolf skull morphometric data (in inches) from Jolicoeur (1959)<sup>3</sup>.

Variable	Description	
location	0 = Rocky Mountain, $1 = $ Arctic	
gender	0 = male, 1 = female	
$x_1$	Palatal length	
$x_2$	Postpalatal length	
$x_3$	Zygomatic width	
$x_4$	Palatal width (outside first upper molars)	
$x_5$	Palatal width (inside second upper molars)	
$x_6$	Width between postglenoid foramina	
$x_7$	Interorbital width	
$x_8$	Least width of the braincase	
$x_9$	Crown length of the first upper molar	

- (a) Try a frequentist logistic regression on the data (in Python, you can use the statsmodels package or sklearn). What are the results?
- (b) Set up a Bayesian logistic regression. Try at least three separate models, changing regression coefficient variance to increasingly informative values for each. What do you observe in the results? How do they differ from the frequentist model and from each other?
- (c) Re-sample the model with only three predictors: gender,  $x_3$ , and  $x_7$ . Give an estimate and credible interval of the probability that a female wolf with measures  $x_3 = 5.28$  and  $x_7 = 1.78$  comes from an Arctic habitat.