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IEMS 304: Statistical Learning for Data Analysis
April 7, 2025

Homework 2

This homework is to give a brief reminder of R, RStudio, and statistical topics covered in IEMS 303.

Note: The homework is scored out of 100 points. The problems add up to 90 points, while the remaining ten points will be graded according to a writing rubric, given at the end of the assignment.

R/RStudio installation If you have not installed R and RStudio, follow the installation instructions outlined in `https://posit.co/download/rstudio-desktop/`. You are strongly encouraged to use R Markdown to integrate text, code, images and mathematics or you can you use the latex code we provide.

Question 1. Linear Regression with Missing Data We consider the standard regression model

$$Y = \beta_0 + \beta_1 X + \epsilon, \quad \epsilon \sim N(0, \sigma^2), \tag{1}$$

with $X \in \mathbb{R}$. In this exercise, 10% of the generated Y values are randomly set to zero. That is, if we denote the observed response by $\tilde{Y}$, then

$$\tilde{Y} = \begin{cases} Y, & \text{with probability } 0.9, \\ 0, & \text{with probability } 0.1. \end{cases} \tag{2}$$

Exercise 1: Bias of the OLS Estimator. When we run OLS on the observed data $\tilde{Y}$, Can $E[\tilde{Y} \mid X]$ be written down as a linear function X? Prove that the bias in the estimators is then given by

$$\text{Bias}(\hat{\beta}_0) = \beta_0 - 0.9\beta_0 = \frac{\beta_0}{10}, \quad \text{Bias}(\hat{\beta}_1) = \beta_1 - 0.9\beta_1 = \frac{\beta_1}{10}.$$

This means both estimators are biased downward by 10% of the true parameter value.

Write down your answer in the `sol` environment.

Exercise 2: Log-Likelihood Formulation. To account for the zero-inflation, we use a likelihood that reflects the two different ways an observation can occur. For each observation i, show that the likelihood is given by:

$$L_i(\beta_0, \beta_1, \sigma) = \begin{cases} 0.1, & \text{if } y_i = 0, \\ 0.9 \cdot \dfrac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\dfrac{(y_i - \beta_0 - \beta_1 x_i)^2}{2\sigma^2}\right), & \text{if } y_i \neq 0. \end{cases}$$

What is the full log-likelihood for the dataset? What is the new objective function you written down for the problem? What is the algorithm looks like?

Question 2. Linear Regression with Censored Data Suppose the true (latent) model is linear:

$$Y^* = \beta_0 + \beta_1 X + \epsilon, \quad \epsilon \sim N(0, \sigma^2). \tag{3}$$

However, instead of observing Y^*, we observe

$$Y = \max\{Y^*, 0\}. \tag{4}$$

This is a censored (or Tobit) model where values below 0 are censored to 0.

Exercise 1: Bias of the OLS Estimator. Compute the Expectation. Even though the latent relationship is linear, show that the observed conditional expectation becomes

$$E[Y \mid X] = (\beta_0 + \beta_1 X)\, \Phi\left(\frac{\beta_0 + \beta_1 X}{\sigma}\right) + \sigma\, \varphi\left(\frac{\beta_0 + \beta_1 X}{\sigma}\right),$$

which is not linear in X. Here φ and Φ denote the standard normal PDF and CDF, respectively. Explain why if one naively applies OLS to Y without accounting for the censoring, the estimated coefficients will be biased.

Exercise 2: Log-Likelihood Formulation. The proper likelihood accounts for whether an observation is censored or not. For each observation i, define $\mu_i = \beta_0 + \beta_1 X_i$. Then the likelihood is given by

$$L_i(\beta_0, \beta_1, \sigma) = \begin{cases} \Phi\Big(\frac{-\mu_i}{\sigma}\Big), & \text{if } Y_i = 0, \\ \dfrac{1}{\sigma}\varphi\Big(\frac{Y_i - \mu_i}{\sigma}\Big), & \text{if } Y_i > 0. \end{cases}$$

What is the full log-likelihood $\ell(\beta_0, \beta_1, \sigma)$ and the new loss function you have?

Exercise 3: Newton Method. We aim to use Newton method to minimize the nagtive log-likelihood $\mathrm{NLL}(\beta_0, \beta_1, \sigma) = -\ell(\beta_0, \beta_1, \sigma)$., we need first to compute the hessian and gradient.

3 a) Gradient Derivation For non-censored observations ($Y_i > 0$), the log-likelihood is $\ell_i = -\log\sigma - \frac{1}{2}\log(2\pi) - \frac{(Y_i-\mu_i)^2}{2\sigma^2}$. (why?) Differentiating with respect to β_j (with $j = 0, 1$):

$$\frac{\partial \ell_i}{\partial \beta_j} = \frac{Y_i - \mu_i}{\sigma^2}\frac{\partial \mu_i}{\partial \beta_j}.$$

Since $\mu_i = \beta_0 + \beta_1 X_i$, $\quad \frac{\partial \mu_i}{\partial \beta_0} = 1$, $\quad \frac{\partial \mu_i}{\partial \beta_1} = X_i$, the contribution to the gradient of the NLL (remember we take the negative derivative) is

$$-\frac{\partial \ell_i}{\partial \beta_j} = -\frac{Y_i - \mu_i}{\sigma^2}\frac{\partial \mu_i}{\partial \beta_j}.$$

Similarly, for censored observations ($Y_i = 0$), the log-likelihood is $\ell_i = \log\Phi\Big(-\frac{\mu_i}{\sigma}\Big)$. (why?) Let $z_i = -\frac{\mu_i}{\sigma}$. Then,using the same steps as before show that $\frac{\partial \ell_i}{\partial \beta_j} = -\frac{1}{\sigma}\frac{\varphi(z_i)}{\Phi(z_i)}\frac{\partial \mu_i}{\partial \beta_j}$ **(provide your calculation to check my result)** and the overall gradient of the NLL is

$$\nabla \mathrm{NLL}(\beta_0, \beta_1) = -\sum_{i:Y_i>0} \frac{Y_i - \mu_i}{\sigma^2}\begin{pmatrix}1 \\ X_i\end{pmatrix} + \sum_{i:Y_i=0} \frac{1}{\sigma}\frac{\varphi(z_i)}{\Phi(z_i)}\begin{pmatrix}1 \\ X_i\end{pmatrix}.$$

3 b) Hessian Derivation for Non-censored observations ($Y_i > 0$) For non-censored observations ($Y_i > 0$), show that the hessian is

$$H_i^{\text{non-cens}} = \frac{1}{\sigma^2}\begin{pmatrix}1 \\ X_i\end{pmatrix}\begin{pmatrix}1 & X_i\end{pmatrix}.$$

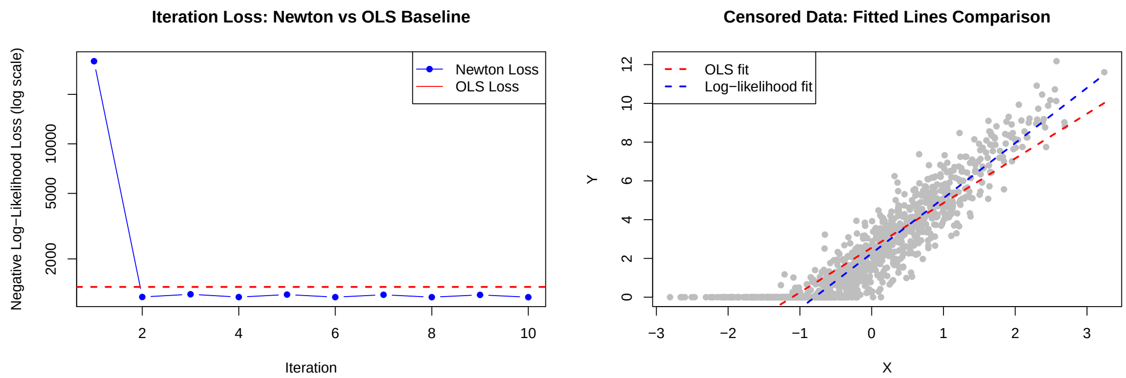
3 c) Hessian Derivation for Censored observations ($Y_i = 0$) For censored observations, we've showed the graident is $\frac{\partial \ell_i}{\partial \beta_j} = -\frac{1}{\sigma}\frac{\varphi(z_i)}{\Phi(z_i)}\frac{\partial \mu_i}{\partial \beta_j}$. Show that the Hessian contribution is

$$H_i^{\text{cens}} = \frac{1}{\sigma^2}\begin{pmatrix}1 \\ X_i\end{pmatrix}\begin{pmatrix}1 & X_i\end{pmatrix}\frac{\varphi(z_i)}{\Phi(z_i)^2}\Big(z_i\Phi(z_i) + \varphi(z_i)\Big)$$

based on the following Fact.

<u>**Fact.**</u> If we define $r(z_i) = \frac{\varphi(z_i)}{\Phi(z_i)}$. Then its derivative is $r'(z_i) = -\frac{\varphi(z_i)}{\Phi(z_i)^2}\Big(z_i\Phi(z_i) + \varphi(z_i)\Big)$.

3 d) Complete the Newton Method's Code. Complete the following code using Newton method for NLL to do linear regression with censored data. If you successfully compelete the code, you are able to generate the following figures. Write down your findings. (You can try different choices of n or other hyperparameter in the code to see what you find.)




```
# -----------------------------
# Data Generation
# -----------------------------
set.seed(123)
n <- 1000
beta0_true <- 2; beta1_true <- 3; sigma <- 1
X <- rnorm(n)
epsilon <- rnorm(n, 0, sigma)
Y_star <- beta0_true + beta1_true * X + epsilon
# Censor at 0
Y <- pmax(Y_star, 0)

# -----------------------------
# Negative Log-Likelihood Function (NLL)
# -----------------------------
nll <- function(params, X, Y, sigma) {
  beta0 <- params[1]
  beta1 <- params[2]
  mu <- beta0 + beta1 * X
  # For censored observations: Y == 0
  cens <- (Y == 0)
  ll_cens <- sum( log(pnorm(-mu[cens] / sigma)) )
  # For non-censored observations: Y > 0
  noncens <- (Y > 0)
  ll_noncens <- sum( -log(sigma) - 0.5 * log(2*pi) - ((Y[noncens] - mu[
   noncens])^2) / (2*sigma^2) )
  return( - (ll_cens + ll_noncens) )
}

# -----------------------------
# Gradient of NLL
# -----------------------------
grad_nll <- function(params, X, Y, sigma) {
  beta0 <- params[1]
  beta1 <- params[2]
  mu <- beta0 + beta1 * X

  noncens <- (Y > 0)
  cens <- (Y == 0)
```

```r

  # For non-censored observations:
  grad_non_cens_0 <- - sum((Y[noncens] - mu[noncens]) / sigma^2)
  grad_non_cens_1 <- - sum((Y[noncens] - mu[noncens]) * X[noncens] / sigma^2)

  # For censored observations:
  z <- -mu[cens] / sigma
  Phi_z <- pnorm(z) + 1e-10  # avoid division by zero
  factor <- dnorm(z) / (sigma * Phi_z)
  grad_cens_0 <- sum(factor)
  grad_cens_1 <- sum(factor * X[cens])

  grad0 <- grad_non_cens_0 + grad_cens_0
  grad1 <- grad_non_cens_1 + grad_cens_1

  return(c(grad0, grad1))
}

# ---------------------------
# Hessian of NLL
# ---------------------------
hessian_nll <- function(params, X, Y, sigma) {
  beta0 <- params[1]
  beta1 <- params[2]
  mu <- beta0 + beta1 * X

  H11 <- 0; H12 <- 0; H22 <- 0

  # Non-censored part:
  noncens <- (Y > 0)
  H11 <- H11 + sum( rep(1, sum(noncens)) / sigma^2 )
  H12 <- H12 + sum( X[noncens] / sigma^2 )
  H22 <- H22 + sum( (X[noncens]^2) / sigma^2 )

  # Censored part:
  cens <- (Y == 0)
  if(sum(cens) > 0){
  # ---------
  # !!!!!!!
  # PUT Your Code here
  # !!!!!!!
  # ---------
  # derivative of r(z)=phi(z)/Phi(z)
    rprime <- - (phi_z / (Phi_z^2)) * ( z * Phi_z + phi_z )

  }

  H <- matrix(c(H11, H12, H12, H22), nrow = 2)
  return(H)
}
```

```

# ---------------------------
# Newton's Method with Loss History
# ---------------------------
params_newton <- c(0, 0)   # initial guess for (beta0, beta1)
num_iter_newton <- 10
loss_history_newton <- numeric(num_iter_newton)

for(i in 1:num_iter_newton) {
  grad <- grad_nll(params_newton, X, Y, sigma)
  H <- hessian_nll(params_newton, X, Y, sigma)
  # ---------
  # !!!!!!!
  # PUT Your Code here
  # !!!!!!!
  # The code would look like params_newton <- ?
  # ---------

  loss_history_newton[i] <- nll(params_newton, X, Y, sigma)
}
newton_est <- params_newton
cat("Newton's Method Estimates (Beta0, Beta1):\n")
print(newton_est)


# ---------------------------
# OLS Estimation (ignoring censoring) as Baseline
# ---------------------------
ols_model <- lm(Y ~ X)
ols_est <- coef(ols_model)
cat("OLS Estimates (Beta0, Beta1):\n")
print(ols_est)
loss_ols <- nll(ols_est, X, Y, sigma)
cat("Negative Log-Likelihood Loss (OLS):\n")
print(loss_ols)

# ---------------------------
# Plot: Newton Iteration Loss vs OLS Baseline
# ---------------------------
# Combined Loss Plot with Log-Scale on Y-Axis: Newton, Gradient Descent
    , and OLS Baseline
plot(1:num_iter_newton, loss_history_newton, type='b', pch=16, col='
    blue', log="y",
     xlab='Iteration', ylab='Negative Log-Likelihood Loss (log scale)',
     main='Iteration Loss: Newton vs OLS Baseline')
abline(h=loss_ols, col='red', lwd=2, lty=2)
legend("topright", legend=c("Newton Loss", "OLS Loss"),
       col=c("blue", "red"), lty=c(1,1,2), pch=c(16, NA, NA))

# ---------------------------
# Plot: Fitted Lines Comparison
```

```r
# ----------------------------
plot(X, Y, pch=16, col='grey',
     main='Censored Data: Fitted Lines Comparison',
     xlab='X', ylab='Y')
curve(ols_est[1] + ols_est[2]*x, add=TRUE, col='red', lwd=2, lty=2)
curve(newton_est[1] + newton_est[2]*x, add=TRUE, col='blue', lwd=2, lty=2)
legend("topleft", legend=c("OLS fit", "Log-likelihood fit"),
       col=c("red","blue","purple"), lty=2, lwd=2)
```

Listing 1. R code: Data generation, Newton's method, and plotting

Question 3. Bias and Variance Trade-off for Newton Method In this question, we use logistic regression as an exmaple. We assume a logistic regression model with one predictor:

$$p_i = \sigma(z_i) = \frac{1}{1 + e^{-z_i}}, \quad \text{with } z_i = \beta_0 + \beta_1 x_i,$$

where p_i is the probability that $y_i = 1$ given x_i. The log-likelihood for n independent observations is

$$\ell(\beta_0, \beta_1) = \sum_{i=1}^{n} \Big[y_i \log p_i + (1 - y_i) \log(1 - p_i) \Big].$$

Exercise 1: Compute the Gradient and Hessian. To derive the gradient, differentiate the log-likelihood with respect to β_j (with $j = 0, 1$). First note that:

$$\frac{\partial p_i}{\partial z_i} = p_i(1 - p_i), \quad \text{and} \quad \frac{\partial z_i}{\partial \beta_j} = \begin{cases} 1, & j = 0, \\ x_i, & j = 1. \end{cases}$$

Thus, using the chain rule, $\frac{\partial p_i}{\partial \beta_j} = p_i(1 - p_i)\, x_{ij}$, where we define $x_{i0} = 1$ and $x_{i1} = x_i$.

Differentiating the log-likelihood yields $\frac{\partial \ell}{\partial \beta_j} = \sum_{i=1}^{n} \left[\frac{y_i}{p_i} - \frac{1 - y_i}{1 - p_i} \right] \frac{\partial p_i}{\partial \beta_j}$. Substituting the derivative of p_i and simplifying gives

$$\frac{\partial \ell}{\partial \beta_j} = \sum_{i=1}^{n} [y_i - p_i]\, x_{ij}.$$

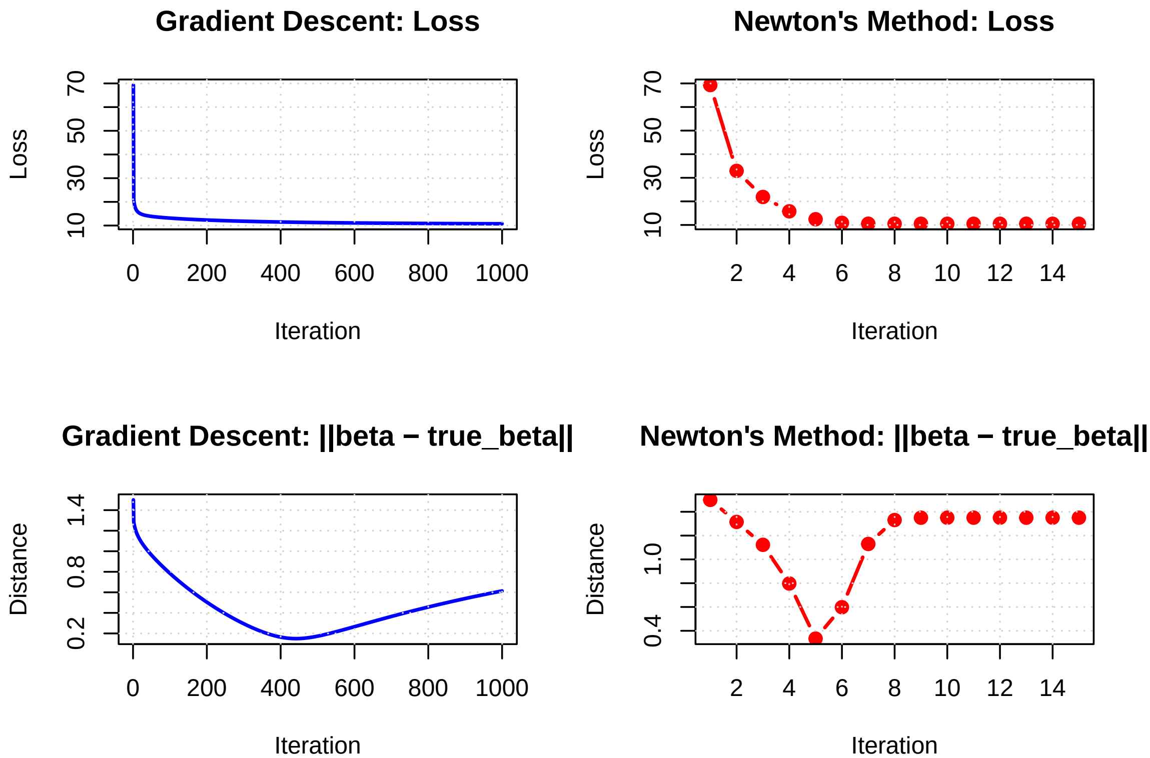
Now you will do the computation for the Hessian, we differentiate the gradient with respect to β_k: $\frac{\partial^2 \ell}{\partial \beta_j \partial \beta_k} = \sum_{i=1}^{n} \frac{\partial}{\partial \beta_k} \{(y_i - p_i) x_{ij}\}$. Show that if X is the $n \times 2$ design matrix with rows $x_i = (1, x_i)$ and $p = (p_1, \ldots, p_n)^\top$, then

- the gradient is $\nabla \ell(\beta) = X^\top (y - p)$,
- the hessian is $H(\beta) = -X^\top W X$, where W is an $n \times n$ diagonal matrix with $W_{ii} = p_i(1 - p_i)$.

More generally, if X is the $n \times 2$ design matrix with rows $x_i = (1, x_i)$ and $p = (p_1, \ldots, p_n)^\top$, and

Hint: Since y_i does not depend on β_k, only p_i does. Thus using the chain rule, we know that $\frac{\partial^2 \ell}{\partial \beta_j \partial \beta_k} = -\sum_{i=1}^{n} \frac{\partial p_i}{\partial \beta_k} x_{ij}$. Then using the earlier derivative, of $\frac{\partial p_i}{\partial \beta_k}$.

Exercise 2: Complete the code. Using the previous computation of gradient and hessian to complete the Newton Method and gradient descent code for solving logisitic regression. If you successfully compelete the code, you are able to generate the following figures. Write down your findings.




```r
# Set seed for reproducibility
set.seed(123)

# ----------------------------
# 1. Create a toy dataset
# ----------------------------
n <- 100                          # number of observations
x1 <- rnorm(n)*10
x2 <- rnorm(n)
X <- cbind(1, x1, x2)              # include intercept

# True coefficients for our logistic model
true_beta <- c(0.5, 1, -1)

# Logistic function
logistic <- function(z) 1 / (1 + exp(-z))

# Compute the probabilities using the logistic function
p <- logistic(X %*% true_beta)

# Generate binary response variable from a Bernoulli distribution
y <- rbinom(n, size = 1, prob = p)

# ----------------------------
# 2. Define the negative log-likelihood and its derivatives
# ----------------------------
nll <- function(beta, X, y) {
  p <- logistic(X %*% beta)
```

```
  # Negative log-likelihood (adding a small constant to avoid log(0))
  -sum(y * log(p + 1e-8) + (1 - y) * log(1 - p + 1e-8))
}

# Gradient of the negative log-likelihood
grad_nll <- function(beta, X, y) {
  # ---------
  # !!!!!!!
  # PUT Your Code here
  # !!!!!!!
  # ---------
}

# Hessian of the negative log-likelihood
hess_nll <- function(beta, X, y) {
  # ---------
  # !!!!!!!
  # PUT Your Code here
  # !!!!!!!
  # ---------
}

# ---------------------------
# 3. Solve using Gradient Descent
# ---------------------------
beta_gd <- rep(0, ncol(X))       # Initialize coefficients
lr <- 0.001                     # Learning rate
num_iter <- 1000                # Number of iterations


loss_gd <- numeric(num_iter)    # Store loss values
dist_gd <- numeric(num_iter)    # Store Euclidean distance to true_beta

for (i in 1:num_iter) {
  loss_gd[i] <- nll(beta_gd, X, y)
  dist_gd[i] <- sqrt(sum((beta_gd - true_beta)^2))
  # ---------
  # !!!!!!!
  # PUT Your Code here
  # !!!!!!!
  # The code would look like beta_gd <- ?
  # ---------
}

# ---------------------------
# 4. Solve using Newton's Method
# ---------------------------
beta_newton <- rep(0, ncol(X))       # Initialize coefficients
num_iter_newton <- 15                # Newton's method converges quickly

```

```r
loss_newton <- numeric(num_iter_newton)
dist_newton <- numeric(num_iter_newton)

for (i in 1:num_iter_newton) {
  loss_newton[i] <- nll(beta_newton, X, y)
  dist_newton[i] <- sqrt(sum((beta_newton - true_beta)^2))
  grad <- grad_nll(beta_newton, X, y)
  H <- hess_nll(beta_newton, X, y)
  # ---------
  # !!!!!!!
  # PUT Your Code here
  # !!!!!!!
  # The code would look like beta_newton <- ?
  # ---------
}

# ---------------------------
# 5. Plot the Loss and Distance Curves
# ---------------------------
# Set up a 2x2 plotting area
par(mfrow = c(2, 2))

# Gradient Descent Loss
plot(loss_gd, type = "l", col = "blue", lwd = 2,
     main = "Gradient Descent: Loss", xlab = "Iteration", ylab = "Loss")
grid()

# Newton's Method Loss
plot(loss_newton, type = "b", col = "red", lwd = 2, pch = 19,
     main = "Newton's Method: Loss", xlab = "Iteration", ylab = "Loss")
grid()

# Gradient Descent Distance
plot(dist_gd, type = "l", col = "blue", lwd = 2,
     main = "Gradient Descent: ||beta - true_beta||", xlab = "Iteration", ylab = "Distance")
grid()

# Newton's Method Distance
plot(dist_newton, type = "b", col = "red", lwd = 2, pch = 19,
     main = "Newton's Method: ||beta - true_beta||", xlab = "Iteration", ylab = "Distance")
grid()
```

Listing 2. R code: Data generation, Newton's method, and plotting

Rubric (10)

- The text is laid out cleanly, with clear divisions between problems and sub-problems. The writing itself is well-organized, free of grammatical and other mechanical errors, and easy to follow.
- Questions which ask for a plot or table are answered with both the figure itself and the command (or commands) use to make the plot. Plots are carefully labeled, with informative and legible titles, axis labels.
- All quantitative and mathematical claims are supported by appropriate derivations, included in the text, or calculations in code. Numerical results are reported to appropriate precision.
- Code is either properly integrated with a tool like R Markdown or included as a separate R file. In the former case, both the knitted and the source file are included. In the latter case, the code is clearly divided into sections referring to particular problems. In either case, the code is indented, commented, and uses meaningful names.
- All parts of all problems are answered with actual coherent sentences, and never with raw computer code or its output. For full credit, all code runs, and the Markdown file knits (if applicable).