MATH 680: Assignment 1

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Question 1

From our definitions of $\tilde{X}$ and $\tilde{Y}$

$$\begin{aligned}\tilde{X} &= X_{-1} - \mathbf{1}_n \bar{x}^T \\ \tilde{Y} &= Y - \mathbf{1}_n^T \bar{Y},\end{aligned}$$

we may decompose $\|\tilde{Y} - \tilde{X}\beta\|_2^2$ as

$$\begin{aligned}\hat{\beta}_{-1} &= \underset{\beta \in \mathbb{R}^{p-1}}{\arg\min}\ \|\tilde{Y} - \tilde{X}\beta\|_2^2 \\ &= \underset{\beta \in \mathbb{R}^{p-1}}{\arg\min}\ \|Y - \mathbf{1}_n \bar{Y} - \left(X_{-1} - \mathbf{1}_n \bar{x}^T\right)\beta_{-1}\|_2^2 \\ &= \underset{\beta \in \mathbb{R}^{p-1}}{\arg\min}\ \|Y - X_{-1}\beta_{-1} - \mathbf{1}_n\left(\bar{Y} - \bar{x}^T \beta_{-1}\right)\|_2^2 \\ &= \underset{\beta \in \mathbb{R}^{p-1}}{\arg\min}\ \|Y - X_{-1}\beta_{-1} - \mathbf{1}_n \beta_1\|_2^2 \quad \text{(by definition of } \beta_1 \text{ above)} \\ &= \underset{\beta \in \mathbb{R}^{p-1}}{\arg\min}\ \|Y - [\mathbf{1}_n,\, X_{-1}]\ [\beta_1,\, \beta_{-1}]\|_2^2 \\ &\equiv \underset{\beta \in \mathbb{R}^{p-1}}{\arg\min}\ \|Y - X\beta\|_2^2.\end{aligned}$$

Therefore, if $\hat{\beta} = \left(\hat{\beta}_1,\, \hat{\beta}_{-1}^T\right)^T \in \mathbb{R}^p$ and

$$\hat{\beta}_1 = \bar{Y} - \bar{x}^T \hat{\beta}_{-1},$$

then $\hat{\beta}$ must also solve the uncentered problem

$$\hat{\beta} = \left(\hat{\beta}_1,\, \hat{\beta}_{-1}^T\right)^T = \underset{\beta \in \mathbb{R}^p}{\arg\min}\ \|Y - X\beta\|_2^2,$$

as desired.

Question 2

(a)

Define our objective function $f : \mathbb{R}^p \to \mathbb{R}$ by

$$
\begin{aligned}
f(\beta) &= \|\tilde{Y} - \tilde{X}\beta\|_2^2 + \lambda\|\beta\|_2^2 \\
&= \left(\tilde{Y} - \tilde{X}\beta\right)^T \left(\tilde{Y} - \tilde{X}\beta\right)^T + \lambda\beta^T\beta \\
&= \tilde{Y}^T\tilde{Y} - \tilde{Y}^T\tilde{X}\beta - \beta^T\tilde{X}^T\tilde{Y} + \beta^T\tilde{X}^T\tilde{X}\beta + \lambda\beta^T\beta \\
&= \tilde{Y}^T\tilde{Y} - 2\beta^T\tilde{X}^T\tilde{Y} + \beta^T\tilde{X}^T\tilde{X}\beta + \lambda\beta^T\beta.
\end{aligned}
$$

Therefore,

$$\nabla f(\beta) = -2\tilde{X}^T\tilde{Y} + 2\tilde{X}^T\tilde{X}\beta + 2\lambda\beta,$$

as desired.

(b)

The Hessian $\nabla^2 f(\beta)$ is given by the $(p-1)\times(p-1)$ matrix

$$\nabla^2 f(\beta) = 2\tilde{X}^T\tilde{X} + 2\lambda\mathbb{I}_{p-1},$$

where $\mathbb{I}_{p-1}$ is the $(p-1)\times(p-1)$ identity matrix. Note that $2\tilde{X}^T\tilde{X} \in \mathbb{S}_+^{p-1}$ (positive semi-definite) and, for $\lambda > 0$, we have $2\lambda\mathbb{I}_{p-1} \in \mathbb{S}_{++}^{p-1}$ (positive definite).[1] Therefore, for all nonzero vectors $v \in \mathbb{R}^{p-1}$,

$$
\begin{aligned}
v^T\left(\nabla^2 f(\beta)\right)v &= v^T\left(2\tilde{X}^T\tilde{X} + 2\lambda\mathbb{I}_{p-1}\right)v \\
&= 2v^T\tilde{X}^T\tilde{X}v + 2\lambda v^T\mathbb{I}_{p-1}v \\
&= 2\left(\underbrace{\|\tilde{X}v\|_2^2}_{\geq 0} + \underbrace{\lambda\|v\|_2^2}_{>0 \text{ when } \lambda>0}\right) \\
&> 0.
\end{aligned}
$$

Hence,

$$\nabla^2 f(\beta) = 2\tilde{X}^T\tilde{X} + 2\lambda\mathbb{I}_{p-1} \in \mathbb{S}_{++}^{p-1},$$

and so, since the Hessian of f is positive definite, f must be strictly convex in β, as desired.

(c)

Suppose a strictly convex function f is globally minimized at distinct points x and y, $x \neq y$. By definition of strict convexity

$$\forall\, t \in (0,1) \quad f(tx + (1-t)y) < tf(x) + (1-t)f(y).$$

Then, since f is minimized at both x and y, we have $f(x) = f(y)$. Hence,

[1] Proof in an appendix.

$$f(tx + (1-t)y) < tf(x) + (1-t)f(x) = f(x).$$

However, this implies that the point $z = tx+(1-t)y$ admits a value of f even *smaller* than $f(x)$, contradicting our assumption that x is a global minimizer. Therefore, we may conclude that strict convexity implies a unique global minimizer. That is, for $\lambda > 0$, we are guaranteed that the above solution will be the unique solution to our penalized least squares problem.

(d)

To write our desired function we first solve $\nabla f(\beta) = 0$ for β, i.e.,

$$\hat{\beta}_{-1}^{(\lambda)} = \left(\tilde{X}^T\tilde{X} + \lambda\mathbb{I}_{p-1}\right)^{-1}\tilde{X}^T\tilde{Y}.$$

For the purpose of computational efficiency we make use of the singular value decomposition of $\tilde{X}$

$$\tilde{X} = UDV^T,$$

for $U \in \mathbb{R}^{n\times n}$ and $V \in \mathbb{R}^{(p-1)\times(p-1)}$ both orthogonal matrices, $U^TU = \mathbb{I}_n$, $V^TV = \mathbb{I}_{p-1}$, and $D \in \mathbb{R}^{n\times(p-1)}$ a diagonal matrix with entries $\{d_j\}_{j=1}^{\min(n,\,p-1)}$ along the main diagonal and zero elsewhere. Therefore,

$$\begin{aligned}\hat{\beta}_{-1}^{(\lambda)} &= \left(\tilde{X}^T\tilde{X} + \lambda\mathbb{I}_{p-1}\right)^{-1}\tilde{X}^T\tilde{Y} \\ &= \left(\left(UDV^T\right)^T UDV^T + \lambda VV^T\right)^{-1}\left(UDV^T\right)^T \\ &= V\left(D^TD + \lambda\mathbb{I}_{p-1}\right)^{-1}D^TU^T\tilde{Y}.\end{aligned}$$

Note that $\left(D^TD + \lambda\mathbb{I}_{p-1}\right)^{-1}D^T$ is diagonal with entries $\frac{d_j}{d_j^2+\lambda}$, $j = 1, ..., p-1$. We exploit this to avoid performing explicit matrix inversions in the function below.

```r
ridge_coef <- function(X, y, lam) {
  # Commented-out scaling parameters represent the transformations
  # used to make the output identical to that of
  # coef(MASS::lm.ridge(y ~ X[,-1], lambda = lam))
  # (left for personal notes)
  Xm1 <- X[,-1]; xbar <- colMeans(Xm1); ybar <- mean(y)

  # center response and each predictor according to their means
  ytilde <- y - ybar
  Xtilde <- (Xm1 - tcrossprod(rep(1, nrow(Xm1)), xbar)) #* sqrt(n/(n - 1))

  # # standardize Xtilde
  # xsds <- apply(Xm1, 2, sd)
  # Xtilde <- sweep(Xtilde, 2, STATS = xsds, FUN = "/")

  # compute the SVD on the centered design matrix
  Xtilde_svd <- svd(Xtilde)
  U <- Xtilde_svd$u; d <- Xtilde_svd$d; V <- Xtilde_svd$v

  # compute the inverse (D^T D + lambda I_{p-1})^{-1} D^T
  Dstar <- diag(d/(d^2 + lam))
  # compute ridge coefficients
  b <- V %*% (Dstar %*% crossprod(U, ytilde)) #* 1/xsds * sqrt(n/(n - 1))
  b1 <- ybar - crossprod(xbar, b)
  list(b1 = b1, b = b)
}
```

(e)

We first take the expectation of $\hat{\beta}_{-1}^{(\lambda)}$

$$\begin{aligned}\mathbb{E}\left[\hat{\beta}_{-1}^{(\lambda)}\right] &= \mathbb{E}\left[\left(\tilde{X}^T\tilde{X} + \lambda\mathbb{I}_{p-1}\right)^{-1}\tilde{X}^T\tilde{Y}\right] \\ &= \left(\tilde{X}^T\tilde{X} + \lambda\mathbb{I}_{p-1}\right)^{-1}\tilde{X}^T\mathbb{E}\left[\tilde{Y}\right] \\ &= \left(\tilde{X}^T\tilde{X} + \lambda\mathbb{I}_{p-1}\right)^{-1}\tilde{X}^T\tilde{X}\beta_{-1}.\end{aligned}$$

We may produce a more elegant expression by once again using the SVD of $\tilde{X}$

$$\begin{aligned}\mathbb{E}\left[\hat{\beta}_{-1}^{(\lambda)}\right] &= \left(\tilde{X}^T\tilde{X} + \lambda\mathbb{I}_{p-1}\right)^{-1}\tilde{X}^T\tilde{X}\beta_{-1} \\ &= V\left(D^TD + \lambda\mathbb{I}_{p-1}\right)^{-1}D^TDV^T\beta_{-1} \\ &= VD^*V^T\beta_{-1},\end{aligned}$$

where D^* is a diagonal matrix with entries $\left\{\frac{d_j^2}{d_j^2+\lambda}\right\}_{j=1}^{\min(n,p-1)}$ along the main diagonal and zero elsewhere. We next take the he variance of our centered ridge estimates,

$$\begin{aligned}\text{Var}\left(\hat{\beta}_{-1}^{(\lambda)}\right) &= \text{Var}\left(\left(\tilde{X}^T\tilde{X} + \lambda\mathbb{I}_{p-1}\right)^{-1}\tilde{X}^T\tilde{Y}\right) \\ &= \left(\tilde{X}^T\tilde{X} + \lambda\mathbb{I}_{p-1}\right)^{-1}\tilde{X}^T\text{Var}\left(\tilde{Y}\right)\left(\left(\tilde{X}^T\tilde{X} + \lambda\mathbb{I}_{p-1}\right)^{-1}\tilde{X}^T\right)^T \\ &= \left(\tilde{X}^T\tilde{X} + \lambda\mathbb{I}_{p-1}\right)^{-1}\tilde{X}^T\text{Var}\left(\tilde{Y}\right)\tilde{X}\left(\tilde{X}^T\tilde{X} + \lambda\mathbb{I}_{p-1}\right)^{-1} \\ &= \sigma_*^2\left(\tilde{X}^T\tilde{X} + \lambda\mathbb{I}_{p-1}\right)^{-1}\tilde{X}^T\tilde{X}\left(\tilde{X}^T\tilde{X} + \lambda\mathbb{I}_{p-1}\right)^{-1}\end{aligned}$$

Again applying the SVD of $\tilde{X}$, we find a more concise expression

$$\text{Var}\left(\hat{\beta}_{-1}^{(\lambda)}\right) = VD^{**}V^T,$$

where D^{**} is a diagonal matrix with entries $\left\{\frac{d_j^2}{\left(d_j^2+\lambda\right)^2}\right\}_{j=1}^{\min(n,p-1)}$ along the main diagonal and zero elsewhere. We now perform a simulation study to compare some sample estimates of the mean and variance with their theoretical values $\mathbb{E}\left[\hat{\beta}_{-1}^{(\lambda)}\right]$ and $\text{Var}\left(\hat{\beta}_{-1}^{(\lambda)}\right)$. We first define functions computing these quantities according to the above expressions,

```r
ridge_coef_true <- function(X, lam, beta, sigma) {
  # Computes the expectation and variance of ridge coefficients
  # given design matrix X, penalty lam, OLS estimates beta,
  # and OLS error standard deviation sigma
  n <- nrow(X); p <- ncol(X)
  betam1 <- beta[-1]; Xm1 <- X[,-1]; xbar <- colMeans(Xm1)

  # center each predictor according to its mean
  Xtilde <- Xm1 - tcrossprod(rep(1, nrow(Xm1)), xbar)

  # compute theoretical expectation and variance/covariance matrix
  inv <- solve(crossprod(Xtilde) + lam * diag(p - 1))
  b <- inv %*% (crossprod(Xtilde) %*% betam1) # expectation
  vcv <- sigma^2 * inv %*% crossprod(Xtilde) %*% inv # variance
  list(b = b, vcv = vcv)
}
```

We may now perform our simulation,

```r
set.seed(124)

# set parameters
nsims <- 1e3
n <- 100
p <- 5
lam <- 4
beta_star <- (-1)^(1:p) * (1:p)
sigma_star <- 1

# generate fixed design matrix
X <- cbind(1, matrix(rnorm(n * (p - 1)), nrow = n))

# compute theoretical mean and variance
true_vals <- ridge_coef_true(X, lam, beta_star, sigma_star)
b_true <- as.vector(true_vals$b) # extract expectation
vcv_true <- true_vals$vcv # extract variance

# simulate ridge coefficients nsims times
# outputs a matrix with row indices corresponding
# to coefficient indices and column indices
# corresponding to simulation number
pt <- proc.time()
b_hat <- replicate(nsims, {
  # generate responses
  y <- X %*% beta_star + rnorm(n, 0, sigma_star)
  # extract, vectorize, and return coefficients, excluding intercept
  as.vector(ridge_coef(X, y, lam)$b)
})
proc.time() - pt
```

```
##    user  system elapsed
##   0.146   0.005   0.153
```

```r
# estimate variance of b1, ..., b_p estimates
vcv_hat <- var(t(b_hat))
```

```r
# print estimated values vs. expected values
b <- rbind(rowMeans(b_hat), b_true, abs(rowMeans(b_hat) - b_true))
rownames(b) <- c("b_hat", "b_true", "abs_err")
round(b, 5)
```

```
##             [,1]     [,2]    [,3]     [,4]
## b_hat   1.84403 -2.92658 3.82497 -4.79001
## b_true  1.85015 -2.92702 3.82712 -4.79042
## abs_err 0.00612  0.00044 0.00215  0.00042
```

```r
# print absolute error between estimated and true variances
round(abs(vcv_true - vcv_hat), 5)
```

```
##         [,1]    [,2]    [,3]    [,4]
## [1,] 0.00006 0.00069 0.00012 0.00021
## [2,] 0.00069 0.00027 0.00045 0.00049
## [3,] 0.00012 0.00045 0.00015 0.00009
## [4,] 0.00021 0.00049 0.00009 0.00072
```

Based on our simulation we find that the empirical sample estimates are very close to their theoretical values, as expected.

Question 3

Note that for the purpose of improved performance we *do not* call our `ridge_coef()` function as was defined above. Calling this implementation would compute the SVD for each value of λ. All else constant, this is unnecessary since the SVD of $\tilde{X}$ is independent of λ. Instead, we perform the SVD prior to separating the vector of λ's, and compute the ridge estimate using the SVD outputs as a (constant) argument across all λ's.

```r
ridge_cv <- function(X, y, lam.vec, K) {
  # Perform K-fold cross-validation on the ridge regression
  # estimation problem over tuning parameters given in lam.vec.
  n <- nrow(X); p <- ncol(X); L <- length(lam.vec)

  # evenly assign a group from 1,..,K to each row index 1,...,n
  folds <- cut(1:n, breaks = K, labels = F)
  # even though our data will be randomly generated, for later
  # portability, shuffle the cross-validation groups randomly
  folds <- sample(folds)

  # get indices of training subset
  train_idxs <- lapply(1:K, function(i) !(folds %in% i))

  # CV errors
  # row index = lambda index
  # col index = fold index
  cv_errs_lams_folds <- matrix(NA, nrow = L, ncol = K)
  cv_errs_lams_folds <- sapply(train_idxs, function(trn_idx) {
    tst_idx <- !trn_idx # find test subset indices

    # extract training data, remove intercept column
    Xm1_trn <- X[trn_idx, -1]; y_trn <- y[trn_idx];
    ybar_trn <- .Internal(mean(y_trn))
    xbar_trn <- colMeans(Xm1_trn); ytilde_trn <- y_trn - ybar_trn

    # center each predictor according to its mean
    Xtilde_trn <- Xm1_trn - tcrossprod(rep(1, nrow(Xm1_trn)), xbar_trn)

    # compute the SVD on the centered design matrix
    # Note: This is done before computing our coefficients for each
    # lambda since the SVD will be identical across the vector of
    # tuning parameters
    Xtilde_trn_svd <- svd(Xtilde_trn)
    U <- Xtilde_trn_svd$u; d <- Xtilde_trn_svd$d; V <- Xtilde_trn_svd$v
    d2 <- d^2

    # CV errors for each value of lambda
    cv_errs_lams <- vector(mode = 'numeric', length = L)
    cv_errs_lams <- sapply(lam.vec, function(lam) {
      # compute the inverse (D^T D + lambda I_{p-1})^{-1} D^T
      Dstar <- diag(d/(d2 + lam))
      # compute ridge coefficients
      b_trn <- V %*% (Dstar %*% crossprod(U, ytilde_trn))
      b1_trn <- ybar_trn - crossprod(xbar_trn, b_trn)

      # fit test data
      yhat_tst <- X[tst_idx,] %*% c(b1_trn, b_trn)
      # compute test error
      sum((y[tst_idx] - yhat_tst)^2)
    })
    cv_errs_lams
  })

  # weighted average according to group size of
  # cross validation error for each value of lambda
  # (some groups may contain +/- 1 member
  # depending on whether or not K divides n evenly)
  cv.error <- apply(cv_errs_lams_folds, 1,
                    function(cv_errs_folds) {
                      sum(cv_errs_folds * tabulate(folds))}) / n

  # extract the optimal value of our tuning parameter lambda
  # and (re)compute the corresponding coefficient estimates
  best.lam <- lam.vec[cv.error == min(cv.error)]
  best.fit <- ridge_coef(X, y, best.lam)
  b1 <- best.fit$b1
  b <- best.fit$b
  list(b1 = b1, b = b, best.lam = best.lam, cv.error = cv.error)
}
```

Question 4

For this problem we first define some global functions

```r
library(doParallel)

rmvn <- function(n, p, mu = 0, S = diag(p)) {
  # Generates n (potentially correlated) p-dimensional normal deviates
  # given mean vector mu and variance-covariance matrix S
  # NOTE: S must be a positive semi-definite matrix
  Z <- matrix(rnorm(n * p), nrow = n, ncol = p) # generate iid normal deviates
  C <- chol(S)
  mu + Z %*% C # compute our correlated deviates
}
loss1 <- function(beta, b) sum((b - beta)^2, na.rm = T)
loss2 <- function(X, beta, b) sum((X %*% (beta - b))^2, na.rm = T)
se <- function(x) sd(x)/sqrt(length(x))
```

and global parameters remaining constant across (a)-(d)

```r
set.seed(680)

# global parameters
nsims <- 50
n <- 100
Ks <- c(5, 10, n)
lams <- 10^seq(-8, 8, 0.5)
sigma_star <- sqrt(1/2)

# preallocate empty data structure to store our results
coef_list <- vector(mode = 'list', length = length(Ks) + 1)
names(coef_list) <- c("OLS", "K5", "K10", "Kn")
```

(a)

$$n = 100$$
$$p = 50$$
$$\theta = 0.5$$

```r
# set parameters
p <- 50
theta <- 0.5

# generate data
beta_star <- rnorm(p, 0, sigma_star)
SIGMA <- outer(1:(p - 1), 1:(p - 1), FUN = function(a, b) theta^abs(a - b))
X <- cbind(1, rmvn(n, p - 1, 0, SIGMA))

# simulation
pt <- proc.time(); registerDoParallel(cores = 4)
sim <- foreach(1:nsims, .combine = cbind) %dopar% {
  # generate response
  y <- X %*% beta_star + rnorm(n, 0, sigma_star)

  # compute OLS estimates (lambda = 0)
  ols_fit <- ridge_coef(X, y, 0)
  coef_list[[1]] <- c(ols_fit$b1, ols_fit$b)

  # compute the cross-validated ridge estimates for each K
  coef_list[2:(length(Ks) + 1)] <- sapply(Ks, function(k) {
    rcv_out <- ridge_cv(X, y, lam.vec = lams, K = k)
    list(coefs = c(rcv_out$b1, rcv_out$b))
  })

  # compute losses
  l1 <- sapply(coef_list, function(b) loss1(beta_star, b))
  l2 <- sapply(coef_list, function(b) loss2(X, beta_star, b))
  list(l1, l2)
}
proc.time() - pt
```

```
##    user  system elapsed
##  26.621   0.505  10.936
```

```
# restructure losses for readability
sim_loss <- lapply(1:nrow(sim), function(i) sapply(sim[i,], function(s) s))
names(sim_loss) <- c("Loss 1", "Loss 2")

# compute loss mean across our sims
sim_means <- t(sapply(sim_loss, function(s) rowMeans(s)))
# compute loss std error across our sims
sim_se <- t(sapply(sim_loss, function(s) apply(s, 1, function(x) se(x))))

# report results
round(sim_means, 4)
```

```
##              OLS      K5     K10      Kn
## Loss 1   0.9142  0.8880  0.8839  0.8922
## Loss 2 25.7169 25.3871 25.3842 25.4274
```

```
round(sim_se, 4)
```

```
##           OLS     K5    K10     Kn
## Loss 1 0.0550 0.0513 0.0495 0.0504
## Loss 2 0.8516 0.8366 0.8240 0.8439
```

(b)

$$n = 100$$
$$p = 50$$
$$\theta = 0.9$$

```
# set parameters
p <- 50
theta <- 0.9

# generate data
beta_star <- rnorm(p, 0, sigma_star)
SIGMA <- outer(1:(p - 1), 1:(p - 1), FUN = function(a, b) theta^abs(a - b))
```

```r
X <- cbind(1, rmvn(n, p - 1, 0, SIGMA))

# simulation
pt <- proc.time(); registerDoParallel(cores = 4)
sim <- foreach(1:nsims, .combine = cbind) %dopar% {
  # generate response
  y <- X %*% beta_star + rnorm(n, 0, sigma_star)

  # compute OLS estimates (lambda = 0)
  ols_fit <- ridge_coef(X, y, 0)
  coef_list[[1]] <- c(ols_fit$b1, ols_fit$b)

  # compute the cross-validated ridge estimates for each K
  coef_list[2:(length(Ks) + 1)] <- sapply(Ks, function(k) {
    rcv_out <- ridge_cv(X, y, lam.vec = lams, K = k)
    list(coefs = c(rcv_out$b1, rcv_out$b))
  })

  # compute losses
  l1 <- sapply(coef_list, function(b) loss1(beta_star, b))
  l2 <- sapply(coef_list, function(b) loss2(X, beta_star, b))
  list(l1, l2)
}
proc.time() - pt
```

```
##    user  system elapsed
##  34.817   0.586  10.251
```

```r
# restructure losses for readability
sim_loss <- lapply(1:nrow(sim), function(i) sapply(sim[i,], function(s) s))
names(sim_loss) <- c("Loss 1", "Loss 2")

# compute loss mean across our sims
sim_means <- t(sapply(sim_loss, function(s) rowMeans(s)))
# compute loss std error across our sims
sim_se <- t(sapply(sim_loss, function(s) apply(s, 1, function(x) se(x))))

# report results
round(sim_means, 4)
```

```
##            OLS      K5     K10      Kn
## Loss 1  4.4842  3.5057  3.4766  3.4847
## Loss 2 23.7086 21.5929 21.4162 21.5129
```

```r
round(sim_se, 4)
```

```
##           OLS    K5    K10     Kn
## Loss 1 0.2155 0.1374 0.1444 0.1309
## Loss 2 0.6807 0.6223 0.6199 0.6222
```

(c)

$$
\begin{aligned}
n &= 100 \\
p &= 200 \\
\theta &= 0.5
\end{aligned}
$$

```r
# set parameters
p <- 200
theta <- 0.5

# generate data
beta_star <- rnorm(p, 0, sigma_star)
SIGMA <- outer(1:(p - 1), 1:(p - 1), FUN = function(a, b) theta^abs(a - b))
X <- cbind(1, rmvn(n, p - 1, 0, SIGMA))

# simulation
pt <- proc.time(); registerDoParallel(cores = 4)
sim <- foreach(1:nsims, .combine = cbind) %dopar% {
  # generate response
  y <- X %*% beta_star + rnorm(n, 0, sigma_star)

  # compute OLS estimates (lambda = 0)
  ols_fit <- ridge_coef(X, y, 0)
  coef_list[[1]] <- c(ols_fit$b1, ols_fit$b)

  # compute the cross-validated ridge estimates for each K
  coef_list[2:(length(Ks) + 1)] <- sapply(Ks, function(k) {
    rcv_out <- ridge_cv(X, y, lam.vec = lams, K = k)
    list(coefs = c(rcv_out$b1, rcv_out$b))
  })

  # compute losses
  l1 <- sapply(coef_list, function(b) loss1(beta_star, b))
  l2 <- sapply(coef_list, function(b) loss2(X, beta_star, b))
  list(l1, l2)
}
proc.time() - pt
```

```
##    user  system elapsed
##  86.156   1.503  57.043
```

```r
# restructure losses for readability
sim_loss <- lapply(1:nrow(sim), function(i) sapply(sim[i,], function(s) s))
names(sim_loss) <- c("Loss 1", "Loss 2")

# compute loss mean across our sims
sim_means <- t(sapply(sim_loss, function(s) rowMeans(s)))
# compute loss std error across our sims
sim_se <- t(sapply(sim_loss, function(s) apply(s, 1, function(x) se(x))))

# report results
round(sim_means, 4)
```

```
##             OLS      K5     K10      Kn
## Loss 1 44.9183 45.5265 45.5286 45.5286
## Loss 2 49.7954 49.7678 49.7954 49.7954
```

```
round(sim_se, 4)
```

```
##           OLS     K5    K10     Kn
## Loss 1 0.0298 0.0220 0.0220 0.0220
## Loss 2 0.8881 0.8837 0.8881 0.8881
```

(d)

$$n = 100$$
$$p = 200$$
$$\theta = 0.9$$

```
# set parameters
p <- 200
theta <- 0.9

# simulation
pt <- proc.time(); registerDoParallel(cores = 4)
sim <- foreach(1:nsims, .combine = cbind) %dopar% {
  # generate response
  y <- X %*% beta_star + rnorm(n, 0, sigma_star)

  # compute OLS estimates (lambda = 0)
  ols_fit <- ridge_coef(X, y, 0)
  coef_list[[1]] <- c(ols_fit$b1, ols_fit$b)

  # compute the cross-validated ridge estimates for each K
  coef_list[2:(length(Ks) + 1)] <- sapply(Ks, function(k) {
    rcv_out <- ridge_cv(X, y, lam.vec = lams, K = k)
    list(coefs = c(rcv_out$b1, rcv_out$b))
  })

  # compute losses
  l1 <- sapply(coef_list, function(b) loss1(beta_star, b))
  l2 <- sapply(coef_list, function(b) loss2(X, beta_star, b))
  list(l1, l2)
}
proc.time() - pt
```

```
##    user  system elapsed
## 198.808   3.161  49.332
```

```
# restructure losses for readability
sim_loss <- lapply(1:nrow(sim), function(i) sapply(sim[i,], function(s) s))
names(sim_loss) <- c("Loss 1", "Loss 2")

# compute loss mean across our sims
sim_means <- t(sapply(sim_loss, function(s) rowMeans(s)))
# compute loss std error across our sims
sim_se <- t(sapply(sim_loss, function(s) apply(s, 1, function(x) se(x))))
```

```r
# report results
round(sim_means, 4)
```

```
##             OLS     K5     K10      Kn
## Loss 1 44.9677 45.5619 45.5528 45.5528
## Loss 2 49.8687 50.3965 49.8687 49.8687
```

```r
round(sim_se, 4)
```

```
##           OLS     K5    K10     Kn
## Loss 1 0.0363 0.0193 0.0192 0.0192
## Loss 2 0.8296 0.8472 0.8296 0.8296
```

Question 5

(a)

Taking the gradient of our objective function g with respect to coefficient vector β yields

$$\begin{aligned}\nabla_\beta g(\beta,\sigma^2) &= \nabla_\beta\left(\frac{n}{2}\log\sigma^2+\frac{1}{2\sigma^2}\|\tilde{Y}-\tilde{X}\beta\|_2^2+\frac{\lambda}{2}\|\beta\|_2^2\right)\\ &= \frac{1}{\sigma^2}\left(-\tilde{X}^T\tilde{Y}+\tilde{X}^T\tilde{X}\beta\right)+\lambda\beta,\end{aligned}$$

while the gradient of g with respect to σ^2 is given by

$$\begin{aligned}\nabla_{\sigma^2} g(\beta,\sigma^2) &= \nabla_{\sigma^2}\left(\frac{n}{2}\log\sigma^2+\frac{1}{2\sigma^2}\|\tilde{Y}-\tilde{X}\beta\|_2^2+\frac{\lambda}{2}\|\beta\|_2^2\right)\\ &= \frac{n}{2\sigma^2}-\frac{1}{2\sigma^4}\|\tilde{Y}-\tilde{X}\beta\|_2^2.\end{aligned}$$

as desired.

(b)

We first consider the convexity of g with respect to β. The corresponding Hessian is given by

$$\begin{aligned}\nabla_\beta^2 g\left(\beta,\sigma^2\right) &= \nabla_\beta^2\left(\frac{n}{2}\log\sigma^2+\frac{1}{2\sigma^2}\|\tilde{Y}-\tilde{X}\beta\|_2^2+\frac{\lambda}{2}\|\beta\|_2^2\right)\\ &= \nabla_\beta\left(\frac{1}{\sigma^2}\tilde{X}^T\left(-\tilde{Y}+\tilde{X}\beta\right)+\lambda\beta\right)\\ &= \tilde{X}^T\tilde{X}+\lambda\mathbb{I}_{p-1}.\end{aligned}$$

As before, the symmetric matrix $\tilde{X}^T\tilde{X}$ will always positive semi-definite, and for $\lambda\geq 0$, the diagonal matrix $\lambda\mathbb{I}_{p-1}$ must also be positive semi-definite (and positive definite when $\lambda>0$). Thus, the Hessian with respect to β must be positive semi-definite

$$\nabla^2_{\beta} g\left(\beta, \sigma^2\right) = \tilde{X}^T \tilde{X} + \lambda \mathbb{I}_{p-1} \in \mathbb{S}^{p-1}_{+},$$

and positive definite when $\lambda > 0$. Therefore, our objective function $g\left(\beta, \sigma^2\right)$ is convex in β. Next, we seek the Hessian of g with respect to σ^2,

$$\begin{aligned}
\nabla^2_{\sigma^2} g\left(\beta, \sigma^2\right) &= \nabla^2_{\sigma^2} \left(\frac{n}{2} \log \sigma^2 + \frac{1}{2\sigma^2} \|\tilde{Y} - \tilde{X}\beta\|_2^2 + \frac{\lambda}{2} \|\beta\|_2^2 \right) \\
&= \nabla_{\sigma^2} \left(\frac{n}{2\sigma^2} - \frac{1}{2\sigma^4} \|\tilde{Y} - \tilde{X}\beta\|_2^2 \right) \\
&= -\frac{n}{2\sigma^4} + \frac{1}{\sigma^6} \|\tilde{Y} - \tilde{X}\beta\|_2^2.
\end{aligned}$$

For g to be convex in σ^2 we require $\nabla^2_{\sigma^2} g\left(\beta, \sigma^2\right) \geq 0$. However, some algebra informs us that such a condition is equivalent to

$$n \geq \frac{2}{\sigma^2} \|\tilde{Y} - \tilde{X}\beta\|_2^2.$$

As a counterexample of this inequality, consider the following data

```r
set.seed(124)
n <- 4
p <- 1
beta <- rep(10, p)
sigma <- 1

Xtilde <- matrix(rnorm(n * p), nrow = n)
ytilde <- Xtilde %*% beta + rnorm(n)

(rhs <- as.numeric(2/sigma^2 * crossprod(ytilde - Xtilde %*% beta)))
```

```
## [1] 6.258667
```

```r
n >= rhs
```

```
## [1] FALSE
```

and so it is *not* the case that $\nabla^2_{\sigma^2} g\left(\beta, \sigma^2\right)$ is (always) nonnegative, implying that our objective function $g\left(\beta, \sigma^2\right)$ is not convex in σ^2.

(c)

Let $\bar{\beta}$ be a solution to our maximum likelihood ridge estimation problem such that, for $\lambda > 0$, we have

$$\tilde{Y} - \tilde{X}\bar{\beta} = 0.$$

Since $\bar{\beta}$ is a solution it must satisfy the first order condition (with respect to β)

$$\nabla_{\beta} g(\beta, \sigma^2) = \frac{1}{\sigma^2} \left(-\tilde{X}^T \tilde{Y} + \tilde{X}^T \tilde{X}\beta \right) + \lambda\beta = 0 \iff \frac{1}{\sigma^2} \left(\tilde{X}^T \left(-\tilde{Y} + \tilde{X}\beta \right) \right) + \lambda\beta = 0.$$

Thus, for such a solution $\bar{\beta}$ and $\lambda > 0$,

$$\begin{aligned} 0 &= \frac{1}{\sigma^2}\left(\tilde{X}^T\left(-\tilde{Y}+\tilde{X}\bar{\beta}\right)\right)+\lambda\bar{\beta} \\ &= \frac{1}{\sigma^2}\left(\tilde{X}^T\left(-\tilde{Y}+\tilde{Y}\right)\right)+\lambda\bar{\beta} \\ &= \lambda\bar{\beta} \\ \iff \bar{\beta} &= 0. \end{aligned}$$

Similarly, using our second first order condition $\nabla_{\sigma^2} g(\beta, \sigma^2) = 0$, at $\beta = \bar{\beta}$,

$$\begin{aligned} 0 = \nabla_{\sigma^2} g(\beta,\sigma^2) &= \frac{n}{2\sigma^2} - \frac{1}{2\sigma^4}\|\tilde{Y}-\tilde{X}\beta\|_2^2 \\ &= \frac{n}{2\sigma^2} - \frac{1}{2\sigma^4}\|\tilde{Y}-\tilde{X}\bar{\beta}\|_2^2 \\ &= \frac{n}{2\sigma^2} - \frac{1}{2\sigma^4}\|\tilde{Y}-\tilde{Y}\|_2^2 \\ &= \frac{n}{2\sigma^2} \end{aligned}$$

This conditions enforces either $n = 0$ or $\sigma^2 \to \infty$. Thus, no such global minimizer could exist.

(d)

Solving our first order conditions

$$\begin{aligned} \frac{1}{\sigma^2}\left(\tilde{X}^T\left(-\tilde{Y}+\tilde{X}\bar{\beta}\right)\right)+\lambda\bar{\beta} &= 0 \\ \frac{n}{2\sigma^2} - \frac{1}{2\sigma^4}\|\tilde{Y}-\tilde{X}\beta\|_2^2 &= 0, \end{aligned}$$

we find the maximum likelihood estimate $\hat{\beta}^{(\lambda,\,ML)}$ to be

$$\hat{\beta}^{(\lambda,\,ML)} = \left(\tilde{X}^T\tilde{X} + \sigma^2\lambda\mathbb{I}_{p-1}\right)^{-1}\tilde{X}^T\tilde{Y}.$$

and the maximum likelihood estimate $\hat{\sigma}^{2\,(\lambda,\,ML)}$ to be

$$\hat{\sigma}^{2\,(\lambda,\,ML)} = \frac{1}{n}\|\tilde{Y} - \tilde{X}\hat{\beta}^{(\lambda,\,ML)}\|_2^2$$

To compute such estimates we may use the following algorithm: Consider some fixed data set $\mathcal{D} = \{X, Y\}$ and a fixed tuning parameter λ.

(1) Center the data: Center each predictor by its mean $X \mapsto \tilde{X}$, center the response vector by its mean $Y \mapsto \tilde{Y}$.

(2) Have some initial proposal for the estimate $\hat{\sigma}_0^{2\,(\lambda,\,ML)} \in \mathbb{R}^+$.

(3) Compute an initial proposal for $\hat{\beta}_0^{(\lambda,\,ML)}$ based on $\hat{\sigma}_0^{2\,(\lambda,\,ML)}$.

(4) Update our variance estimate $\hat{\sigma}_i^{2\,(\lambda,\,ML)}$ using the previous estimate of $\hat{\beta}_{i-1}^{(\lambda,\,ML)}$.

(5) Update our coefficient estimate $\hat{\beta}_i^{(\lambda,\,ML)}$ using the new estimate of $\hat{\sigma}_i^{2\,(\lambda,\,ML)}$.

(6) Repeat steps (5)-(6) until some convergence criteria is met, say $\|\hat{\sigma}_i^{2\,(\lambda,\,ML)} - \hat{\sigma}_{i-1}^{2\,(\lambda,\,ML)}\|$, is small.

(e)

Our function is as follows

```r
ridge_coef_mle <- function(X, y, lam, tol = 1e-16) {
  # Compute ML estimates of ridge coefficients with penalty lam

  # remove leading column, find means
  Xm1 <- X[,-1]; xbar <- colMeans(Xm1); ybar <- mean(y)
  # center response and predictors according to their means
  ytilde <- y - ybar
  Xtilde <- sweep(Xm1, 2, xbar)

  # compute the SVD on the centered design matrix
  Xtilde_svd <- svd(Xtilde)
  U <- Xtilde_svd$u; d <- Xtilde_svd$d; V <- Xtilde_svd$v

  # generate some initial guess for sigma and beta
  sig0 <- rexp(1)
  Dstar <- diag(d/(d^2 + sig0^2 * lam))
  b0 <- V %*% (Dstar %*% crossprod(U, ytilde))

  i <- 1
  repeat {
    # update sigma and beta
    sig_new <- sqrt(1/n * crossprod(ytilde - Xtilde %*% b0))
    Dstar <- diag(d/(d^2 + sig_new^2 * lam))
    b_new <- V %*% (Dstar %*% crossprod(U, ytilde))

    if (abs(sig_new^2 - sig0^2) < tol)
      break
    sig0 <- sig_new; b0 <- b_new; i <- i + 1
  }

  list(niter = i, sigma = as.numeric(sig_new), b = b_new)
}
grad_mle <- function(X, y, lam, b, s) {
  # Compute the gradient of our (unconstrained) ridge
  # objective function

  # remove leading column, find means
  n <- nrow(X); Xm1 <- X[,-1]; xbar <- colMeans(Xm1); ybar <- mean(y)
  # center response and predictors according to their means
  ytilde <- y - ybar
  Xtilde <- sweep(Xm1, 2, xbar)

  gb <- 1/s^2 * crossprod(Xtilde, Xtilde %*% b - ytilde) + lam * b
  gs <- n/(2 * s^2)  - 1/(2 * s^4) * crossprod(ytilde - Xtilde %*% b)
  c(grad_b = gb, grad_s = gs)
}
```

(f)

```r
set.seed(124)
n <- 100
p <- 5
lam <- 1
beta_star <- (-1)^(1:p) * rep(5, p)
sigma_star <- sqrt(1/2)

X <- cbind(1, matrix(rnorm(n * (p - 1)), nrow = n))
y <- X %*% beta_star + rnorm(n, 0, sigma_star)

(rcm <- ridge_coef_mle(X, y, lam))
```

```
## $niter
## [1] 9
##
## $sigma
## [1] 0.6559084
##
## $b
##           [,1]
## [1,]  4.976904
## [2,] -5.000078
## [3,]  4.888082
## [4,] -5.017066
```

```r
grad_mle(X, y, lam, rcm$b, rcm$sigma)
```

```
##       grad_b1       grad_b2       grad_b3       grad_b4        grad_s
##  5.178080e-13 -1.419309e-12  4.849454e-13 -9.281464e-13  1.421085e-14
```

as desired.

Question 6

(a)

Consider our objective function

$$f(\beta) = \frac{1}{2}\|\tilde{Y} - \tilde{X}\beta\|_2^2 + \frac{\lambda_1}{2}\|\beta\|_2^2 + \frac{\lambda_2}{2}\sum_{j=2}^{p}(\beta_j - \beta_{j-1})^2 .$$

To show convexity we wish to show $\nabla^2 f(\beta) \in \mathbb{S}_+^{p-1}$. However, it's not immediately obvious how to take such a gradient with our fused sum terms $(\beta_j - \beta_{j-1})^2$. In order to be able to take the gradient we wish to express the objective function strictly in terms of the vector β. One way to accomplish this is to define vector $B \in \mathbb{R}^{p-1}$ given by

$$B = \begin{bmatrix} \beta_2 - \beta_1 \\ \vdots \\ \beta_p - \beta_{p-1} \end{bmatrix},$$

so that

$$\sum_{j=2}^{p} (\beta_j - \beta_{j-1})^2 = B^T B.$$

Next, define matrix $A \in \mathbb{R}^{(p-2)\times(p-1)}$ with entries -1 along the main diagonal and 1 along the upper diagonal, i.e.,

$$A = \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{bmatrix}.$$

Using this matrix A permits us to express our fused sum $\sum_{j=2}^{p} (\beta_j - \beta_{j-1})^2 = B^T B$ in terms of the vector β, i.e.,

$$\begin{aligned} \sum_{j=2}^{p} (\beta_j - \beta_{j-1})^2 &= B^T B \\ &= \beta^T A^T A \beta \\ &\equiv \|A\beta\|_2^2. \end{aligned}$$

Therefore, our objective function is expressible as

$$\begin{aligned} f(\beta) &= \frac{1}{2}\|\tilde{Y} - \tilde{X}\beta\|_2^2 + \frac{\lambda_1}{2}\|\beta\|_2^2 + \frac{\lambda_2}{2}\|A\beta\|_2^2 \\ &\equiv \frac{1}{2}\tilde{Y}^T\tilde{Y} - \beta^T\tilde{X}^T\tilde{Y} + \frac{1}{2}\beta^T\tilde{X}^T\tilde{X}\beta + \frac{\lambda_1}{2}\beta^T\beta + \frac{\lambda_2}{2}\beta^T A^T A\beta. \end{aligned}$$

Hence,

$$\nabla f(\beta) = -\tilde{X}^T\tilde{Y} + \tilde{X}^T\tilde{X}\beta + \lambda_1\beta + \lambda_2 A^T A\beta,$$

admitting the Hessian

$$\nabla^2 f(\beta) = \tilde{X}^T\tilde{X} + \lambda_1\mathbb{I}_{p-1} + \lambda_2 A^T A.$$

Recalling that a matrix multiplied with its transpose must always be positive semi-definite, we find that $\tilde{X}^T X$ and $A^T A$ must be positive semi-definite. Thus, since $\lambda_1 > 0$, the sum $\tilde{X}^T\tilde{X} + \lambda_1\mathbb{I}_{p-1} + \lambda_2 A^T A = \nabla^2 f(\beta)$ is positive definite, and so $f(\beta)$ must be strictly convex in β, as desired.

(b)

We first solve for $\hat{\beta}_{-1}^{(\lambda_1,\lambda_2)}$ in (a) by setting $\nabla f(\beta) = 0$

$$
\begin{aligned}
0 &= -\tilde{X}^T\tilde{Y} + \tilde{X}^T\tilde{X}\beta + \lambda_1\beta + \lambda_2 A^T A\beta \\
\tilde{X}^T\tilde{Y} &= \left(\tilde{X}^T\tilde{X} + \lambda_1\mathbb{I}_{p-1} + \lambda_2 A^T A\right)\beta \\
\implies \hat{\beta}_{-1}^{(\lambda_1,\,\lambda_2)} &= M\tilde{X}^T\tilde{Y},
\end{aligned}
$$

where we have set $M = \left(\tilde{X}^T\tilde{X} + \lambda_1\mathbb{I}_{p-1} + \lambda_2 A^T A\right)^{-1}$ for brevity. Therefore

$$
\begin{aligned}
\mathbb{E}\left[\hat{\beta}_{-1}^{(\lambda_1,\,\lambda_2)}\right] &= \mathbb{E}\left[M\tilde{X}^T\tilde{Y}\right] \\
&= M\tilde{X}^T\mathbb{E}\left[\tilde{Y}\right] \\
&= M\tilde{X}^T\beta_{*,\,-1},
\end{aligned}
$$

and

$$
\begin{aligned}
\mathrm{Var}\left(\hat{\beta}_{-1}^{(\lambda_1,\,\lambda_2)}\right) &= \mathrm{Var}\left(M\tilde{X}^T Y\right) \\
&= M\tilde{X}^T\mathrm{Var}\left(\tilde{Y}\right)\tilde{X}M^T \\
&= \sigma_*^2 M\tilde{X}^T\tilde{X}M^T,
\end{aligned}
$$

as desired. We now perform our fused ridge simulation study to test the theoretical values with some empirical estimates. We first define our fused ridge coefficient estimation function (as well as functions permitting us to easily compute the theoretical means and variances of the fused ridge problem)

```r
fused_ridge_coef <- function(X, y, lam1, lam2) {
  n <- nrow(X); p <- ncol(X)

  # remove leading column, find predictor means, center response
  Xm1 <- X[,-1]; xbar <- colMeans(Xm1); ytilde <- y - mean(y)
  # center each predictor according to its mean
  Xtilde <- Xm1 - tcrossprod(rep(1, nrow(Xm1)), xbar)

  I <- diag(p - 1)
  UD <- cbind(rep(0, p - 2), diag(p - 2)) # upper diagonal matrix
  J <- -1 * cbind(diag(p - 2), rep(0, p - 2)) # diag (p - 2)*(p - 1) matrix
  A <- J + UD

  b <- solve(crossprod(Xtilde) + lam1 * I + lam2 * crossprod(A),
             crossprod(Xtilde, ytilde))
  b0 <- mean(y) - crossprod(xbar, b)
  list(b0 = b0, b = b)
}
fused_ridge_coef_true <- function(X, lam1, lam2, beta, sigma) {
  # Returns theoretical means and variances for the fused ridge problem
  # Note: Omits intercept term b0
  n <- nrow(X); p <- ncol(X)

  # remove leading column, remove intercept, center predictors
  Xm1 <- X[,-1]; betam1 <- beta[-1]; xbar <- colMeans(Xm1)
  # center each predictor according to its mean
  Xtilde <- Xm1 - tcrossprod(rep(1, nrow(Xm1)), xbar)

  I <- diag(p - 1)
  UD <- cbind(rep(0, p - 2), diag(p - 2)) # upper diagonal matrix
  J <- -1 * cbind(diag(p - 2), rep(0, p - 2)) # diag (p - 2)*(p - 1) matrix
  A <- J + UD

  M <- solve(crossprod(Xtilde) + lam1 * I + lam2 * crossprod(A))
  b <- M %*% crossprod(Xtilde, (Xtilde %*% betam1))
  vcv <- sigma^2 * M %*% tcrossprod(crossprod(Xtilde), M)
  list(b = b, vcv = vcv)
}
```

We now simulate some data to test our estimates

```r
set.seed(124)

# set parameters
nsims <- 1e3
n <- 1e2
p <- 5
lam1 <- 1; lam2 <- 1;
sigma_star <- 1
beta_star <- rnorm(p)

# generate (fixed) design matrix
X <- cbind(rep(1, n), matrix(rnorm(n * (p - 1)), nrow = n, ncol = p - 1))

# compute expected parameter values
par_true <- fused_ridge_coef_true(X, lam1, lam2, beta_star, sigma_star)
b_true <- as.vector(par_true$b)
vcv_true <- par_true$vcv

# simulate our fused ridge coefficients nsims times
# outputs a matrix with rows corresponding to coefficients
# and columns correspond to simulation number
pt <- proc.time()
b_hat <- replicate(nsims, {
  y <- X %*% beta_star + rnorm(n, 0, sigma_star) # generate response
  as.vector(fused_ridge_coef(X, y, lam1, lam2)$b)
})
proc.time() - pt
```

```
##    user  system elapsed
##   0.122   0.003   0.127
```

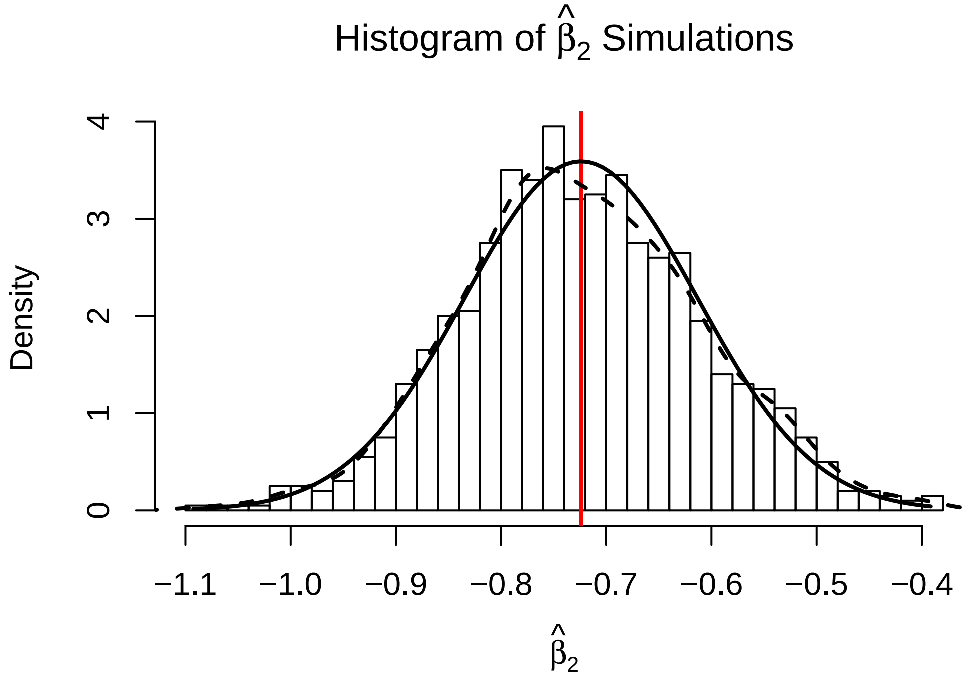
```r
# estimate variance of b2, ..., b_p estimates
vcv_hat <- var(t(b_hat))

# print estimated fused ridge coefficients vs. expected values
b <- rbind(rowMeans(b_hat), b_true)
rownames(b) <- c("b_hat", "b_true")
round(b, 4)
```

```
##           [,1]    [,2]    [,3]    [,4]
## b_hat  0.0248 -0.7232 0.2214 1.3927
## b_true 0.0313 -0.7240 0.2235 1.3920
```

```r
# print absolute error between estimated and true fused ridge variances
round(abs(vcv_true - vcv_hat), 4)
```

```
##        [,1]  [,2]  [,3]  [,4]
## [1,] 0e+00 7e-04 4e-04 2e-04
## [2,] 7e-04 6e-04 6e-04 8e-04
## [3,] 4e-04 6e-04 2e-04 0e+00
## [4,] 2e-04 8e-04 0e+00 5e-04
```

As a final point, we may look at the simulations of $\hat{\beta}_2^{(\lambda_1,\lambda_2)}$ and compare it with its theoretical distribution. Note that the estimates $\hat{\beta}^{(\lambda_1,\lambda_2)} = M\tilde{X}^T\tilde{Y}$ are normally distributed because they are a linear combination of $\tilde{Y} \sim \mathcal{N}(\tilde{X}\beta, \sigma^2)$ (when our noise terms $\epsilon \sim \mathcal{N}(0, \sigma^2)$). We visualize the histogram of the $\hat{\beta}_2^{(\lambda_1,\lambda_2)}$ simulations with its empirical and theoretical densities overlaid (dashed, solid), along with its expected value (vertical line) below.



Appendix

2 (b)

Proposition: Suppose $X \in \mathbb{R}^{n \times p}$, then $X^T X$ is positive semi-definite.

Proof: Suppose X is a real-valued $n \times p$ matrix and let v be an arbitrary real-valued $p \times 1$ vector. Let X_i denote the i^{th} row of X. Then,

$$\begin{aligned} v^T X^T X v &= (Xv)^T (Xv) \\ &= \|Xv\|_2^2 \\ &= \sum_{i=1}^{n} (X_i \bullet v)^2 \\ &\geq 0 \end{aligned}$$

which satisfies the definition of positive semi-definiteness, as desired.

Proposition: Let $\mathbb{I}_p$ be a $p \times p$ identity matrix and λ a positive nonzero real number, then $\lambda \mathbb{I}_p$ is positive definite.

Proof: Suppose $\lambda > 0$ and let v be an arbitrary real-valued $p \times 1$ vector. Then,

$$\begin{aligned} v^T (\lambda \mathbb{I}_p) v &= \lambda \left(v^T \mathbb{I}_p v\right) \\ &= \lambda \left(v^T v\right) \\ &= \lambda \|v\|_2^2 \\ &= \lambda \sum_{i=1}^{p} v_i^2 \\ &> 0, \quad \text{when } \lambda > 0 \end{aligned}$$

which satisfies the definition of positive definiteness, as desired.