MATH 680: Assignment 1

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To do... Run the full Q4

check what to do for the OLS/lambda = 0 case for p > n (Q4) remove longwinded answers (expected values/variance estimates)

Question 1

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

$$\tilde{X} = X_{-1} - \mathbf{1}_n \bar{x}^T$$

$$\tilde{Y} = Y - \mathbf{1}_n^T \bar{Y},$$

we find

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

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 $\hat{\beta}$ also solves the uncentered problem

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

as desired.

(a)

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

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

Therefore, by taking the gradient we find

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

as desired.

(b)

The Hessian $\nabla^2 f(\beta)$ is given by

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

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). Therefore, for all nonzero vectors $v\in\mathbb{R}^{p-1}$,

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

$$= 2v^{T} \tilde{X}^{T} \tilde{X} v + 2\lambda v^{T} \mathbb{I}_{p-1} v$$

$$= 2 \left(\underbrace{\|\tilde{X}v\|_{2}^{2}}_{\geq 0} + \underbrace{\lambda \|v\|_{2}^{2}}_{> 0 \text{ when } \lambda > 0} \right)$$

Hence,

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

and so f must be strictly convex in β .

(c)

Suppose a strictly convex function f is globally minimized at distinct points x and y. By strict convexity

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

Since f is minimized at both x and y we have f(x) = f(y), so

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

However, this implies that the point z = tx + (1-t)y yields a value of f even *smaller* than at x, contradicting our assumption that x is a global minimizer. Therefore, strict convexity implies that the global minimizer must be unique, and so 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 function computing the ridge coefficients we first set $\nabla f(\beta) = 0$

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

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, $U^T U = \mathbb{I}_n$, $V^T V = \mathbb{I}_{p-1}$, 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. Hence,

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

Note that $D^TD + \lambda \mathbb{I}_{p-1}$ is a diagonal $(p-1) \times (p-1)$ matrix with entries $d_j^2 + \lambda$, j = 1, ..., p-1, and so the inverse $(D^TD + \lambda \mathbb{I}_{p-1})^{-1}$ must also be diagonal with entries $(d_j^2 + \lambda)^{-1}$, j = 1, ..., p-1. We exploit this to avoid performing a matrix inversion in our function. For brevity, let

$$D^* = (D^T D + \lambda I_{p-1})^{-1} D^T,$$

so that

$$\hat{\beta}^{(\lambda)} = V D^* U^T \tilde{Y}.$$

We present a function written in R performing such calculations below.

```
ridge_coef <- function(X, y, lam) {</pre>
  Xm1 \leftarrow X[,-1] # remove leading column of 1's marking the intercept
  ytilde <- y - mean(y) # center response</pre>
  xbar <- colMeans(Xm1) # find predictor means</pre>
  # center each predictor according to its mean
  Xtilde <- Xm1 - tcrossprod(rep(1, nrow(Xm1)), xbar)</pre>
  # compute the SVD on the centered design matrix
  Xtilde_svd <- svd(Xtilde)</pre>
  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 \leftarrow diag(d/(d^2 + lam))
  # compute ridge coefficients
  b <- V %*% (Dstar %*% crossprod(U, ytilde)) # slopes
  b1 <- mean(y) - crossprod(xbar, b) # intercept
  list(b1 = b1, b = b)
}
```

It turns out the following implementation will be considerably quicker

```
scale_faster <- function(x,</pre>
                        center = TRUE,
                        scale = TRUE,
                        add_attr = TRUE,
                        rows = NULL,
                        cols = NULL) {
  # adapted from
  # https://www.r-bloggers.com/a-faster-scale-function/
  if (!is.null(rows) && !is.null(cols)) {
    x <- x[rows, cols, drop = FALSE]</pre>
  } else if (!is.null(rows)) {
   x \leftarrow x[rows, drop = FALSE]
  } else if (!is.null(cols)) {
    x \leftarrow x[, cols, drop = FALSE]
  # Get the column means
  cm = colMeans(x, na.rm = TRUE)
  # Get the column sd
  if (scale) {
   csd = colSds(x, center = cm)
  } else {
    # just divide by 1 if not
    csd = rep(1, length = length(cm))
  if (!center) {
    # just subtract 0
    cm = rep(0, length = length(cm))
  x = t((t(x) - cm) / csd)
```

```
if (add_attr) {
    if (center) {
      attr(x, "scaled:center") <- cm</pre>
    }
    if (scale) {
      attr(x, "scaled:scale") <- csd</pre>
  }
  return(x)
}
ridge_coef_faster <- function(X, y, lam) {</pre>
  # Commented-out scaling parameters represent the transformations
  # used to make the output identical to that of
  # coef(MASS::lm.ridge(X, y, lam))
  Xm1 \leftarrow X[,-1]
  n \leftarrow nrow(X); ybar \leftarrow mean(y); #sqrt_sc \leftarrow sqrt(n/(n-1))
  #Xtilde <- scale_faster(Xm1) * sqrt_sc</pre>
  Xtilde <- scale_faster(Xm1, scale = F)</pre>
  ytilde <- y - ybar
  b <- chol2inv(chol(crossprod(Xtilde) + lam * diag(ncol(Xm1)))) %*%
    crossprod(Xtilde, ytilde) #*
    #sqrt sc * 1/attr(Xtilde, "scaled:scale")
  b1 <- ybar - sum(attr(Xtilde, "scaled:center") * b)</pre>
  list(b1 = b1, b = b)
```

(e)

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

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

If p >> n then using the SVD on \tilde{X} may yield some speed improvements, that is, with $\tilde{X} = UDV^T$ as above, we find

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

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

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

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

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

$$= \sigma_*^2 \left(\tilde{X}^T \tilde{X} + \lambda \mathbb{I}_{p-1}\right)^{-1} \tilde{X}^T \tilde{X} \left(\tilde{X}^T \tilde{X} + \lambda \mathbb{I}_{p-1}\right)^{-1}$$

as desired. We once again may be interested in applying the SVD on \tilde{X} as we had done before. Such a decomposition gives us a more concise solution

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

where D^{**} is a diagonal min $(n, p-1) \times \min(n, p-1)$ matrix with diagonal entries $\left\{\frac{d_j^2}{\left(d_j^2 + \lambda\right)^2}\right\}_{j=1}^{\min(n, p-1)}$ and zero elsewhere.

We now wish to perform a simulation study to estimate our theoretical values $\mathbb{E}\left[\hat{\beta}_{-1}^{(\lambda)}\right]$ and $\operatorname{Var}\left(\hat{\beta}_{-1}^{(\lambda)}\right)$. For readability we first define functions computing the theoretical mean and variance according to our above expressions.

```
ridge_coef_params <- function(X, lam, beta, sigma) {</pre>
  n \leftarrow nrow(X); p \leftarrow ncol(X)
  betam1 <- beta[-1] # remove intercept term</pre>
  Xm1 \leftarrow X[,-1] # remove leading column of 1's in our design matrix
  xbar <- colMeans(Xm1) # find prector means</pre>
  # center each predictor according to its mean
  Xtilde <- sweep(Xm1, 2, xbar)</pre>
  if (n \ge p) {
    I \leftarrow diag(p - 1)
    inv <- solve(crossprod(Xtilde) + lam * I)</pre>
    b <- solve(crossprod(Xtilde) + lam * I) %*% (crossprod(Xtilde) %*% betam1)
    vcv <- sigma^2 * inv %*% crossprod(Xtilde) %*% inv</pre>
    list(b = b, vcv = vcv)
  } else {
    # compute SVD on the centered design matrix
    Xtilde svd <- svd(Xtilde)</pre>
    d <- Xtilde svd$d
    V <- Xtilde_svd$v</pre>
    Dstar \leftarrow diag(d^2/(d^2 + lam))
    Dstar2 \leftarrow diag(d^2/(d^2 + lam)^2)
    b <- V ** (Dstar ** crossprod(V, betam1))
    vcv <- V ** tcrossprod(Dstar2, V)
    list(b = b, vcv = vcv)
  }
}
```

We may now perform our simulation.

```
set.seed(124)
# set parameters
nsims <- 1e3
n <- 25
p < -7
lam < -4
beta_star <- 1:p
sigma_star <- 1
# generate fixed design matrix
X \leftarrow cbind(1, matrix(rnorm(n * (p - 1)), nrow = n))
# compute theoretical mean and variance
par_true <- ridge_coef_params(X, lam, beta_star, sigma_star)</pre>
b_true <- as.vector(par_true$b)</pre>
vcv_true <- par_true$vcv
# simulate ridge coefficients nsims times
# outputs a matrix with rows corresponding to coefficients
# and columns correspond to simulation number
b_hat <- replicate(nsims, {</pre>
 y <- X %*% beta_star + rnorm(n, 0, sigma_star)
 as.vector(ridge coef faster(X, y, lam)$b)
})
# estimate variance of b1, ..., b_p estimates
vcv_hat <- var(t(b_hat))</pre>
# print estimated fused ridge coefficients vs. expected values
b <- rbind(rowMeans(b_hat), b_true)</pre>
rownames(b) <- c("b_hat", "b_true")</pre>
round(b, 4)
            [,1]
                    [,2]
                           [,3]
                                  [,4]
                                          [,5]
## b_hat 0.7861 1.6595 3.2916 3.8786 4.2007 6.3650
## b_true 0.7797 1.6636 3.2936 3.8779 4.2025 6.3689
# print absolute error between estimated and true fused ridge variances
round(abs(vcv_true - vcv_hat), 4)
          [,1]
                 [,2]
                         [,3]
                                [,4]
                                        [,5]
## [1,] 0.0010 0.0008 0.0013 0.0012 0.0008 0.0009
## [2,] 0.0008 0.0008 0.0009 0.0017 0.0011 0.0003
## [3,] 0.0013 0.0009 0.0012 0.0006 0.0015 0.0015
## [4,] 0.0012 0.0017 0.0006 0.0014 0.0005 0.0001
## [5,] 0.0008 0.0011 0.0015 0.0005 0.0007 0.0012
## [6,] 0.0009 0.0003 0.0015 0.0001 0.0012 0.0013
```

We see that the empirical sample estimates are very close to their theoretical values, as expected.

Prior to writing our cross-validation function we create some helper functions for the sake of readability

```
ridge_cv_lam <- function(X, y, lam, K) {</pre>
  # Helper function for ridge_cv()
  # perform K-fold cross-validation on the ridge regression
  # estimation problem over a single tuning parameter lam
  n \leftarrow nrow(X)
  if (K > n) {
    stop(paste0("K > ", n, "."))
  } else if (K < 2) {</pre>
    stop("K < 2.")
  }
  # groups to cross-validate over
  folds <- cut(1:n, breaks = K, labels = F)</pre>
  # get indices of training subset
  train_idxs <- lapply(1:K, function(i) !(folds %in% i))</pre>
  cv_err <- sapply(train_idxs, function(tr_idx) {</pre>
    # train our model, extract fitted coefficients
    b_train <- unlist(ridge_coef_faster(X[tr_idx,], y[tr_idx], lam))</pre>
    # fit testing data
    yhat <- X[!tr_idx,] %*% b_train</pre>
    # compute test error
    sum((y[!tr_idx] - yhat)^2)
  })
  # weighted average (according to group size, some groups may have
  # +/- 1 member depending on whether sizes divided unevenly) of
  # cross validation error for a fixed lambda
  sum((cv err * table(folds)))/n
```

Then, our cross-validation function is as follows:

```
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)

cv.error <- sapply(lam.vec, function(1) ridge_cv_lam(X, y, 1, K))

# extract best tuning parameter and corresponding coefficient estimates
best.lam <- lam.vec[cv.error == min(cv.error)]
best.fit <- ridge_coef_faster(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)
}</pre>
```

For this problem we first set some global libraries/functions

```
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-semidefinite 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)</pre>
```

and global parameters which remain constant across (a)-(d)

```
# global parameters
nsims <- 3
n <- 100
Ks <- c(5, 10, n)
lams <- 10^seq(-8, 8, 0.5)
sigma_star <- sqrt(1/2)

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

(a)

```
# 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% {
    y <- X %*% beta_star + rnorm(n, 0, sigma_star)

# compute OLS estimates (lambda = 0)
    ols_fit <- ridge_coef_faster(X, y, 0)
    coef_list[[1]] <- c(ols_fit$b1, ols_fit$b)</pre>
```

```
\# compute the cross-validated ridge estimates for each K
  coef_list[2:(length(Ks) + 1)] <- sapply(Ks, function(k) {</pre>
    rcv <- ridge_cv(X, y, lam.vec = lams, K = k)</pre>
    list(coefs = c(rcv$b1, rcv$b))
  })
 11 <- sapply(coef_list, function(b) loss1(beta_star, b))</pre>
 12 <- sapply(coef list, function(b) loss2(X, beta star, b))
 list(11, 12)
sim_loss <- lapply(1:nrow(sim), function(i) sapply(sim[i,], function(s) s))</pre>
names(sim_loss) <- c("Loss 1", "Loss 2")</pre>
sim_means <- t(sapply(sim_loss, function(s) rowMeans(s)))</pre>
sim_se <- t(
  sapply(sim_loss, function(s) apply(s, 1, function(x) sd(x)/sqrt(length(x)))))
proc.time() - pt
##
      user system elapsed
     6.323
            0.233
                      4.372
# report results
round(sim_means, 4)
##
              OLS
                        K5
                               K10
                                         Kn
## Loss 1 0.8535 0.7168 0.6461 0.7168
## Loss 2 27.3800 25.8764 25.6029 25.8764
round(sim se, 4)
##
             OLS
                      K5
                            K10
                                     Kn
## Loss 1 0.2155 0.1494 0.0687 0.1494
## Loss 2 1.8833 2.0970 2.2944 2.0970
(b)
# set parameters
p < -50
theta <- 0.9
# generate data
beta_star <- rnorm(p, 0, sigma_star)</pre>
SIGMA <- outer(1:(p - 1), 1:(p - 1), FUN = function(a, b) theta^abs(a - b))
X \leftarrow cbind(1, rmvn(n, p - 1, 0, SIGMA))
# simulation
pt <- proc.time()</pre>
registerDoParallel(cores = 4)
sim <- foreach(1:nsims, .combine = cbind) %dopar% {</pre>
 y <- X ** beta_star + rnorm(n, 0, sigma_star)
  # compute OLS estimates (lambda = 0)
ols_fit <- ridge_coef_faster(X, y, 0)</pre>
```

```
coef_list[[1]] <- c(ols_fit$b1, ols_fit$b)</pre>
  # compute the cross-validated ridge estimates for each K
  coef_list[2:(length(Ks) + 1)] <- sapply(Ks, function(k) {</pre>
    rcv <- ridge_cv(X, y, lam.vec = lams, K = k)</pre>
    list(coefs = c(rcv$b1, rcv$b))
  })
  11 <- sapply(coef_list, function(b) loss1(beta_star, b))</pre>
  12 <- sapply(coef_list, function(b) loss2(X, beta_star, b))</pre>
  list(11, 12)
}
sim_loss <- lapply(1:nrow(sim), function(i) sapply(sim[i,], function(s) s))</pre>
names(sim_loss) <- c("Loss 1", "Loss 2")</pre>
sim_means <- t(sapply(sim_loss, function(s) rowMeans(s)))</pre>
sim_se <- t(
  sapply(sim_loss, function(s) apply(s, 1, function(x) sd(x)/sqrt(length(x)))))
proc.time() - pt
##
      user system elapsed
     9.413
            0.319
                      4.089
# report results
round(sim_means, 4)
##
               OLS
                        K5
                                K10
                                          Kn
## Loss 1 4.0450 2.9931 3.0588 3.0588
## Loss 2 23.4672 21.1195 21.9358 21.9358
round(sim_se, 4)
##
             OLS
                      K5
                             K10
                                     Kn
## Loss 1 0.0835 0.2739 0.1987 0.1987
## Loss 2 1.4640 1.2852 0.2253 0.2253
(c)
# set parameters
p < -200
theta \leftarrow 0.5
# generate data
beta_star <- rnorm(p, 0, sigma_star)</pre>
SIGMA <- outer(1:(p - 1), 1:(p - 1), FUN = function(a, b) theta^abs(a - b))
X \leftarrow cbind(1, rmvn(n, p - 1, 0, SIGMA))
# simulation
pt <- proc.time()</pre>
registerDoParallel(cores = 4)
sim <- foreach(1:nsims, .combine = cbind) %dopar% {</pre>
  y <- X %*% beta_star + rnorm(n, 0, sigma_star)
```

```
\# compute OLS estimates (lambda = 0)
  ols_fit <- ridge_coef(X, y, 0)</pre>
  coef_list[[1]] <- c(ols_fit$b1, ols_fit$b)</pre>
  \# compute the cross-validated ridge estimates for each K
  coef_list[2:(length(Ks) + 1)] <- sapply(Ks, function(k) {</pre>
    rcv <- ridge_cv(X, y, lam.vec = lams, K = k)</pre>
    list(coefs = c(rcv$b1, rcv$b))
  })
  11 <- sapply(coef_list, function(b) loss1(beta_star, b))</pre>
  12 <- sapply(coef_list, function(b) loss2(X, beta_star, b))</pre>
  list(11, 12)
sim_loss <- lapply(1:nrow(sim), function(i) sapply(sim[i,], function(s) s))</pre>
names(sim_loss) <- c("Loss 1", "Loss 2")</pre>
sim_means <- t(sapply(sim_loss, function(s) rowMeans(s)))</pre>
sim_se <- t(
  sapply(sim_loss, function(s) apply(s, 1, function(x) sd(x)/sqrt(length(x)))))
proc.time() - pt
      user system elapsed
##
## 87.765
            3.161 59.303
# report results
round(sim_means, 4)
##
               OLS
                        К5
                                K10
                                          Kn
## Loss 1 47.2441 47.0716 47.1331 47.4372
## Loss 2 49.3878 49.3879 50.2006 60.9522
round(sim_se, 4)
##
              OLS
                      K5
                            K10
                                     Kn
## Loss 1 0.2667 0.0476 0.0387 0.2027
## Loss 2 4.3178 4.3177 4.1894 5.7437
(d)
# set parameters
p <- 200
theta <- 0.9
# generate data
beta_star <- rnorm(p, 0, sigma_star)</pre>
SIGMA <- outer(1:(p - 1), 1:(p - 1), FUN = function(a, b) theta^abs(a - b))
X \leftarrow cbind(1, rmvn(n, p - 1, 0, SIGMA))
# simulation
pt <- proc.time()
registerDoParallel(cores = 4)
sim <- foreach(1:nsims, .combine = cbind) %dopar% {</pre>
```

```
y <- X ** beta_star + rnorm(n, 0, sigma_star)
  # compute OLS estimates (lambda = 0)
  ols_fit <- ridge_coef(X, y, 0)</pre>
  coef_list[[1]] <- c(ols_fit$b1, ols_fit$b)</pre>
  # compute the cross-validated ridge estimates for each K
  coef list[2:(length(Ks) + 1)] <- sapply(Ks, function(k) {</pre>
    rcv <- ridge_cv(X, y, lam.vec = lams, K = k)</pre>
    list(coefs = c(rcv$b1, rcv$b))
  })
  11 <- sapply(coef_list, function(b) loss1(beta_star, b))</pre>
  12 <- sapply(coef_list, function(b) loss2(X, beta_star, b))
  list(11, 12)
}
sim_loss <- lapply(1:nrow(sim), function(i) sapply(sim[i,], function(s) s))</pre>
names(sim_loss) <- c("Loss 1", "Loss 2")</pre>
sim_means <- t(sapply(sim_loss, function(s) rowMeans(s)))</pre>
sim_se <- t(
  sapply(sim_loss, function(s) apply(s, 1, function(x) sd(x)/sqrt(length(x)))))
proc.time() - pt
      user system elapsed
## 123.455
             4.517 44.646
# report results
round(sim_means, 4)
##
               OLS
                        K5
                               K10
## Loss 1 47.0701 46.7023 47.0125 46.6204
## Loss 2 43.5539 41.6447 43.9821 40.9527
round(sim se, 4)
##
             OI.S
                      K5
                            K10
                                     Kn
## Loss 1 0.1591 0.2718 0.2520 0.2054
## Loss 2 1.2297 0.2172 3.6758 0.8716
```

(a)

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

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

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

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

as desired.

(b)

We first consider the objective function in terms of β . We find the Hessian with respect to β

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

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

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

and so our objective function $g(\beta, \sigma^2)$ is convex in β . Now, considering the Hessian with respect to σ^2 ,

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

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

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

As a counterexample consider the following data

```
set.seed(124)
n <- 20
p <- 100
beta <- rep(0.1, p)
sigma <- sqrt(2)

Xtilde <- matrix(rnorm(n * p), nrow = n)
eps <- rnorm(n, 0, sigma^2)</pre>
```

```
ytilde <- Xtilde %*% beta + eps

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

[1] 55.03599

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 our first order condition

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

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

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

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

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

$$= \frac{n}{2\sigma^2} - \frac{1}{2\sigma^4} \|\tilde{Y} - \tilde{X}\bar{\beta}\|_2^2$$

$$= \frac{n}{2\sigma^2} - \frac{1}{2\sigma^4} \|\tilde{Y} - \tilde{Y}\|_2^2$$

$$= \frac{n}{2\sigma^2} = 0$$

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

(d)

Solving our first order conditions

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

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

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

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

```
ridge_coef_mle <- function(X, y, lam, tol = 1e-16) {
   Xm1 <- X[,-1] # remove leading column of 1's marking the intercept

ytilde <- y - mean(y) # center response
   xbar <- colMeans(Xm1) # find predictor means
   Xtilde <- sweep(Xm1, 2, xbar) # center each predictor according to its mean

# compute the SVD on the centered design matrix

Xtilde_svd <- svd(Xtilde)
   U <- Xtilde_svd$d
   V <- Xtilde_svd$d
   V <- Xtilde_svd$v

## generate some initial guess for sigma and beta
   sig0 <- rexp(1)
   Dstar <- diag(d/(d^2 + sig0^2 * lam))</pre>
```

```
b0 <- V ** (Dstar ** crossprod(U, ytilde))
  i <- 1
  repeat {
    # update sigma and beta
    sig_new <- sqrt(1/n * crossprod(ytilde - Xtilde %*% b0))</pre>
    Dstar <- diag(d/(d^2 + sig_new^2 * lam))</pre>
    b_new <- V %*% (Dstar %*% crossprod(U, ytilde))</pre>
    if (abs(sig_new^2 - sig0^2) < tol)</pre>
      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) {</pre>
  n \leftarrow nrow(X)
  Xm1 <- X[,-1] # remove leading column of 1's marking the intercept
  ytilde <- y - mean(y) # center response</pre>
  xbar <- colMeans(Xm1) # find predictor means</pre>
 Xtilde <- sweep(Xm1, 2, xbar) # center each predictor according to its mean</pre>
  gb <- 1/s^2 * crossprod(Xtilde, Xtilde %*% b - ytilde) + lam * b
  gs \langle -n/(2 * s^2) - 1/(2 * s^4) * crossprod(ytilde - Xtilde %*% b)
  c(grad_b = gb, grad_s = gs)
```

(f)

```
set.seed(124)
n <- 100
p <- 5
lam <- 1
beta_star <- (-1)^{(1:p)} * rep(5, p)
sigma_star <- sqrt(1/2)
X \leftarrow 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)</pre>
rcm
## $niter
## [1] 9
##
## $sigma
## [1] 0.6559084
##
## $b
```

```
## [1,1]
## [1,] 4.976904
## [2,] -5.000078
## [3,] 4.888082
## [4,] -5.017066
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.

(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 $(b_j - \beta_{j-1})^2$. One way to get around this is to define vector $B \in \mathbb{R}^{p-1}$ given by

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

Then

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

In order to achieve our task of expressing the fused sum in terms of the vector β we must next decompose B into a product of β and some matrix. To this end we 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.,

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

Then

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

Therefore, our objective function can be expressed as

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

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 \tilde{X}^TX and A^TA must be positive semi-definite. Thus, since $\lambda_1 > 0$, we find that our sum $\tilde{X}^T\tilde{X} + \lambda_1\mathbb{I}_{p-1} + \lambda_2A^TA = \nabla^2 f(\beta)$ is positive semi-definite, and so $f(\beta)$ must be strictly convex, as desired.

(b)

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

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

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

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

and

$$\operatorname{Var}\left(\hat{\beta}_{-1}^{(\lambda_{1}, \lambda_{2})}\right) = \operatorname{Var}\left(M\tilde{X}^{T}Y\right)$$
$$= M\tilde{X}^{T}\operatorname{Var}\left(\tilde{Y}\right)\tilde{X}M^{T}$$
$$= \sigma_{*}^{2}M\tilde{X}^{T}\tilde{X}M^{T}$$

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)

```
fused_ridge_coef <- function(X, y, lam1, lam2) {</pre>
  n \leftarrow nrow(X); p \leftarrow ncol(X)
  Xm1 \leftarrow X[,-1] # remove leading column of 1's marking the intercept
  ytilde <- y - mean(y) # center response</pre>
  xbar <- colMeans(Xm1) # find predictor means</pre>
  Xtilde <- sweep(Xm1, 2, xbar) # center each predictor according to its mean
  I \leftarrow diag(p - 1)
  UD <- cbind(rep(0, p - 2), diag(p - 2)) # upper diagonal matrix
  J \leftarrow -1 * cbind(diag(p - 2), rep(0, p - 2)) # diag(p - 2)*(p - 1) matrix
  A \leftarrow J + UD
  M <- solve(crossprod(Xtilde) + lam1 * I + lam2 * crossprod(A))</pre>
  b <- M %*% crossprod(Xtilde, y)
  b0 <- mean(y) - crossprod(xbar, b)
  return(list(b0 = b0, b = b))
fused_ridge_coef_params <- function(X, lam1, lam2, beta, sigma) {</pre>
  # omits intercept term b0
  # returns theoretical means and variances for the fused ridge problem
  n <- nrow(X); p <- ncol(X)</pre>
  Xm1 \leftarrow X[,-1] # remove leading column of 1's marking the intercept
  betam1 <- beta[-1] # remove intercept term</pre>
  xbar <- colMeans(Xm1) # find predictor means</pre>
  Xtilde <- sweep(Xm1, 2, xbar) # center each predictor according to its mean
  I \leftarrow diag(p - 1)
  UD <- cbind(rep(0, p - 2), diag(p - 2)) # upper diagonal matrix
  J \leftarrow -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 <pre>%*% crossprod(Xtilde, (Xtilde %*% betam1))
  vcv \leftarrow matrix(0, nrow = p - 1, ncol = p - 1)
  if (n > p) { # when n > p this matrix multiplication routine is quicker
    vcv <- sigma^2 * M %*% tcrossprod(crossprod(Xtilde), M)</pre>
  \} else { # when p > n this matrix multiplication routine is quicker
   vcv <- sigma^2 * tcrossprod(M, Xtilde) %*% tcrossprod(Xtilde, M)</pre>
  list(b = b, vcv = vcv)
```

}

We now simulate some data to test our estimates:

```
set.seed(124)
# set parameters
nsims <- 1e4
n <- 1e2
p <- 5
lam1 <- 1
lam2 <- 1
sigma star <- 1
beta_star <- rnorm(p)</pre>
# generate (fixed) design matrix
X \leftarrow cbind(rep(1, n), matrix(rnorm(n * (p - 1)), nrow = n, ncol = p - 1))
# compute expected parameter values
par_true <- fused_ridge_coef_params(X, lam1, lam2, beta_star, sigma_star)</pre>
b_true <- as.vector(par_true$b)</pre>
vcv_true <- par_true$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()</pre>
b_hat <- replicate(nsims, {</pre>
  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
##
     1.636
            0.016
                    1.664
# estimate variance of b2, ..., b_p estimates
vcv_hat <- var(t(b_hat))</pre>
# print estimated fused ridge coefficients vs. expected values
b <- rbind(rowMeans(b_hat), b_true)</pre>
rownames(b) <- c("b_hat", "b_true")</pre>
round(b, 4)
##
            [,1]
                     [,2]
                            [,3]
                                    [,4]
## b hat 0.0316 -0.7226 0.2226 1.3899
## b_true 0.0313 -0.7240 0.2235 1.3920
# print absolute error between estimated and true fused ridge variances
round(abs(vcv_true - vcv_hat), 4)
##
         [,1] [,2] [,3] [,4]
## [1,] 2e-04 1e-04 1e-04 1e-04
## [2,] 1e-04 1e-04 1e-04 2e-04
## [3,] 1e-04 1e-04 0e+00 1e-04
## [4,] 1e-04 2e-04 1e-04 3e-04
```

As a case study, we may look at the simulations of $\hat{\beta}_2^{(\lambda_1,\lambda_2)}$ and compare it with it's 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.



