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 find

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

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

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

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, 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 $v \in \mathbb{R}^{p-1}$,

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

Hence,

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

and so 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, $U^TU = \mathbb{I}_n$, $V^TV = \mathbb{I}_{p-1}$, 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. Hence,

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

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

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

so that

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

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

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

  ytilde <- y - mean(y) # center response
  xbar <- colMeans(Xm1) # find predictor means
  # center each predictor according to its mean
  Xtilde <- Xm1 - tcrossprod(rep(1, nrow(Xm1)), 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

  # 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)) # slopes
  b1 <- mean(y) - crossprod(xbar, b) # intercept
  list(b1 = b1, b = b)
}
```

Note the choice to use `V %*% (Dstar %*% crossprod(U, ytilde))` to compute the matrix product $VD^*U^T\tilde{Y}$ as opposed to (the perhaps more intuitive) `V %*% Dstar %*% t(U) %*% ytilde`. Such a choice is empirically justified in an appendix.

(e)

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

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

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

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

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

We next compute the variance of our centered ridge estimates

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

[1] Benchmarks are provided in an appendix for the cases of large n, large p, and $n \approx p$.

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

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

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 $\text{Var}\left(\hat{\beta}_{-1}^{(\lambda)}\right)$. 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) {
  n <- nrow(X); p <- ncol(X)
  betam1 <- beta[-1] # remove intercept term
  Xm1 <- X[,-1] # remove leading column of 1's in our design matrix

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

  if (n >= p) {
    I <- diag(p - 1)
    inv <- solve(crossprod(Xtilde) + lam * I)

    b <- solve(crossprod(Xtilde) + lam * I) %*% (crossprod(Xtilde) %*% betam1)
    vcv <- sigma^2 * inv %*% crossprod(Xtilde) %*% inv
    list(b = b, vcv = vcv)

  } else {
    # compute SVD on the centered design matrix
    Xtilde_svd <- svd(Xtilde)
    d <- Xtilde_svd$d
    V <- Xtilde_svd$v

    Dstar <- diag(d^2/(d^2 + lam))
    Dstar2 <- 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
```

```r
beta_star <- 1:p
sigma_star <- 1

# generate fixed design matrix
X <- 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)
b_true <- as.vector(par_true$b)
vcv_true <- par_true$vcv

# simulate ridge coefficients nsims times
# outputs a matrix with rows corresponding to coefficients
# and columns correspond to simulation number
b_hat <- replicate(nsims, {
  y <- X %*% beta_star + rnorm(n, 0, sigma_star)
  as.vector(ridge_coef(X, y, lam)$b)
})

# estimate variance of b1, ..., 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]   [,5]   [,6]
## 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
```

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

```
##        [,1]   [,2]   [,3]   [,4]   [,5]   [,6]
## [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.

Question 3

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

```r
ridge_cv_lam <- function(X, y, lam, K) {
  # Helper function for ridge_cv()
  # perform K-fold cross-validation on the ridge regression
  # estimation problem over a single tuning parameter lam
  n <- nrow(X)
```

```r
  if (K > n) {
    stop(paste0("K > ", n, "."))
  } else if (K < 2) {
    stop("K < 2.")
  }

  # groups to cross-validate over
  folds <- cut(1:n, breaks = K, labels = F)
  # get indices of training subset
  train_idxs <- lapply(1:K, function(i) !(folds %in% i))

  cv_err <- sapply(train_idxs, function(tr_idx) {
    # train our model, extract fitted coefficients
    b_train <- unlist(ridge_coef(X[tr_idx,], y[tr_idx], lam))

    # fit testing data
    yhat <- X[!tr_idx,] %*% b_train
    # 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:

```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)

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

  # extract best tuning parameter and 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 set some global libraries/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
```

```r
  # 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)
loss2 <- function(X, beta, b) sum((X %*% (beta - b))^2)
```

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

```r
set.seed(124)

# 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")
```

(a)

```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 = 3)

sim <- foreach(1:nsims, .combine = cbind) %dopar% {
  y <- X %*% beta_star + rnorm(n, 0, sigma_star)

  ols_fit <- ridge_coef(X, y, 0)
  coef_list[[1]] <- c(ols_fit$b1, ols_fit$b)

  coef_list[2:(length(Ks) + 1)] <- sapply(Ks, function(k) {
    rcv <- ridge_cv(X, y, lam.vec = lams, K = k)
    list(coefs = c(rcv$b1, rcv$b))
  })

  l1 <- sapply(coef_list, function(b) loss1(beta_star, b))
  l2 <- sapply(coef_list, function(b) loss2(X, beta_star, b))
  list(l1, l2)
}
```

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

sim_means <- t(sapply(sim_loss, function(s) rowMeans(s)))
sim_se <- t(
  sapply(sim_loss, function(s) apply(s, 1, function(x) sd(x)/sqrt(length(x)))))
proc.time() - pt
```

```
##    user  system elapsed
##  28.568   0.460  21.108
```

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

```
##            OLS      K5     K10      Kn
## Loss 1  0.9810  0.9019  0.8464  0.9275
## Loss 2 23.9665 22.8950 22.2139 23.5021
```

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

```
##           OLS     K5    K10     Kn
## Loss 1 0.3363 0.2786 0.2068 0.2676
## Loss 2 4.6200 4.0621 3.6654 3.6523
```

(b)

```r
# 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))
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)

  ols_fit <- ridge_coef(X, y, 0)
  coef_list[[1]] <- c(ols_fit$b1, ols_fit$b)

  coef_list[2:(length(Ks) + 1)] <- sapply(Ks, function(k) {
    rcv <- ridge_cv(X, y, lam.vec = lams, K = k)
    list(coefs = c(rcv$b1, rcv$b))
  })

  l1 <- sapply(coef_list, function(b) loss1(beta_star, b))
  l2 <- sapply(coef_list, function(b) loss2(X, beta_star, b))
  list(l1, l2)
}
```

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

sim_means <- t(sapply(sim_loss, function(s) rowMeans(s)))
sim_se <- t(
  sapply(sim_loss, function(s) apply(s, 1, function(x) sd(x)/sqrt(length(x)))))
proc.time() - pt
```

```
##    user  system elapsed
##  39.548   0.574  15.063
```

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

```
##            OLS      K5     K10      Kn
## Loss 1  4.8646  3.5062  3.5062  3.5062
## Loss 2 26.9360 24.3441 24.3441 24.3441
```

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

```
##           OLS     K5    K10     Kn
## Loss 1 1.1021 0.2385 0.2385 0.2385
## Loss 2 2.2743 2.6142 2.6142 2.6142
```

(c)

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

  ols_fit <- ridge_coef(X, y, 0)
  coef_list[[1]] <- c(ols_fit$b1, ols_fit$b)

  coef_list[2:(length(Ks) + 1)] <- sapply(Ks, function(k) {
    rcv <- ridge_cv(X, y, lam.vec = lams, K = k)
    list(coefs = c(rcv$b1, rcv$b))
  })

  l1 <- sapply(coef_list, function(b) loss1(beta_star, b))
  l2 <- sapply(coef_list, function(b) loss2(X, beta_star, b))
  list(l1, l2)
}
```

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

sim_means <- t(sapply(sim_loss, function(s) rowMeans(s)))
sim_se <- t(
  sapply(sim_loss, function(s) apply(s, 1, function(x) sd(x)/sqrt(length(x)))))
proc.time() - pt
```

```
##    user  system elapsed
## 152.209   2.752  80.261
```

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

```
##            OLS      K5     K10      Kn
## Loss 1 47.8517 47.1939 47.2239 47.5534
## Loss 2 46.7702 46.7702 46.4305 56.4192
```

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

```
##           OLS     K5    K10      Kn
## Loss 1 0.3406 0.1585 0.1803  0.3893
## Loss 2 4.9703 4.9703 5.2712 13.0995
```

(d)

```r
# set parameters
p <- 200
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))
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)

  ols_fit <- ridge_coef(X, y, 0)
  coef_list[[1]] <- c(ols_fit$b1, ols_fit$b)

  coef_list[2:(length(Ks) + 1)] <- sapply(Ks, function(k) {
    rcv <- ridge_cv(X, y, lam.vec = lams, K = k)
    list(coefs = c(rcv$b1, rcv$b))
  })

  l1 <- sapply(coef_list, function(b) loss1(beta_star, b))
  l2 <- sapply(coef_list, function(b) loss2(X, beta_star, b))
  list(l1, l2)
}
```

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

sim_means <- t(sapply(sim_loss, function(s) rowMeans(s)))
sim_se <- t(
  sapply(sim_loss, function(s) apply(s, 1, function(x) sd(x)/sqrt(length(x)))))
proc.time() - pt
```

```
##    user  system elapsed
## 204.336   4.321  80.208
```

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

```
##            OLS      K5     K10      Kn
## Loss 1 47.0857 46.7890 47.3856 47.1591
## Loss 2 56.5290 54.1721 58.2390 55.9134
```

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

```
##           OLS     K5    K10     Kn
## Loss 1 0.0478 0.0916 0.0829 0.2342
## Loss 2 5.6920 5.5685 4.2870 6.3636
```

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

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

as desired.

(b)

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

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

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

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

and so our objective function $g\left(\beta, \sigma^2\right)$ is convex in β. Now, considering the Hessian 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, such a condition is equivalent to

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

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)
ytilde <- Xtilde %*% beta + eps

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

```
## [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 $\lambda > 0$,

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

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

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

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

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

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) {
  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$u
  d <- Xtilde_svd$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
  }
```

```r
  list(niter = i, sigma = as.numeric(sig_new), b = b_new)
}
grad_mle <- function(X, y, lam, b, s) {
  n <- nrow(X)
  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

  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)
rcm
```

```
## $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 $(b_j - \beta_{j-1})^2$. 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

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

Therefore, our objective function can be expressed 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 $\tilde{X}^T X$ and $A^T A$ must be positive semi-definite. Thus, since $\lambda_1 > 0$, we find that our sum $\tilde{X}^T\tilde{X} + \lambda_1\mathbb{I}_{p-1} + \lambda_2 A^T A = \nabla^2 f(\beta)$ 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 $\nabla f(\beta) = 0$

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

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)
  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

  I <- diag(p - 1)
  UD <- cbind(rep(0, p - 2), diag(p - 2)) # upper diagonal matrix
```

```r
  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, y)
  b0 <- mean(y) - crossprod(xbar, b)
  return(list(b0 = b0, b = b))
}
fused_ridge_coef_params <- function(X, lam1, lam2, beta, sigma) {
  # omits intercept term b0
  # returns theoretical means and variances for the fused ridge problem
  n <- nrow(X); p <- ncol(X)
  Xm1 <- X[,-1] # remove leading column of 1's marking the intercept
  betam1 <- beta[-1] # remove intercept term

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

  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 <- 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)
  } else { # when p > n this matrix multiplication routine is quicker
   vcv <- sigma^2 * tcrossprod(M, Xtilde) %*% tcrossprod(Xtilde, M)
  }

  return (list(b = b, vcv = vcv))
}
```

We now simulate some data to test our estimates:

```r
set.seed(124)

# set parameters
nsims <- 1e4
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_params(X, lam1, lam2, beta_star, sigma_star)
```

```r
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
  return (as.vector(fused_ridge_coef(X, y, lam1, lam2)$b))
})
proc.time() - pt
```

```
##    user  system elapsed
##   2.008   0.038   2.228
```

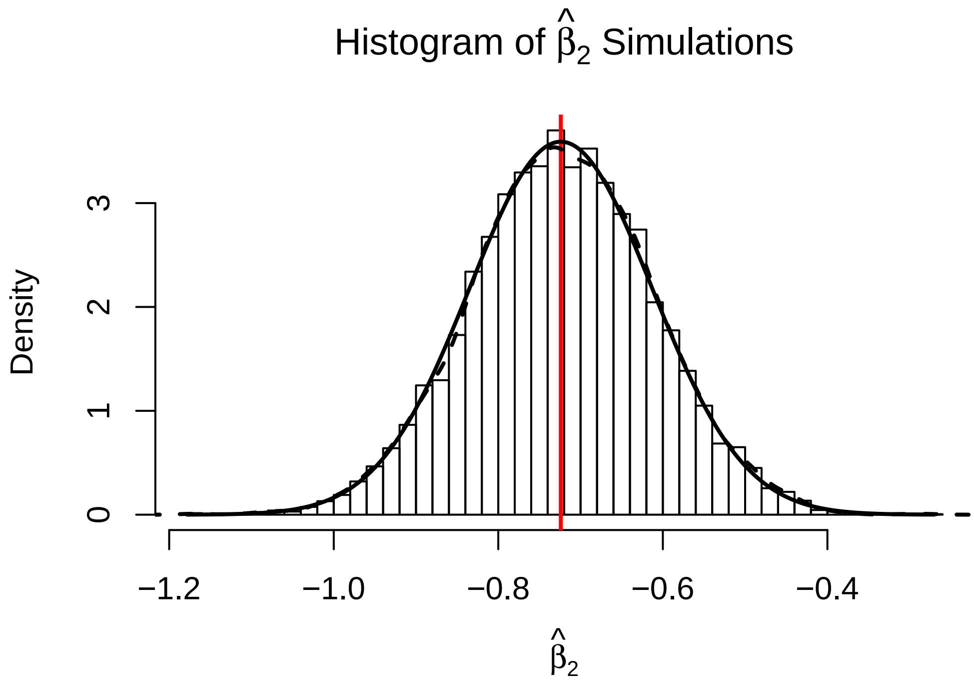
```r
# estimate variance of b2, ..., b_p estimates
vcv_hat <- var(t(b_hat))

# 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  0.0316 -0.7226 0.2226 1.3899
## 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,] 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.



Histogram of $\hat{\beta}_2$ Simulations
Density
0
1
2
3
−1.2
−1.0
−0.8
−0.6
−0.4
$\hat{\beta}_2$

Appendix

Computing $\mathbb{E}\left[\hat{\beta}^{(\lambda)}\right]$

Consider the case of $n >> p$

```
library(microbenchmark)
set.seed(124)

#===== Large n case =====#
# parameters
n <- 1e2
p <- 1e1
lam <- 1

# generate data
beta <- rnorm(p)
X <- matrix(rnorm(n * p), nrow = n)
I <- diag(p)

# define functions
f1 <- function() solve(crossprod(X) + lam * I) %*% (crossprod(X) %*% beta)
f2 <- function() {
  X_svd <- svd(X)
  V <- X_svd$v
  d <- X_svd$d
  Dstar <- diag(d^2/(d^2 + lam))
  V %*% (Dstar %*% crossprod(V, beta))
}

# test speed
microbenchmark(f1(), f2(), times = 1e3, unit = "us")
```

```
## Unit: microseconds
##  expr     min       lq      mean   median       uq      max neval
##  f1()  40.406  45.2640  59.62362  50.5840  60.1195 1507.324  1000
##  f2() 135.495 143.4655 188.29019 152.0155 185.9305 3465.140  1000
```

and the case for $p >> n$

```
#===== Large p case =====#
# parameters
n <- 1e1
p <- 1e2
lam <- 1

# generate data
beta <- rnorm(p)
X <- matrix(rnorm(n * p), nrow = n)
I <- diag(p)

# define functions
f1 <- function() solve(crossprod(X) + lam * I) %*% (crossprod(X) %*% beta)
f2 <- function() {
  X_svd <- svd(X)
```

```r
  V <- X_svd$v
  d <- X_svd$d
  Dstar <- diag(d^2/(d^2 + lam))
  V %*% (Dstar %*% crossprod(V, beta))
}

# test speed
microbenchmark(f1(), f2(), times = 1e3, unit = "us")
```

```
## Unit: microseconds
##  expr      min       lq      mean   median       uq       max neval
##  f1() 2506.339 2664.658 3283.0828 2926.610 3512.609 47840.314  1000
##  f2()  145.535  163.293  265.3074  204.044  254.235  3354.482  1000
```

and $n \approx p$

```r
#===== n ~ p case =====#
# parameters
n <- 1e2
p <- 1e2
lam <- 1

# generate data
beta <- rnorm(p)
X <- matrix(rnorm(n * p), nrow = n)
I <- diag(p)

# define functions
f1 <- function() solve(crossprod(X) + lam * I) %*% (crossprod(X) %*% beta)
f2 <- function() {
  X_svd <- svd(X)
  V <- X_svd$v
  d <- X_svd$d
  Dstar <- diag(d^2/(d^2 + lam))
  V %*% (Dstar %*% crossprod(V, beta))
}

# test speed
microbenchmark(f1(), f2(), times = 1e3, unit = "us")
```

```
## Unit: microseconds
##  expr      min       lq     mean   median       uq      max neval
##  f1() 3301.427 3531.346 4304.499 3859.514 4423.801 49950.40  1000
##  f2() 6352.193 6967.011 8418.279 7594.422 8421.103 78342.53  1000
```

Matrix Multiplication Timing

Consider the following matrix multiplication benchmarks (for the cases of $n >> p$ and $p >> n$).

```r
set.seed(124)
#===== Large n case =====#

# set parameters
n <- 1e3
p <- 1e2
```

```r
lam <- 1

# generate data
X <- matrix(rnorm(n * p), nrow = n)
beta <- rnorm(p)
eps <- rnorm(n)
y <- X %*% beta + eps

ytilde <- y - mean(y)
xbar <- colMeans(X)
Xtilde <- sweep(X, 2, xbar)

# compute decomposition
Xtilde_svd <- svd(Xtilde)
U <- Xtilde_svd$u
d <- Xtilde_svd$d
V <- Xtilde_svd$v
Dstar <- diag(d/(d^2 + lam))

# define multiplication functions
f1 <- function() V %*% Dstar %*% t(U) %*% ytilde
f2 <- function() V %*% Dstar %*% (t(U) %*% ytilde)
f3 <- function() V %*% (Dstar %*% (t(U) %*% ytilde))
f4 <- function() V %*% (Dstar %*% crossprod(U, ytilde))
f5 <- function() V %*% crossprod(Dstar, crossprod(U, ytilde))

# test speed
microbenchmark(f1(), f2(), f3(), f4(), f5(), times = 100, unit = "us")
```

```
## Unit: microseconds
##   expr      min        lq       mean     median         uq       max neval
##   f1() 8720.848 9472.4135 10389.9466 10122.5155 10707.7265 16967.431   100
##   f2() 1114.408 1237.5495  1891.0480  1337.1565  1558.2230 40934.177   100
##   f3()  372.685  430.0735  1103.3505   499.9840   691.5555 42471.462   100
##   f4()  130.378  137.2480   173.1447   148.9335   166.1345   894.318   100
##   f5()  126.691  132.2650   161.7938   146.5435   158.6385   622.646   100
```

```r
#===== Large p case =====#
set.seed(124)

# set parameters
n <- 1e2
p <- 1e3
lam <- 1

# generate data
X <- matrix(rnorm(n * p), nrow = n)
beta <- rnorm(p)
eps <- rnorm(n)
y <- X %*% beta + eps

# define multiplication functions
f1 <- function() V %*% Dstar %*% t(U) %*% ytilde
f2 <- function() V %*% Dstar %*% (t(U) %*% ytilde)
```

```r
f3 <- function() V %*% (Dstar %*% (t(U) %*% ytilde))
f4 <- function() V %*% (Dstar %*% crossprod(U, ytilde))
f5 <- function() V %*% crossprod(Dstar, crossprod(U, ytilde))

# test speed
microbenchmark(f1(), f2(), f3(), f4(), f5(), times = 100, unit = "us")
```

```
## Unit: microseconds
##  expr      min        lq       mean     median         uq       max neval
##  f1() 8576.944 9480.5695 10784.6446 10185.4260 10963.1265 21535.895   100
##  f2() 1106.382 1233.4500  2057.1389  1390.1810  1664.4140 52760.203   100
##  f3()  370.962  433.2255   728.0709   508.0305   617.6325  6043.718   100
##  f4()  130.610  137.8785   161.3811   150.8340   165.2900   280.387   100
##  f5()  126.571  134.1715   165.9973   151.9625   168.1125   553.625   100
```