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
  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

  # 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
  return (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.

```r
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
  Xtilde <- sweep(Xm1, 2, xbar) # center each predictor according to its mean

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

We may now perform our simulation.

```r
set.seed(124)

# set parameters
nsims <- 1e3
n <- 25
p <- 7
lam <- 4
beta_star <- 1:p
```

```r
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)
  return (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_fit <- function(X, y, lam) {
  # fully fit a ridge regression model given predictors, response, and penalty

  b <- unlist(ridge_coef(X, y, lam)) # extract coefficient estimates
  yhat <- X %*% b # fit a response estimate given fitted coefficients
  res <- sum((y - yhat)^2) # find prediction error

  return (list(X = X, y = y, lam = lam, coef = b, fit = yhat, res = res))
}

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

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

  # groups to cross-validate over
  folds <- cut(1:nrow(X), breaks = K, labels = F)
  train_grps <- lapply(1:K, function(i) which(!(1:K %in% i)))
  # get indices of our training subsets
  train_idxs <- lapply(train_grps, function(tgs) which(folds %in% tgs))

  cv_err <- sapply(train_idxs, function(tis) {
    # train our model
    train_fit <- ridge_fit(X[tis,], y[tis], lam)

    # find observations needed for testing fits
    test_idx <- which(!((1:n) %in% tis))

    # extract fitted coefficients
    b <- train_fit$coef
    # fit data
    yhat <- X[test_idx,] %*% b
    # compute test error
    sum((y[test_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
}
```

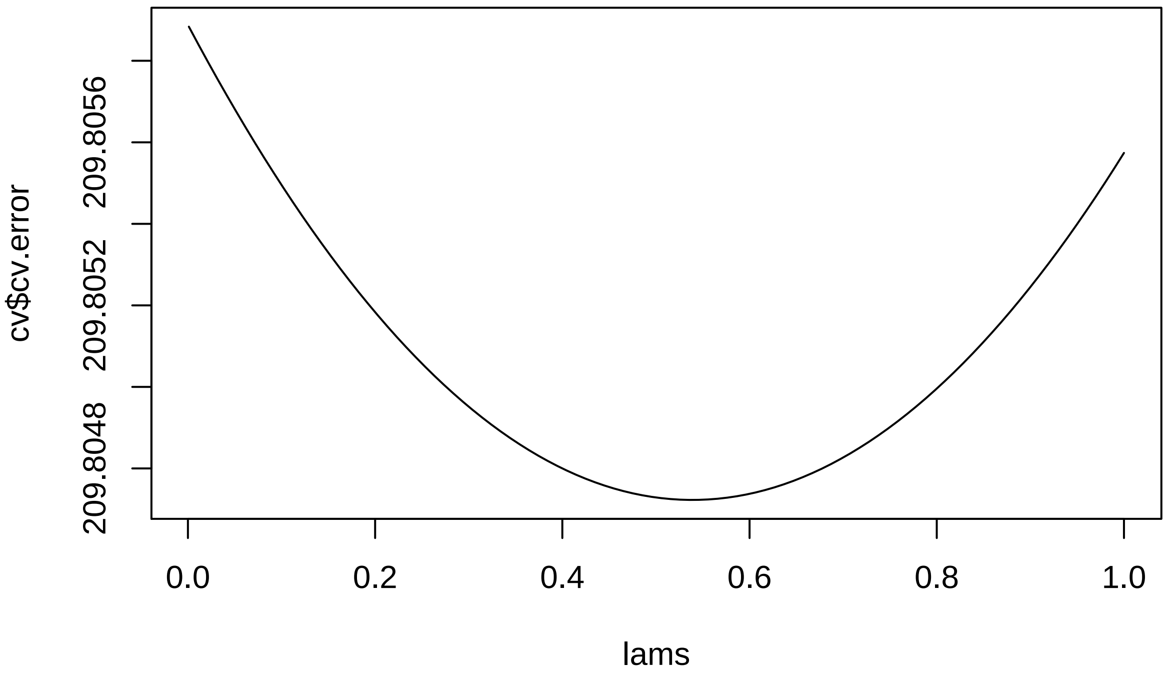
Then, our cross-validation function is as follows:

```
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); L <- length(lam.vec)

  cv.error <- vector(mode = "numeric", length = L)
  for (i in 1:L) {
    cv.error[i] <- ridge_cv_lam(X, y, lam.vec[i], K)
  }

  best.lam <- lam.vec[which(cv.error == min(cv.error))]
  best.fit <- ridge_fit(X, y, best.lam)
  b1 <- best.fit$coef[1]
  b <- best.fit$coef[-1]

  return (list(b1 = b1, b = b, best.lam = best.lam, cv.error = cv.error))
}
```

```
set.seed(124)
n <- 1e3
p <- 3
beta <- 1:p
sigma <- 1
K <- 5
lams <- seq(0.001, 1, length.out = 100)

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

pt <- proc.time()
cv <- ridge_cv(X, y, lams, K)
proc.time() - pt
```

```
##    user  system elapsed
##   0.342   0.008   0.364
```

```
plot(cv$cv.error ~ lams, type = 'l')
```



Question 4

For this problem we first define some additional functions and set some global parameters which remain constant across (a)-(d)

```r
set.seed(124)

# global parameters
nsims <- 50
lams <- 10^seq(-8, 8, 0.5)
sigma_star <- sqrt(1/2)
```

(a)

```r
# set parameters
n <- 100
p <- 50
theta <- 0.5

# generate data
beta_star <- rnorm(p, 0, sigma_star)
Z <- matrix(rnorm(n * (p - 1)), nrow = n, ncol = p - 1) # indep. normal deviates
SIGMA <- outer(1:(p - 1), 1:(p - 1), FUN = function(a, b) theta^abs(a - b))
C <- chol(SIGMA)
X <- cbind(rep(1, n), Z %*% C) # correlated normal deviates

# simulate noise and response
sim <- replicate(nsims, {
  eps <- rnorm(n, 0, sigma_star)
  y <- X %*% beta_star + eps

})
```

(b)

(c)

(d)

Question 5

(a)

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

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

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

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

(b)

(c)

(d)

(e)

(f)

Question 6

(a)

Consider our objective function

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

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 $\left(b_j - \beta_{j-1}\right)^2$. 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

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

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
  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)
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
##   1.728   0.025   1.790
```

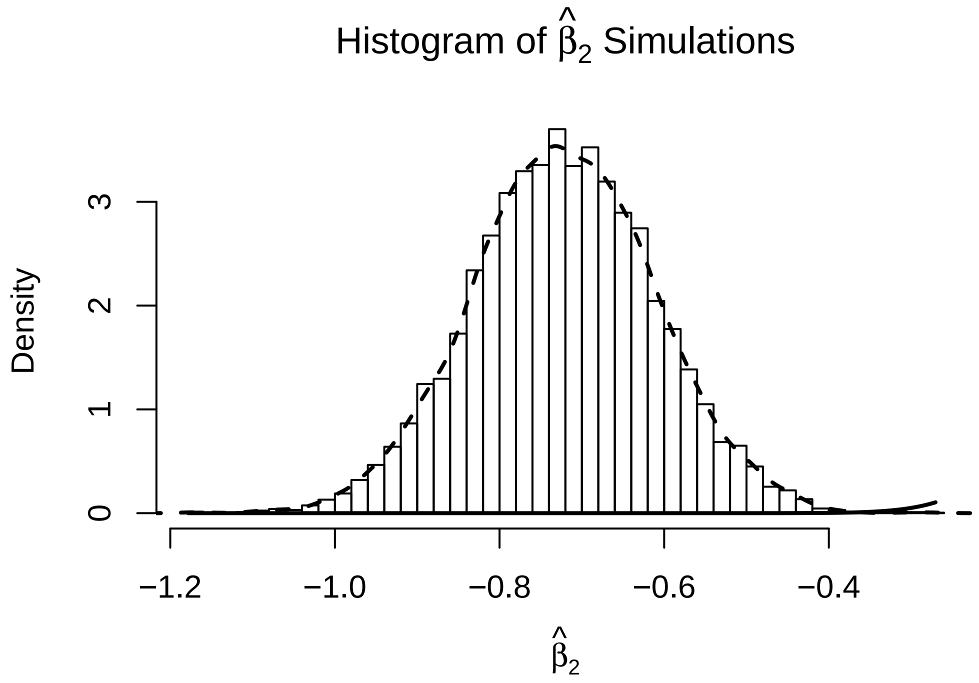
```r
# estimate variance of b2, ..., b_p estimates
vcv_hat <- var(t(b_hat))

# 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.



Appendix

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

Consider the case of $n >> p$

```r
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()  40.134  43.8105  55.05968  47.9220  52.669 1123.733  1000
##   f2() 134.212 140.1685 172.32382 143.8035 153.872 2612.723  1000
```

and the case for $p >> n$

```r
#===== 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)
  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() 2502.892 2670.0440 3108.3987 2882.606 3236.966 39843.969  1000
##  f2()  143.744  159.3665  214.3261  187.310  235.229  1420.855  1000
```

and $n \approx p$

```
#===== 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() 3296.854 3472.305 3966.685 3750.748 4173.743 40217.25  1000
##  f2() 6316.863 6732.056 7388.102 7087.233 7721.514 43120.50  1000
```

Matrix Multiplication Timing

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

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

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

```
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() 8664.317 9653.2800 10880.7200 10213.2025 11094.3265 47260.812   100
##   f2() 1102.176 1250.0655  1948.5505  1409.0820  1793.5275 37734.267   100
##   f3()  366.983  436.9275   670.0132   504.2995   678.0130  1868.955   100
##   f4()  129.898  148.2585   172.6657   160.0640   173.4555   368.257   100
##   f5()  127.400  143.3425   162.5338   151.1950   162.2450   580.183   100
```

```
#===== 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)
```

```
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() 8724.069 9712.4400 10415.9528 10367.2740 10988.8920 13098.456   100
##  f2() 1099.808 1185.5055  1886.2096  1325.1940  1561.3610 37591.452   100
##  f3()  359.874  427.9355  1386.9447   491.8890   610.4375 37465.479   100
##  f4()  130.079  142.3410   168.1796   155.1185   170.4025   671.296   100
##  f5()  126.181  133.7765   164.1720   147.9280   161.5120   997.785   100
```