Assignment 1

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DON'T FORGET TO UNCOMMENT Q4

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

  # compute the SVD on the centered design matrix
  Xtilde_svd <- svd(Xtilde)
```

```r
  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 $\left\{\frac{d_j^2}{(d_j^2+\lambda)^2}\right\}_{j=1}^{\min(n,p-1)}$ 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
  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
    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
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)
  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)

  if (K > n) {
```

```r
    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(tis) {
    # train our model, extract fitted coefficients
    b_train <- unlist(ridge_coef(X[tis,], y[tis], lam))

    # find observations needed for testing fits
    test_idx <- !((1:n) %in% tis)
    # fit data
    yhat <- X[test_idx,] %*% b_train
    # 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:

```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

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

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

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 $g\left(\beta, \sigma^2\right)$ is convex in β. Now, considering the Hessian with respect to σ^2,

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

For g to be convex in σ^2 we require $\nabla_{\sigma^2}^2 g\left(\beta, \sigma^2\right) \geq 0$. 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

```r
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))
n >= rhs
```

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

and so it is not the case that $\nabla^2_{\sigma^2} g\left(\beta, \sigma^2\right)$ is 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

```
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))
```

```r
  b0 <- V %*% (Dstar %*% crossprod(U, ytilde))

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

    if (abs(sig_new^2 - sig0^2) < tol)
      break

    sig0 <- sig_new
    b0 <- b_new
    i <- i + 1
  }
  list(niter = i, sigma = as.numeric(sig_new), b = b_new)
}
grad_mle <- function(X, y, lam, b, s) {
  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)

```
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
##   1.862   0.023   1.927
```

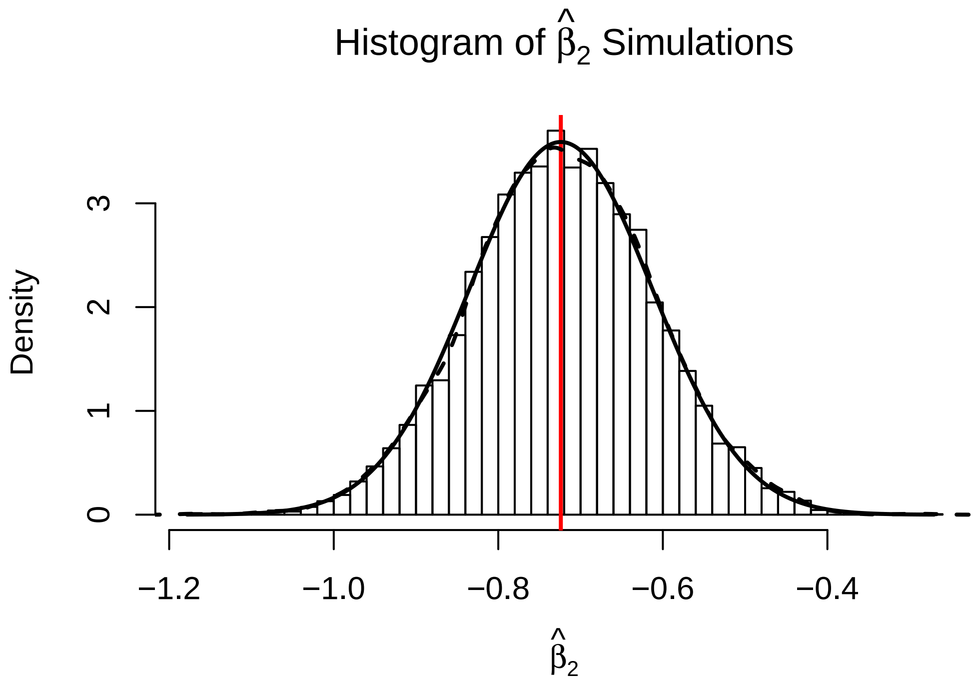
```r
# estimate variance of b2, ..., b_p estimates
vcv_hat <- var(t(b_hat))

# 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 $n >> p$

```
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()  40.372  44.2995  61.40828  49.5850  65.5915  437.949  1000
##  f2() 133.436 142.1035 192.80813 150.4875 192.9895 1808.623  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() 2508.989 2793.9725 3235.0076 3014.476 3376.9035 47197.359  1000
##  f2()  144.755  168.1655  251.1069  222.317  272.2155  2082.819  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() 3297.960 3592.409 4541.548 3931.411 4524.395 61611.97  1000
##  f2() 6325.234 6986.127 8254.252 7667.305 8528.119 62919.38  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() 8583.400 9425.3555 10699.1601 10104.0675 10990.2105 45616.497   100
##  f2() 1106.389 1240.4895  2028.6171  1396.7560  2073.7475 37677.972   100
##  f3()  366.287  418.3830   688.5485   494.5440   658.9570  2238.895   100
##  f4()  129.725  137.0815   171.1268   151.6555   168.7945  1051.026   100
##  f5()  126.731  131.0305   157.9678   148.3220   162.3690   413.771   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() 8543.140 9405.967 10143.3669 10144.878 10907.813 12869.605   100
##  f2() 1101.534 1183.899  2147.7061  1276.919  1573.379 35488.036   100
##  f3()  369.646  414.184   926.5855   487.932   561.038 35247.893   100
##  f4()  129.664  137.932   157.4483   149.375   165.022   363.137   100
##  f5()  126.205  131.436   157.5801   146.959   159.629   764.477   100
```