Model selection, unbiased estimators, and the Gauss-Markov theorem

MATH 697 AM:ST

Tuesday, September 19th
Let us recall a fundamental linear algebra fact

\[ M \text{ a self-adjoint linear operator } (M^t = M) \]

\[ \implies M \text{ is diagonal in some orthonormal basis} \]

In other words, symmetric matrices \( M \) are equivalent to a diagonal matrix under an orthogonal change of basis.
A symmetric matrix $M$ is said to be non-negative if all of its eigenvalues are non-negative.

Equivalently, $M$ is non-negative if

$$(Mv, v) \geq 0 \text{ for all } v \in \mathbb{R}^n.$$ 

Likewise, we say that $M \geq N$ if $M - N$ is non-negative.

In summary

$$M \geq N \iff (Mv, v) \geq (Nv, v) \text{ for all } v \in \mathbb{R}^n.$$
An important example: Covariance matrices of random vectors.

Let $X$ be a random vector in $\mathbb{R}^n$. Then, for $v, w \in \mathbb{R}^n$ define

$$\text{Cov}_X(v, w) = \mathbb{E}[(X - \mathbb{E}[X], v)(X - \mathbb{E}[X], w)]$$

This is a bilinear form that can be written as $(\Sigma_X v, w)$, where

$$(\Sigma_X)_{ij} = \mathbb{E}[(X_i - \mathbb{E}[X_i])(X_j - \mathbb{E}[X_j])]$$

(note that $\Sigma_X^t = \Sigma_X$ follows immediately from this formula)
Observe that given $v \in \mathbb{R}^d$, then the real random variable $(X, v)$ has mean $(\mathbb{E}[(X), v])$ and variance $\text{Cov}_X(v, v)$, since

$$\text{Cov}_X(v, v) = \mathbb{E}[((X, v) - (\mathbb{E}[X], v))^2]$$

In particular, given two random vectors $X$ and $X'$ in $\mathbb{R}^n$, when we say $X$ has smaller variance than $X'$, written as

$$\text{Cov}_X \leq \text{Cov}_{X'}$$

this simply means that for any $v$ we have the inequality

$$\text{Var}((X, v)) \leq \text{Var}((X', v))$$
Example: If $X = (X_1, X_2)$ where $X_i \sim N(0, \sigma^2)$ and the $X_i$ are uncorrelated, then

$$\Sigma_X = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

If $X' := (2X_1, 3X_2)$, then clearly $\text{Cov}(X') \geq \text{Cov}(X)$. 
Model Selection

**Problem:** All of the structures we have seen in the past two weeks come with some kind of complexity parameter. Once we decide on one of these structures, we face the following question: What is a judicious choice for

- ... the penalty parameter $\lambda$?
- ... the number and nature of basis functions?
- ... the size of the support for the kernel?
- ... the number of nearest neighbors considered?

In other words, what is the right amount of **smoothing**?
Higher Model Complexity $\Rightarrow$ Higher variance, lower bias.

For least squares the larger $p$, the more complexity. For $k$-NN the smaller the $k$, the more complexity.

Complexity is intrinsically connected with smoothness: their relationship is a tense one where one pulls against the other.
Model Selection
Training error versus Test error

Fix $N$ points $x_1, \ldots, x_N$, which are fixed and known. (so for simplicity we are assuming no randomness in the $x_i$).

Along with this, we have a training data set modeled by random observations

$$Y_1, \ldots, Y_N$$

yielding training data $\{(x_i, Y_i)\}_{i=1}^N$. A particular realization of this data $\{(x_i, y_i)\}_{i=1}^N$, we denote by $\mathcal{T}$.

Alternatively, we think of $\mathcal{T}$ as the event given by

$$\{Y_1 = y_1, \ldots, Y_N = y_n\}$$
We also fix a loss function $L(\hat{y}, y)$, typically it’s just the squared error

$$L(\hat{y}, y) = |\hat{y} - y|^2$$
Let $\hat{f}$ be a function which intends to estimate an unknown $f$.

The **training error** for $\hat{f}$ is defined as the quantity

$$
\frac{1}{N} \sum_{i=1}^{N} L(\hat{f}(x_i), y_i)
$$

Most commonly, in the case $L(\hat{y}, y) = |\hat{y} - y|^2$, it is given by

$$
\frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{f}(x_i))^2
$$
What is important to remember is the training error quantifies how closely $\hat{f}$ matches the training data it was used in its selection.

One can imagine a situation where the $\hat{f}$ we choose may have a very small training error, but tends to give large errors when tested against predictions outside the training data set.

This issue leads us to the notion of test error.
The **test error** for \( \hat{f} \), also known as the **generalization error** is a more subtle notion which is also more useful in assessing the accuracy of a predictive model.

It pressuposes a statistical model for the data, and it is given by

\[
\mathbb{E}[L(Y, \hat{f}(X)) \mid \mathcal{T}]
\]

Where \( \mathcal{T} \) corresponds to the training data \((x_i, y_i)\).

The quantity above corresponds to the average error we make when using \( \hat{f}(X) \) to estimate \( Y \), having sampled the training data \( \mathcal{T} \) and used it to select the function \( \hat{f} \).
...of course, if we take $L(\hat{y}, y) = |\hat{y} - y|^2$, then we obtain the expected squared prediction error, conditioned on $\mathcal{T}$,

$$E[|Y - \hat{f}(X)|^2 | \mathcal{T}]$$
Model Selection
Training error versus Test error

By the total expectation formula, we have in any case

$$\mathbb{E}[L(Y, \hat{f}(X))] = \mathbb{E}[\mathbb{E}[L(Y, \hat{f}(X)) \mid \mathcal{T}]]$$

Thus: the Expected Prediction Error ought to be understood as the expected value for the generalization error for $\mathcal{T}$, this being a random variable computed from the model $(X, Y)$ we have for our data, as well as the predictive model which generates $\hat{f}$ from a training set.
As the model becomes more and more complex, it uses the training data more and is able to adapt to more complicated underlying structures...
Model Selection

From Tibshirani, Hastie, and Friedman (p. 220-221):

...Hence there is a decrease in bias but an increase in variance. There is some intermediate model complexity that gives minimum expected test error.
Model Selection

From Tibshirani, Hastie, and Friedman (p. 220-221):

Unfortunately training error is not a good estimate of the test error, as seen in Figure 7.1.
They conclude, thusly:

*Training error consistently decreases with model complexity, typically dropping to zero if we increase the model complexity enough. However, a model with zero training error is overfit to the training data and will typically generalize poorly.*
Now, a more in-depth look at linear regression
Let us consider the additive model

\[ Y = f(X) + \varepsilon \]

and approximate \( f \) among affine functions

\[ \hat{f}(x) = \beta_0 + x \cdot \beta, \quad \beta_0 \in \mathbb{R}, \beta \in \mathbb{R}^p \]

(the "real" \( f \) may or may not be affine).

By data, we mean \( N \) samples \((X_i, Y_i)\ i = 1, \ldots, N\).
That is, there are random variables $Y_i, X_i$ and $\varepsilon_i$ satisfying

$$Y_i = \beta_0 + X_i \cdot \beta + \varepsilon_i$$

**Assumptions:** Assume that the $X_i$ are known and fixed (not random) and that the $\varepsilon_i$ all have mean zero, common variance $\sigma^2$ and are uncorrelated.
Least Squares’ Statistics

Distribution of $\hat{\beta}$

From the data $(X_i, Y_i)$ we recall the $N \times p$ matrix $X$

$$Xv = (X_1 \cdot v, \ldots, X_N \cdot v)$$

and the random vectors

$$y = (Y_1, \ldots, Y_N)$$
$$\bar{\varepsilon} = (\varepsilon_1, \ldots, \varepsilon_N)$$

Under these assumptions, we have the equation

$$y = X\beta + \bar{\varepsilon}$$
The least squares estimator for $\beta$, is the random vector

$$\hat{\beta} = (X^t X)^{-1} X^t y$$

A number of facts can be gleaned from the formula for $\hat{\beta}$, depending on what model assumptions we make about the data $$\{(x_1, y_1), \ldots, (x_N, y_N)\}$$
Least Squares’ Statistics
Distribution of $\hat{\beta}$

First, under the current assumptions (namely the $x_i$ being fixed and known and the $y_i$ being uncorrelated and with common variance $\sigma^2$) one can show that

$$E[\hat{\beta}] = \beta, \quad \text{Var}(\hat{\beta}) = (X^tX)^{-1}\sigma^2$$
Second, if one further assumes that $\varepsilon \sim \mathcal{N}(0, \sigma^2)$ and the $\varepsilon_i$ are independent, then

$$\hat{\beta} \sim \mathcal{N}(\beta, (X^t X)^{-1} \sigma^2)$$
The celebrated Gauss-Markov Theorem
This theorem says that the least squares estimator has the least variance among all linear estimators.

Let us explain what we mean by this.
First, let us repeat the assumptions.

For some $N$, we have $x_1, \ldots, x_N \in \mathbb{R}^p$, fixed and known vectors. Then, we have $N$ random variables

$$Y_i = x_i \cdot \beta + \varepsilon_i$$

The $\varepsilon_i$ are of mean zero and are pairwise uncorrelated. Then, our goal is to infer $\beta$ from the $Y_i$. Concretely, we are looking at estimators for $\beta$. 

The Gauss-Markov Theorem

Setup
Let us repeat the assumptions.

For some $N$, we have $x_1, \ldots, x_N \in \mathbb{R}^p$, fixed and known vectors. Then, we have the vector random variable $y$

$$y = X\beta + \bar{\varepsilon}$$

The $\bar{\varepsilon}$ is a zero-mean vector with covariance matrix $\sigma^2 I$

Then, our goal is to infer $\beta$ from $y$. Concretely, we are looking at estimators for $\beta$. 
The Gauss-Markov Theorem
Linear & unbiased estimators

An estimator $\tilde{\beta}$ is said to be **linear** if it has the form

$$\tilde{\beta} = Cy, \quad y = (Y_1, \ldots, Y_N) \in \mathbb{R}^N$$

where $C$ is some $p \times N$ matrix.

Recall that an estimator for a parameter is said to be **unbiased** if its expectation returns the parameter for all values of the parameter. In this context, this means that we always have

$$\mathbb{E}[Cy] = \beta$$
Going forward, let us use the notation

\[ L := (X^t X)^{-1} X^t \]

(the \( L \) stands for Least Squares). In this notation then, we have

\[ \hat{\beta} := Ly \]
The Gauss-Markov Theorem
Linear & unbiased estimators

As mentioned earlier, the least squares estimator is unbiased

**Proposition**

*If the \( x_i \) are fixed and \( \hat{\beta} \) is as above then for any \( \beta \) we have*

\[
\mathbb{E}[\hat{\beta}] = \beta
\]
The Gauss-Markov Theorem
Linear & unbiased estimators

**Proof.** Observe that $LX = I$, so

$$
\hat{\beta} = Ly = L(X\beta + \bar{\varepsilon})
= \beta + L\bar{\varepsilon}
$$

Since the entries of $L$ are non-random, we have

$$
\mathbb{E}[L\bar{\varepsilon}] = L\mathbb{E}[\bar{\varepsilon}] = 0
$$

Therefore, we always have $\mathbb{E}[\hat{\beta}] = \beta$. 
The Gauss-Markov Theorem

<table>
<thead>
<tr>
<th>Theorem</th>
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<tbody>
<tr>
<td>Among all unbiased linear estimators for $\beta$, the least squares estimator has the least variance.</td>
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</table>
The Gauss-Markov Theorem

In other words: if $C$ is a $p \times N$ matrix such that

$$\mathbb{E}[Cy] = \beta$$

Then,

$$\text{Cov}(Cy) \geq \text{Cov}(\hat{\beta}).$$
The Gauss-Markov Theorem

Equivalently, we have that for any vector \( v \in \mathbb{R}^p \),

\[
\text{Var}( (\tilde{\beta}, v) ) \geq \text{Var}( (\hat{\beta}, v) ) .
\]

where we are writing \( \tilde{\beta} = Cy \) and \( \hat{\beta} = Ly \)

Let us prove the theorem by showing the above inequality.
The Gauss-Markov Theorem

Fix $v \in \mathbb{R}^p$, then

$$E[(\tilde{\beta}, v)] = E[(\beta, v)] = (\beta, v)$$

Therefore,

$$Var((\tilde{\beta}, v)) = E[(\tilde{\beta} - \beta, v)^2]$$
$$Var((\hat{\beta}, v)) = E[(\hat{\beta} - \beta, v)^2]$$
Recall that \( y = X\beta + \bar{\epsilon} \), where \( \bar{\epsilon} = (\epsilon_1, \ldots, \epsilon_N) \).

Then,

\[
Cy = CX\beta + C\bar{\epsilon} \Rightarrow \mathbb{E}[Cy] = CX\beta
\]

It follows then that \( C \) yields an unbiased estimator if and only if

\[
CX = I
\]

(Note that, as it should be, we have \( LX = (X^tX)^{-1}X^tX = I \))
The Gauss-Markov Theorem

In any case, going forward, we keep in mind this:

\[ CX = I \]

We have also established that

\[ \hat{\beta} = \beta + L\bar{\epsilon}, \quad \tilde{\beta} = \beta + C\bar{\epsilon} \]

Let us use this to compute the variances of \((\hat{\beta}, v)\) and \((\tilde{\beta}, v)\)
The Gauss-Markov Theorem

We have that

\[ \text{Var}((\hat{\beta}, v)) = \mathbb{E}[(\hat{\beta} - \beta, v)^2] = \mathbb{E}[(\mathbf{L}\bar{\varepsilon}, v)^2] \]
\[ \text{Var}((\tilde{\beta}, v)) = \mathbb{E}[(\tilde{\beta} - \beta, v)^2] = \mathbb{E}[(\mathbf{C}\bar{\varepsilon}, v)^2] \]

what we need to prove is that

\[ \mathbb{E}[(\mathbf{L}\bar{\varepsilon}, v)^2] \leq \mathbb{E}[(\mathbf{C}\bar{\varepsilon}, v)^2] \]
The Gauss-Markov Theorem

Let us write one expectation in terms of the other:

\[
\mathbb{E}[(C\bar{\epsilon}, v)^2] = \mathbb{E}[(L\bar{\epsilon} + (C - L)\bar{\epsilon}, v)^2]
\]

\[
= \mathbb{E}[(L\bar{\epsilon}, v)^2] + \mathbb{E}[((C - L)\bar{\epsilon}, v)^2] + 2\mathbb{E}[(L\bar{\epsilon}, v)((C - L)\bar{\epsilon}, v)]
\]

**Claim:** In these circumstances, we have that

\[
\mathbb{E}[(L\bar{\epsilon}, v)((C - L)\bar{\epsilon}, v)] = 0
\]

and this immediately proves the theorem, since \(\mathbb{E}[(C\bar{\epsilon}, v)^2]\) is then equal to \(\mathbb{E}[(L\bar{\epsilon}, v)^2]\) plus a non-negative term!
The Gauss-Markov Theorem

It remains to prove the claim – here is where the assumption that the $\varepsilon_i$ are uncorrelated and have the same variance is used!

First, note that

$$E[(L\bar{\varepsilon}, v)((C - L)\bar{\varepsilon}, v)] = E[(\bar{\varepsilon}, L^tv)(\bar{\varepsilon}, (C - L)^tv)]$$

Therefore, from the definition of the Covariance matrix

$$E[(L\bar{\varepsilon}, v)((C - L)\bar{\varepsilon}, v)] = \text{Cov}_{\bar{\varepsilon}}(L^tv, (C - L)^tv)$$

$$= \sigma^2(L^tv, (C - L)^tv)$$

The latter beign simply because $\Sigma_{\bar{\varepsilon}} = \sigma^2 I$. 
The Gauss-Markov Theorem

Now,

\[(L^tv, (C - L)^tv) = (v, L(C - L)^tv)\]

Finally, we make use of two facts \(CX = I\) and the form of \(L\)

\[
L L^t = (X^t X)^{-1} X^t X (X^t X)^{-1} = (X^t X)^{-1} \\
L C^t = (X^t X)^{-1} X^t C^t = (X^t X)^{-1}
\]

This means that \(L(C - L)^t = 0\), and therefore

\[(L^tv, (C - L)^tv) = 0 \ \forall \ v\]

as we wanted!
The biased estimators: ridge regression

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Warm up
Polar factorization

Let $M$ be a $n \times n$ invertible matrix. Then the matrix

$$MM^t$$

is symmetric, non-negative, and invertible.

Thusly, there is a unique symmetric, positive $P$ such that

$$P^2 = MM^t$$
Warm up
Polar factorization

In this case, moreover, the matrix

\[ V := M^{-1}P \]

is orthogonal and moreover, one has that

\[ M = PV^t \]

This expression for \( M \) is known as its polar factorization.
Warm up

Singular Value Decomposition of a matrix

What happens for general matrices? What we have is the Singular Value Decomposition (SVD):

It says that given a $n \times m$ matrix $M$, there exists

- $U$ a $n \times m$ matrix whose columns yield an orthonormal basis for the image of $M$,
- $D$ a $n \times n$ diagonal non-negative matrix,
- $V$ a $n \times n$ orthogonal matrix,

all such that $M$ is decomposed as

$$M = UDV^t$$
Warm up
The SVD and Least Squares

Let $X$ be a $N \times p$ matrix (as considered in least squares), and let us consider it’s SVD

$$X = UDV^t$$

Then, a brief computation yields the identity

$$(X^tX)^{-1} = V^{-t}D^{-2}V^{-1}$$

as well as the important identity,

$$(X^tX)^{-1}X^t = V^{-t}D^{-1}U^t$$

$$X(X^tX)^{-1}X^t = UU^t$$
Warm up
The SVD and Least Squares

Let us denote by \( u_1, \ldots, u_p \) the non-zero columns of \( \mathbf{U} \).

Now, given \( y \in \mathbb{R}^N \), the entries of

\[
\mathbf{U}^t y
\]

are either zero or of the form \( (u_i, y) \), thus, they represent the components of \( \hat{y} \) in the basis \( u_1, \ldots, u_r \). Accordingly,

\[
\hat{y} = \sum_{i=1}^{p} (u_i, y) u_i
\]
Univariate v. Multivariate regression

When doing a regression where the input space has dimension \( p = 1 \) we say the regression is **univariate**.

Then, suppose we are given data \((x_1, y_1), \ldots, (x_N, y_N)\) with \( x_i, y_i \in \mathbb{R} \), and write

\[
\mathbf{x} = (x_1, \ldots, x_N), \quad \mathbf{y} = (y_1, \ldots, y_N)
\]
The least square regression reduces to finding $\beta_0$ minimizing

$$|x \beta - y|^2$$

It is immediate that the solution is given by

$$\hat{\beta} = \frac{\sum_{i=1}^{N} x_i y_i}{\sum_{i=1}^{N} x_i^2} = \frac{x \cdot y}{|x|^2}$$
Univariate v. Multivariate regression

It is illustrative to compare the univariate formula

\[ \hat{\beta} = |x|^{-2} x \cdot y \]

with the multivariate one

\[ \hat{\beta} = (X^t X)^{-1} X^t y \]

The multivariate regression can be decomposed into several independent univariate regressions, in the right system of coordinates.
Univariate v. Multivariate regression

Suppose for a moment that the matrix $X^tX$ is diagonal

$$(X^tX)_{ij} = d_i^2 \delta_{ij}$$

where $d_i^2 = x_{1i}^2 + \ldots + x_{Ni}^2$

$\hat{\beta} = (X^tX)^{-1}X^ty$

becomes

$$\hat{\beta}_j = d_i^{-2} \sum_{i=1}^{N} x_{ji} y_j$$
Univariate v. Multivariate regression

When the matrix $X^tX$ is not diagonal, since it is in any case symmetric and positive, we may use the Gram-Schmidt process to select a new orthonormal system of coordinates where $X^tX$ is diagonal.

Therefore, up to “just” a change of orthonormal basis, multivariate regression is the same as $p$ separate univariate regressions.
Univariate v. Multivariate regression
Centering and the intercept

Let us add a word about ways of dealing with $\beta_0$.

First, the way we have dealt with so far more or less implicitly: we think of the numbers

\[(x_i, \beta) + \beta_0\]

as the dot product between \((1, x_i)\) and \((\beta_0, \beta)\), vectors in $\mathbb{R}^{p+1}$.

Then, by adding an extra column to $\mathbf{X}$, we make $\beta_0$ part of the $\beta$ parameter, increasing its dimension by 1.
Another option is to center the data before applying the least squares algorithm

\[
\sum_{i=1}^{N} |y_i - (x_i, \beta) - \beta_0|^2
\]

Meaning the following: thinking first of \( \beta \) as fixed, minimize the above as a function of \( \beta_0 \).
This is a parabola with respect to $\beta_0$, so finding the minimum is simple...

Differentiating, we have

$$\frac{d}{d\beta_0} \sum_{i=1}^{N} |y_i - (x_i, \beta) - \beta_0|^2 = 2 \sum_{i=1}^{N} (y_i - (x_i, \beta) - \beta_0)$$

Therefore, the minimizer $\hat{\beta}_0$ is given by

$$\sum_{i=1}^{N} (y_i - (x_i, \beta) - \hat{\beta}_0) = 0$$
Univariate v. Multivariate regression
Centering and the intercept

This, would yield the solution

$$\hat{\beta}_0 = \frac{1}{N} \sum_{i=1}^{N} y_i - (x_i, \beta) = \frac{1}{N} \sum_{i=1}^{N} y_i - \left( \frac{1}{N} \sum_{i=1}^{N} x_i, \beta \right)$$

However, this does not mean we choose this $\hat{\beta}_0$.

Instead we change the $y_i$ and $x_i$ to make $\hat{\beta}_0 = 0$

$$y'_i = y_i - \bar{y}, \quad x'_i = x_i - \bar{x}$$
where $\bar{y}$ and $\bar{x}$ are

$$\bar{y} = \frac{1}{N} \sum_{i=1}^{N} y_i, \quad \bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i$$

This means that $y'_1 + \ldots + y'_N = 0$ and $x'_1 + \ldots + x'_N = 0$, and thus, $\hat{\beta}_0 = 0$ regardless of $\beta$.

The process of changing the variables $y_i$ and $x_i$ for $y_i - \bar{y}$ is what is known as centering the data.
We have already seen that the EPE is given by the addition of the bias squared, the variance underlying to the data, and the variance inherent to the estimator.

What if a great deal of the variance appearing above is due to a component $\hat{\beta}_j$ of $\hat{\beta}$ with small mean ($=\beta_j$) and large variance?

Well, if we replaced $\hat{\beta}_j$ with 0, then the bias of $\hat{\beta}$ would change from zero to something small, while at the same time the variance would decrease by a lot. Yielding a net improvement on the EPE. This means that unbiased estimators are preferable under the right circumstances.
Variable subset selection

1. Best-subset selection via *leaps and bounds* algorithm.
2. Forward and backward stepwise selection.
3. Forward-stagewise regression.

The above involve a discrete selection process. What if instead of altogether eliminating a variable, we diminished, in a continuous manner, its influence on our prediction model?

This is the idea behind shrinking methods, which are by now more widely used than selection methods. We start with Ridge regression and the Lasso.
Ridge regression

So, in least squares, we have an affine structure

\[ y = (x, \beta) + \beta_0 \]

and data \( X \) and \( y \), leading to

\[ \hat{\beta} = (X^tX)^{-1}X^ty \]

For random data, what may cause \( \hat{\beta} \) to have high variance?
Ridge regression
Ridge regression

Hoerl and Kennard (1970):
Add $\lambda \mathbf{I}$ to $\mathbf{X}^t \mathbf{X}$ before taking the inverse, then set

$$\hat{\beta}_{\text{ridge}} = (\mathbf{X}^t \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^t \mathbf{y}$$

For $\lambda > 0$, $\mathbf{X}^t \mathbf{X} + \lambda$ is always invertible, even if $\mathbf{X}^t \mathbf{X}$ is not.
Ridge regression

On the other hand, we have

\[ H_\lambda = X (X^t X + \lambda I)^{-1} X^t \]

Let us use the SVD for \( X \), \( X = UDV^t \), then

\[ X^t X + \lambda I = VD^2 V^t + \lambda I \]

Now, since \( V(\lambda I)V^t = \lambda I \), we have

\[ X^t X + \lambda I = V(D^2 + \lambda I)V^t \]

\[ \Rightarrow (X^t X + \lambda I)^{-1} = V(D^2 + \lambda I)^{-1} V^t \]
Ridge regression

Therefore,

$$H_\lambda = (UDV^t)V(D^2 + \lambda I)^{-1}V^t(VDU^t)$$

$$= U(D(D^2 + \lambda I)^{-1}D)U^t$$

In terms of the column vectors of $U$, this is

$$\hat{y}_{\text{ridge}} = \sum_{i=1}^{p} (u_i, y) \frac{d_i^2}{d_i^2 + \lambda} u_i$$
Ridge regression

What about $\hat{\beta}_{\text{ridge}}$?

Well, we saw from the SVD for $X$, $UDV^t$ that

$$(X^tX + \lambda I)^{-1} = V(D^2 + \lambda I)^{-1}V^t$$

from where it follows that

$$(X^tX + \lambda I)^{-1}X^t = V(D^2 + \lambda I)^{-1}V^t(VDU^t)$$

$$= V(D^2 + \lambda I)^{-1}DU^t$$
Ridge regression

What about $\hat{\beta}_{\text{ridge}}$?

We conclude that

$$\hat{\beta}_{\text{ridge}} = V(D^2 + \lambda I)^{-1}DU^t y$$

which, it’s convenient to write as

$$\hat{\beta}_{\text{ridge}} = \sum_{i=1}^{p} \frac{d_i}{d_i^2 + \lambda} (u_i, y)v_i$$

$$= \sum_{i=1}^{p} \frac{d_i^2}{d_i^2 + \lambda d_i} \frac{1}{d_i} (u_i, y)v_i$$
Ridge regression

... or, in the more suggestive form

$$\hat{\beta}_{\text{ridge}} = \sum_{i=1}^{p} \frac{d_i^2}{d_i^2 + \lambda} \frac{1}{d_i} (u_i, y) v_i$$

Compare this with the least squares solution $\hat{\beta}$, which is

$$\hat{\beta}_{\text{ridge}} = \sum_{i=1}^{p} \frac{1}{d_i} (u_i, y) v_i$$

The numbers $d_i^2/(d_i^2 + \lambda)$ are all $< 1$ when $\lambda > 0$ and $d_i > 0$, therefore, ridge regression shrinks the components of $\hat{\beta}$ in the basis $v_1, \ldots, v_p$. 

Ridge regression

More so,

$$\hat{\beta}_{\text{ridge}} = \sum_{i=1}^{p} \frac{d_i^2}{d_i^2 + \lambda d_i} \frac{1}{(u_i, y)} v_i$$

Those components corresponding to smaller $d_i$ are shrunk way more than the components corresponding to larger $d_i$.

It is helpful to think of ridge regression as diminishing the effects corresponding to the directions along which the sample points $x_i$ exhibit the smaller variance.
Ridge regression

Suppose for a second that the sample point data $\mathbf{X}$ is such that

$$\mathbf{D} = d \mathbf{I}$$

Then, ridge regression yields smaller multiples of the least squares solution

$$\hat{\beta}_{\text{ridge}} = \frac{d^2}{d^2 + \lambda} \hat{\beta}, \quad \hat{\mathbf{y}}_{\text{ridge}} = \frac{d^2}{d^2 + \lambda} \hat{\mathbf{y}}$$
Ridge regression
The variational side of ridge regression

Problem:

Given \( \{(x_i, y_i)\}_{i=1}^{N} \) find \( \beta_0 \in \mathbb{R}, \beta \in \mathbb{R}^p \) minimizing

\[
\sum_{i=1}^{N} (y_i - \beta_0 - (x_i, \beta))^2 + \lambda|\beta|^2
\]

Note the "penalization" term does not involve \( \beta_0 \).
We do the usual centering,

\[
y_i \rightarrow y_i - \bar{y}, \quad x_i \rightarrow x_i - \bar{x}
\]

Where \( \bar{y} \) and \( \bar{x} \) are the respective means.
Ridge regression
The variational side of ridge regression

Having done this centering, we aim to minimize

\[ \text{RSS}_\lambda(\beta) = \sum_{i=1}^{N} (y_i - (x_i, \beta))^2 + \lambda|\beta|^2 \]

As in standard least squares, we may rewrite this in vector form

\[ |X\beta - y|^2 + \lambda|\beta|^2 \]
Ridge regression
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Computing the gradient of $\text{RSS}_\lambda$

$$\nabla (|X\beta - y|^2 + \lambda|\beta|^2) = 2X^t (X\beta - y) + 2\lambda \beta$$

$$= 2(X^tX + \lambda I)\beta - 2X^ty$$

Therefore, the minimizer is given by

$$(X^tX + \lambda I)^{-1}X^ty$$

That is, by $\hat{\beta}^{\text{ridge}}$! This shows ridge regression is simply least squares plus a quadratic penalization term for $\beta$ having coefficient $\lambda$. 
Let us make a brief comment about the norms

$$|x|_{\ell^2} = \left( \sum_{j=1}^{p} |x_j|^2 \right)^{\frac{1}{2}}, \quad |x|_{\ell^1} = \sum_{j=1}^{p} |x_j|$$

The “unit ball” for the $\ell^2$ is the standard Euclidean ball in $\mathbb{R}^p$, meanwhile, the “unit ball” for $\ell^1$ is a diamond shape with flat faces and corners.
The Lasso

\( \ell^2 \) and \( \ell^1 \)

This fact about “flat sides” and “corners” for \( B_{1}^{\ell^1} (0) \) has a very important consequence, which we state as a lemma

**Lemma**

Let \( f : \mathbb{R}^p \to \mathbb{R} \) be a linear functional, then, the maximum of \( f \) over \( B_{1}^{\ell^1} (0) \) is always attained at least at a vector \( x = (x_1, \ldots, x_p) \in B_{1}^{\ell^1} (0) \) having at least one zero component, i.e. \( x_j = 0 \) for some \( j \).
The Lasso

The Least Absolute Shrinkage and Selection Operator

Given \( \{(x_i, y_i)\}_{i=1}^{N} \) find \( \beta_0 \in \mathbb{R}, \beta \in \mathbb{R}^p \) minimizing

\[
\frac{1}{2} \sum_{i=1}^{N} (y_i - \beta_0 - x_i \cdot \beta)^2 + \lambda \sum_{j=1}^{p} |\beta_j|
\]

or, equivalently

\[
\sum_{i=1}^{N} (y_i - \beta_0 - x_i \cdot \beta)^2 + \lambda |\beta|_{\ell^1}
\]
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The Least Absolute Shrinkage and Selection Operator

After the proper centering, we find ourselves with the problem of minimizing

\[ J(\beta) = \frac{1}{2} \sum_{i=1}^{N} (y_i - x_i \cdot \beta)^2 + \lambda |\beta|_{\ell 1} \]

\[ = \frac{1}{2} |X\beta - y|^2 + \lambda |\beta|_{\ell 1} \]

This functional \( J \) is \textbf{convex}, and second order differentiable away from \( \beta = 0 \), at which point it fails to be differentiable of first order.
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The Least Absolute Shrinkage and Selection Operator

We observe that for \( \beta \)'s such that \( \beta_j \neq 0 \ \forall \ j \)

\[
\nabla|\beta|_{\ell_1} = \text{sign}(\beta) := (\text{sign}(\beta_1), \ldots, \text{sign}(\beta_p))
\]

Then, for such \( \beta \), we have

\[
\nabla J(\beta) = X^t(X\beta - y) + \lambda \text{sign}(\beta)
\]

Trying to solve \( \nabla J(\beta) = 0 \) is not as straightforward now as in least squares! The resulting equation is not linear.
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Example:
Consider the case $p = 1$ and with data $x_1, \ldots, x_N$ such that

$$x_1^2 + \ldots + x_N^2 = 1$$

Then, if we consider the function of the real variable $\beta$

$$J(\beta) = \frac{1}{2} \sum_{i=1}^{N} |x_i \beta - y_i|^2 + \lambda |\beta|$$

it’s minimizer is given by

$$\text{sign}(\hat{\beta})(|\hat{\beta}| - \lambda)_+$$

where $\hat{\beta}$ is the least squares solution.
The Lasso

The Least Absolute Shrinkage and Selection Operator

Example: (continued)
This means that the lasso estimator takes the least square solution \( \hat{\beta} \) and returns zero if \( |\hat{\beta}| \) is no larger than \( \lambda \), and otherwise returns the \( \beta - \lambda \) or \( \beta + \lambda \) according to the sign of \( \beta \). The function

\[
\beta \mapsto \text{sign}(\beta)(|\beta| - \lambda)_+
\]

is known as a shrinkage operator.
1. When selecting a predictive model, one may judge it by looking at the training error and the test error. Of these, the training error is by the better evaluation metric.

2. A biased algorithm is often preferable to an unbiased one: the tradeoff may lead to a reduced mean squared error.

3. The Gauss-Markov Theorem says that among linear, unbiased estimators, least squares has the least variance.

4. Ridge regression is an alternative linear estimator with bias. It diminishes the components $\beta_j$ according to the degeneracy associated to each direction.

5. The Lasso takes advantage of the geometry of the $\ell^1$ metric to shrink the components of an estimation for $\beta$ in a more dramatic manner than ridge regression.