Assignment 2

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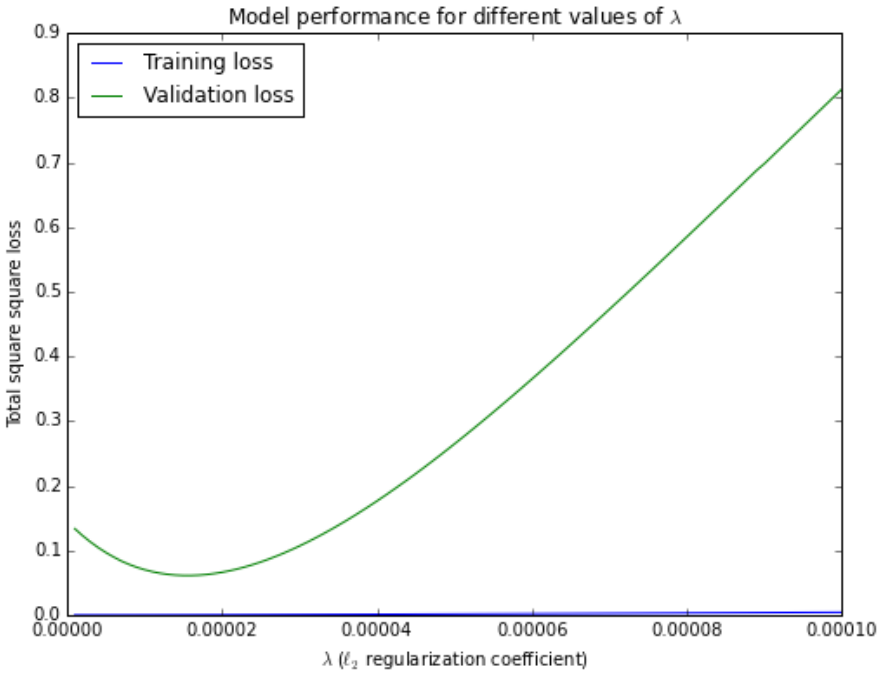
1. Preliminaries

1.1 Dataset construction

See attached iPython notebook.

1.2 Experiments with Ridge Regression

Ridge regression was run on the simulated dataset for a range of λ values, and performance was evaluated using validation set square loss. The optimal λ_{opt} (i.e. validation set square loss minimizing λ) was found to be 1.6×10^{-5}. A plot showing results (near λ_{opt}) is shown below:



Next, let's examine the minimizing weight vector $\boldsymbol{w}$ found when $\lambda = 1.6 \times 10^{-5}$; specifically, we're interested in the number of coefficients w_j at or near zero. These results are presented in the table below:

- $w_j = 0$:

	Predicted zero	Predicted non-zero
True non-zero ($\boldsymbol{w}$[0:10])	0	10
True zero ($\boldsymbol{w}$[10:])	0	65

- $w_j < 10^{-3}$:

	Predicted zero	Predicted non-zero
True non-zero ($\boldsymbol{w}$[0:10])	0	10
True zero ($\boldsymbol{w}$[10:])	0	65

- $w_j < 10^{-2}$:

	Predicted zero	Predicted non-zero
True non-zero ($\boldsymbol{w}$[0:10])	0	10
True zero ($\boldsymbol{w}$[10:])	5	60

- $w_j < 10^{-1}$:

	Predicted zero	Predicted non-zero
True non-zero ($\boldsymbol{w}$[0:10])	0	10
True zero ($\boldsymbol{w}$[10:])	37	28

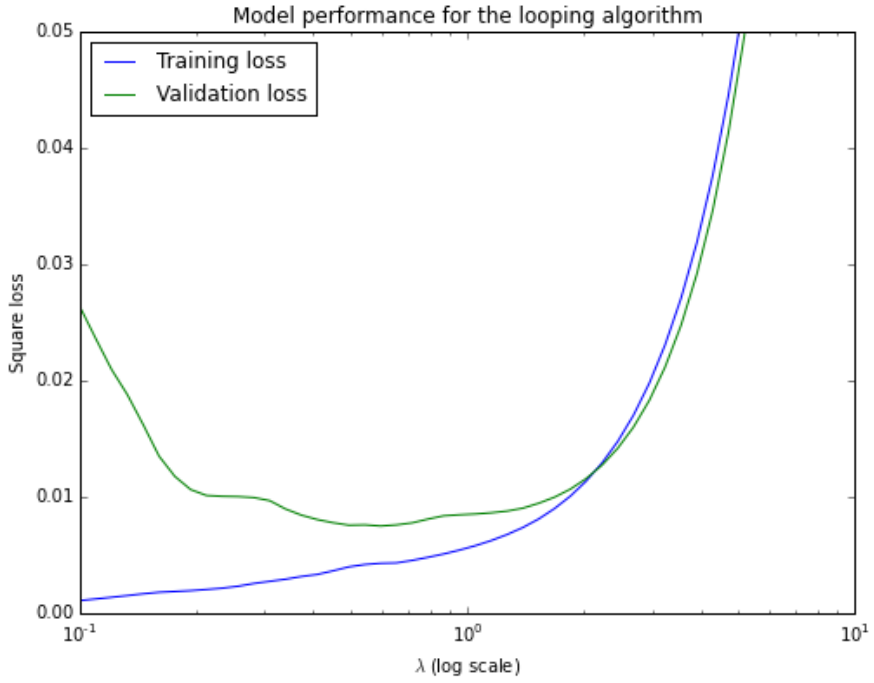
It is apparent that ridge regression is achieving shrinkage, but not promoting sparsity (i.e. setting coefficients to 0).

2. Coordinate Descent for Lasso (Shooting Algorithm)

2.1 Experiments with the Shooting Algorithm

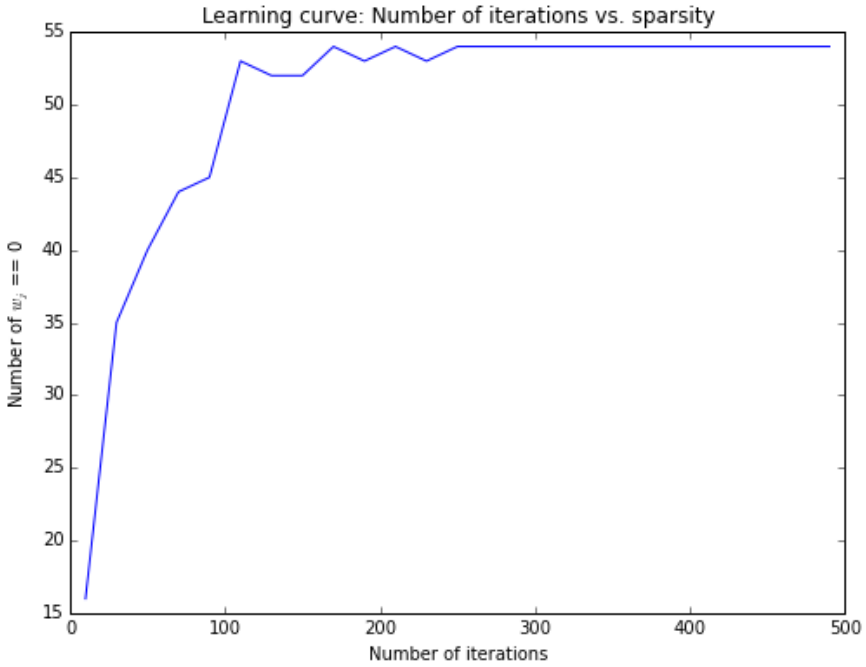
2.1.1 Finding an optimal λ

First, the (non-vectorized, i.e. looping) lasso coordinate descent algorithm was implemented (see attached iPython notebook). Using this implementation, the optimal (i.e. validation set square error minimizing) λ was found to be 0.596, with a corresponding validation set square error of 7.51×10^{-3}. Loss values for λ in a neighborhood of $\lambda_{opt} = 0.596$ are shown in the plot below:



2.1.2 Sparsity analysis of $\boldsymbol{w}_{\boldsymbol{\lambda}_{opt}}$

First, prior to analyzing the sparsity of our solution, we present a learning curve showing the number of zero coefficients versus the number of iterations of the cyclic coordinate descent algorithm.



Based on this learning curve, it appears the sparsity of our solution stabilizes when the number of iterations is greater than 250. Thus, setting the number of iterations to 300, we report a "confusion matrix" for the zero/non-zero coefficients of $\boldsymbol{w}$.

	Predicted zero	Predicted non-zero
True non-zero ($\boldsymbol{w}$[0:10])	0	10
True zero ($\boldsymbol{w}$[10:])	54	11

Importantly, the maximum absolute value of the 15 predicted non-zero, true zero coefficients was 0.0548. Thus, compared to the true non-zero weights (which ranged in absolute value between 9.9 and 10.04), the lasso essentially assigned no weight to the true zero features.

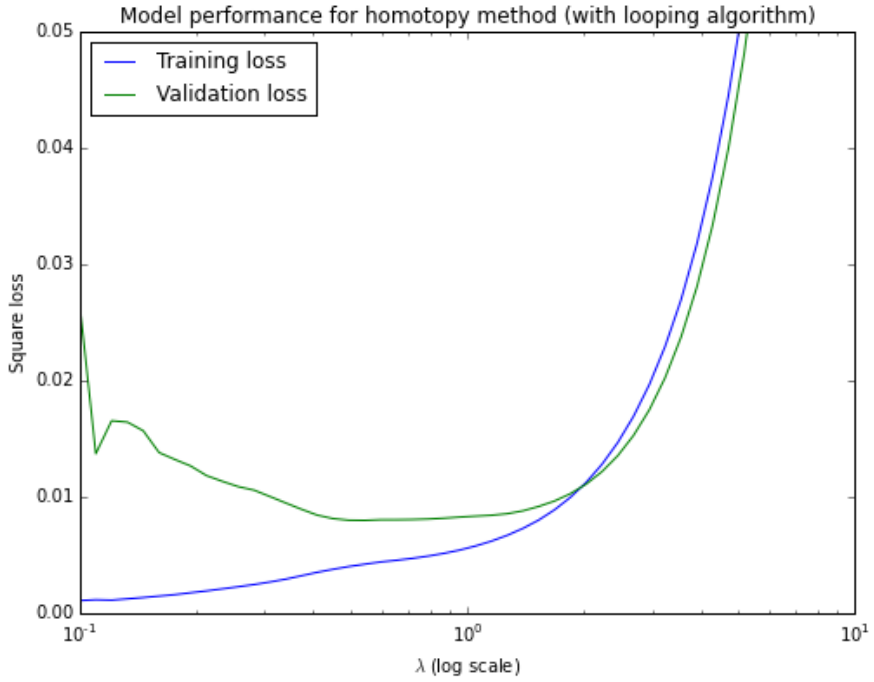
2.1.3 Implementing the homotopy method

The homotopy method was implemented as follows:

- The same candidate set for λ was chosen as in 2.1.1 (specifically the set defined by `np.logspace(-1,1, 50)`).
- The homotopy algorithm was initialized with the same starting weight vector as the looping algorithm (namely the optimal $\boldsymbol{w}$ found using ridge regression), and with $\lambda = \max($`np.logspace(-1,1, 50)`$)$.

- For each $\lambda \in$ `np.logspace(-1,1, 50)`, the optimal weight vector found in the previous iteration was used as the starting point for the coordinate descent.

Results from the homotopy method (used with the looping algorithm) are presented below



Next, runtimes for the two algorithms were compared:

Implementation (tolerance $= 10^{-6}$**)**	**Runtime**
Looping with homotopy method	`1 loops, best of 3: 4min 5s per loop`
Looping without homotopy method	`1 loops, best of 3: 4min 17s per loop`

Thus, it appears the homotopy method achieved marginal runtime gains. Note this result might be due to the termination conditions used for both algorithms. Both algorithms terminated after either:

- 100 iterations (cycles through each coordinate)
- $\boldsymbol{w_{i+1}}$ - $\boldsymbol{w_i}$ $<$ tolerance $= 10^{-6}$

Perhaps the tolerance was too strict, so termination was essentially determined by the fixed maximum number of iterations- if so, the homotopy wouldn't produce any runtime gains.
To test this hypothesis, the test was re-run with tolerance $= 10^{-3}$. Runtime results from this test are given below:

Implementation (tolerance $= 10^{-3}$**)**	**Runtime**
Looping with homotopy method	`1 loops, best of 3: 4min 44s per loop`
Looping without homotopy method	`1 loops, best of 3: 1min 16s per loop`

Thus, with the tolerance set to a lower value (10^{-3}), we see the homotopy method producing a substantial runtime improvement.

2.1.4 Vectorizing the coordinate descent algorithm

First we present matrix expressions for computing a_j and c_j in the coordinate descent algorithm. Recall

$$a_j = 2\sum_{i=1}^{n} x_{ij}^2$$
$$c_j = 2\sum_{i=1}^{n} x_{ij}(y_i - w^T x_i + w_j x_{ij})$$

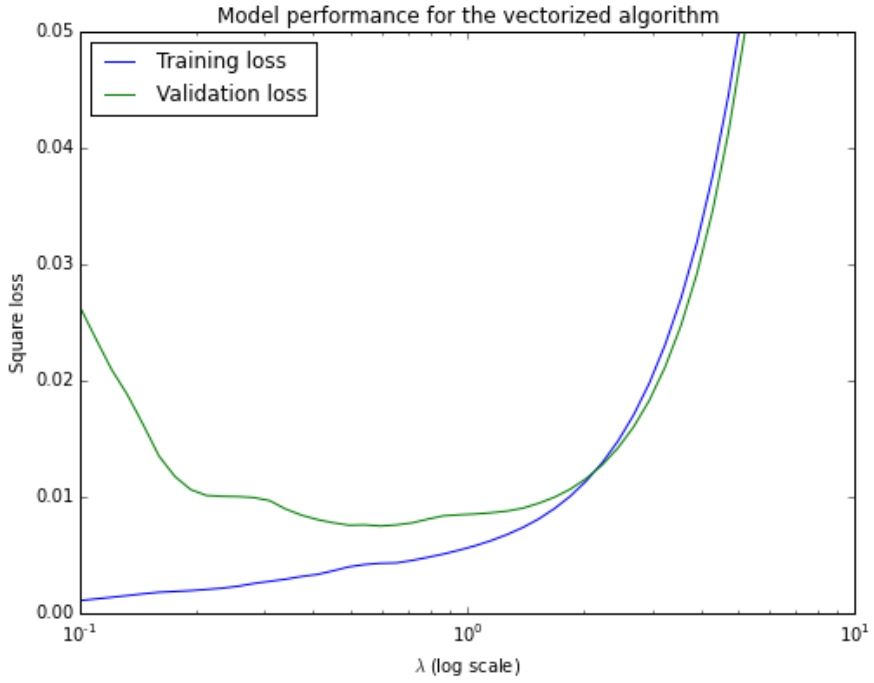
Then, first letting

- $X_{\cdot j}$ be the j^{th} column (i.e. feature) of matrix X
- $X_{\cdot -j}$ be the matrix X without the j^{th} column (feature)
- w_{-j} be the weight vector w without the j^{th} entry

we can expressed a_j and c_j in matrix/vector notation as:

$$a_j = 2X_{\cdot j}^T X_{\cdot j}$$
$$c_j = 2X_{\cdot j}^T \ (y - X_{\cdot -j} w_{-j})$$

After implementing the vectorized algorithm, the following results were obtained:



First, it is important to note the model performance (i.e. square loss for a given λ) is equivalent under the looping and the vectorized versions of the looping algorithm. However, the runtimes are very different. Using `%timeit` magic in iPython for $\lambda = 0.596$, with a maximum of 100 iterations and tolerance $= 10^{-6}$, and initializing with the solution to the ridge regression problem, the following runtimes were obtained:

Implementation	**Runtime**
Vectorized	`1 loops, best of 3:  332 ms per loop`
Looping	`1 loops, best of 3:  4.62 s per loop`

Obviously the vectorization produces dramatic runtime gains.

2.2 Deriving the Coordinate Minimizer for Lasso

2.2.1 Trivial case: $\boldsymbol{x}_{\cdot j} = 0$

Note we are trying to derive the coordinate minimizer for the Lasso. First, consider the case where $\boldsymbol{x}_{\cdot j} = 0$. In this trivial case, we are trying to minimize:

$$\begin{aligned} ||Xw - y||_2^2 - \lambda||w||_1 &= ||\sum_k \boldsymbol{x}_{\cdot k} w[k] - y||_2^2 - \lambda(\sum_k |w[k]|) \\ &= ||\sum_{k \neq j} \boldsymbol{x}_{\cdot k} w[k] - y||_2^2 - \lambda(\sum_{k \neq j} |w[k]| + |w[j]|) \end{aligned}$$

where $w[k]$ is the k^{th} entry of w. Thus, to minimize this expression we clearly set $w[j] = 0$.

2.2.2 Expression for the derivative of $f(w_j)$

Now, as we proceed, assume there is no j such that $\boldsymbol{x}_{\cdot j} = 0$.
For $w_j \neq 0$,

$$
\begin{aligned}
f(w_j) &= \sum_{i=1}^{n} \left[w_j x_{ij} + \sum_{k \neq j} w_k x_{ik} - y_i \right]^2 + \lambda |w_j| + \lambda \sum_{k \neq j} |w_k| \\
\frac{\mathrm{d}}{\mathrm{d}w_j} f(w_j) &= \sum_{i=1}^{n} \frac{\mathrm{d}}{\mathrm{d}w_j} \left[w_j x_{ij} + \sum_{k \neq j} w_k x_{ik} - y_i \right]^2 + \frac{\mathrm{d}}{\mathrm{d}w_j} \lambda |w_j| + \frac{\mathrm{d}}{\mathrm{d}w_j} \lambda \sum_{k \neq j} |w_k| \\
&= \sum_{i=1}^{n} 2 x_{ij} \left(w_j x_{ij} + \sum_{k \neq j} w_k x_{ik} - y_i \right) + \lambda \ \mathrm{sign}(w_j) \\
&= w_j 2 \sum_{i=1}^{n} x_{ij}^2 - 2 \sum_{i=1}^{n} \left[x_{ij} (y_i - \sum_{k \neq k} w_k x_{ik}) \right] + \lambda \ \mathrm{sign}(w_j)
\end{aligned}
$$

Now let

$$
\begin{aligned}
a_j &:= 2 \sum_{i=1}^{n} x_{ij}^2 \\
c_j &:= 2 \sum_{i=1}^{n} \left[x_{ij} (y_i - \sum_{k \neq j} w_k x_{ik}) \right]
\end{aligned}
$$

Then

$$
\frac{\mathrm{d}}{\mathrm{d}w_j} f(w_j) = w_j a_j - c_j + \lambda \ \mathrm{sign}(w_i)
$$

2.2.3 Expressions for minimizing $w_j \neq 0$

I If $w_j > 0$ and minimizes f, then

$$
\begin{aligned}
& & 0 &= w_j a_j - c_j + \lambda \ \mathrm{sign}(w_i) \\
& & 0 &= w_j a_j - c_j + \lambda \\
\implies & & w_j &= -\frac{1}{a_j} (\lambda - c_j)
\end{aligned}
$$

If $w_j < 0$ and minimizes f, then

$$
\begin{aligned}
& & 0 &= w_j a_j - c_j + \lambda \ \mathrm{sign}(w_i) \\
& & 0 &= w_j a_j - c_j - \lambda \\
\implies & & w_j &= \frac{1}{a_j} (\lambda + c_j)
\end{aligned}
$$

Next, we give conditions on c_j that imply the minimizer $w_j > 0$ and $w_j < 0$, respectively. Assume w_j is the minimizer, and $w_j \neq 0$. Then, from above,

$$\begin{aligned} & & 0 &= w_j a_j - c_j + \lambda \operatorname{sign}(w_j) \\ &\implies & 0 &= \operatorname{sign}(w_j)|w_j|a_j - c_j + \lambda \operatorname{sign}(w_j) \\ \implies & & c_j - \lambda \operatorname{sign}(w_j) &= \operatorname{sign}(w_j)|w_j|a_j \end{aligned}$$

Now we use contradiction to give a condition on c_j that implies $w_j > 0$. First noting $|w_j|a_j \geq 0$, let $0 < \lambda < c_j$ and assume sign(w_j) = -1. Then

$$c_j - \lambda \operatorname{sign}(w_j) = c_j - \lambda(-1) = c_j + \lambda > 0 \qquad (\text{by } 0 < \lambda < c_j)$$

Then, since $c_j - \lambda \operatorname{sign}(w_j) = \operatorname{sign}(w_j)|w_j|a_j$, we have

$$\begin{aligned} & & \operatorname{sign}(w_j)|w_j|a_j &> 0 \\ &\implies & \operatorname{sign}(w_j) &= +1 \end{aligned}$$

which is a contraction.

Therefore, if $0 < \lambda < c_j, w_j > 0$.

Similarly, let $c_j < -\lambda < 0$ and assume sign(w_j) = +1. Then

$$c_j - \lambda \operatorname{sign}(w_j) = c_j - \lambda(+1) = c_j - \lambda < 0 \qquad (\text{by } c_j < -\lambda < 0)$$

Then, since $c_j - \lambda \operatorname{sign}(w_j) = \operatorname{sign}(w_j)|w_j|a_j$, we have

$$\begin{aligned} & & \operatorname{sign}(w_j)|w_j|a_j &< 0 \\ &\implies & \operatorname{sign}(w_j) &= -1 \end{aligned}$$

which is a contraction.

Therefore, if $c_j < -\lambda < 0, w_j < 0$.

2.2.4 One-sided derivatives at $f(0)$, etc.

Now let's consider the two one-sided derivatives at $f(0)$. First let's find an expression for

$$\lim_{\epsilon \downarrow 0} \frac{f(\epsilon) - f(0)}{\epsilon}$$

First, let's tackle just the numerator:

$$\begin{aligned}
f(\epsilon) - f(0) &= \left[\sum_{i=1}^{n}\left(\epsilon x_{ij} + \sum_{k\neq j} w_k x_{ik} - y_i\right)^2 + \lambda|\epsilon| + \lambda\sum_{k\neq j}|w_k|\right] \\
&\quad - \left[\sum_{i=1}^{n}\left(0 x_{ij} + \sum_{k\neq j} w_k x_{ik} - y_i\right)^2 + \lambda|0| + \lambda\sum_{k\neq j}|w_k|\right] \\
&= \sum_{i=1}^{n}\left(\epsilon x_{ij} + \sum_{k\neq j} w_k x_{ik} - y_i\right)^2 + \lambda|\epsilon| - \sum_{i=1}^{n}\left(\sum_{k\neq j} w_k x_{ik} - y_i\right)^2 \\
&= \sum_{i=1}^{n}\left[\left(\epsilon x_{ij} + \sum_{k\neq j} w_k x_{ik} - y_i\right)^2 - \left(\sum_{k\neq j} w_k x_{ik} - y_i\right)^2\right] + \lambda|\epsilon| \\
&= \sum_{i=1}^{n}\left[\epsilon^2 x_{ij}^2 + 2\epsilon x_{ij}\left(\sum_{k\neq j} w_k x_{ik} - y_i\right)\right] + \lambda|\epsilon| \\
&= \epsilon^2\sum_{i=1}^{n} x_{ij}^2 + 2\epsilon\sum_{i=1}^{n} x_{ij}\left(\sum_{k\neq j} w_k x_{ik} - y_i\right) + \lambda|\epsilon|
\end{aligned}$$

Now, let's substitute in a_j and c_j, as defined previously. Then

$$f(\epsilon) - f(0) = \frac{1}{2}\epsilon^2 a_j + \epsilon c_j + \lambda|\epsilon|$$

Now let's return to the limit (noting, under $\epsilon \downarrow 0, |\epsilon| = \epsilon$):

$$\begin{aligned}
\lim_{\epsilon\downarrow 0}\frac{f(\epsilon) - f(0)}{\epsilon} &= \lim_{\epsilon\downarrow 0}\frac{\frac{1}{2}\epsilon^2 a_j + \epsilon c_j + \lambda|\epsilon|}{\epsilon} \\
&= \lim_{\epsilon\downarrow 0}\left[\frac{1}{2}\epsilon a_j + c_j + \lambda\right] \\
&= c_j + \lambda
\end{aligned}$$

The other limit is similar- except now we replace all the ϵ's with $-\epsilon$. This yields

$$\begin{aligned}
\lim_{\epsilon\downarrow 0}\frac{f(-\epsilon) - f(0)}{\epsilon} &= \frac{(-\epsilon)^2\sum_{i=1}^{n} x_{ij}^2 + 2(-\epsilon)\sum_{i=1}^{n} x_{ij}\left(\sum_{k\neq j} w_k x_{ik} - y_i\right) + \lambda|(-\epsilon)|}{\epsilon} \\
&= \lim_{\epsilon\downarrow 0}\left[\frac{1}{2}\epsilon a_j - c_j + \lambda\right] \\
&= -c_j + \lambda
\end{aligned}$$

Now, using the given optimality conditions, we know 0 is a minimizer if and only if:

$$\lim_{\epsilon \downarrow 0} \frac{f(-\epsilon) - f(0)}{\epsilon} = c_j + \lambda \geq 0 \implies c_j \geq -\lambda$$

$$\lim_{\epsilon \downarrow 0} \frac{f(\epsilon) - f(0)}{\epsilon} = -c_j + \lambda \geq 0 \implies c_j \leq \lambda$$

Stated more succinctly, 0 is a minimizer if and only if $c_j \in [-\lambda, \lambda]$.

By way of justification, note in this one dimensional case, having both one-sided derivatives (of our convex function) be positive implies there is no descent direction, so we have a global minimizer.

2.2.5 Putting it it all together: expression for minimizer w_j

Putting together the conditions from 2.2.2 and 2.2.3, we immediately get

$$w_j = \begin{cases} \frac{1}{a_j}(c_j - \lambda) & c_j > \lambda \\ 0 & c_j \in [-\lambda, \lambda] \\ \frac{1}{a_j}(c_j + \lambda) & c_j < -\lambda \end{cases}$$

Finally, we show this is equivalent to the expression given in the original formulation of the algorithm, specifically:

$$\begin{aligned} w_j &= \text{soft}\left(\frac{c_j}{a_j}, \frac{\lambda}{a_j}\right) \\ &= \text{sign}\left(\frac{c_j}{a_j}\right)\left(\left|\frac{c_j}{a_j}\right| - \frac{\lambda}{a_j}\right)_+ \end{aligned}$$

Now, if $c_j \in [-\lambda, \lambda]$, $\left(\left|\frac{c_j}{a_j}\right| - \frac{\lambda}{a_j}\right) \leq 0$, so $\left(\left|\frac{c_j}{a_j}\right| - \frac{\lambda}{a_j}\right)_+ = 0$, and $w_j = 0$.
Next, since $a_j \geq 0, \text{sign}\left(\frac{c_j}{a_j}\right) = \text{sign}(c_j)$.

Thus, if $c_j > \lambda \geq 0$, then

$$\text{sign}\left(\frac{c_j}{a_j}\right)\left(\left|\frac{c_j}{a_j}\right| - \frac{\lambda}{a_j}\right)_+ = \left(\frac{c_j}{a_j} - \frac{\lambda}{a_j}\right) = \frac{1}{a_j}(c_j - \lambda)$$

Finally, if $c_j < \lambda \leq 0$, then

$$\text{sign}\left(\frac{c_j}{a_j}\right)\left(\left|\frac{c_j}{a_j}\right| - \frac{\lambda}{a_j}\right)_+ = -\left(\frac{-c_j}{a_j} - \frac{\lambda}{a_j}\right) = \frac{1}{a_j}(c_j + \lambda)$$

Thus, the piecewise expression derived above is in fact equivalent to the original expression $w_j = \text{soft}\left(\frac{c_j}{a_j}, \frac{\lambda}{a_j}\right)$.

3. Lasso Properties

3.1 Deriving λ_{max}

3.1.1 One-sided directional derivative of $L(w)$

First, note we are trying to derive an expression for λ_{max}, i.e. the maximum λ such that $\boldsymbol{w} = 0$.
To start, we find the one-sided directional derivative of $L(0)$ in the direction v, where

$$L(w) = ||Xw - y||_2^2 + \lambda||w||_1$$

.
This one-sided directional derivative is

$$\begin{aligned}
L'(0;v) &= \lim_{h\downarrow 0} \frac{L(0+hv) - L(0)}{h} \\
&= \lim_{h\downarrow 0} \frac{L(0+hv) - L(0)}{h} \\
&= \lim_{h\downarrow 0} \frac{||X(0+hv) - y||_2^2 + \lambda||(0+hv)|_1 - (||X(0) - y||_2^2 + \lambda||(0)|_1)}{h} \\
&= \lim_{h\downarrow 0} \frac{||hXv - y||_2^2 + \lambda h||v||_1 - || - y||_2^2}{h} \\
&= \lim_{h\downarrow 0} \frac{(hXv - y)^T(hXv - y) + \lambda h||v||_1 - ||y||_2^2}{h} \\
&= \lim_{h\downarrow 0} \frac{(hv^TX^T - y^T)(hXv - y) + \lambda h||v||_1 - ||y||_2^2}{h} \\
&= \lim_{h\downarrow 0} \frac{h^2v^TX^TXv - hv^TX^Ty - hy^TXv - y^ty + \lambda h||v||_1 - ||y||_2^2}{h} \\
&= \lim_{h\downarrow 0} \frac{h^2v^TX^TXv - 2hv^TX^Ty + \lambda h||v||_1}{h} \\
&= \lim_{h\downarrow 0} \left[hv^TX^TXv - 2v^TX^Ty + \lambda||v||_1\right] \\
&= -2v^TX^Ty + \lambda||v||_1
\end{aligned}$$

3.1.2 Lower bound on λ

Now, since $L'(0;v) \geq 0$ for all v is 0 is the minimizer, we can rearrange the directional derivative to get a lower bound on λ:

$$\begin{aligned}
-2v^TX^Ty + \lambda||v||_1 &\geq 0 \\
\lambda||v||_1 &\geq 2v^TX^Ty \\
\lambda &\geq \frac{2v^TX^Ty}{||v||_1}
\end{aligned}$$

3.1.3 Maximizing the lower bound

Finally, we want to compute the maximum lower bound (so it holds for all v). First, note:

$$\max_v \frac{2v^T X^T y}{||v||_1}$$

is equivalent to:

$$\begin{aligned} \max_w \quad & 2wX^T y \\ \text{subject to} \quad & ||w||_1 = 1 \end{aligned}$$

(where, to ease notation, we let w be a row vector). Now, let k be the index of the absolute maximum entry of $X^T y$ (so $||X^T y||_\infty = |(X^T y)[k]|$).

We show the maximizer $w^* = \text{sign}((X^T y)[k])e_k$, were e_k is the standard basis vector with

$$e_k[j] = \begin{cases} 0 & \text{if } j \neq k \\ 1 & \text{if } j = k \end{cases}$$

Assume not. Then there exists some $w' \neq w^*, ||w'||_1 = 1$ such that

$$\begin{aligned} 2w'X^T y &> 2w^* X^T y \\ w'X^T y &> \text{sign}((X^T y)[k])(X^T y)[k] \\ w'X^T y &> |(X^T y)[k]| \\ w'[k](X^T y)[k] + \sum_{i \neq k} w'[i](X^T y)[i] &> |(X^T y)[k]| \end{aligned}$$

Before we proceed, note that since w' maximizes $2w^T X^T y$, we know for every i, $w'[i](X^T y)[i] \geq 0$ (i.e., $\text{sign}(w'[i]) = \text{sign}((X^T y)[i])$) since, if not, we could construct a vector $w'', w''[i] = -w'[i]$ such that $w''X^T y > w'X^T y$.

Thus we can proceed using absolute values of all terms (and recalling $||w'||_1 = 1$):

$$
\begin{aligned}
|w'[k]||(X^T y)[k]| + \sum_{i \neq k} |w'[i]||(X^T y)[i]| &> |(X^T y)[k]| \\
|w'[k]||(X^T y)[k]| + \sum_{i \neq k} |w'[i]||(X^T y)[i]| &> \left(|w'[k]| + \sum_{i \neq k} |w'[i]| \right) |(X^T y)[k]| \\
\sum_{i \neq k} |w'[i]||(X^T y)[i]| &> \left(\sum_{i \neq k} |w'[i]| \right) |(X^T y)[k]| \\
\implies \quad |w'[i]||(X^T y)[i]| &> |w'[i]||(X^T y)[k]| \text{ for some } i \neq k \\
\implies \quad |(X^T y)[i]| &> |(X^T y)[k]| \text{ for some } i \neq k
\end{aligned}
$$

This is our contradiction since, by assumption, $||X^T y||_\infty = |(X^T y)[k]|$. Hence, we know there is no $w' \neq w^*$ such that $2w'X^T y > 2w^* X^T y$, and the maximum lower bound is $||X^T y||_\infty$.

3.2 Feature Correlation

3.2.1 Relation between $\hat{\theta}_i$ and $\hat{\theta}_j$ for lasso

Now consider the design matrix $X \in \mathbb{R}^{m \times d}$, where $X_{\cdot a} = X_{\cdot b}$ for some a and b. Then note

$$
\begin{aligned}
\hat{\theta} &= \arg\min_{\theta \in \mathbb{R}^d} ||X\theta - y||_2^2 + \lambda |\theta|_1 \\
&= \arg\min_{\theta \in \mathbb{R}^d} || \sum_{i=1}^{d} \theta_i X_{\cdot i} - y||_2^2 + \lambda |\theta|_1 \\
&= \arg\min_{\theta \in \mathbb{R}^d} || \sum_{i=1, i \neq a,b}^{d} \theta_i X_{\cdot i} + \theta_a X_{\cdot a} + \theta_b X_{\cdot b} - y||_2^2 + \lambda |\theta|_1 \\
&= \arg\min_{\theta \in \mathbb{R}^d} || \sum_{i=1, i \neq a,b}^{d} \theta_i X_{\cdot i} + \theta_a X_{\cdot a} + \theta_b X_{\cdot b} - y||_2^2 + \lambda \left(\sum_{i=1, i \neq a,b}^{d} |\theta_i| + |\theta_a| + |\theta_b| \right) \\
&= \arg\min_{\theta \in \mathbb{R}^d} || \sum_{i=1, i \neq a,b}^{d} \theta_i X_{\cdot i} + (\theta_a + \theta_b) X_{\cdot a} - y||_2^2 + \lambda \left(\sum_{i=1, i \neq a,b}^{d} |\theta_i| + |\theta_a| + |\theta_b| \right)
\end{aligned}
$$

Now let $\hat{\theta}_a = a$ and $\hat{\theta}_b = b$ be the coefficients for these features in the ℓ_1 regularized LS optimal weight vector. Then note we must have $\text{sign}(a) = \text{sign}(b)$. To see this, note that (if not), we can find θ' such that

$$
||X\theta' - y||_2^2 + \lambda |\theta'|_1 \; < ||X\hat{\theta} - y||_2^2 + \lambda |\hat{\theta}|_1
$$

Specifically, let $\theta'_a = (a+b)$ and $\theta'_b = 0$. Then (by $|a+b| < |a| + |b|$):

$$\begin{aligned}
||X\theta' - y||_2^2 + \lambda|\theta'|_1 &= || \sum_{i=1, i\neq a,b}^{d} \theta'_i X_{\cdot i} + (\theta'_a + \theta'_b)X_{\cdot a} - y||_2^2 + \lambda \left(\sum_{i=1, i\neq a,b}^{d} |\theta'_i| + |\theta'_a| + |\theta'_b| \right) \\
&= || \sum_{i=1, i\neq a,b}^{d} \theta'_i X_{\cdot i} + (a+b)X_{\cdot a} - y||_2^2 + \lambda \left(\sum_{i=1, i\neq a,b}^{d} |\theta'_i| + |a+b| + |0| \right) \\
&< || \sum_{i=1, i\neq a,b}^{d} \theta'_i X_{\cdot i} + (a+b)X_{\cdot a} - y||_2^2 + \lambda \left(\sum_{i=1, i\neq a,b}^{d} |\theta'_i| + |a| + |b| \right) \\
&= ||X\hat{\theta} - y||_2^2 + \lambda|\hat{\theta}|_1
\end{aligned}$$

This is a contradiction, since $\hat{\theta} = \arg\min \hat{\mathcal{R}}(\theta)$, the lasso empirical risk.
Now, since $\text{sign}(a) = \text{sign}(b)$, we have $|a| + |b| = |a+b|$. Thus, letting $a + b = c$, we can rewrite the optimization problem as:

$$\begin{aligned}
\hat{\theta} &= \arg\min_{\theta \in \mathbb{R}^d} ||X\theta - y||_2^2 + \lambda|\theta|_1 \\
&= \arg\min_{\theta \in \mathbb{R}^d} || \sum_{i=1, i\neq a,b}^{d} \theta_i X_{\cdot i} + \theta_a X_{\cdot a} + \theta_b X_{\cdot b} - y||_2^2 + \lambda \left(\sum_{i=1, i\neq a,b}^{d} |\theta_i| + |\theta_a| + |\theta_b| \right) \\
&= \arg\min_{\theta \in \mathbb{R}^{d-2}, c \in \mathbb{R}} || \sum_{i=1, i\neq a,b}^{d} \theta_i X_{\cdot i} + cX_{\cdot a} - y||_2^2 + \lambda \left(\sum_{i=1, i\neq a,b}^{d} |\theta_i| + |c| \right)
\end{aligned}$$

Thus we conclude that (for the Lasso), if two features are identical, there may not be a unique minimizer- instead the set of optimal weights for those two features is the line segment $\{a, b | a + b = c_{opt}\}$.

3.2.2 Relation between $\hat{\theta}_i$ and $\hat{\theta}_j$ for ridge regression

Again consider the design matrix $X \in \mathbb{R}^{m \times d}$, where $X_{\cdot a} = X_{\cdot b}$ for some a and b. Then note for ridge regression:

$$\begin{aligned}
\hat{\theta} &= \arg\min_{\theta \in \mathbb{R}^d} ||X\theta - y||_2^2 + \lambda||\theta||_2^2 \\
&= \arg\min_{\theta \in \mathbb{R}^d} || \sum_{i=1}^{d} \theta_i X_{\cdot i} - y||_2^2 + \lambda||\theta||_2^2 \\
&= \arg\min_{\theta \in \mathbb{R}^d} || \sum_{i=1, i\neq a,b}^{d} \theta_i X_{\cdot i} + (\theta_a + \theta_b)X_{\cdot a} - y||_2^2 + \lambda \left(\sum_{i=1, i\neq a,b}^{d} \theta_i^2 + \theta_a^2 + \theta_b^2 \right)
\end{aligned}$$

Again, letting $\hat{\theta}_a = a$ and $\hat{\theta}_b = b$ be the coefficients for these features in the ℓ_2 regularized LS optimal weight vector. Then note we must have $a = b$. Otherwise we can construct θ' with $\theta'_a = \theta'_b = \frac{a+b}{2}$ such that

$$\begin{aligned}
\hat{\mathcal{R}}(\theta') &= || \sum_{i=1, i\neq a,b}^{d} \theta'_i X_{\cdot i} + (\theta'_a + \theta'_b) X_{\cdot a} - y||_2^2 + \lambda \left(\sum_{i=1, i\neq a,b}^{d} {\theta'_i}^2 + {\theta'_a}^2 + {\theta'_b}^2 \right) \\
&= || \sum_{i=1, i\neq a,b}^{d} \theta'_i X_{\cdot i} + \left(\frac{a+b}{2} + \frac{a+b}{2} \right) X_{\cdot a} - y||_2^2 + \lambda \left(\sum_{i=1, i\neq a,b}^{d} {\theta'_i}^2 + \left(\frac{a+b}{2} \right)^2 + \left(\frac{a+b}{2} \right)^2 \right) \\
&= || \sum_{i=1, i\neq a,b}^{d} \theta'_i X_{\cdot i} + (a+b) X_{\cdot a} - y||_2^2 + \lambda \left(\sum_{i=1, i\neq a,b}^{d} {\theta'_i}^2 + \frac{(a+b)^2}{2} \right)
\end{aligned}$$

Now, note the first term (the squared loss term) is the same for $\hat{\theta}$ and θ'. Thus, restricting our attention to only the second term (the regularization term) and recalling that

$$\frac{1}{2}(a+b)^2 \leq a^2 + b^2$$

yields

$$\hat{\mathcal{R}}(\theta') \leq \hat{\mathcal{R}}(\hat{\theta}) = || \sum_{i=1, i\neq a,b}^{d} \hat{\theta}_i X_{\cdot i} + (a+b) X_{\cdot a} - y||_2^2 + \lambda \left(\sum_{i=1, i\neq a,b}^{d} \hat{\theta}_i^2 + a^2 + b^2 \right)$$

Which is a contradiction- therefore, we conclude $a = b$.

4. The ellipsoids in the ℓ_1/ℓ_2 regularization picture

a. 4.1 Empirical risk of LS solution

Let $\hat{w} = (X^T X)^{-1} X^T y$ (note this is just the OLS solution).
We proceed to show $\hat{R}_n(\hat{w}) = \frac{1}{n}(-y^T X \hat{w} + y^T y)$

$$
\begin{aligned}
\hat{R}_n(\hat{w}) &= \frac{1}{n}\left(X(X^TX)^{-1}X^Ty - y\right)^T\left(X(X^TX)^{-1}X^Ty - y\right) \\
&= \frac{1}{n}\left(y^TX\left((X^TX)^{-1}\right)^TX^T - y^T\right)\left(X(X^TX)^{-1}X^Ty - y\right) \\
&= \frac{1}{n}\left(y^TX(X^TX)^{-1}X^T - y^T\right)\left(X(X^TX)^{-1}X^Ty - y\right) \\
&= \frac{1}{n}\left(y^TX(X^TX)^{-1}X^TX(X^TX)^{-1}X^Ty - 2y^TX(X^TX)^{-1}X^Ty - y^Ty\right) \\
&= \frac{1}{n}\left(y^TX(X^TX)^{-1}X^Ty - 2y^TX(X^TX)^{-1}X^Ty - y^Ty\right) \\
&= \frac{1}{n}\left(-y^TX(X^TX)^{-1}X^Ty - y^Ty\right) \\
&= \frac{1}{n}\left(-y^TX\hat{w} - y^Ty\right)
\end{aligned}
$$

B. 4.2 Empirical risk for an arbitrary w

Now let w be an arbitrary estimator. Then

$$
\begin{aligned}
\hat{R}_n(w) &= \frac{1}{n}(Xw - y)^T(Xw - y) \\
&= \frac{1}{n}(w^TX^T - y^T)(Xw - y) \\
&= \frac{1}{n}(w^TX^TXw - 2y^TXw + y^Ty) \\
&= \frac{1}{n}(w^TX^TXw - 2(X^Ty)^Tw) + \frac{1}{n}y^Ty
\end{aligned}
$$

Now, completing the square yields

$$
\begin{aligned}
\hat{R}_n(w) &= \frac{1}{n}(w^TX^TXw - 2(X^Ty)^Tw) + \frac{1}{n}y^Ty \\
&= \frac{1}{n}\left((w - (X^TX)^{-1}X^Ty)^TX^TX(w - (X^TX)^{-1}X^Ty) - (X^Ty)^T(X^TX)^{-1}X^Ty\right) + \frac{1}{n}y^Ty \\
&= \frac{1}{n}(w - \hat{w})^TX^TX(w - \hat{w}) + \frac{1}{n}(-y^TX\hat{w} + y^Ty) \\
&= \frac{1}{n}(w - \hat{w})^TX^TX(w - \hat{w}) + \hat{R}_n(\hat{w})
\end{aligned}
$$

C. 4.3 $\hat{w}$ is the empirical risk minimizer

From 2, we have

$$
\hat{R}_n(w) = \frac{1}{n}(w - \hat{w})^TX^TX(w - \hat{w}) + \hat{R}_n(\hat{w})
$$

Now, since X^TX is positive semidefinite,

$$\frac{1}{n}(w-\hat{w})^TX^TX(w-\hat{w}) \geq 0 \text{ for all } w \in \mathbb{R}^d$$

Hence, for all $w \in \mathbb{R}^d$,

$$\hat{R}_n(w) = \frac{1}{n}(w-\hat{w})^TX^TX(w-\hat{w}) + \hat{R}_n(\hat{w}) \geq \hat{R}_n(\hat{w})$$

Hence $\hat{R}_n(\hat{w})$ is the minimum empirical risk, and $\hat{w}$ is the empirical risk minimizer.

D. Set of w exceeding $\hat{R}_n(\hat{w})$ by c

Let $S_c := \{w|\hat{R}_n(w) + \hat{R}_n(\hat{w}) + c\}$. Then, by 2, for any $w \in S_c$,

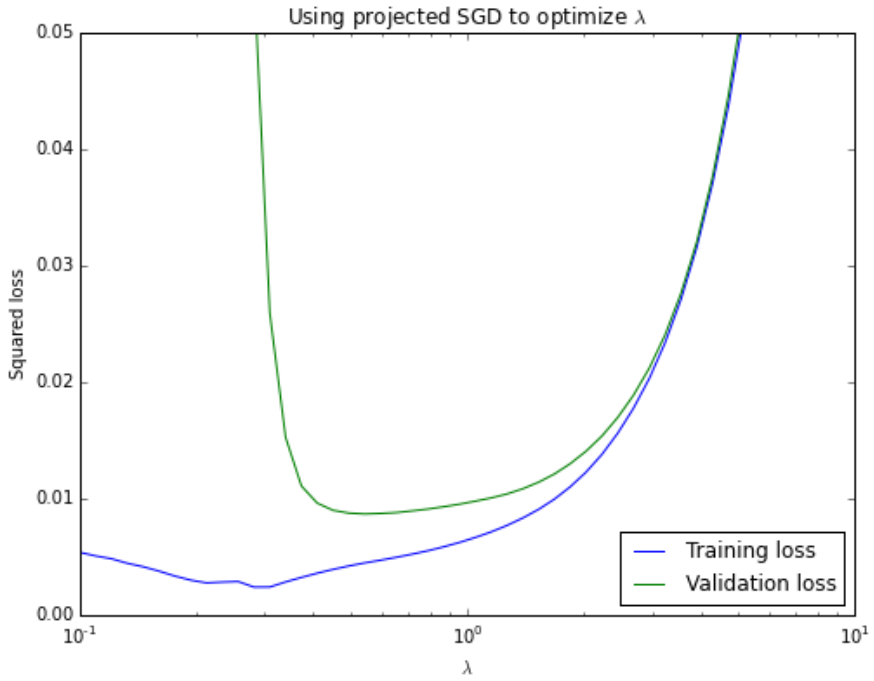
$$\frac{1}{n}(w-\hat{w})^TX^TX(w-\hat{w}) = c$$

We conclude by simply noting (by X^TX positive semi-definite) this is simply an ellipsoid with center at $\hat{w}$.

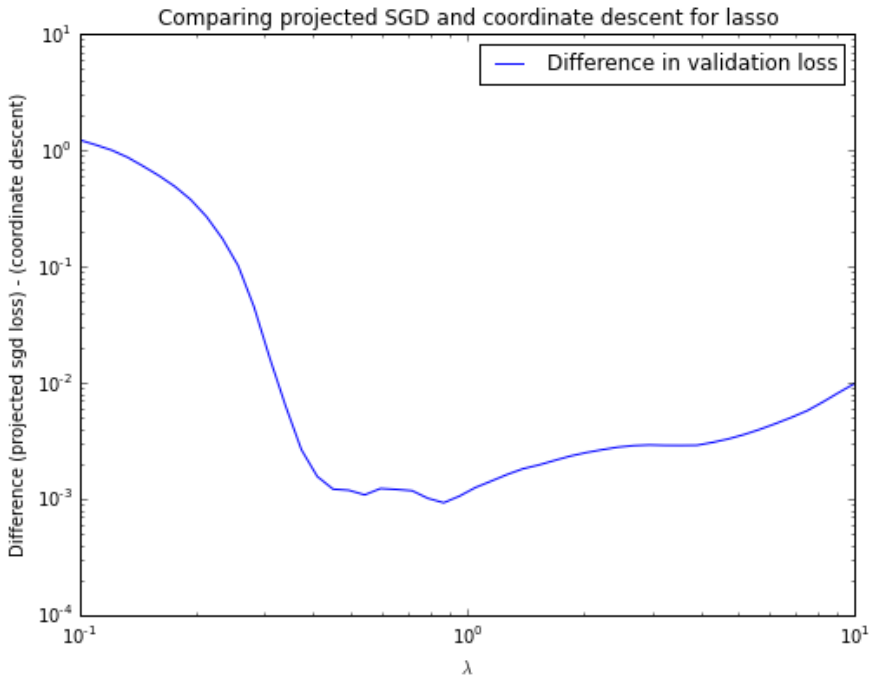
5. Projected SGD

5.1 Implementing projected SGD

After implementing projected SGD in python (using a fixed stepsize of $\alpha = 0.0001$, the following training and test set loss values were obtained:



Note that projected SGD and coordinate descent find essentially the same solution. However, the validation set loss values obtained for projected SGD is much worse than those obtained for coordinate descent for λ values that are not near $\lambda_{optimal}$.



This behavior is likely due to lack of convergence (i.e. a function of the fixed stepsize in SGD, and the number of iterations for both algorithms).

5.2 Comparing projected SGD and coordinate descent

Finally, the sparsity of the SGD solution is analyzed (using several thresholds for w_j near zero):

- $w_j = 0$:

	Predicted zero	Predicted non-zero
True non-zero ($\boldsymbol{w}$[0:10])	0	10
True zero ($\boldsymbol{w}$[10:])	0	65

- $w_j < 10^{-3}$:

	Predicted zero	Predicted non-zero
True non-zero ($\boldsymbol{w}$[0:10])	0	10
True zero ($\boldsymbol{w}$[10:])	14	51

- $w_j < 10^{-2}$:

	Predicted zero	Predicted non-zero
True non-zero ($\boldsymbol{w}$[0:10])	0	10
True zero ($\boldsymbol{w}$[10:])	57	8

Comparing our results to coordinate descent, it appears the coordinate descent algorithm finds the optimal solution more quickly (both in terms of minimum squared validation error and maximum sparsity). However, it is important to note the projected SGD algorithm has not been optimized- specifically, it was only run with a fixed step size of $\alpha = 0.0001$, which was selected since it found the correct λ.