

S&DS 365 / 665

Intermediate Machine Learning

Sparse Regression

Friday, September 1
(aka Monday, September 4)

Welcome back!

- Course page: <http://interml.ydata123.org>
- iML page:
<https://ydata123.org/fa22/introml/calendar.html>
- Quiz 1 posted on September 6
- Assignment 1 posted on September 13
- OH posted on Canvas / EdD
- Install IML environment (available from the course page)

Preliminary OH

John Lafferty: Monday 11 am–12 pm

Ruixiao Wang: Monday 4 pm–5 pm

Zehao Dou: Tuesday 4 pm–5 pm

Chris Xu: Wednesday 10 am–11 am

Andy Yang: Friday 1 pm–2 pm

Room(s) TBA; we'll post a Zoom link as well

Topics for today

- *Regression*
- High dimensional regression
- Sparsity and the lasso

Regression

We observe pairs $(X_1, Y_1), \dots, (X_n, Y_n)$.

$\mathcal{D} = \{(X_1, Y_1), \dots, (X_n, Y_n)\}$ is called the *training data*

$Y_i \in \mathbb{R}$ is the *response*; $X_i \in \mathbb{R}^p$ is the *covariate* (or feature) vector

For example, suppose we have n subjects and Y_i is the blood pressure of subject i and $X_i = (X_{i1}, \dots, X_{ip})$ is a vector of $p = 5,000$ gene expression levels for subject i

Remember: $Y_i \in \mathbb{R}$ and $X_i \in \mathbb{R}^p$

Given a new pair (X, Y) , we want to predict Y from X .

Regression

Let \hat{Y} be a prediction of Y . The *prediction error* or *risk* is

$$R = \mathbb{E}(Y - \hat{Y})^2$$

where \mathbb{E} is the expected value (mean).

The best predictor is the *regression function*

$$m(x) = \mathbb{E}(Y|X = x) = \int y p(y | x) dy.$$

However, the true regression function $m(x)$ is not known. We need to estimate $m(x)$.

Regression

Given the training data $\mathcal{D} = \{(X_1, Y_1), \dots, (X_n, Y_n)\}$ we want to construct \hat{m} to make

$$\text{prediction risk} = R(\hat{m}) = \mathbb{E}(Y - \hat{m}(X))^2$$

small. Here, (X, Y) is a new pair.

Bias-variance decomposition

$$R(\hat{m}) = \int \text{bias}^2(x)p(x)dx + \int \text{var}(x)p(x) + \sigma^2$$

where

$$\text{bias}(x) = \mathbb{E}(\hat{m}(x)) - m(x)$$

$$\text{var}(x) = \text{Variance}(\hat{m}(x))$$

$$\sigma^2 = \mathbb{E}(Y - m(X))^2$$

Bias-Variance Tradeoff

Prediction Risk = $\text{Bias}^2 + \text{Variance}$

Prediction methods with **low bias** tend to have **high variance**.

Prediction methods with **low variance** tend to have **high bias**.

For example, the predictor $\hat{m}(x) \equiv 0$ has 0 variance but will be badly biased.

To predict well, we need to balance the bias and the variance.

Bias-Variance Tradeoff

More generally, we need to tradeoff **approximation error** against **estimation error**:

$$R(\hat{f}) - R^* = \underbrace{R(\hat{f}) - \inf_{f \in \mathcal{F}} R(f)}_{\text{estimation error}} + \underbrace{\inf_{f \in \mathcal{F}} R(f) - R^*}_{\text{approximation error}}$$

where R^* is the smallest possible risk and $\inf_{f \in \mathcal{F}} R(f)$ is smallest possible risk using class of estimators \mathcal{F} .

- Approximation error is a generalization of squared bias
- Estimation error is a generalization of variance

Linear Regression

Try to find the **best linear predictor**:

$$m(x) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p.$$

Important: We do *not* assume the true regression function is linear.

Can always define $x_1 = 1$; then the intercept is β_1 and we can write

$$m(x) = \beta_1 x_1 + \cdots + \beta_p x_p = \beta^T x$$

where $\beta = (\beta_1, \dots, \beta_p)$ and $x = (x_1, \dots, x_p)$.

Low Dimensional Linear Regression

Assume for now that p (= length of each X_i) is small. To find a good linear predictor we choose β to minimize the *training error*:

$$\text{training error} = \frac{1}{n} \sum_{i=1}^n (Y_i - \beta^T X_i)^2$$

The minimizer $\hat{\beta} = (\hat{\beta}_1, \dots, \hat{\beta}_p)$ is called the *least squares estimator*.

Low Dimensional Linear Regression

The least squares estimator is:

$$\hat{\beta} = (\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T \mathbb{Y}$$

where

$$\mathbb{X}_{n \times p} = \begin{pmatrix} X_{11} & X_{12} & \cdots & X_{1p} \\ X_{21} & X_{22} & \cdots & X_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ X_{n1} & X_{n2} & \cdots & X_{np} \end{pmatrix}$$

and

$$\mathbb{Y} = (Y_1, \dots, Y_n)^T.$$

Exercise: Show this

Low Dimensional Linear Regression

Summary: the least squares estimator is $m(x) = \hat{\beta}^T x = \sum_j \hat{\beta}_j x_j$
where

$$\hat{\beta} = (\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T \mathbb{Y}.$$

When we observe a new X , we predict Y to be

$$\hat{Y} = \hat{m}(X) = \hat{\beta}^T X.$$

We can try to improve this by:

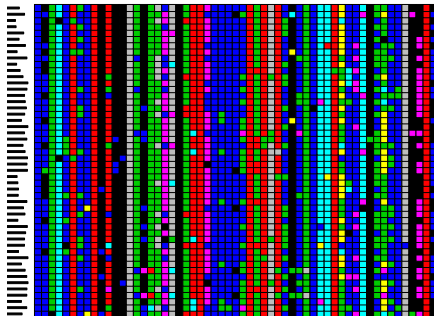
- (i) dealing with high dimensions
- (ii) using something more flexible than linear predictors.

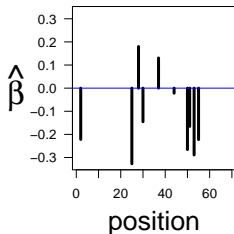
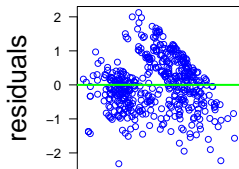
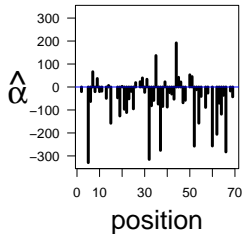
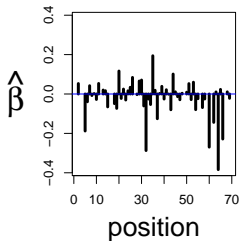
Example

Y = HIV resistance

X_j = amino acid in position j of the virus.

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_{100} X_{100} + \epsilon$$





Top left: $\hat{\beta}$ fitted values

Top right: marginal regression coefficients (one-at-a-time)

Bottom left: $\hat{Y}_i - Y_i$ versus \hat{Y}_i

Bottom right: a sparse regression (coming up soon)

Topics

- Regression
- *High dimensional regression*
- Sparsity and the lasso

High Dimensional Linear Regression

Now suppose p is large. We even might have $p > n$ (more predictors than data points).

The least squares estimator is not defined since $\mathbb{X}^T \mathbb{X}$ is not invertible. The variance of the least squares prediction is huge.

Recall the **bias-variance tradeoff**:

$$\text{Prediction Error} = \text{Bias}^2 + \text{Variance}$$

We need to increase the bias so that we can decrease the variance.

Ridge Regression

Recall that the least squares estimator minimizes the training error $\frac{1}{n} \sum_{i=1}^n (Y_i - \beta^T X_i)^2$.

Instead, we can minimize the *penalized training error*:

Ridge regression

$$\hat{\beta} = \arg \min_{\beta} \frac{1}{n} \sum_{i=1}^n (Y_i - \beta^T X_i)^2 + \frac{\lambda}{n} \|\beta\|_2^2$$

where $\|\beta\|_2 = \sqrt{\sum_j \beta_j^2}$. The solution is:

$$\hat{\beta} = (\mathbb{X}^T \mathbb{X} + \lambda I)^{-1} \mathbb{X}^T \mathbb{Y}$$

Ridge Regression

The tuning parameter λ controls the bias-variance tradeoff:

$\lambda = 0 \implies$ least squares.

$\lambda = \infty \implies \hat{\beta} = 0.$

We choose λ to minimize $\hat{R}(\lambda)$ where $\hat{R}(\lambda)$ is an estimate of the prediction risk.

Ridge Regression

To estimate the prediction risk, do *not* use training error:

$$R_{\text{training}} = \frac{1}{n} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2, \quad \hat{Y}_i = \mathbf{x}_i^T \hat{\beta}$$

because it is biased: $\mathbb{E}(R_{\text{training}}) < R(\hat{\beta})$

Instead, we use *leave-one-out cross-validation*:

1. leave out (X_i, Y_i)
2. find $\hat{\beta}$
3. predict Y_i : $\hat{Y}_{(-i)} = \hat{\beta}^T \mathbf{x}_i$
4. repeat for each i

Leave-one-out cross-validation

Can be shown that

$$\begin{aligned}\hat{R}(\lambda) &= \frac{1}{n} \sum_{i=1}^n (Y_i - \hat{Y}_{(-i)})^2 = \frac{1}{n} \sum_{i=1}^n \frac{(Y_i - \hat{Y}_i)^2}{(1 - H_{ii})^2} \\ &\approx \frac{R_{\text{training}}}{\left(1 - \frac{p_\lambda}{n}\right)^2} \\ &\approx R_{\text{training}} + \frac{2p_\lambda \hat{\sigma}^2}{n}\end{aligned}$$

where

$$\begin{aligned}H &= \mathbb{X}(\mathbb{X}^T \mathbb{X} + \lambda I)^{-1} \mathbb{X}^T \\ p_\lambda &= \text{trace}(H) = H_{11} + H_{22} + \cdots + H_{nn} \\ &\quad \text{"effective dimension" of the model}\end{aligned}$$

Example

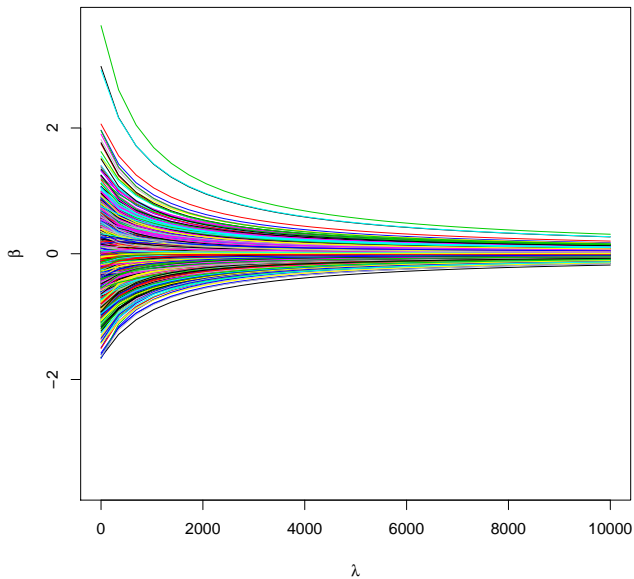
$$Y = 3X_1 + \cdots + 3X_5 + 0X_6 + \cdots + 0X_{1000} + \epsilon$$

$$n = 100, \quad p = 1,000.$$

So there are 1000 covariates but only 5 are relevant.

What does ridge regression do in this case?

Ridge Regularization Paths



Sparse Linear Regression

Ridge regression does not take advantage of **sparsity**.

Maybe only a small number of covariates are important predictors.
How do we find them?

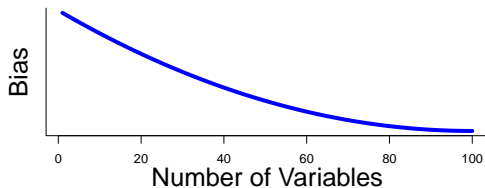
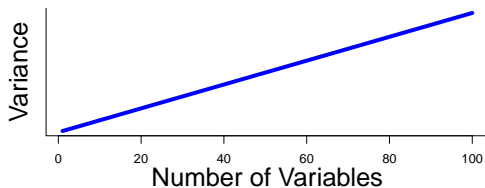
We could fit many submodels (with a small number of covariates) and choose the best one. This is called *model selection*.

The inaccuracy is

$$\text{prediction error} = \text{bias}^2 + \text{variance}$$

Now the bias is the error due to omitting important variables. The variance is the error due to having to estimate many parameters.

The Bias-Variance Tradeoff



The Bias-Variance Tradeoff

This is a Goldilocks problem: Can't use too few or too many variables.

Have to choose just the right variables.

If there are p variables then there are 2^p models.

Suppose we have 30,000 genes.

It seems we have to search through $2^{30,000}$ models.

Two things that save us

Two key ideas to make this feasible are **sparsity** and **convex relaxation**.

Sparsity: probably only a few genes are needed to predict some disease Y . In other words, of $\beta_1, \dots, \beta_{30,000}$ most $\beta_j \approx 0$.

But which ones? (Needle in a haystack.)

Convex Relaxation: Replace model search with something easier.

It is the marriage of these two concepts that makes it all work.

Topics

- Regression
- High dimensional regression
- *Sparsity and the lasso*

Sparsity

Consider estimating $\beta = (\beta_1, \dots, \beta_p)$ by minimizing

$$\sum_{i=1}^n \left(Y_i - (\beta_0 + \beta_1 X_{i1} + \dots + \beta_p X_{ip}) \right)^2$$

subject to the constraint on the “size” of β : $\|\beta\|_q \leq \text{small}$.

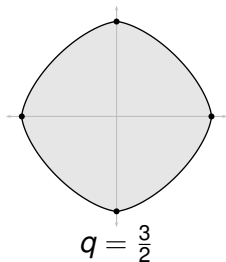
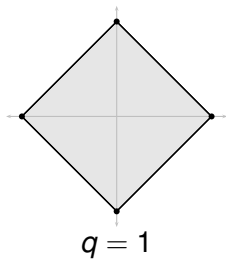
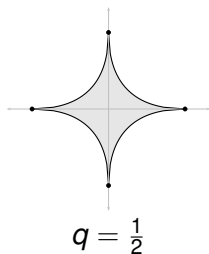
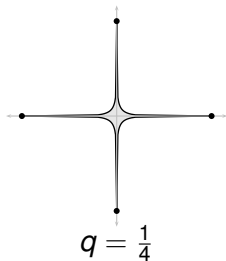
Can we do this minimization?

If we use $q = 0$ this is same as searching through all 2^p models, because $\|\beta\|_q^q$ is the number of nonzero coefficients as $q \rightarrow 0$.

What about other values of q ?

What does the set $\{\beta : \|\beta\|_q \leq \text{small}\}$ look like?

The set $\|\beta\|_q \leq 1$ when $p = 2$



Sparsity Meets Convexity

We need these sets to have a nice shape (convex). If so, the minimization is no longer computationally hard. In fact, it is easy.

Sensitivity to sparsity: $q \leq 1$

Convexity (niceness): $q \geq 1$

This means we should use $q = 1$.

Sparsity Meets Convexity

Lasso regression

$$\hat{\beta} = \arg \min_{\beta} \frac{1}{2n} \sum_{i=1}^n (Y_i - \beta^T X_i)^2 + \lambda \|\beta\|_1$$

where $\|\beta\|_1 = \sum_j |\beta_j|$.

Lasso

The result is an estimated vector

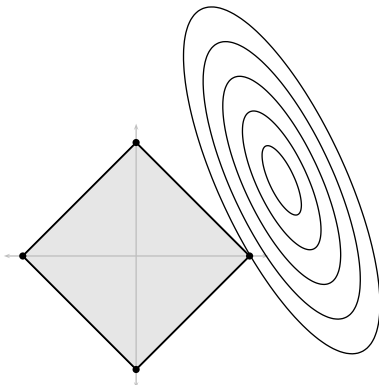
$$\hat{\beta}_1, \dots, \hat{\beta}_p$$

Most are zero!

Magically, we have done model selection without searching (thanks to sparsity plus convexity).

The next picture gives intuition for why some $\hat{\beta}_j = 0$.

Sparsity: How corners create sparse estimators



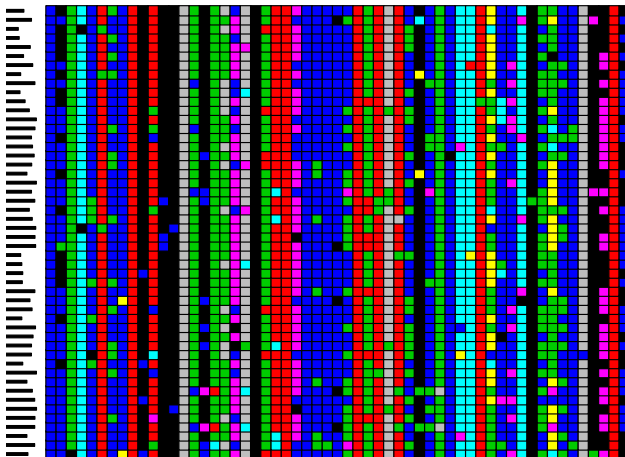
Standardization

Note that, for both lasso and ridge regression, it's important to standardize the features — scale so that the standard deviation of each feature (column) is a constant.

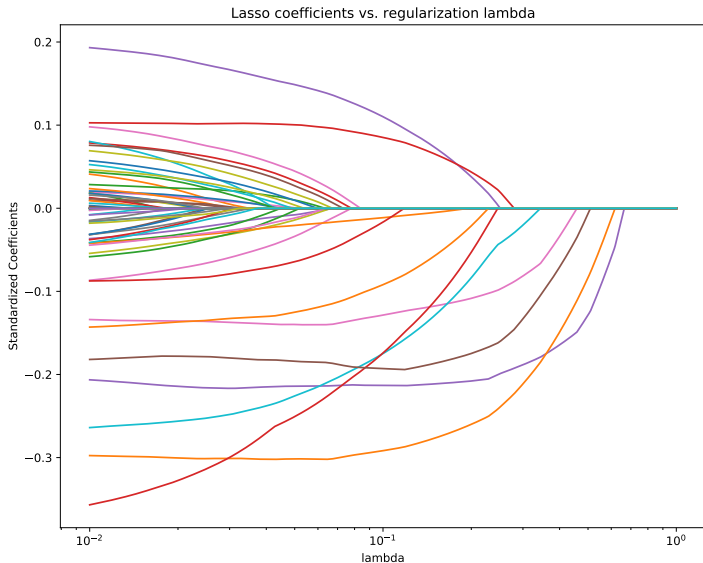
Let's go to the notebook!

The lasso: HIV example again

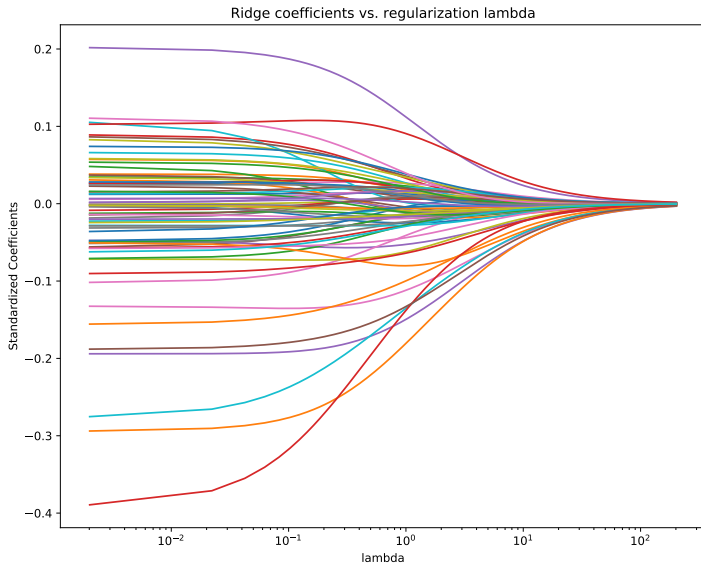
- Y is resistance to HIV drug.
- X_j = amino acid in position j of the virus.
- $p = 99$, $n \approx 100$.



The lasso: HIV example

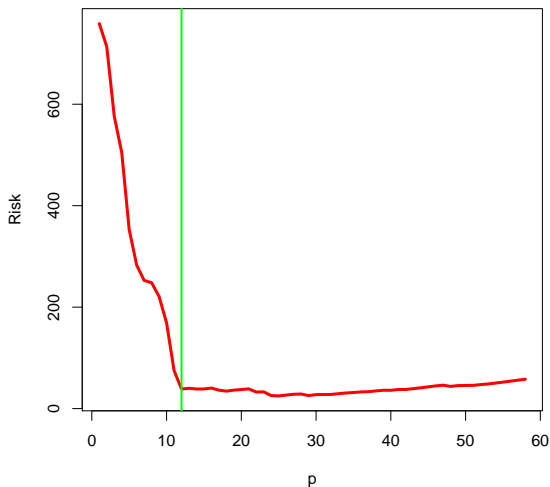


Contrast with ridge regression

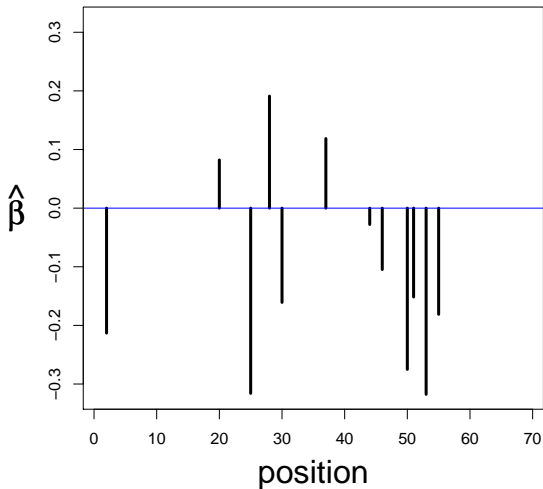


Selecting λ

We choose the sparsity level by estimating prediction error.



The lasso: An example



Sparsity and convexity

Marriage of sparsity and convexity was one of biggest developments in statistics and machine learning in last 10-20 years

The lasso

- $\hat{\beta}(\lambda)$ is called the **lasso** estimator. Then define

$$\hat{S}(\lambda) = \left\{ j : \hat{\beta}_j(\lambda) \neq 0 \right\}.$$

- After you find $\hat{S}(\lambda)$, you should re-fit the model by doing least squares on the sub-model $\hat{S}(\lambda)$.

The lasso

Choose λ by risk estimation.

Re-fit the model with the non-zero coefficients. Then apply leave-one-out cross-validation:

$$\hat{R}(\lambda) = \frac{1}{n} \sum_{i=1}^n (Y_i - \hat{Y}_{(i)})^2 = \frac{1}{n} \sum_{i=1}^n \frac{(Y_i - \hat{Y}_i)^2}{(1 - H_{ii})^2} \approx \frac{1}{n} \frac{RSS}{(1 - \frac{s}{n})^2}$$

where H is the hat matrix and $s = \#\{j : \hat{\beta}_j \neq 0\}$.

Choose $\hat{\lambda}$ to minimize $\hat{R}(\lambda)$.

The lasso

The complete steps are:

- 1 Find $\hat{\beta}(\lambda)$ and $\hat{S}(\lambda)$ for each λ .
- 2 Choose $\hat{\lambda}$ to minimize estimated risk.
- 3 Let \hat{S} be the selected variables.
- 4 Let $\hat{\beta}$ be the least squares estimator using only \hat{S} .
- 5 Prediction: $\hat{Y} = X^T \hat{\beta}$.

Summary

- For low dimensional (linear) prediction, we can use least squares.
- For high dimensional linear regression, we face a bias-variance tradeoff: omitting too many variables causes bias while including too many variables causes high variance.
- The key is to select a good subset of variables.
- The *lasso* (ℓ_1 -regularized least squares) is a fast way to select variables.
- If there are good, sparse linear predictors, lasso will work well.

Some computational details (optional)



Some convexity theory for the lasso

Consider a simpler model than regression: Suppose $Y \sim N(\mu, 1)$. Let $\hat{\mu}$ minimize

$$A(\mu) = \frac{1}{2}(Y - \mu)^2 + \lambda|\mu|.$$

How do we minimize $A(\mu)$?

- Since A is convex, we set the subderivative = 0. Recall that c is a *subderivative* of $f(x)$ at x_0 if

$$f(x) - f(x_0) \geq c(x - x_0).$$

- The *subdifferential* $\partial f(x_0)$ is the set of subderivatives. Also, x_0 minimizes f if and only if $0 \in \partial f$.

ℓ_1 and soft thresholding

- If $f(\mu) = |\mu|$ then

$$\partial f = \begin{cases} \{-1\} & \mu < 0 \\ [-1, 1] & \mu = 0 \\ \{+1\} & \mu > 0. \end{cases}$$

- Hence,

$$\partial A = \begin{cases} \{\mu - Y - \lambda\} & \mu < 0 \\ \{\mu - Y + \lambda z : -1 \leq z \leq 1\} & \mu = 0 \\ \{\mu - Y + \lambda\} & \mu > 0. \end{cases}$$

ℓ_1 and soft thresholding

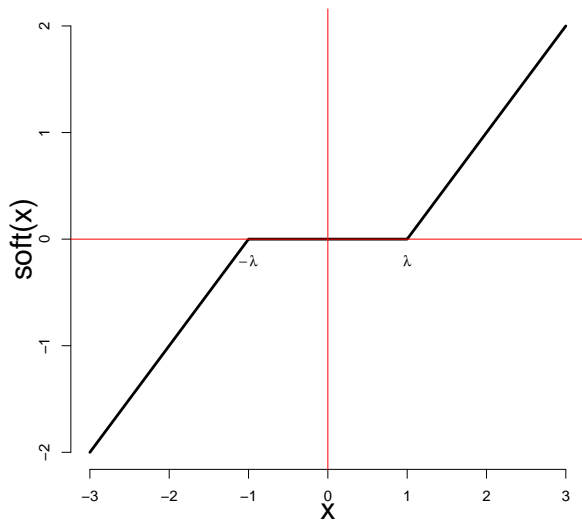
- $\hat{\mu}$ minimizes $A(\mu)$ if and only if $0 \in \partial A$.
- So

$$\hat{\mu} = \begin{cases} Y + \lambda & Y < -\lambda \\ 0 & -\lambda \leq Y \leq \lambda \\ Y - \lambda & Y > \lambda. \end{cases}$$

- This can be written as

$$\hat{\mu} = \text{soft}(Y, \lambda) \equiv \text{sign}(Y) (|Y| - \lambda)_+.$$

ℓ_1 and soft thresholding



The lasso: Computing $\hat{\beta}$

To minimize $\frac{1}{2n} \sum_{i=1}^n (Y_i - \beta^T X_i)^2 + \lambda \|\beta\|_1$ by *coordinate descent*:

- Set $\hat{\beta} = (0, \dots, 0)$ then iterate the following
- for $j = 1, \dots, p$:
 - ▶ set $R_i = Y_i - \sum_{s \neq j} \hat{\beta}_s X_{si}$
 - ▶ Set $\hat{\beta}_j$ to be least squares fit of R_i 's on X_j .
 - ▶ $\hat{\beta}_j \leftarrow \text{Soft}_{\lambda_j}(\hat{\beta}_j)$ where $\lambda_j = \frac{\lambda}{\frac{1}{n} \sum_i X_{ij}^2}$.
- Then use least squares $\hat{\beta}$ on selected subset S .

Variations on the lasso

- “Elastic net”: minimize

$$\sum_{i=1}^n (Y_i - \beta^T X_i)^2 + \lambda_1 \|\beta\|_1 + \lambda_2 \|\beta\|_2^2$$

- Group lasso:

$$\beta = (\underbrace{\beta_1, \dots, \beta_k}_{v_1}, \dots, \underbrace{\beta_t, \dots, \beta_p}_{v_m})$$

minimize:

$$\sum_{i=1}^n (Y_i - \beta^T X_i)^2 + \lambda \sum_{j=1}^m \|v_j\|$$