S&DS 365 / 665

Intermediate Machine Learning

Lasso, Smoothing and Kernels

Wednesday, September 7

Yale

Reminders

- OH posted to Canvas / EdD
- Reminder: Slides updated often; please refresh
- Quiz 1
  - Available after class on Canvas
  - Complete before Friday at 10:30am (48 hours)
  - Topics: Bias, variance, risk
- Assignment 1 next week
- Questions?

Reminders: OH

John Lafferty	Monday	2:00 pm-3:00 pm
Sophia Zhu	Monday	7:00 pm-8:00 pm
Chris Xu	Tuesday	2:00 pm-3:00 pm
Ben Christensen	Tuesday	6:30 pm - 7:30 pm
Jacques Morris	Wednesday	11:00 am-12:00 pm
Louis Deschuttere	Friday	11:00 am-12:00 pm
Eric Sun	Sunday	9:00 am-10:00 am

Topics for today

- Recap of lasso
- A simple algorithm for the lasso
- Nonparametric regression
- Smoothing methods
- Bias, variance, and curse of dimensionality

Recall from last time

- 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.

Regression

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

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

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

Key fact: Bias-variance decomposition:

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

where

$$\begin{aligned}
\text{bias}(x) &= \mathbb{E}(\widehat{m}(x)) - m(x) \\
\text{var}(x) &= \text{Variance}(\widehat{m}(x)) \\
\sigma^2 &= \mathbb{E}(Y - m(X))^2
\end{aligned}$$

Bias-Variance Tradeoff

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

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

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
- Decomposition holds more generally, even for classification

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

prediction error = bias^2 + variance + σ^2

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

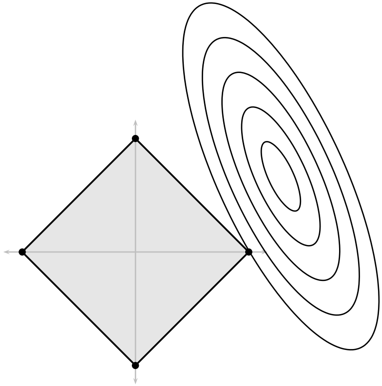
Sparsity Meets Convexity

Lasso regression

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

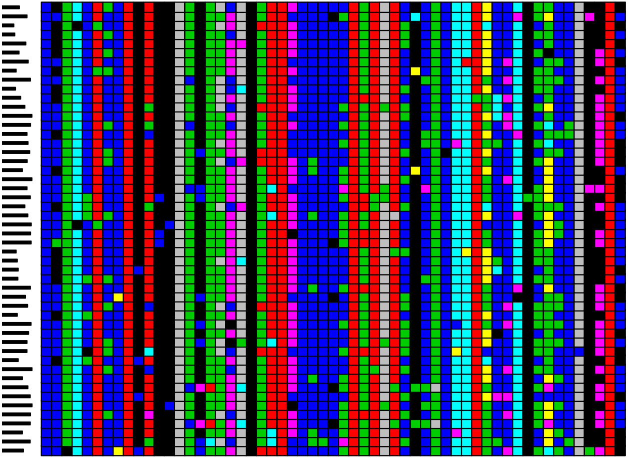
where $\|\beta\|_1 = \sum_j |\beta_j|$.

Sparsity: How corners create sparse estimators

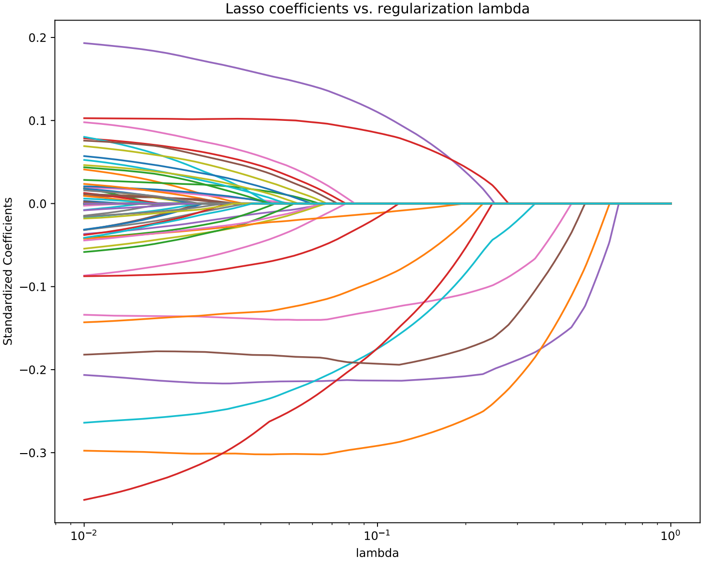


The lasso: HIV example

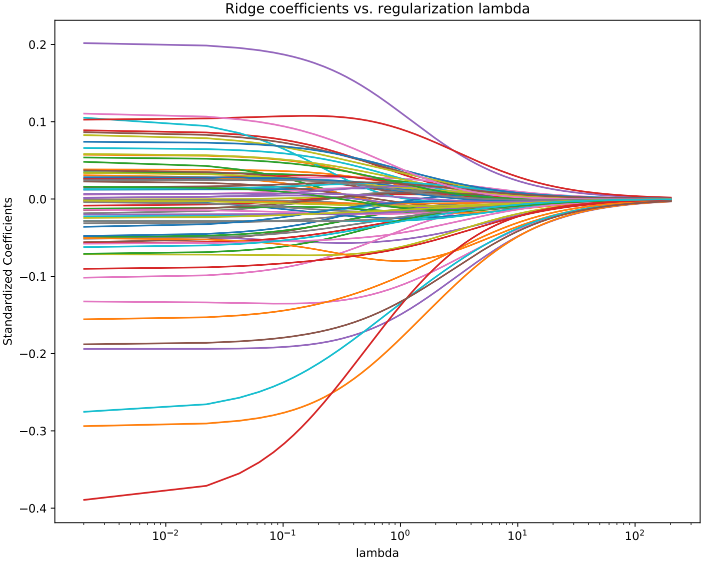
- Y is resistance to HIV drug.
- X_j = amino acid in position j of the virus.
- $p = 99$, $n \approx 100$.



The lasso: HIV example



Contrast with ridge regression



The lasso

- $\widehat{\beta}(\lambda)$ is called the lasso estimator. Selected set of variables is

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

Selecting λ

To choose λ by risk estimation:

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

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

where RSS is residual sum of squares and H is the hat matrix and $s = \|\widehat{\beta}\|_0 = \#\{j : \ \widehat{\beta}_j \neq 0\}$.

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

The lasso

The complete steps are:

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

An algorithm for the lasso: Derived in steps

We'll derive a simple algorithm for computing the lasso solution in steps.

I'll do the first step in detail. The next steps only require simple calculations that I'll leave to you.

An algorithm for the lasso

First consider minimizing

$$\frac{1}{2}(y-\beta)^2 + \lambda|\beta|$$

where y is a single number.

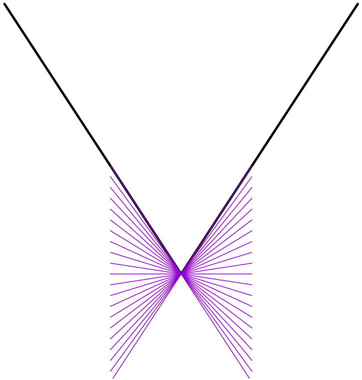
Taking the derivative and setting to zero, we get

$$\beta - y + \lambda v = 0$$

where

$$v \quad \begin{cases} = \text{sign}(\beta) & \text{if } |\beta| > 0 \\ \in [-1, 1] & \text{if } \beta = 0. \end{cases}$$

Subdifferential for $|\cdot|$



The set of vectors v pass through the tip at 0 and have slope between -1 and 1.

An algorithm for the lasso

Solution can be written as

$$\widehat{\beta} = \begin{cases} y - \lambda & \text{if } \beta > 0 \\ y + \lambda & \text{if } \beta < 0 \\ y - \lambda \left(\frac{y}{\lambda}\right) & \text{if } \beta = 0. \end{cases}$$

Equivalently:

$$\widehat{\beta} = \begin{cases} y - \lambda & \text{if } y > \lambda \\ y + \lambda & \text{if } y < -\lambda \\ 0 & \text{if } |y| \leq \lambda. \end{cases}$$

An algorithm for the lasso

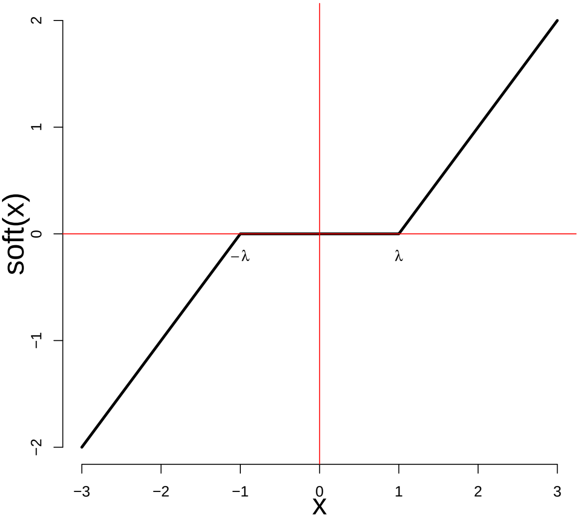
Equivalently:

$$\widehat{\beta} = \begin{cases} y - \lambda & \text{if } y > \lambda \\ y + \lambda & \text{if } y < -\lambda \\ 0 & \text{if } |y| \le \lambda. \end{cases}$$

Soft thresholding

$$\begin{aligned} \widehat{\beta} &= \mathrm{Soft}_\lambda(y) \\ &\equiv \mathrm{sign(y)}\,(|y| - \lambda)_+ = \left(1 - \frac{\lambda}{|y|}\right)_+ y \end{aligned}$$

Soft thresholding



An algorithm for the lasso: Next step

Next consider minimizing

$$\frac{1}{2}(y - x\beta)^2 + \lambda|\beta|$$

where y and x are a single numbers.

Exercise: Show that

$$\widehat{\beta} = \text{Soft}_{\frac{\lambda}{x^2}}\left(\frac{xy}{x^2}\right)$$

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

To minimize $\frac{1}{2n}\sum_i (y_i - \beta^T x_i)^2 + \lambda\|\beta\|_1$, we apply this algorithm one coordinate at a time:

Lasso by coordinate descent

- Set $\widehat{\beta} = (0, \ldots, 0)$, then iterate until convergence:
- for $j = 1, \ldots, p$:
  - set $r_i = y_i - \sum_{s \neq j} \widehat{\beta}_s x_{si}$
  - Set $\widehat{\beta}_j$ to be least squares fit of r_i's on x_j.
  - $\widehat{\beta}_j \leftarrow \text{Soft}_{\lambda_j}(\widehat{\beta}_j)$ where $\lambda_j = \frac{\lambda}{\frac{1}{n}\sum_i x_{ij}^2}$.
- Then use least squares $\widehat{\beta}$ on selected subset $\widehat{S}(\lambda)$.

Next up

Nonparameteric regression by smoothing

Nonparametric Regression

Given $(X_1, Y_1), \ldots, (X_n, Y_n)$ predict Y from X.

Assume only that $Y_i = m(X_i) + \epsilon_i$ where where $m(x)$ is a smooth function of x.

The most popular methods are *kernel methods*. However, there are two types of kernels:

1. Smoothing kernels
2. Mercer kernels

Smoothing kernels involve local averaging.
Mercer kernels involve regularization.

Smoothing kernel estimator

$$\widehat{m}_h(x) = \frac{\sum_{i=1}^n Y_i \, K_h(X_i, x)}{\sum_{i=1}^n K_h(X_i, x)}$$

where $K_h(x, z)$ is a *kernel* such as

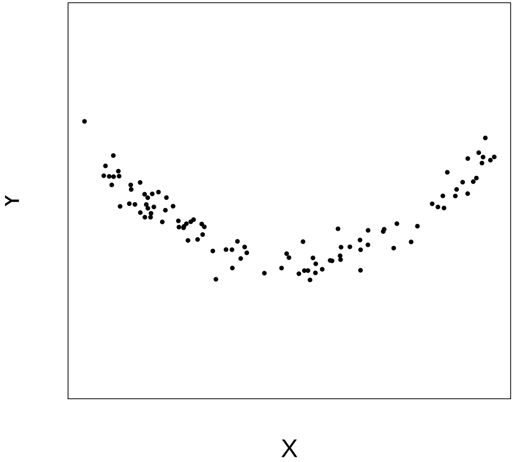
$$K_h(x, z) = \exp\left(-\frac{\|x - z\|^2}{2h^2}\right)$$

and $h > 0$ is called the *bandwidth*

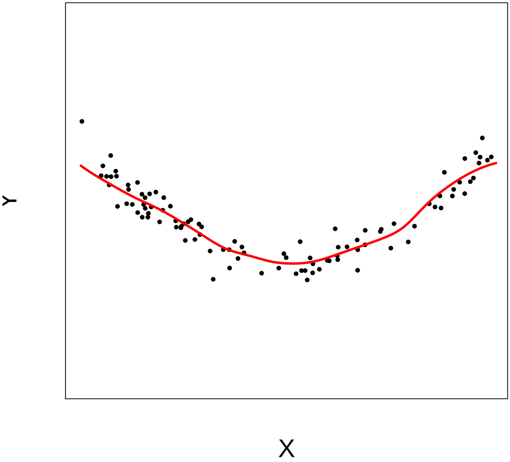
- $\widehat{m}_h(x)$ is just a local average of the Y_i's near x.

- The bandwidth h controls the bias-variance tradeoff:
Small h = large variance while *large h = large bias*.

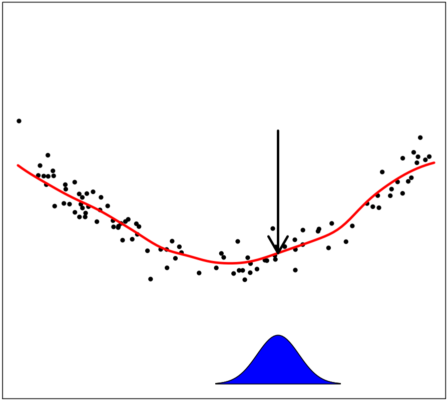
Example: Some Data – Plot of Y_i versus X_i



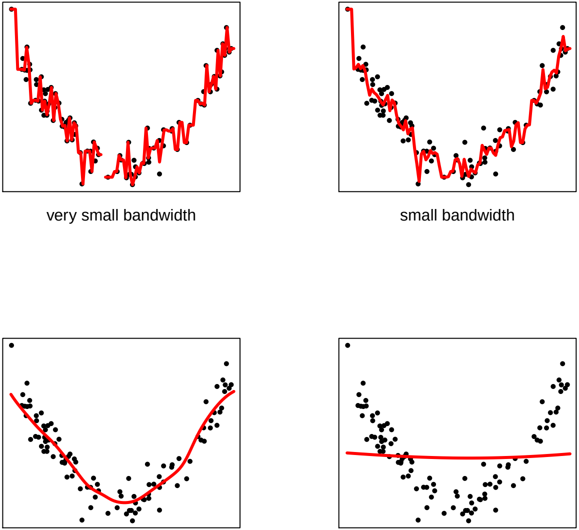
Example: $\widehat{m}(x)$



$\widehat{m}(x)$ is a local average



Effect of the bandwidth h



very small bandwidth

small bandwidth

medium bandwidth

large bandwidth

Let's go to the notebook

Smoothing Kernels

$$\text{Risk} = \mathbb{E}(Y - \widehat{m}_h(X))^2 = \text{bias}^2 + \text{variance} + \sigma^2.$$

Under mild assumptions on the distribution of the data:

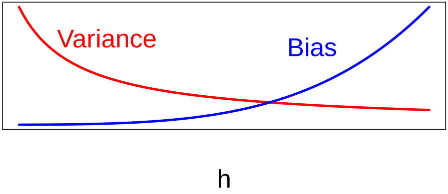
$$\text{bias}^2 \approx h^4$$
$$\text{variance} \approx \frac{1}{nh^p}$$

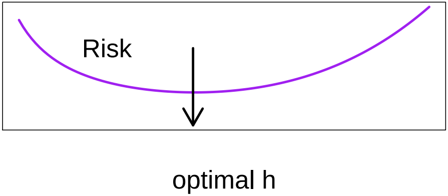
where p = dimension of X.

$\sigma^2 = \mathbb{E}(Y - m(X))^2$ is the unavoidable prediction error.

small h: low bias, high variance (undersmoothing)
large h: high bias, low variance (oversmoothing)

Risk Versus Bandwidth





Estimating the Risk: Cross-Validation

To choose h we need to estimate the risk $R(h)$. We can estimate the risk by using *cross-validation*.

1. Omit (X_i, Y_i) to get $\widehat{m}_{h,(i)}$, then predict: $\widehat{Y}_{(i)} = \widehat{m}_{h,(i)}(X_i)$.
2. Repeat this for all observations.
3. The cross-validation estimate of risk is:

$$\widehat{R}(h) = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \widehat{Y}_{(i)})^2.$$

Shortcut formula:

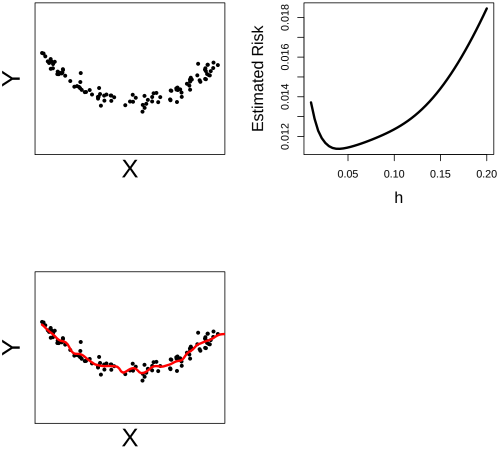
$$\widehat{R}(h) = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{Y_i - \widehat{Y}_i}{1 - L_{ii}}\right)^2$$

where $L_{ii} = K_h(X_i, X_i)/\sum_{i'=1}^{n} K_h(X_i, X_{i'})$.

Summary so far

1. Compute $\widehat{m}_h$ for each h.
2. Estimate the risk $\widehat{R}(h)$.
3. Choose bandwidth $\widehat{h}$ to minimize $\widehat{R}(h)$.
4. Let $\widehat{m}(x) = \widehat{m}_{\widehat{h}}(x)$.

Example



The curse of dimensionality

The method is easily applied in high dimensions — but it doesn't work well.

- The squared bias scales as h^4 and the variance scales as $\frac{1}{nh^p}$
- As a result, the risk goes down no faster than $n^{-4/(4+p)}$ (Exercise)
- Suppose we want to make this small, of size ϵ—how many data points do we need?

$$n \geq \left(\frac{1}{\epsilon}\right)^{1+p/4}$$

- Grows exponentially with dimension—*the curse of dimensionality*

Additive models

A compromise is to use *additive models* of the form

$$\widehat{m}(x) = \widehat{m}_1(x_1) + \widehat{m}_2(x_2) + \cdots \widehat{m}_p(x_p)$$

- Each function $\widehat{m}_j(x_j)$ is estimated by smoothing, holding the other functions fixed
- Soft thresholding can be used in high dimensions, leading to a generalization of the lasso

https://rss.onlinelibrary.wiley.com/doi/abs/10.1111/j.1467-9868.2009.00718.x

Summary for today

- The lasso can be computed by iterative soft thresholding
- Smoothing methods compute local averages, weighting points by a kernel
- The curse of dimensionality limits use of smoothing methods to low dimensions