VIASM Lectures on

Statistical Machine Learning for High Dimensional Data

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References

- *Statistical Machine Learning.* Lafferty, Liu and Wasserman (2012).
- *The Elements of Statistical Learning*. Hastie, Tibshirani and Friedman (2009).
  (`www-stat.stanford.edu/~tibs/ElemStatLearn/`)
- *Pattern Recognition and Machine Learning* Bishop (2009).

Outline

1. Regression
   - predicting Y from X
2. Structure and Sparsity
   - finding and using hidden structure
3. Nonparametric Methods
   - using statistical models with weak assumptions
4. Latent Variable Models
   - making use of hidden variables

Introduction

- Machine learning is statistics with a focus on *prediction*, *scalability* and *high dimensional problems*.
- Regression: predict $Y \in \mathbb{R}$ from X.
- Classification: predict $Y \in \{0, 1\}$ from X.
  - Example: Predict if an email X is real $Y = 1$ or spam $Y = 0$.
- Finding structure. Examples:
  - Clustering: find groups.
  - Graphical Models: find conditional independence structure.

Three Main Themes

Convexity

Convex problems can be solved quickly. If necessary, approximate the problem with a convex problem.

Sparsity

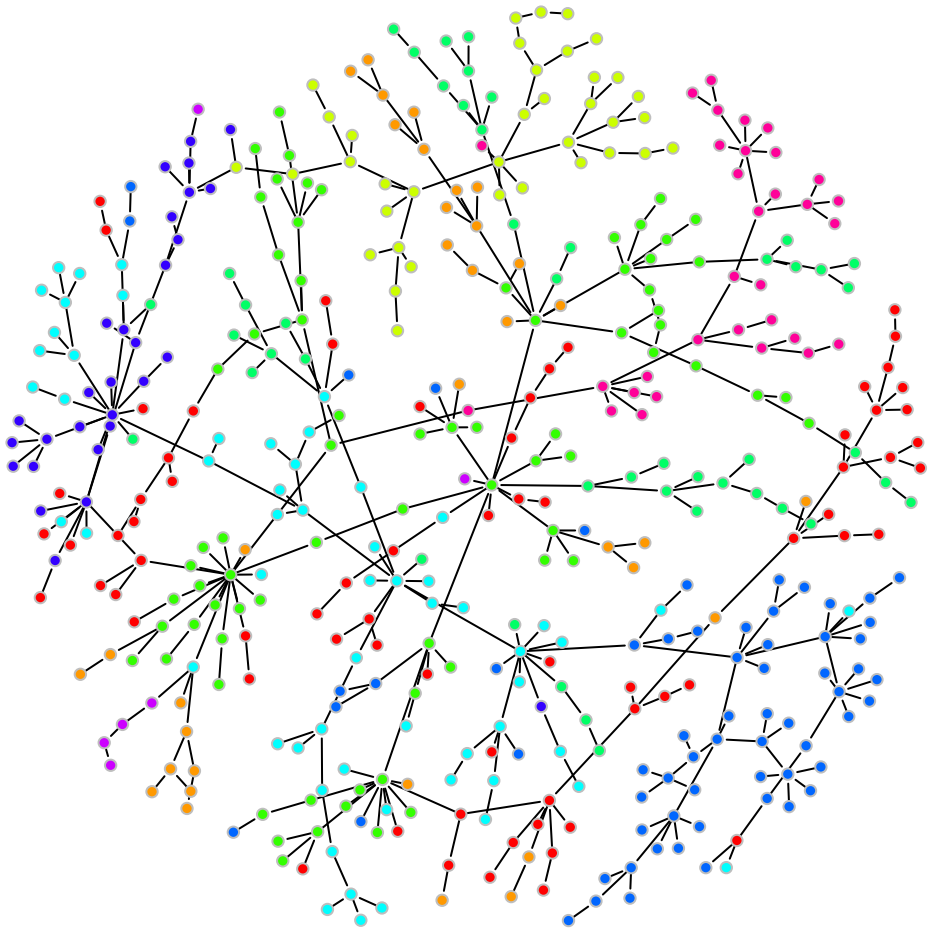
Many interesting problems are high dimensional. But often, the relevant information is effectively low dimensional.

Nonparametricity

Make the weakest possible assumptions.

Preview: Graphs on Equities Data

Preview: Finding relations between stocks in the S&P 500:



By the end of the lectures, you'll know what this is!

Lecture 1

Regression

How to predict Y from X

Topics

- *Regression*
- High dimensional regression
- Sparsity
- The lasso
- Some extensions

Regression

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

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

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

For example, suppose we have n subjects. Y_i is the blood pressure of subject i. $X_i = (X_{i1}, \ldots, X_{ip})$ 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 $\widehat{Y}$ be a prediction of Y. The *prediction error* or *risk* is

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

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

The best predictor is the *regression function*

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

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

Regression

Given the training data $\mathcal{D} = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ 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

Prediction Risk = Bias^2 + 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 $\widehat{m}(x) \equiv 0$ has 0 variance but will be terribly biased.

To predict well, we need to balance the bias and the variance. We begin with linear methods.

Bias-Variance Tradeoff

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

$$R(\widehat{f}, g) = R(\widehat{f}, f^*) + R(\widehat{f}^*, g)$$

- Approximation error is generalization of squared bias
- Estimation error is generalization like variance.
- Decomposition holds more generally, even for classification

Linear Regression

Try to find the best linear predictor, that is, a predictor of the form:

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

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

We 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 $\beta = (\beta_1, \ldots, \beta_p)$ and $x = (x_1, \ldots, x_p)$.

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 $\widehat{\beta} = (\widehat{\beta}_1, \ldots, \widehat{\beta}_p)$ is called the *least squares estimator*.

Low Dimensional Linear Regression

The least squares estimator is:

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

where

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

and

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

In R: lm(y $\sim$ x)

Low Dimensional Linear Regression

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

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

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

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

Our goals are to improve this by:

(i) dealing with high dimensions

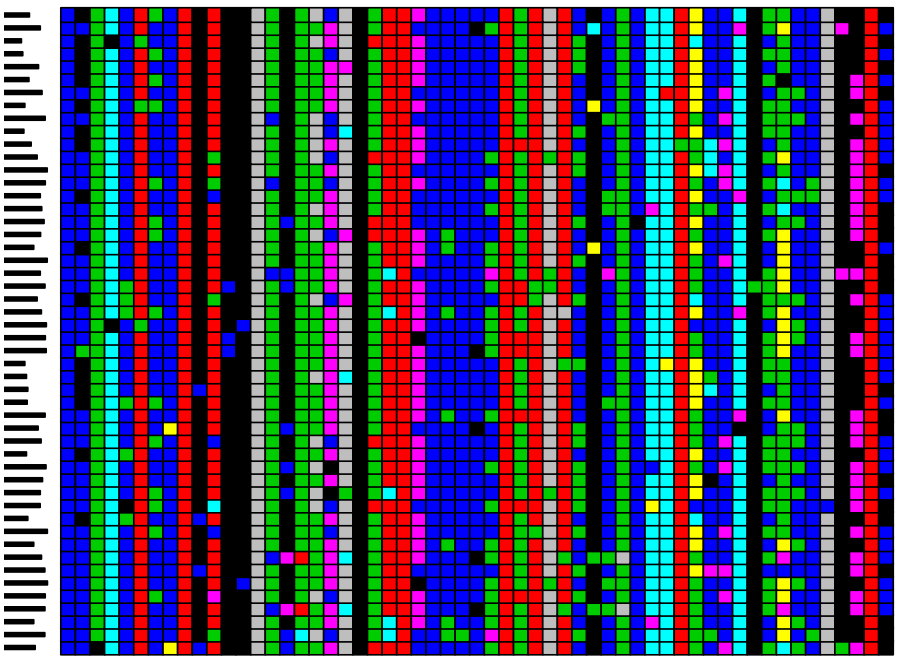
(ii) using something more flexible than linear predictors.

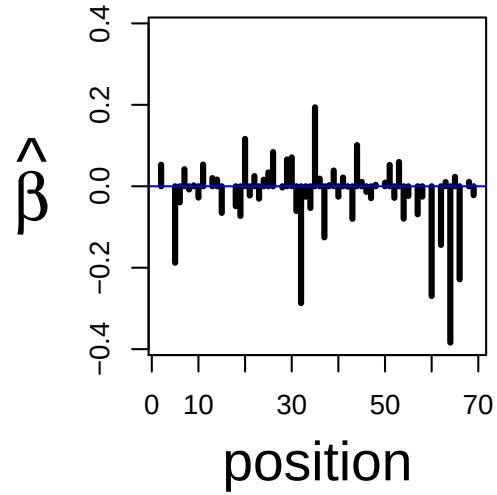
Example

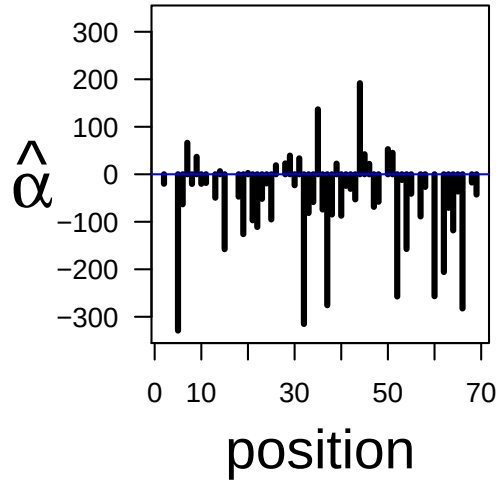
$Y =$ HIV resistance

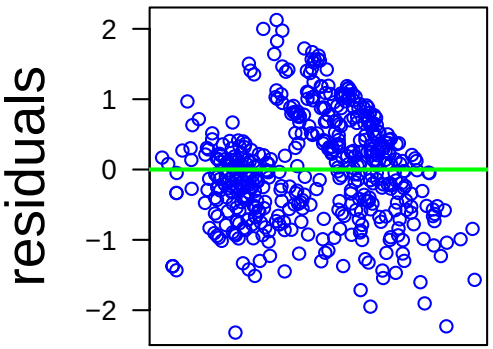
X_j = amino acid in position j of the virus.

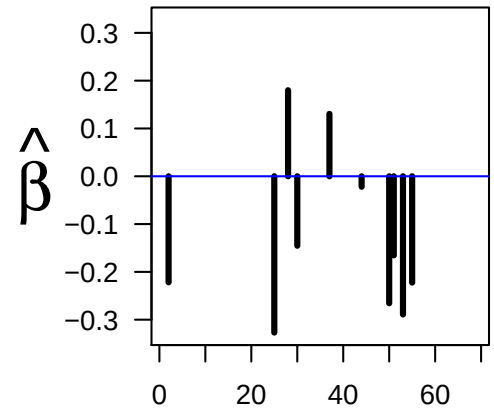
$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_{100} X_{100} + \epsilon$$











Top left: $\widehat{\beta}$

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

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

Bottom right: a sparse regression (coming up soon)

Topics

- Regression
- *High dimensional regression*
- Sparsity
- The lasso
- Some extensions

High Dimensional Linear Regression

Now suppose p is large. We even might have $p > n$ (more covariates 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:

Prediction Error = Bias^2 + 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*:

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

where $\|\beta\|_2 = \sqrt{\sum_j \beta_j^2}$.

The solution is:

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

Ridge Regression

The tuning parameter λ controls the bias-variance tradeoff:

$$\begin{aligned} \lambda = 0 &\implies \text{least squares.} \\ \lambda = \infty &\implies \widehat{\beta} = 0. \end{aligned}$$

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

Ridge Regression

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

$$R_{\text{training}} = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \widehat{Y}_i)^2, \qquad \widehat{Y}_i = X_i^T\widehat{\beta}$$

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

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

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

Leave-one-out cross-validation

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

where

$$\begin{aligned}
H &= \mathbb{X}(\mathbb{X}^T\mathbb{X} + \lambda I)^{-1}\mathbb{X}^T \\
p &= \text{trace}(H)
\end{aligned}$$

Example

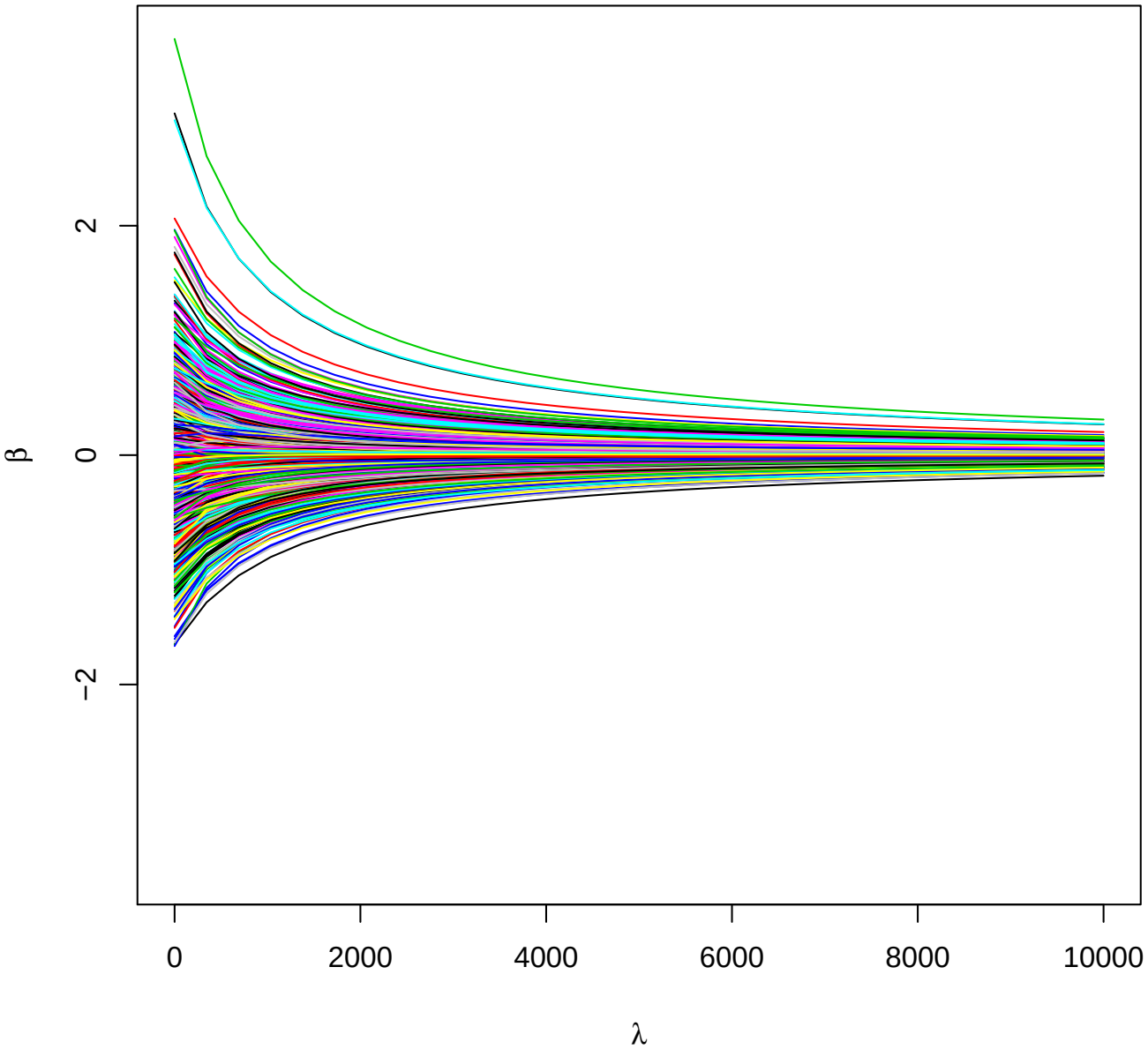
$$Y = 3X_1 + \cdots + 3X_5 + 0X_6 + \cdots + 0X_{1000} + \epsilon$$

$n = 100,\ p = 1{,}000.$

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?

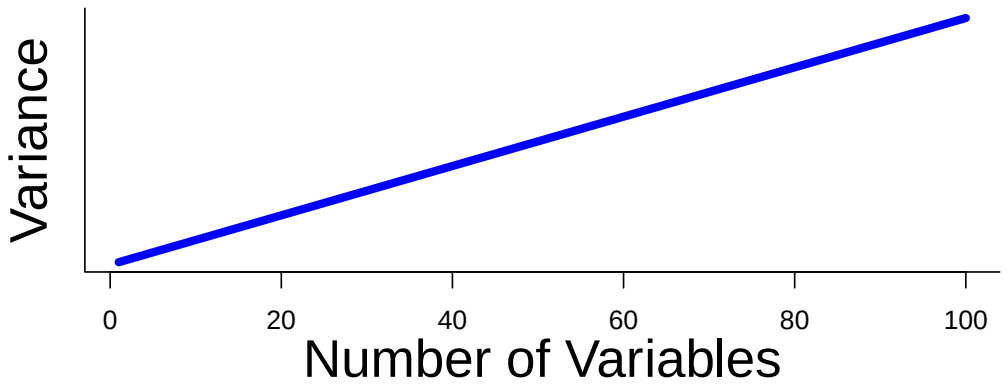
We could fit many submodels (with a small number of covariates) and choose the best one. This is called *model selection*.

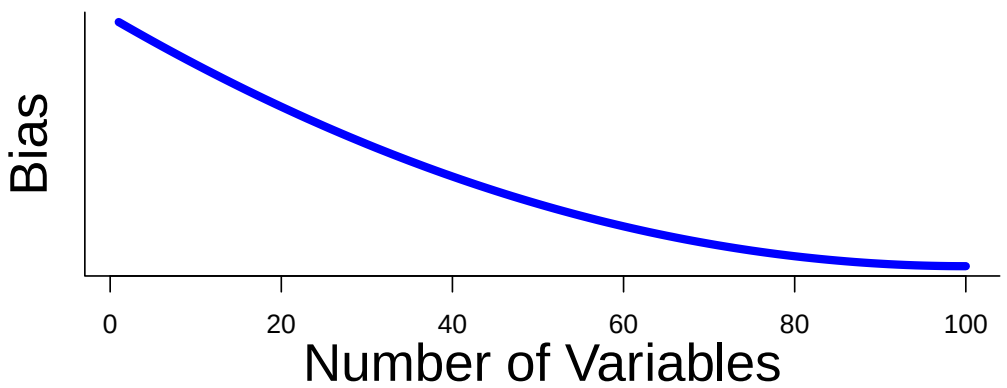
Now the inaccuracy is

prediction error = bias^2 + variance

The bias is the errors 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.

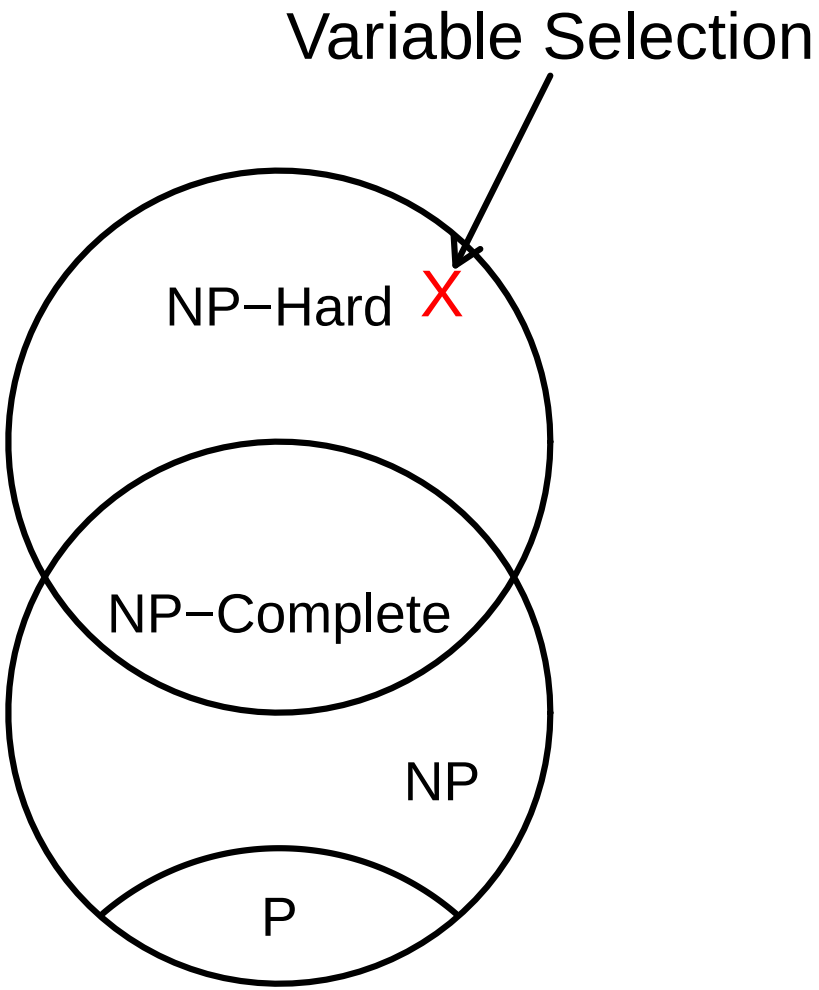
Have to try all models with one variable, two variables,...

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

Suppose we have 50,000 genes. We have to search through $2^{50,000}$ models. But $2^{50,000} >$ number of atoms in the universe.

This problem is NP-hard. This was a major bottleneck in statistics for many years.

You are Here



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 $\beta_1, \ldots, \beta_{50,000}$ 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*
- The lasso
- Some extensions

Sparsity

Look at this:

$$\beta = (5, 5, 5, 0, 0, 0, \ldots, 0).$$

This vector is high-dimensional but it is sparse.

Here is a less obvious example:

$$\beta = (50, 12, 6, 3, 2, 1.4, 1, 0.8., 0.6, 0.5, \ldots)$$

It turns out that, if the β_j's die off fairly quickly, then β behaves a like a sparse vector.

Sparsity

We measure the (lack of) sparsity of $\beta = (\beta_1, \ldots, \beta_p)$ with the q-norm

$$\|\beta\|_q = \left(|\beta_1|^q + \cdots + |\beta_p|^q\right)^{1/q} = \left(\sum_j |\beta_j|^q\right)^{1/q}.$$

Which values of q measure (lack of) sparsity?

sparse:	$a =$	1	0	0	0	$\cdots$	0
not sparse:	$b =$	.001	.001	.001	.001	$\cdots$	.001

	$\sqrt{}$ $q = 0$	$\sqrt{}$ $q = 1$	$\times$ $q = 2$
$\|a\|_q$	1	1	1
$\|b\|_q$	d	$\sqrt{p}$	1

Lesson: Need to use $q \leq 1$ to measure sparsity. (Actually, $q < 2$ ok.)

Sparsity

So we estimate $\beta = (\beta_1, \ldots, \beta_p)$ by minimizing

$$\sum_{i=1}^{n} (Y_i - [\beta_0 + \beta_1 X_{i1} + \cdots + \beta_p X_{ip}])^2$$

subject to the constraint that β is sparse i.e. $\|\beta\|_q \leq$ small.

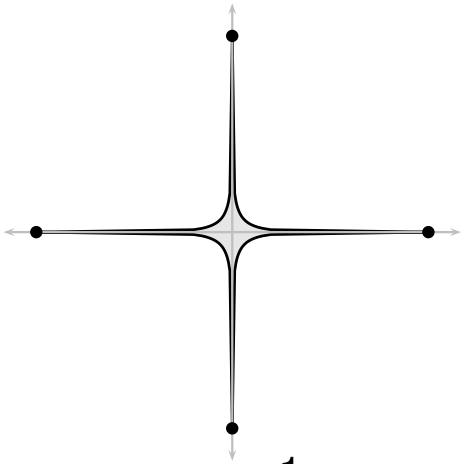
Can we do this minimization?

If we use $q = 0$ this turns out to be the same as searching through all 2^p models. Ouch!

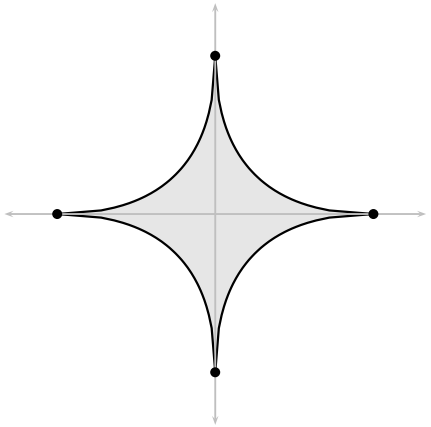
What about other values of q?

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

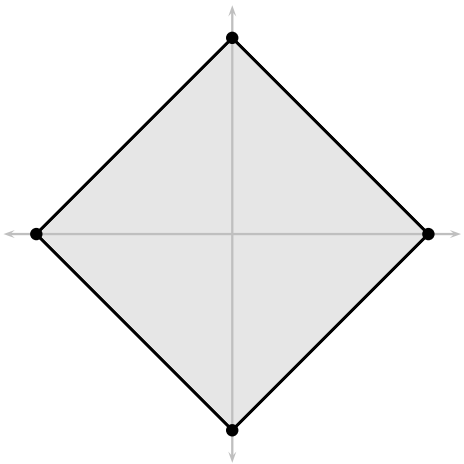
The set $\|\beta\|_q \leq 1$ when $p = 2$



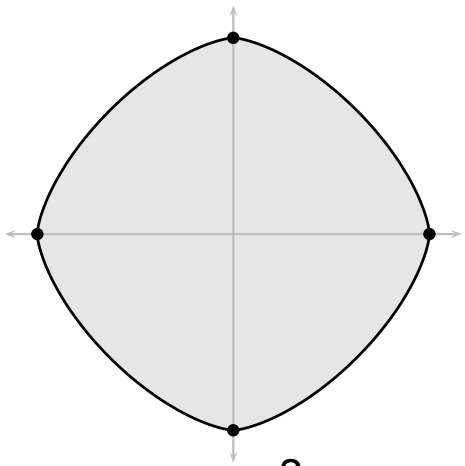
$q = \frac{1}{4}$



$q = \frac{1}{2}$



$q = 1$



$q = \frac{3}{2}$

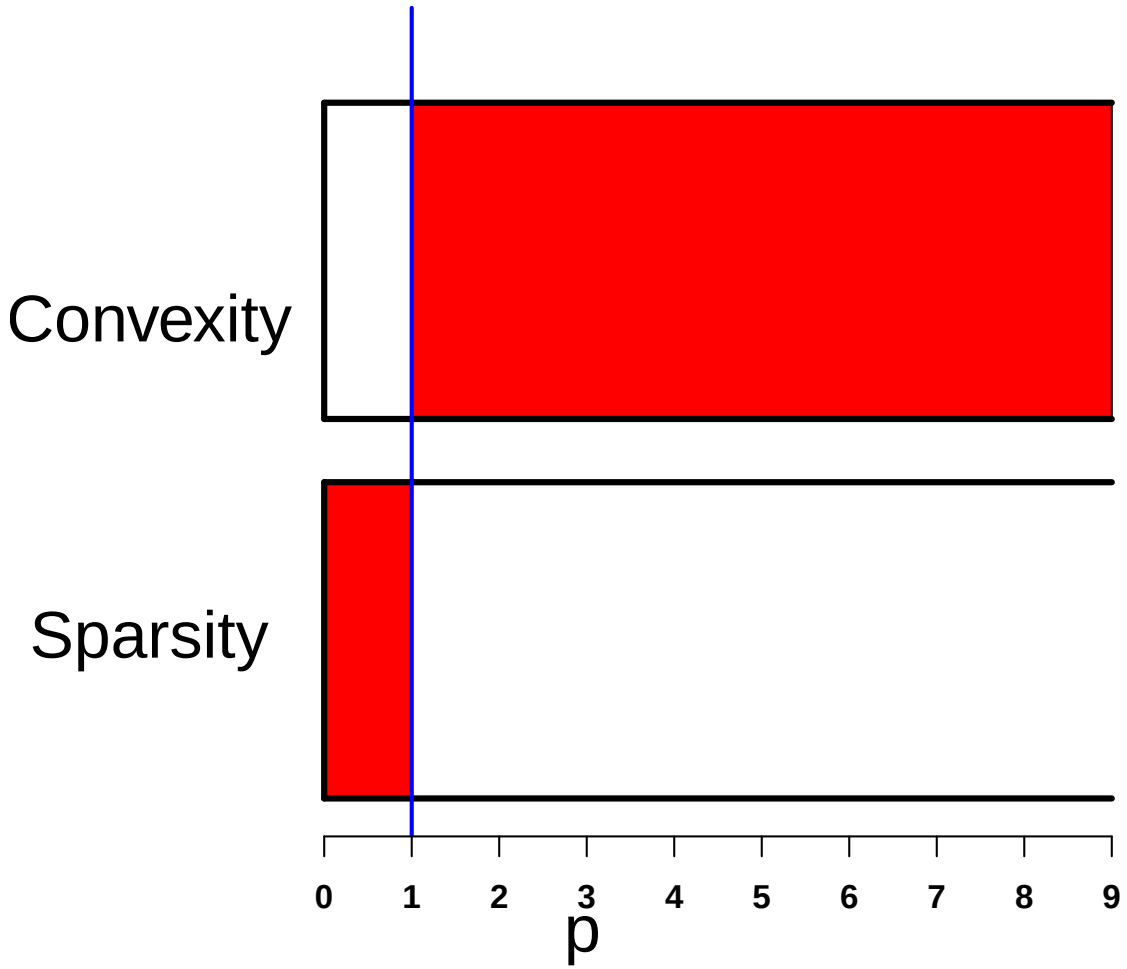
Sparsity Meets Convexity

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

Sensitivity to sparsity: $q \leq 1$ (actually, $q < 2$ suffices)
Convexity (niceness): $q \geq 1$

This means we should use $q = 1$.

Where Sparsity and Convexity Meet



Topics

- Regression
- High dimensional regression
- Sparsity
- *The lasso*
- Some extensions

Sparsity Meets Convexity

So we estimate $\beta = (\beta_1, \ldots, \beta_p)$ by minimizing

$$\sum_{i=1}^{n} (Y_i - [\beta_0 + \beta_1 X_{i1} + \cdots + \beta_p X_{ip}])^2$$

subject to the constraint that β is sparse i.e. $\|\beta\|_1 = \sum_j |\beta_j| \leq$ small.

This is called the lasso. Invented by Rob Tibshirani in 1996. (Related work by Donoho and others around the same time).

Lasso

The result is an estimated vector

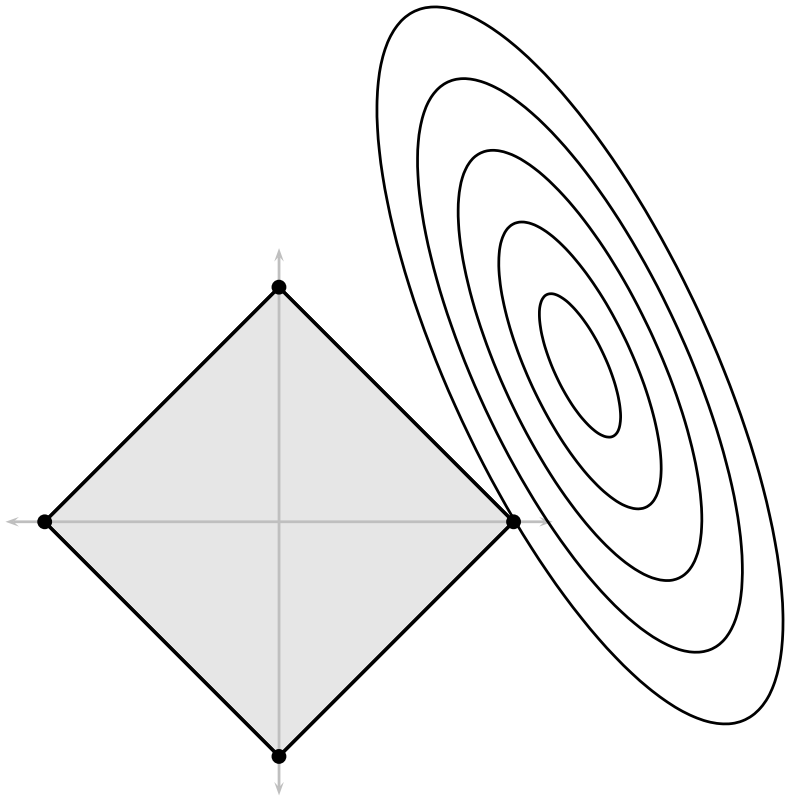
$$\widehat{\beta}_1, \ldots, \widehat{\beta}_p$$

Most are 0!

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

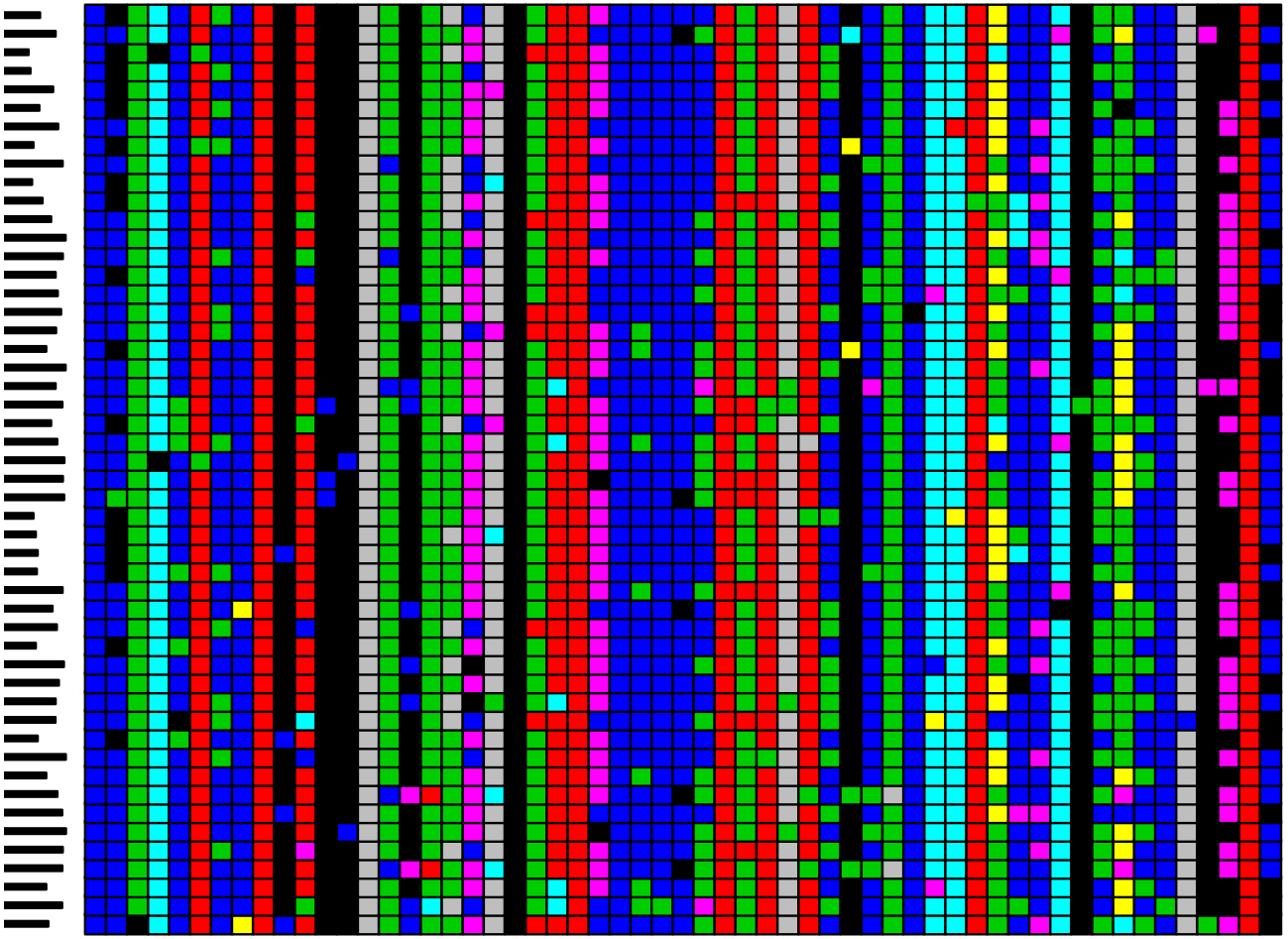
The next picture explains why some $\widehat{\beta}_j = 0$.

Sparsity: How Corners Create Sparse Estimators

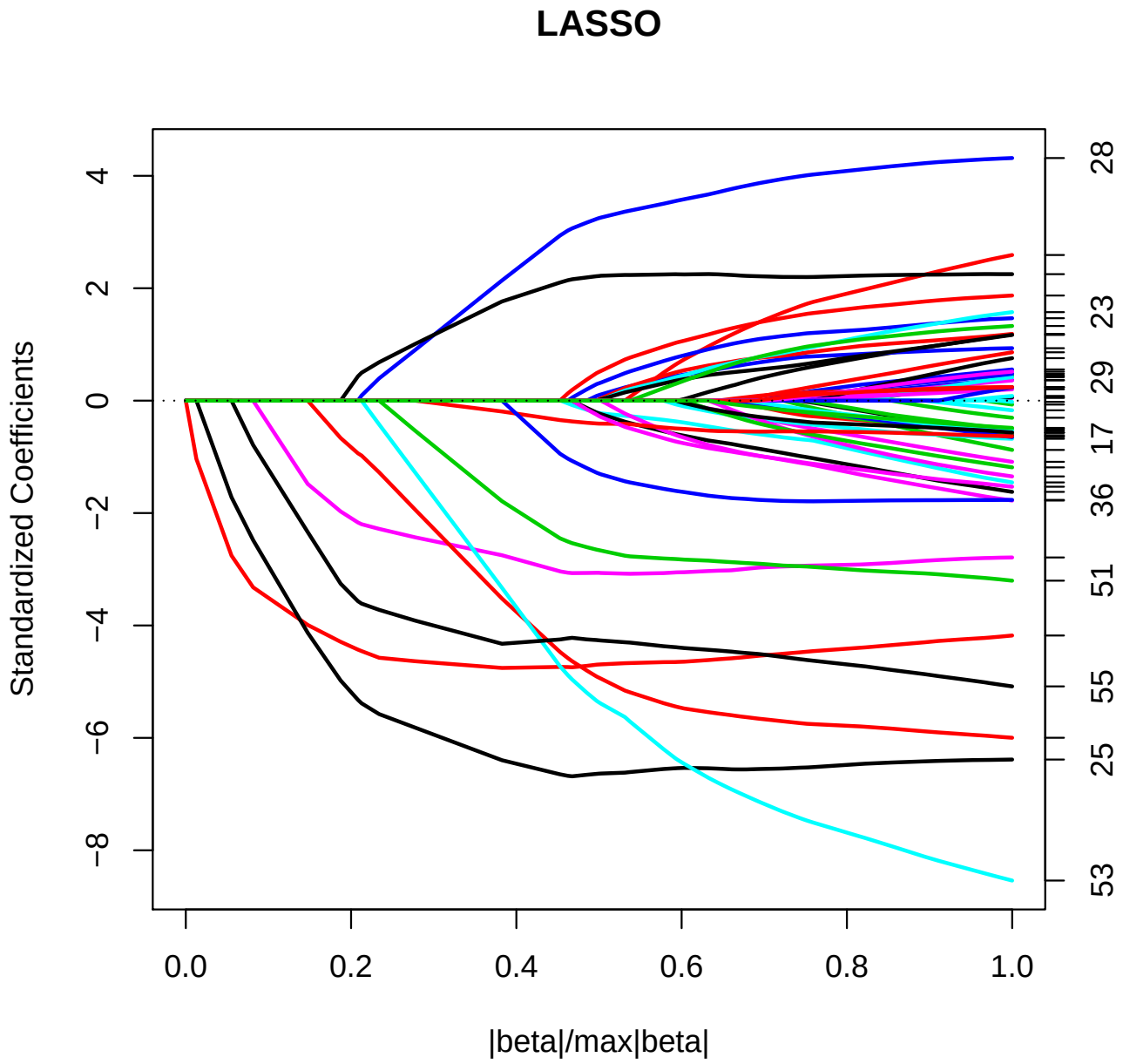


The Lasso: HIV Example Again

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

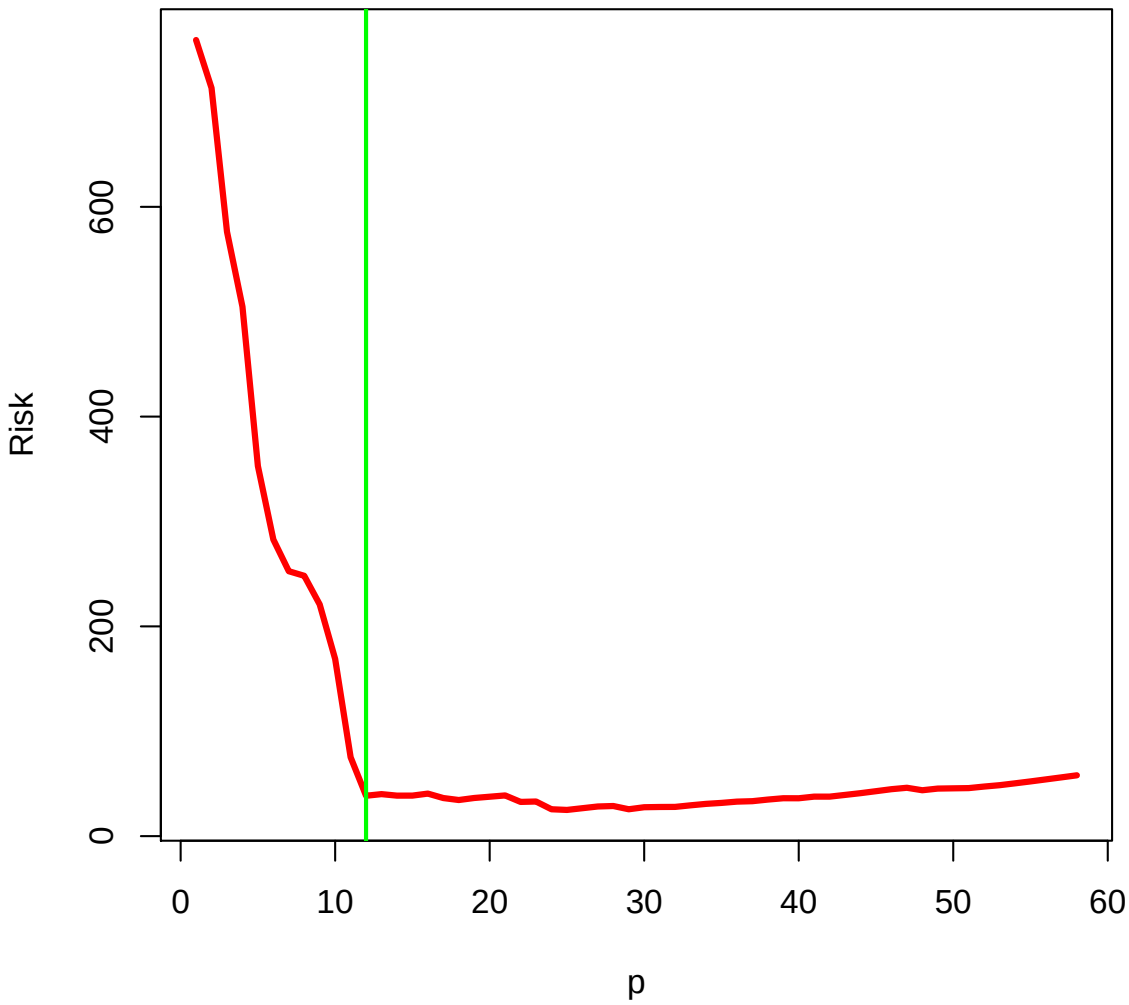


The Lasso: An Example

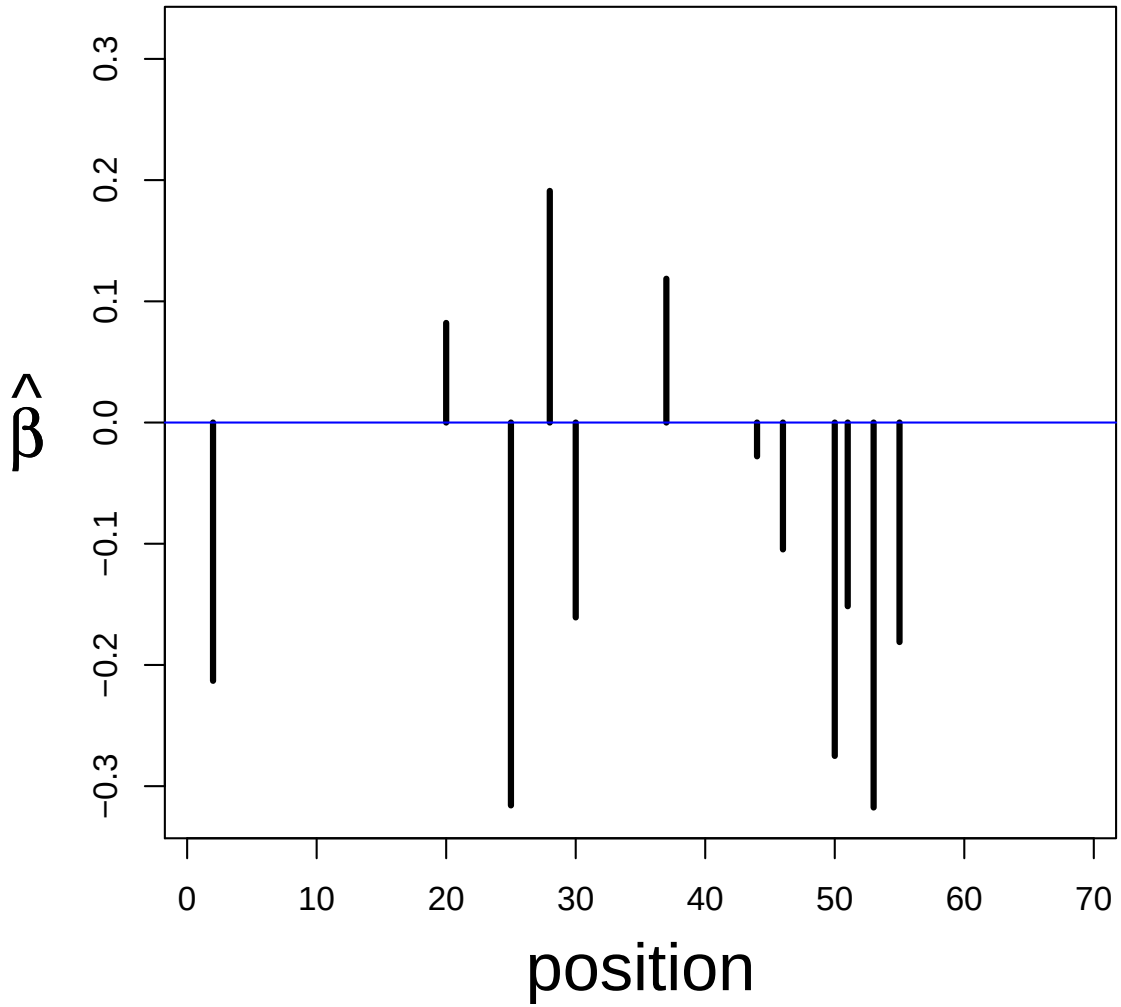


Selecting λ

We choose the sparsity level by estimating prediction error.



The Lasso: An Example



Sparsity and Convexity

To summarize: we penalize the sums of squares with

$$\|\beta\|_q = \left(\sum_j |\beta_j|^q \right)^{1/q}.$$

To get a sparse answer: $q < 2$.

To get a convex problem: $q \geq 1$.

So $q = 1$ works.

The marriage of sparsity and convexity is one of the biggest developments in statistics and machine learning.

The Lasso

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

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

  R: lars (y,x) or glmnet (y,x)

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

The Lasso

Choose λ by risk estimation.

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

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

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

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: $\widehat{Y} = X^T \widehat{\beta}$.

Some Convexity Theory for the Lasso

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

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

- 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

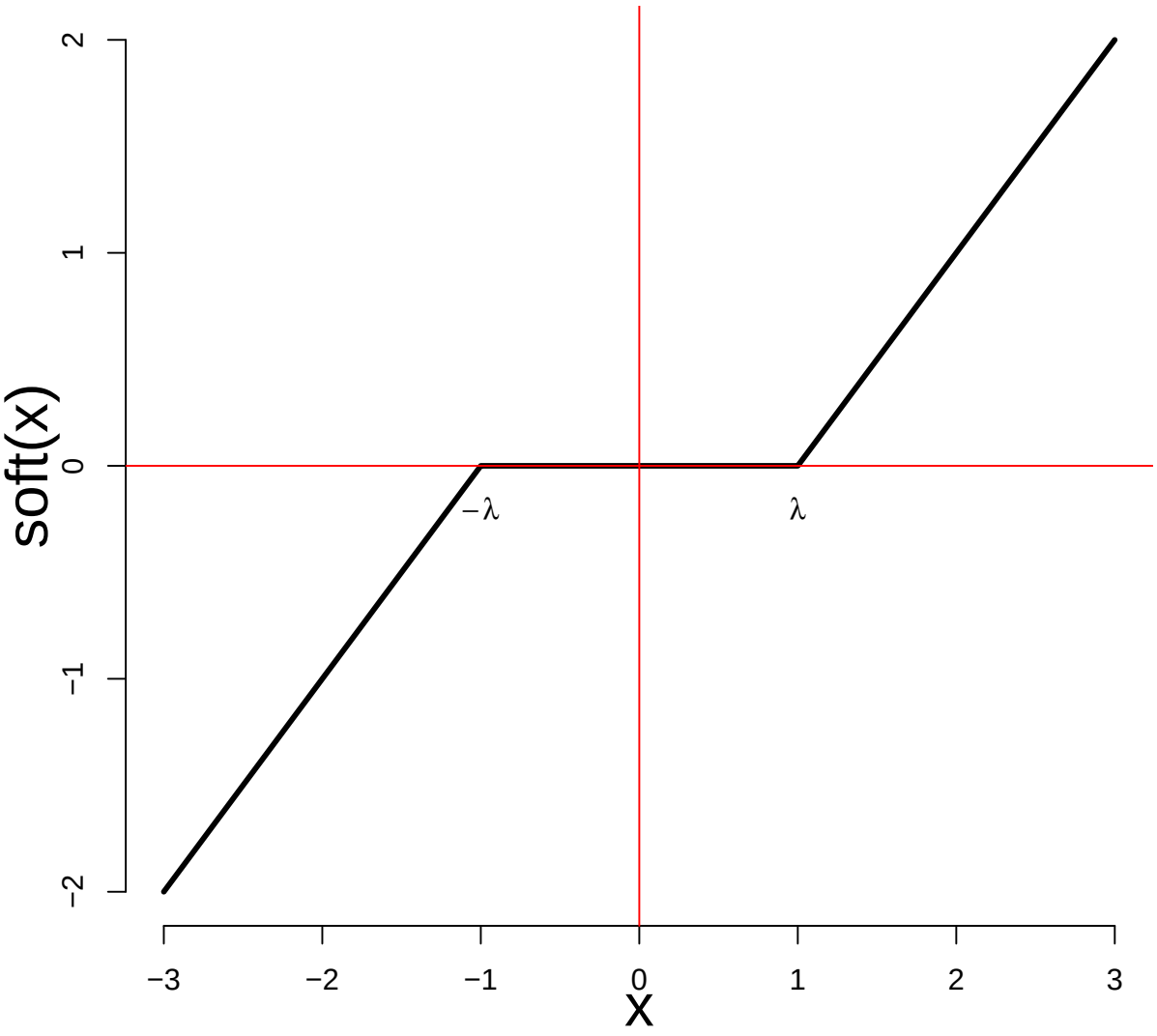
- $\widehat{\mu}$ minimizes $A(\mu)$ if and only if $0 \in \partial A$.
- So

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

- This can be written as

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

ℓ_1 and Soft Thresholding



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

- Minimize $\sum_i (Y_i - \beta^T X_i)^2 + \lambda \|\beta\|_1$.
  - use lars (least angle regression) or
  - coordinate descent: set $\widehat{\beta} = (0, \ldots, 0)$ then iterate the following:
    - for $j = 1, \ldots, d$:
    - set $R_i = Y_i - \sum_{s \neq j} \widehat{\beta}_s X_{si}$
    - $\widehat{\beta}_j$ = least squares fit of R_i's in X_j.
    - $\widehat{\beta}_j \leftarrow \text{soft}(\widehat{\beta}_{j,LS}, \lambda / \sum_i X_{ij}^2)$
- Then use least squares $\widehat{\beta}$ on selected subset S.

R: glmnet

Variations on the Lasso

- Elastic Net: minimize

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

- Group Lasso:

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

minimize:

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

Some Theory: Persistence

Population risk

$$R(\beta) = \mathbb{E}(Y - \beta^T X)^2$$

Let $\widehat{\beta}_n$ be the empirical risk minimizer. Then

$$R(\widehat{\beta}_n) - R(\beta_*) \xrightarrow{P} 0$$

if minimization is over all β with

$$\|\beta\|_1 = o\left(\frac{n}{\log n}\right)^{1/4}$$

Multivariate Regression

$Y \in \mathbb{R}^q$ and $X \in \mathbb{R}^p$. Regression function $M(X) = \mathbb{E}(Y \mid X)$.

Linear model $M(X) = BX$ where $B \in \mathbb{R}^{q \times p}$.

Reduced rank regression: $r = \text{rank}(B) \leq C$.

Recent work has studied properties and high dimensional scaling of reduced rank regression where nuclear norm

$$\|B\|_* := \sum_{j=1}^{\min(p,q)} \sigma_j(B)$$

as convex surrogate for rank constraint (Yuan et al., 2007; Negahban and Wainwright, 2011)

Multivariate Regression

Example: “Mind reading,” predicting brain response patterns from semantic features, or vice-versa.

- 10 subjects
- Each shown 60 words while brain activity is imaged
- Word features from semantic hierarchy, $p = 200$ features
- Subsampled images, $q = 400$ voxels.
- Can be thought of as a type of “multi-task learning”

More on this when we talk about dictionary learning, or sparse coding.

Nuclear Norm Regularization

Nuclear norm $\|X\|_*$ of $p \times q$ matrix X

$$\|X\|_* = \sum_{j=1}^{\min(p,q)} \sigma_j(X)$$

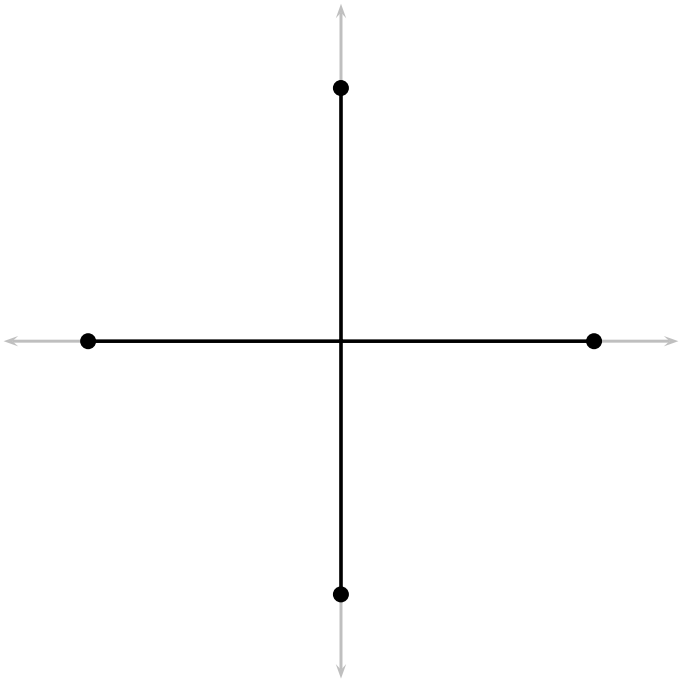
Sum of singular values. (a.k.a. *trace norm* or *Ky-Fan norm*)

Generalization to matrices of ℓ_1 norm for vectors.

Recall: Sparse Vectors and ℓ_1 Relaxation

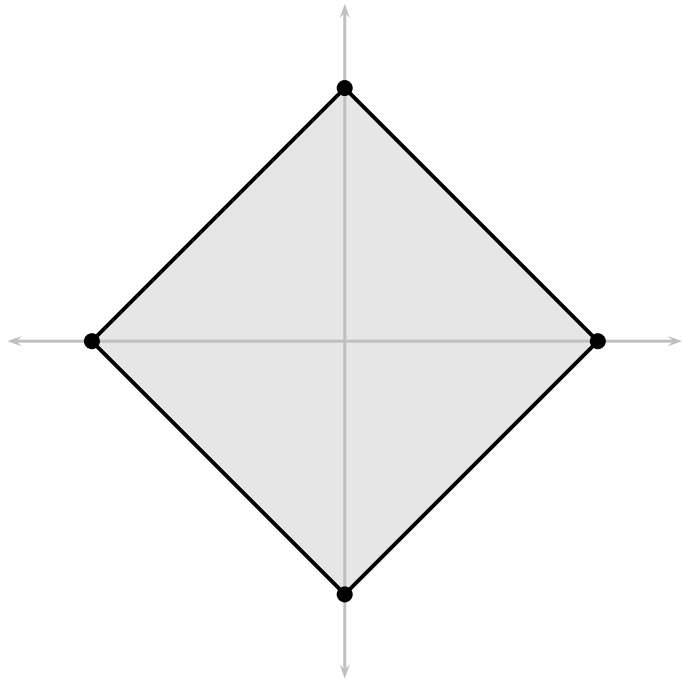
sparse vectors

$\|X\|_0 \leq t$



convex hull

$\|X\|_1 \leq t$



Low-Rank Matrices

- 2×2 symmetric matrices:

$$X = \begin{pmatrix} x & y \\ y & z \end{pmatrix}$$

- By scaling, can assume $|x + z| = 1$.

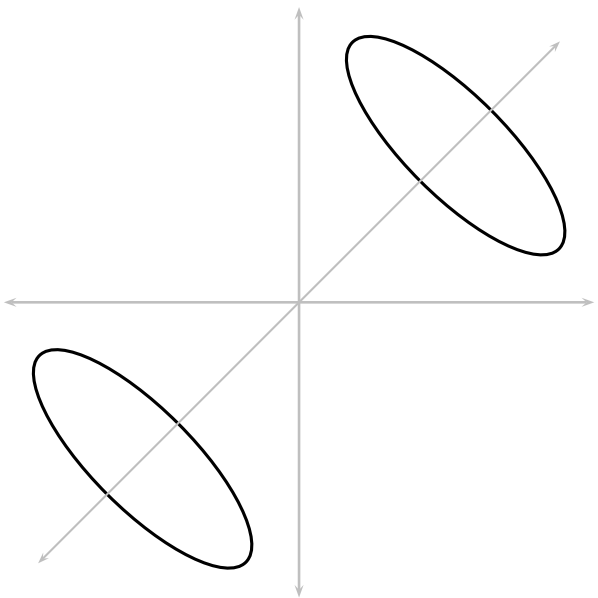
$$X \text{ has rank one iff } x^2 + 2y^2 + z^2 = 1$$

- Union of two ellipses in $\mathbb{R}^3$.
- Convex hull is a cylinder.

Low-Rank Matrices and Convex Relaxation

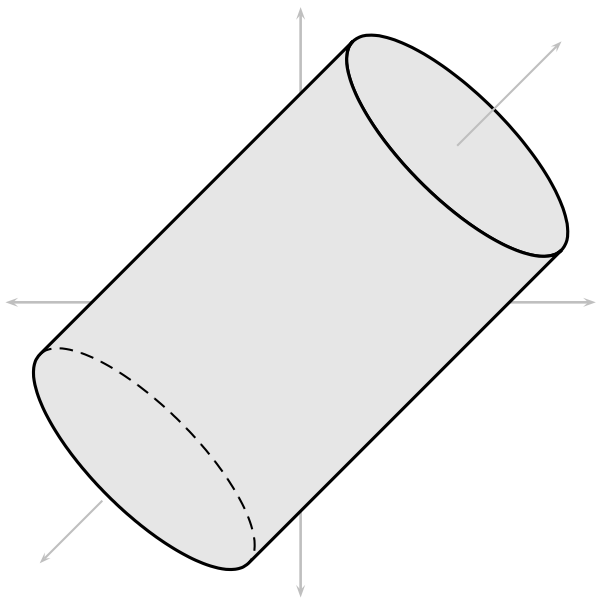
low rank matrices

$\text{rank}(X) \leq t$



convex hull

$\|X\|_* \leq t$



Nuclear Norm Regularization

Algorithms for nuclear norm minimization are a lot like iterative soft thresholding for lasso problems.

To project a matrix B onto the nuclear norm ball $\|X\|_* \leq t$:

- Compute the SVD:

$$B = U \operatorname{diag}(\sigma) V^T$$

- Soft threshold the singular values:

$$B \leftarrow U \operatorname{diag}(\operatorname{Soft}_\lambda(\sigma)) V^T$$

Reduced Rank Regression

- Recent theory has established consistency for reduced rank regression in high dimensions.
- We have results on “persistency” or risk consistency
- These results describe the rate of decay of “excess risk” relative to the oracle
- Do not assume model is correct

Excess Risk for Reduced Rank Regression

- Oracle inequality of Xu and Lafferty (ICML, 2012)
- Uses concentration of measure for covariance matrices in the spectral norm (e.g., Vershynin, 2010)

$$R(\widehat{B}) - R(B_*) = O_P\left(L^2\sqrt{\frac{(p+q)\log n}{n}}\right)$$

- Minimized over class of matrices with $\|B\|_* \leq L$

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, the lasso will work well.
- Low-rank assumption is different type of structure for high dimensional problems.