Lecture 12: Shrinkage

Reading: Section 3.4

GU4241/GR5241 Statistical Machine Learning

y E R^p
y1 ~ N(Θ,σ^2Ip)
EIIΘ_hat - θII^2 = E(IIΘ_hat - EΘII^2 + (EΘ_hat - Θ)^2
= variance + bias

θmle_hat = y1

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February 28, 2016

when p ≥3
Θjs_hat = (1 - (p-2)σ^2/IIyII^2) * y1
js_style performance better. because it shrink the obsevation

Issues with Least Squares

Robustness

- Least squares works only if $\mathbf{X}$ has full column rank, i.e. if $\mathbf{X}^T\mathbf{X}$ is invertible.
- If $\mathbf{X}^T\mathbf{X}$ *almost* not invertible, least squares is numerically unstable.
  Statistical consequence: High variance of predictions.

Not suited for high-dimensional data

- Modern problems: Many dimensions/features/predictors (possibly thousands)
- Only a few of these may be important
  $\rightarrow$ need some form of feature selection
- Least squares:
  - Treats all dimensions equally
  - Relevant dimensions are averaged with irrelevant ones
  - Consequence: Signal loss

$Y = x\beta + \varepsilon$

$\beta\_hat = (XtX)^{-1}\ XtY$

Regularity of Matrices

Regularity

A square matrix is singular if and only if its determinant is 0.

A matrix which is not invertible is also called a **singular** matrix. A matrix which is invertible (not singular) is called **regular**.

In computations

Numerically, matrices can be "almost singular". Intuition:

- A singular matrix maps an entire linear subspace into a single point.
- If a matrix maps points far away from each other to points very close to each other, it almost behaves like a singular matrix.

Regularity of Symmetric Matrices

A positive semi-definite matrix A is singluar $\Leftrightarrow$ smallest EValue is 0

Illustration

If smallest EValue $\lambda_{\text{min}} > 0$ but very small (say $\lambda_{\text{min}} \approx 10^{-10}$):

- Suppose x_1, x_2 are two points in subspace spanned by ξ_{min} with $\|x_1 - x_2\| \approx 1000$.
- Image under A: $\|Ax_1 - Ax_2\| \approx 10^{-7}$

In this case

- A has an inverse, but A behaves almost like a singular matrix
- The inverse A^{-1} can map almost identical points to points with large distance, i.e.

$$\text{small change in input} \quad \rightarrow \quad \text{large change in output}$$

Consequence for Statistics

If a statistical prediction involves the inverse of an almost-singular matrix, the predictions become unreliable (high variance).

Implications for Linear Regression

Recall: Prediction in linear regression

For a point $\mathbf{x}_{\text{new}} \in \mathbb{R}^p$, we predict the corresponding function value as

$$\hat{y}_{\text{new}} = \left\langle \hat{\beta}, \mathbf{x}_{\text{new}} \right\rangle = \mathbf{x}_{\text{new}} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Effect of unstable inversion

- Suppose we choose an arbitrary training point $\mathbf{x}_i$ and make a small change to its response value y_i.
- Intuitively, that should not have a big impact on $\hat{\beta}$ or on prediction.
- If $\mathbf{X}^T \mathbf{X}$ is almost singular, a small change to y_i can prompt a huge change in $\hat{\beta}$, and hence in the predicted value $\hat{y}_{\text{new}}$.

Measuring Regularity (of Symmetric Matrices)

Symmetric matrices

Denote by λ_{max} and λ_{min} the eigenvalues of A with largest/smallest *absolute* value. If A is symmetric, then

$$A \text{ regular} \quad \Leftrightarrow \quad |\lambda_{\mathsf{min}}| > 0 \, .$$

Idea

- We can use $|\lambda_{\mathsf{min}}|$ as a measure of regularity:

  $$\text{larger value of } \lambda_{\mathsf{min}} \quad \leftrightarrow \quad \text{"more regular" matrix } A$$

- We need a notion of scale to determine whether $|\lambda_{\mathsf{min}}|$ is large.
- The relevant scale is how A scales a vector. Maximal scaling coefficient: λ_{max}.

Regularity measure

$$c(A) := \frac{|\lambda_{\mathsf{max}}|}{|\lambda_{\mathsf{min}}|}$$

The function $c(\,.\,)$ is called the **spectral condition** ("spectral" since the set of eigenvalues is also called the "spectrum").

Ridge Regression

Objective

Ridge regression is a modification of least squares. We try to make least squares more robust if $\mathbf{X}^T\mathbf{X}$ is almost singular.

Ridge regression solution

The ridge regression solution to a linear regression problem is defined as

$$\hat{\boldsymbol{\beta}}^{\text{ridge}} := (\mathbf{X}^T\mathbf{X} + \lambda\mathbb{I})^{-1}\mathbf{X}^T\mathbf{y}$$

λ is a tuning parameter.

Explanation

Recall

$\mathbf{X}^T\mathbf{X} \in \mathbb{R}^{p\times p}$ is positive definite.

Spectral shift

Suppose $\xi_1, \ldots, \xi_p$ are EVectors of $\mathbf{X}^T\mathbf{X}$ with EValues $\lambda_1, \ldots, \lambda_p$. Then:

$$(\mathbf{X}^T\mathbf{X} + \lambda\mathbb{I})\xi_i = (\mathbf{X}^T\mathbf{X})\xi_i + \lambda\mathbb{I}\xi_i = (\lambda_i + \lambda)\xi_i$$

Hence: $(\mathbf{X}^T\mathbf{X} + \lambda\mathbb{I})$ is positive definite with EValues $\lambda_1 + \lambda, \ldots, \lambda_p + \lambda$.

Conclusion

$\mathbf{X}^T\mathbf{X} + \lambda\mathbb{I}$ is a *regularized* version of $\mathbf{X}^T\mathbf{X}$.

Implications for statistics

Effect of regularization

- We deliberately distort prediction:
  - If least squares ($\lambda = 0$) predicts perfectly, the ridge regression prediction has an error that increases with λ.
  - Hence: Biased estimator, bias increases with λ.
- Spectral shift regularizes matrix $\rightarrow$ decreases variance of predictions.

Bias-variance trade-off

- We decrease the variance (improve robustness) at the price of incurring a bias.
- λ controls the trade-off between bias and variance.

Cost Function

- Linear regression solution was defined as minimizer of $L(\boldsymbol{\beta}) := \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2$
- We have so far defined ridge regression only directly in terms of the estimator $\hat{\boldsymbol{\beta}}^{\text{ridge}} := (\mathbf{X}^T\mathbf{X} + \lambda\mathbb{I})^{-1}\mathbf{X}^T\mathbf{y}$.
- To analyze the method, it is helpful to understand it as an optimization problem.
- We ask: Which function L' does $\hat{\boldsymbol{\beta}}^{\text{ridge}}$ minimize?

Ridge regression

Ridge regression solves the following optimization:

$$\min_{\beta} \quad \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{i,j} \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

In blue, we have the RSS of the model.

In red, we have the squared ℓ_2 norm of $\boldsymbol{\beta}$, or $\|\boldsymbol{\beta}\|_2^2$. It is called a **penalty term**.

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The parameter λ is a tuning parameter. It modulates the importance of fit vs. shrinkage.

We find an estimate $\hat{\beta}_\lambda^{\text{ridge}}$ for many values of λ and then choose it by cross-validation. Fortunately, this is no more expensive than running a least-squares regression.

Ridge regression

In least-squares linear regression, scaling the variables has no effect on the fit of the model:

$$Y = X_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p.$$

Multiplying X_1 by c can be compensated by dividing $\hat{\beta}_1$ by c, ie. after doing this we have the same RSS.

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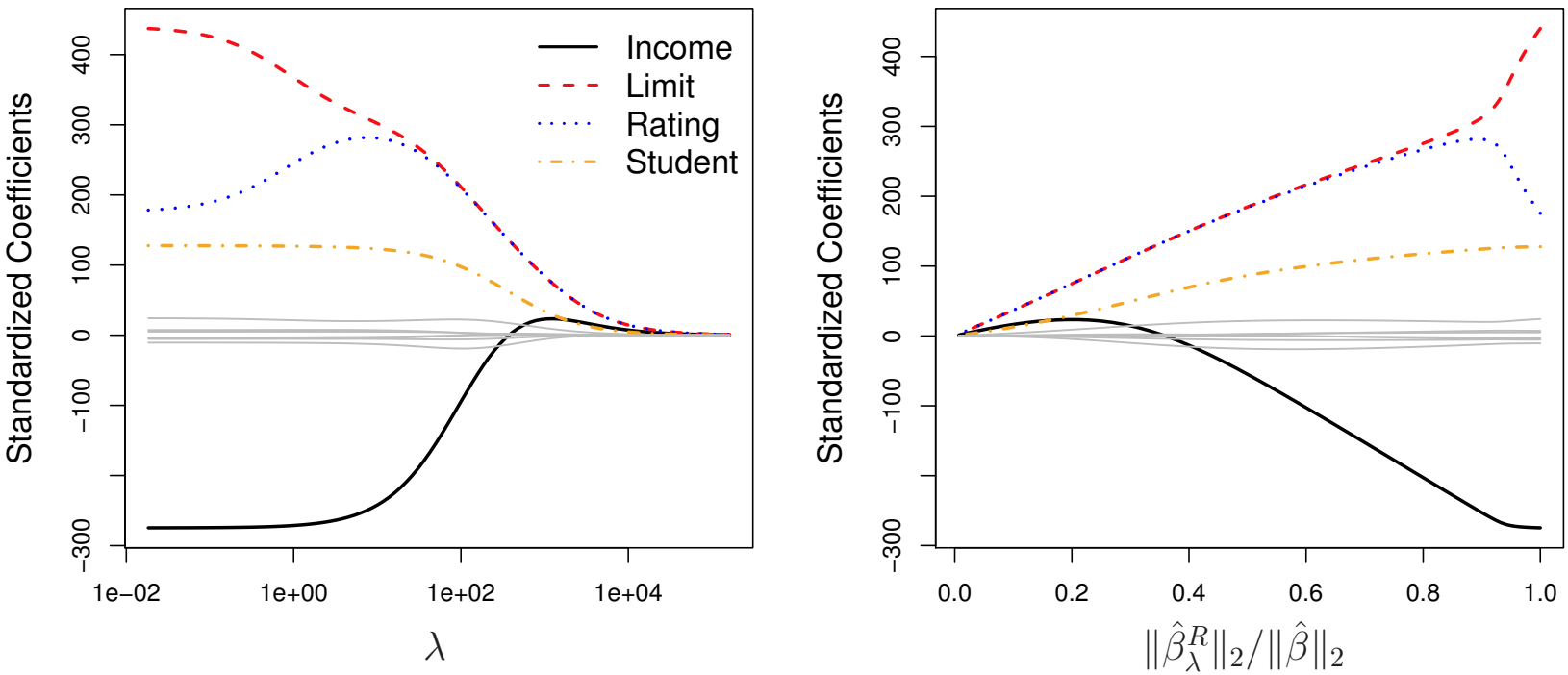
In practice, what do we do?

- Scale each variable such that it has sample variance 1 before running the regression.
- This prevents penalizing some coefficients more than others.

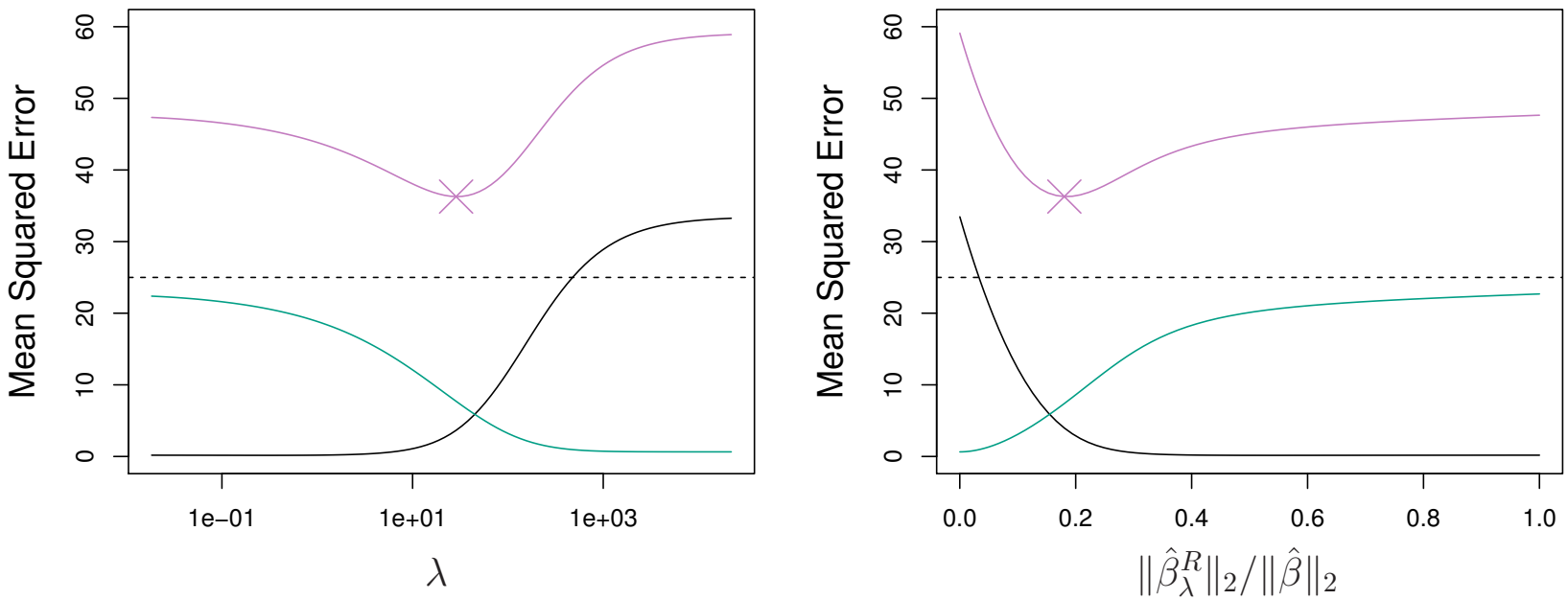
Example. Ridge regression

Ridge regression of `default` in the Credit dataset.



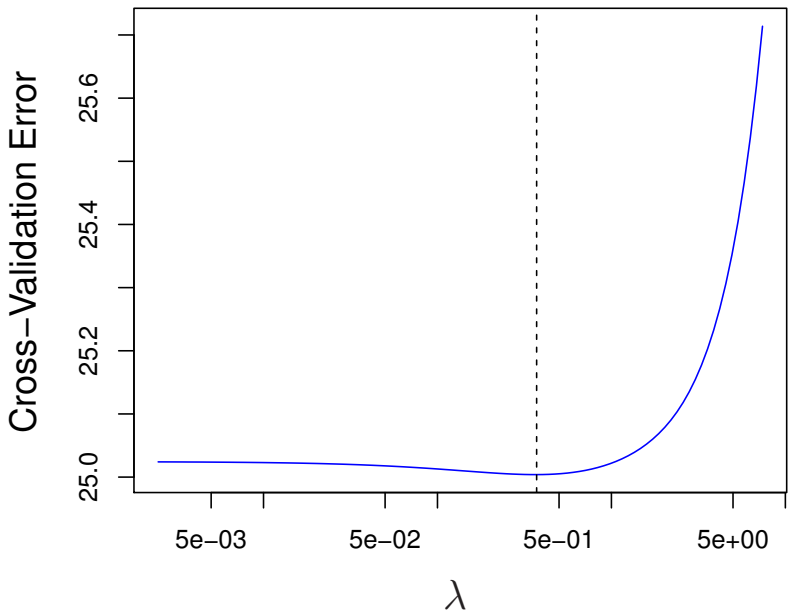
Bias-variance tradeoff

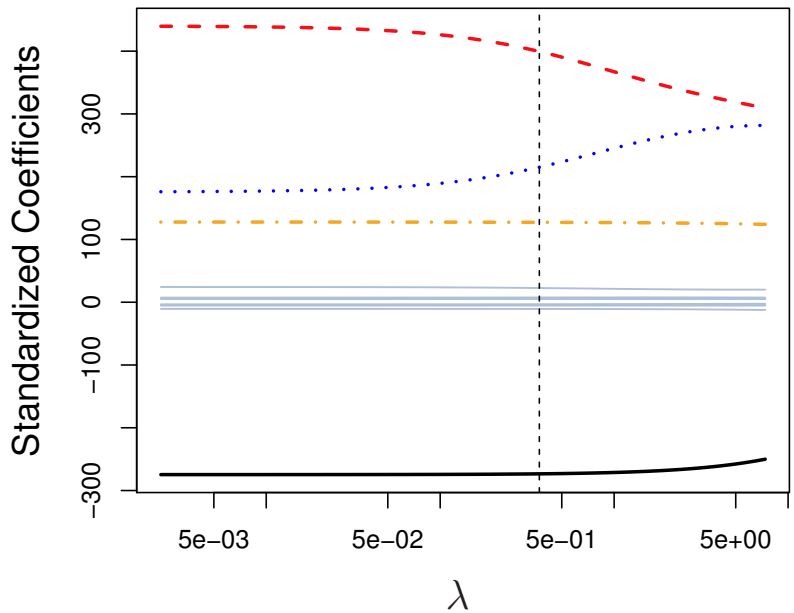
In a simulation study, we compute bias, variance, and test error as a function of λ.



Cross validation would yield an estimate of the test error.

Selecting λ by cross-validation





The Lasso

Lasso regression solves the following optimization:

$$\min_{\beta} \quad \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{i,j} \right)^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

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Why would we use the Lasso instead of Ridge regression?

we dont put any penalty on the intercept

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- Ridge regression shrinks all the coefficients to a non-zero value.

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Why would we use the Lasso instead of Ridge regression?

- Ridge regression shrinks all the coefficients to a non-zero value.
- The Lasso shrinks some of the coefficients all the way to zero. Alternative to best subset selection or stepwise selection!

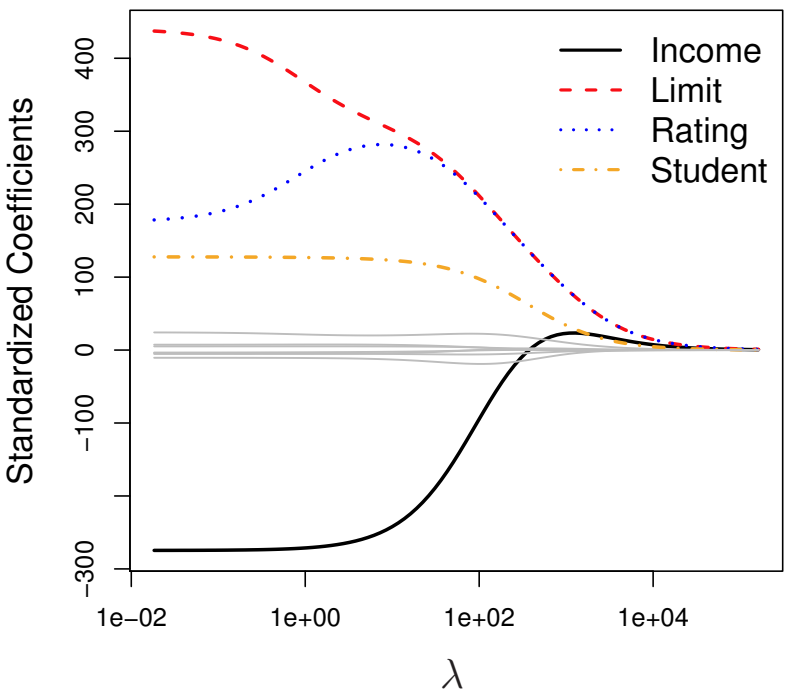
Example. Ridge regression

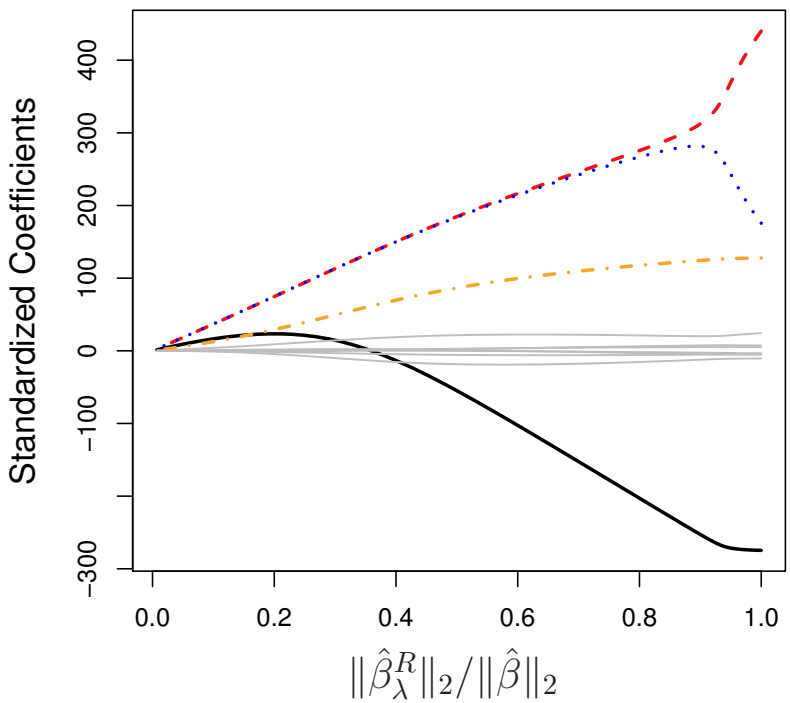
lasso: the gradient will always be a constant

redge: the gradient will adjust with the Bj

Ridge regression of `default` in the Credit dataset.

both will shrink coef to 0;
ridge will shrink non-o value;
lasso will shrink to 0





A lot of pesky small coefficients throughout the regularization path.

Example. The Lasso

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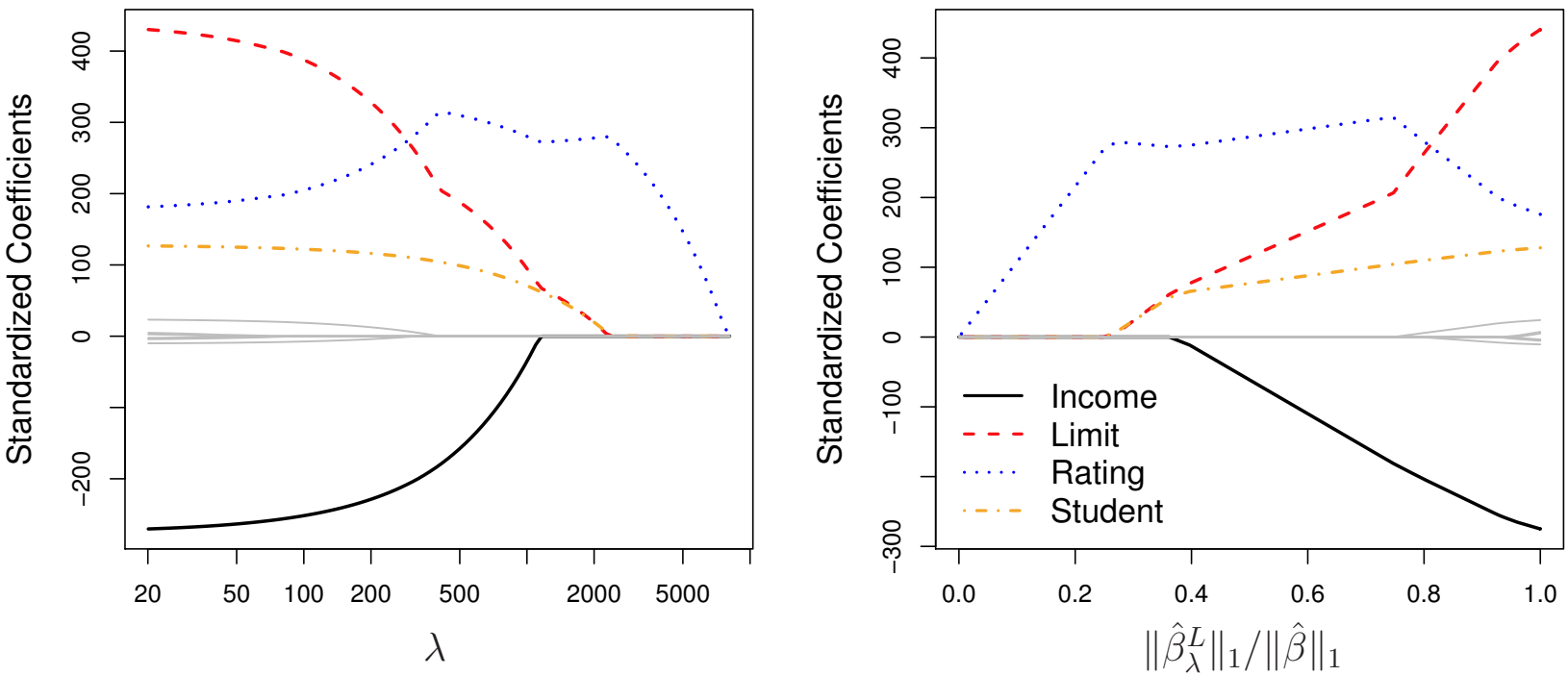

Those coefficients are shrunk to zero.

An alternative formulation for regularization

- **Ridge:** for every λ, there is an s such that $\hat{\boldsymbol{\beta}}_{\lambda}^{\text{ridge}}$ solves:

$$\underset{\beta}{\text{minimize}} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{i,j} \right)^2 \right\} \text{ subject to } \sum_{j=1}^{p} \beta_j^2 < s.$$

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redget: min(β): RSS + λ∑βi^2 ≤ S
laso： min RSS + λ∑| βi| ≤ S
if the β is small, then the gradient will be samll.
For lasso, the sign(Bi) is always a constance,
the gradiant will be larger, and we can drag solution to 0
lasso can do model selection autimatically

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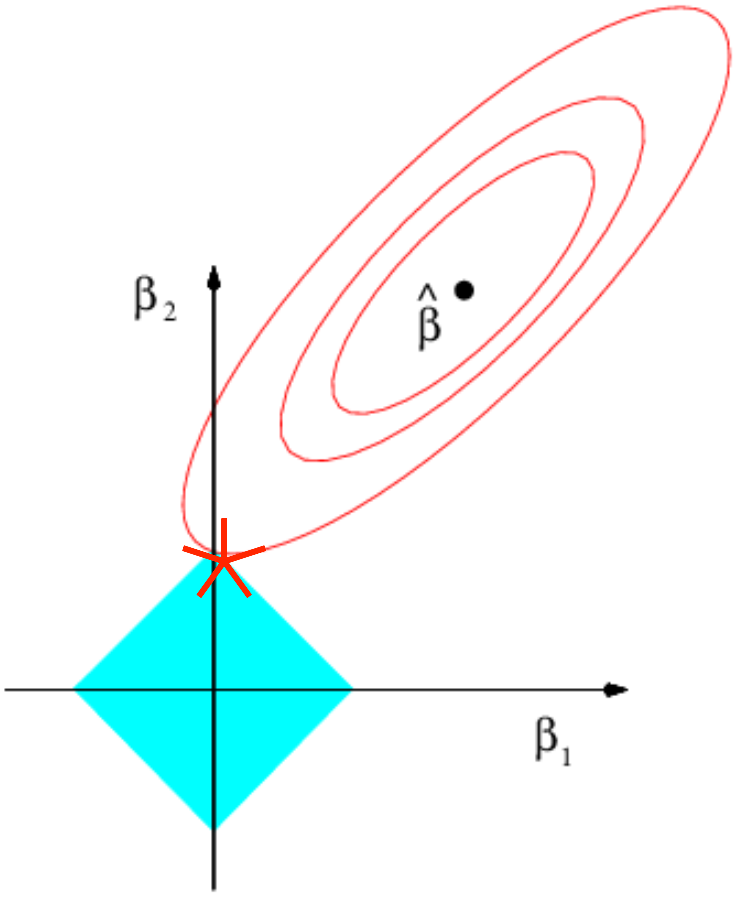
- **Best subset:**

$$\underset{\beta}{\text{minimize}} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{i,j} \right)^2 \right\} \quad \text{s.t.} \quad \sum_{j=1}^{p} \mathbf{1}(\beta_j \neq 0) < s.$$

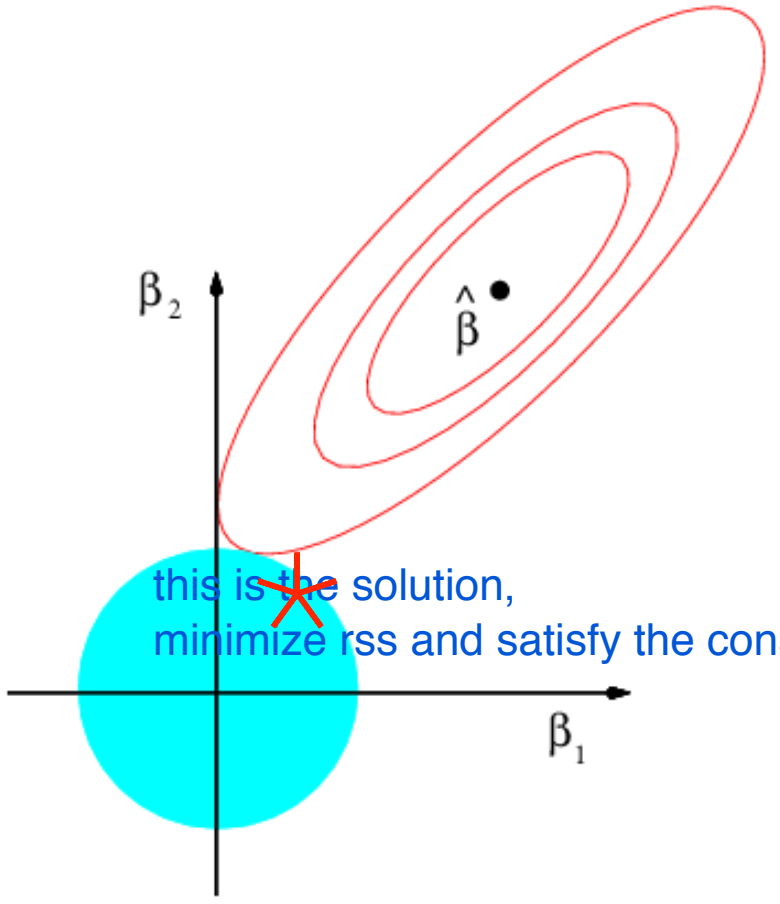
Visualizing Ridge and the Lasso with 2 predictors



we prefer coeff to be 0 in lasso

The Lasso

◆ : $\sum_{j=1}^{p} |\beta_j| < s$



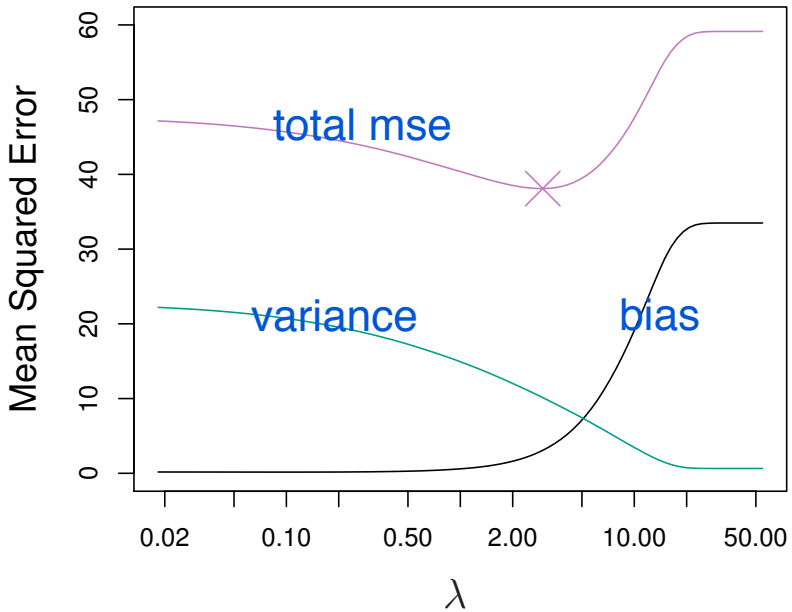
this is the solution,
minimize rss and satisfy the constraint

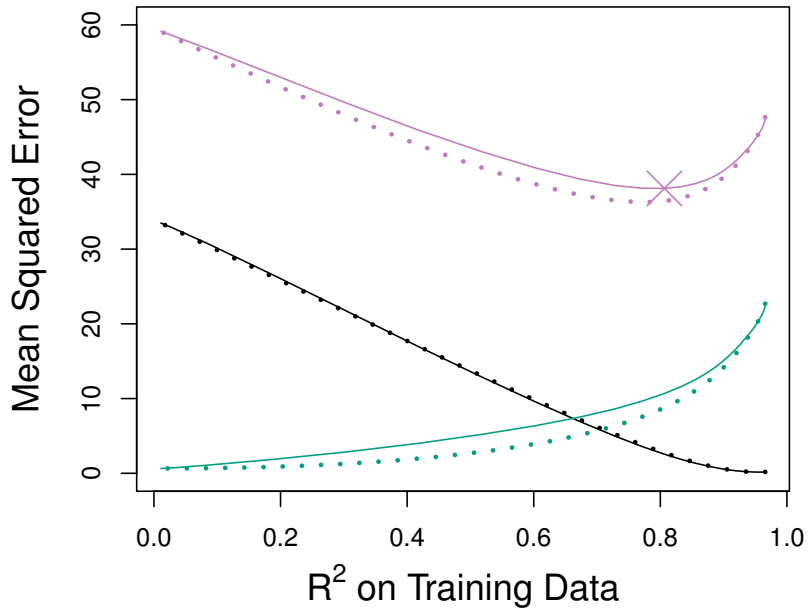
Ridge Regression

● : $\sum_{j=1}^{p} \beta_j^2 < s$

When is the Lasso better than Ridge?

Example 1. Most of the coefficients are non-zero.





$Y = X\beta + \varepsilon$

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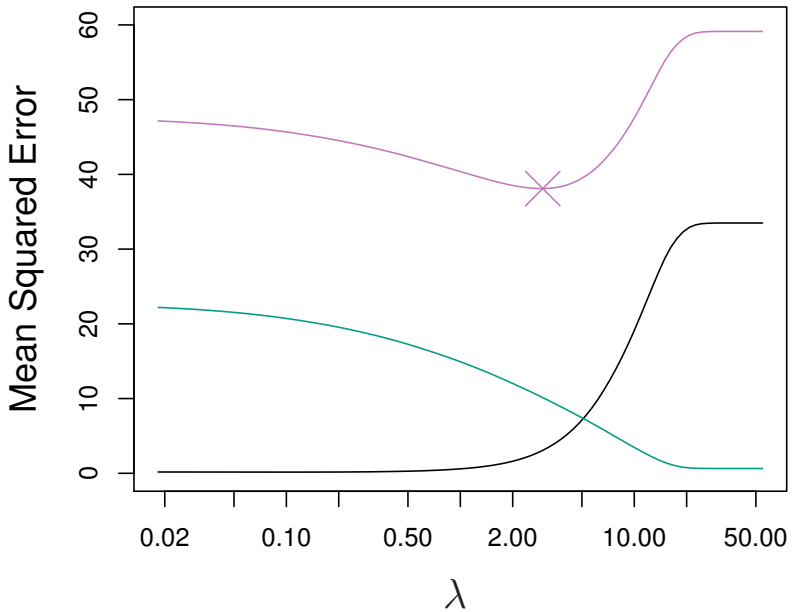

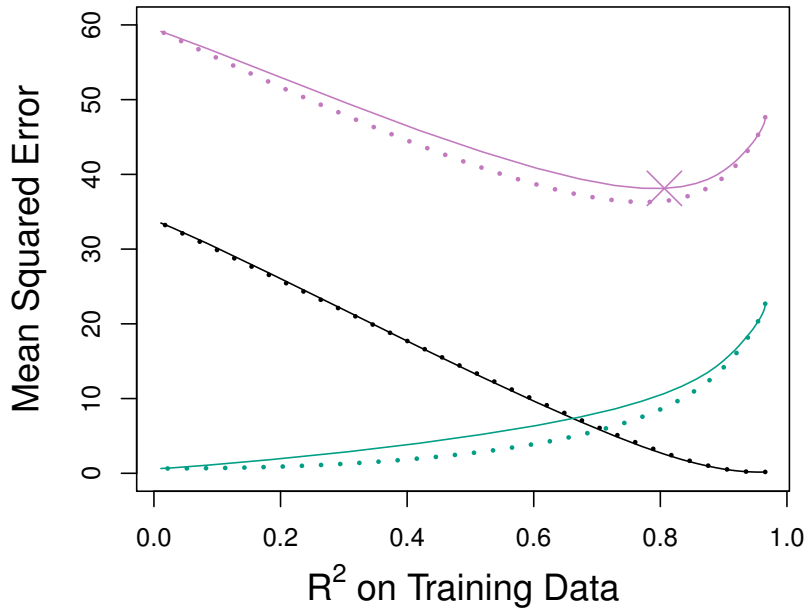

- Bias, Variance, MSE.

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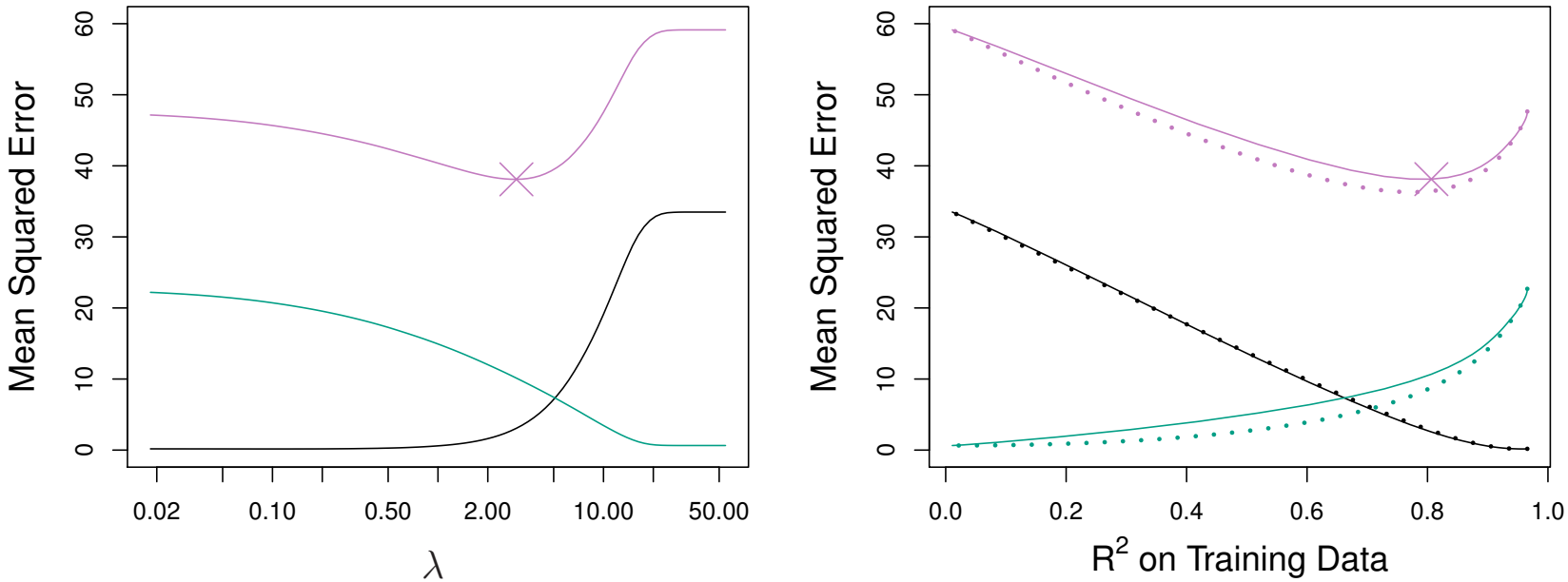

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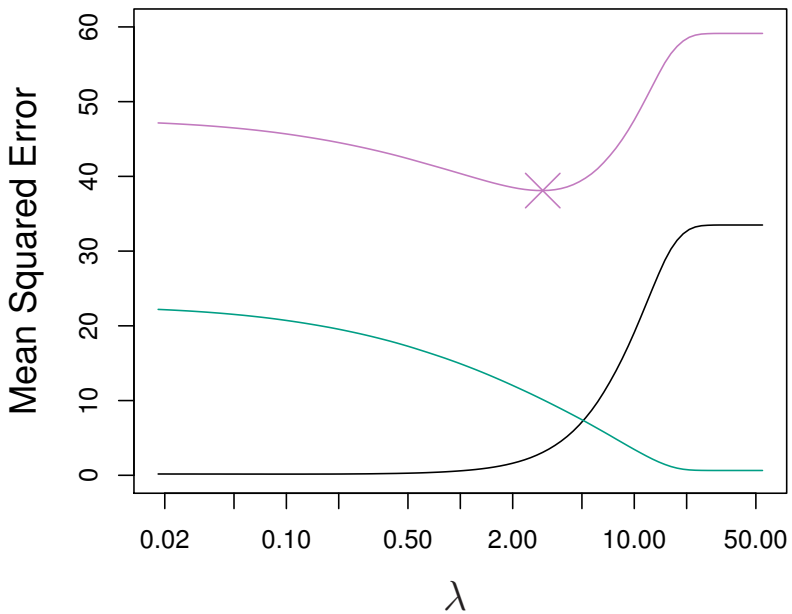

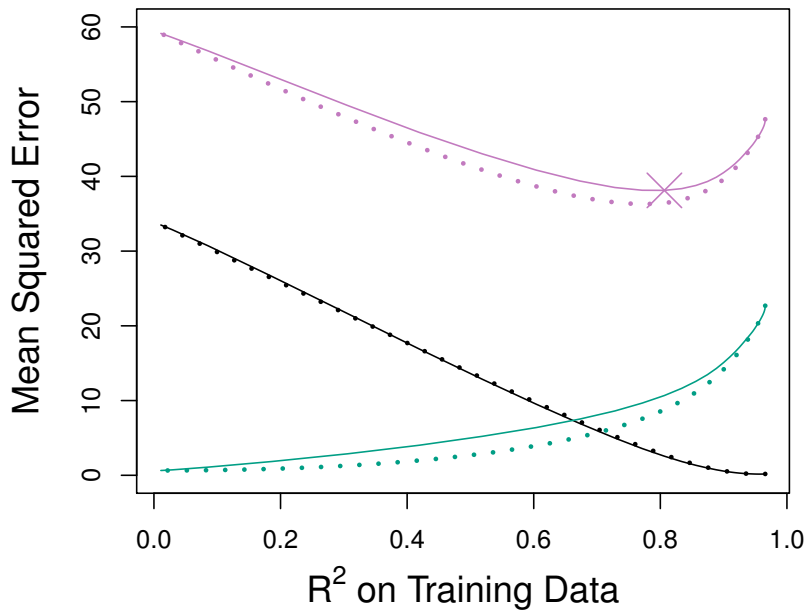

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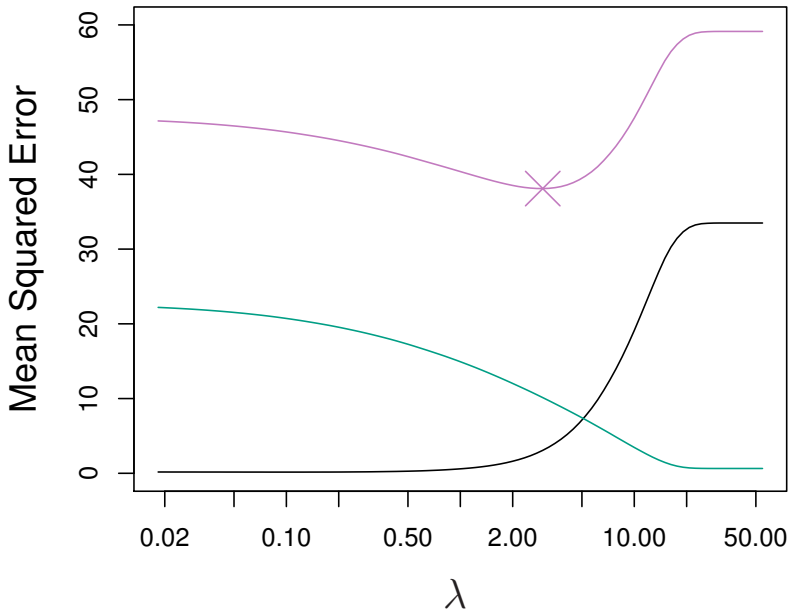
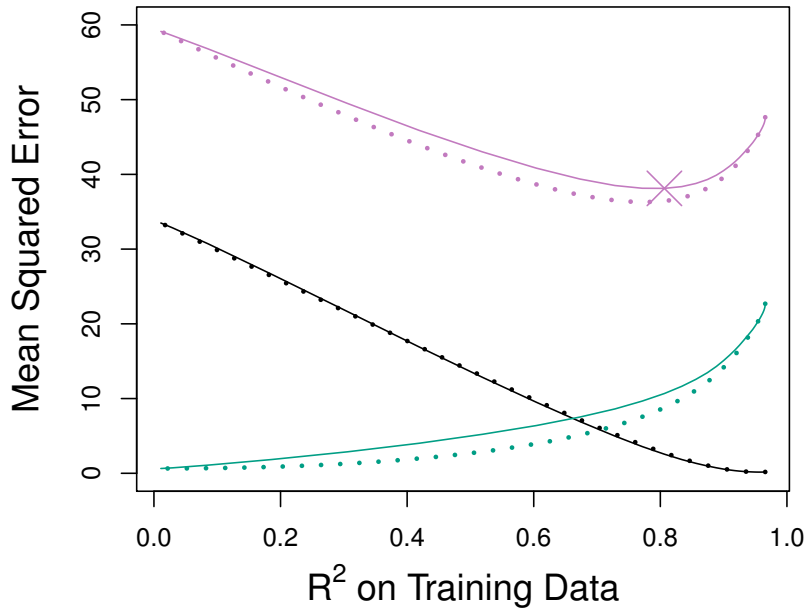


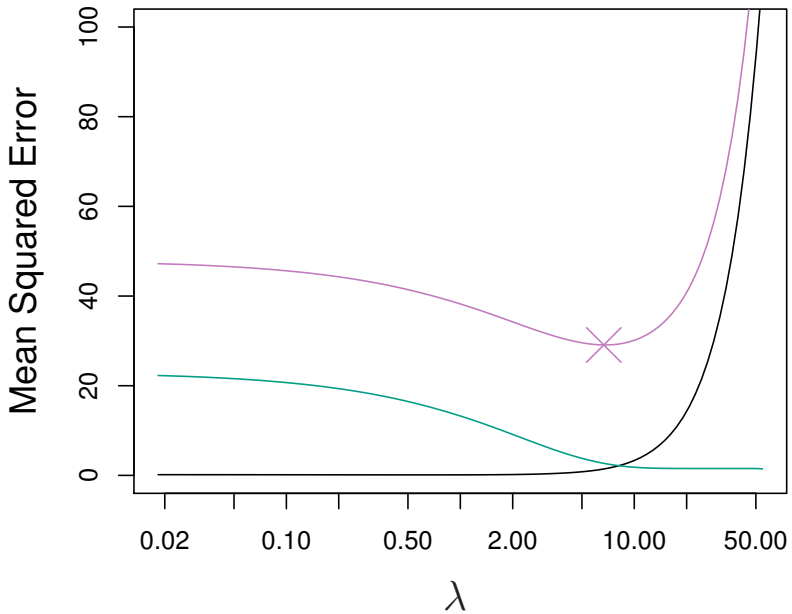


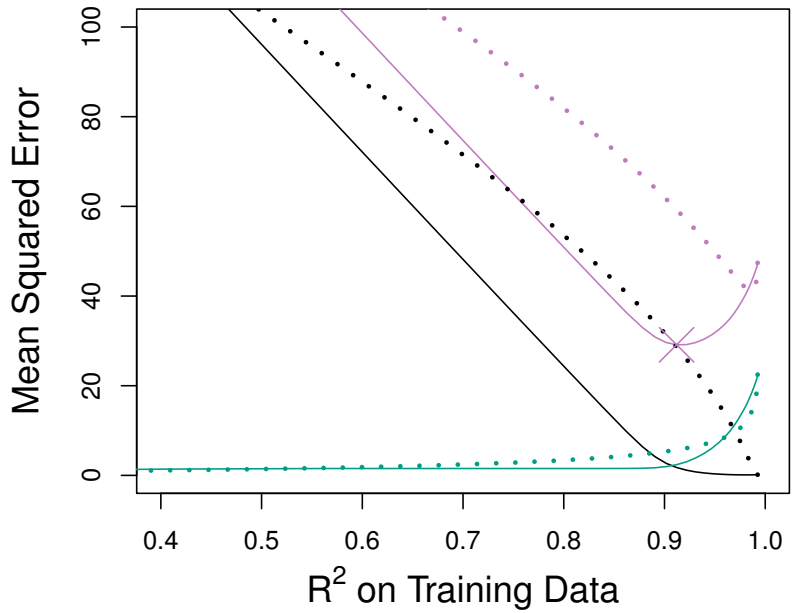
we choose lamda by cross validation, pack glmnet

- Bias, Variance, MSE. The Lasso (—), Ridge ($\cdots$).
- The bias is about the same for both methods.
- The variance of Ridge regression is smaller, so is the MSE.

When is the Lasso better than Ridge?

Example 2. Only 2 coefficients are non-zero.





if (xTx)^-1 perform well in ridge

Y_hat = x(xTx + λI)^-1xT*y

(sy)

y_hat = sλy

df = tr(sy)# use aic or bic to select

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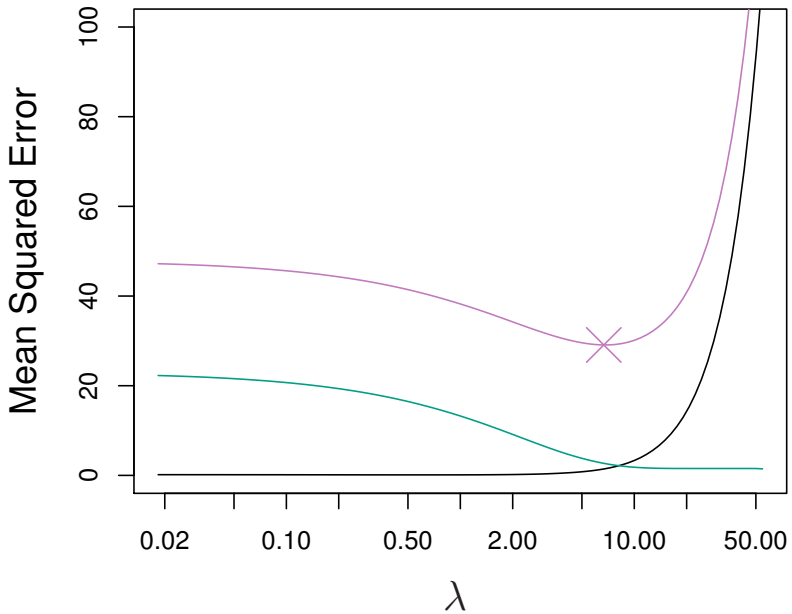

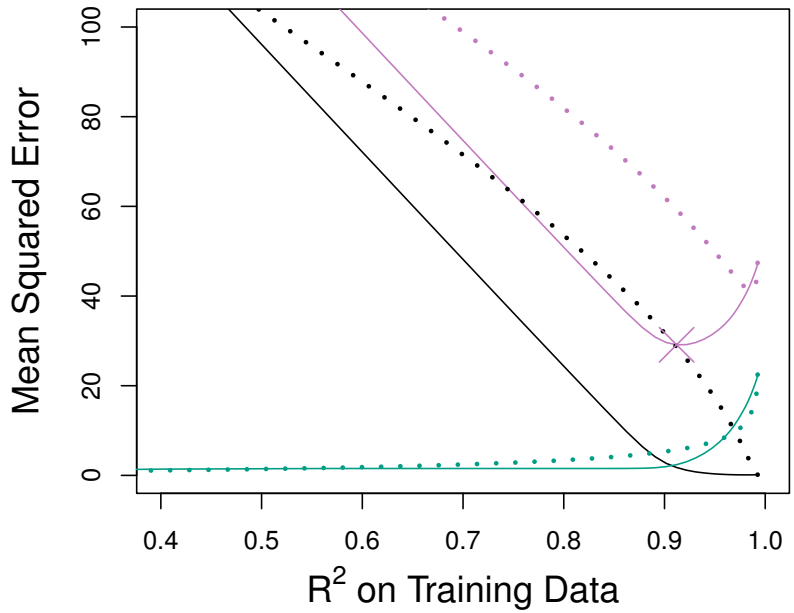

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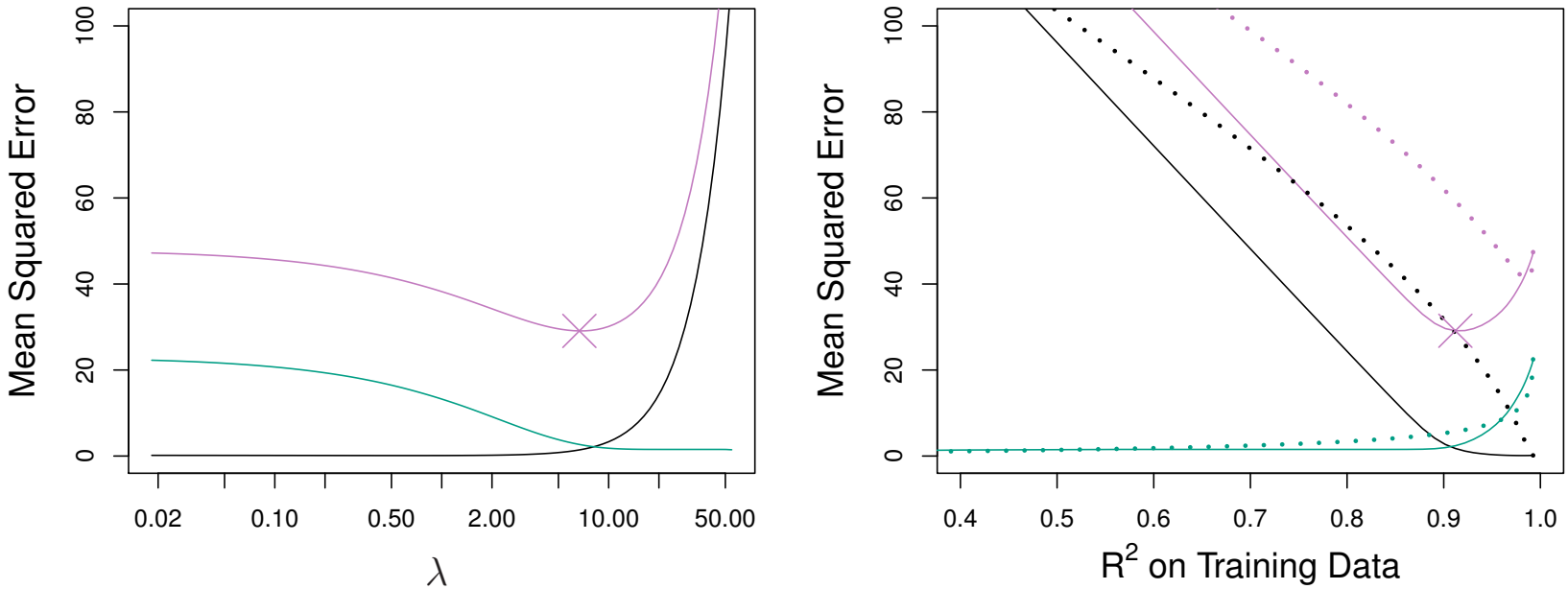

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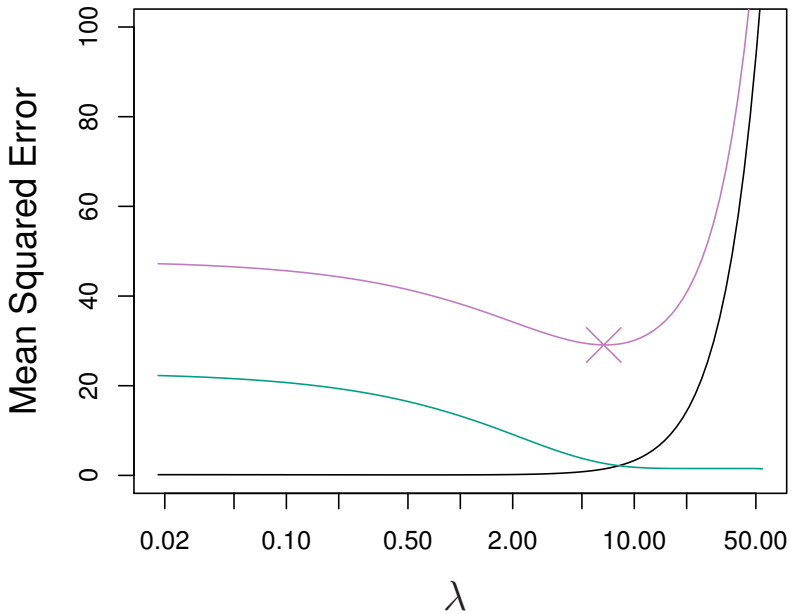
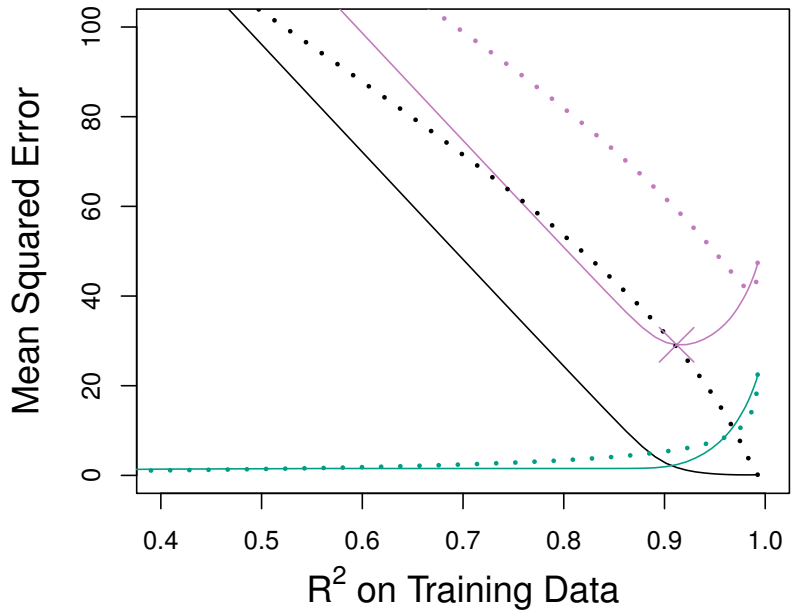
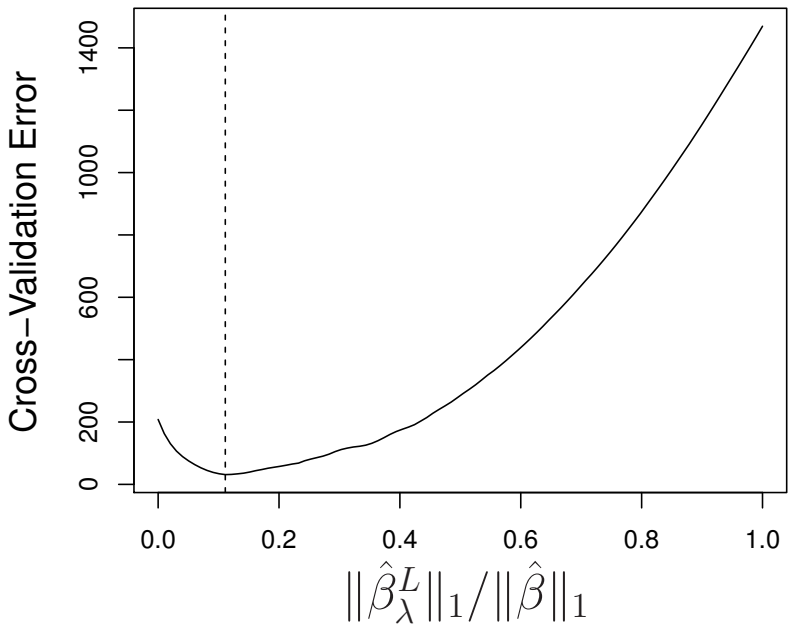
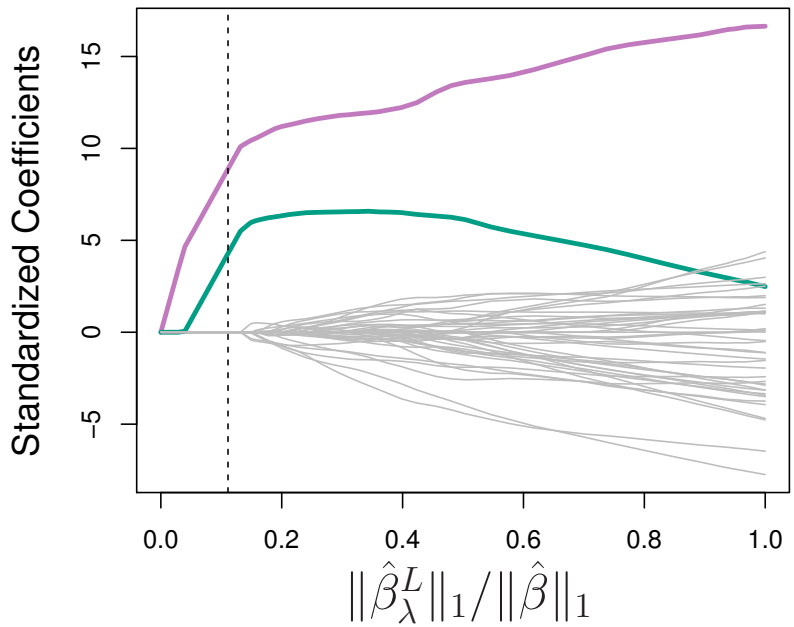




- Bias, Variance, MSE. The Lasso (—), Ridge ($\cdots$).
- The bias, variance, and MSE are lower for the Lasso.

Choosing λ by cross-validation





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It is easy to show that

$$\hat{\beta}_j^{\text{ridge}} = \frac{y_j}{1 + \lambda}.$$

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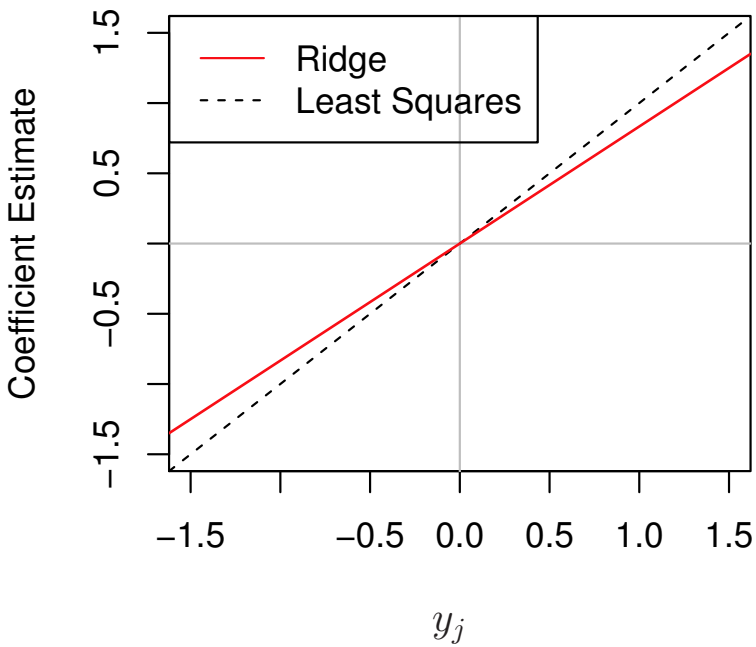
It is easy to show that

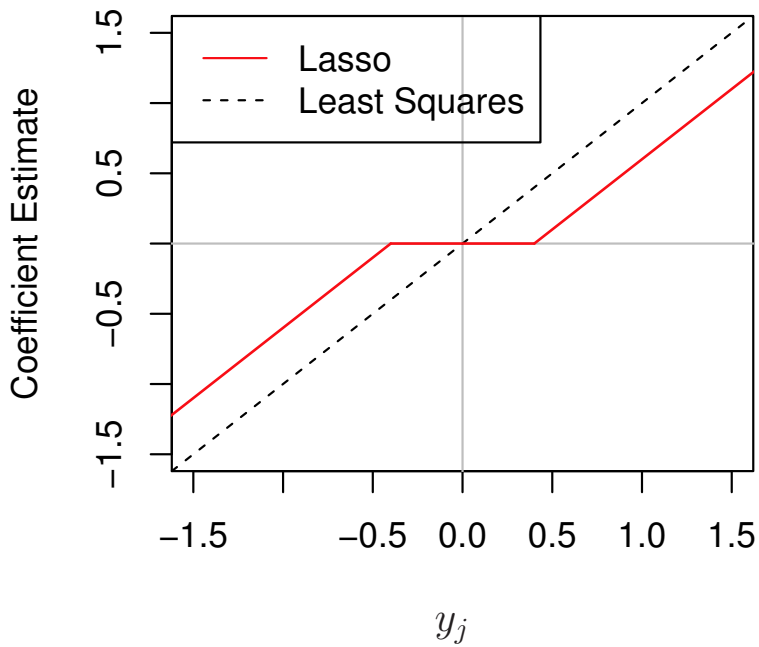
$$\hat{\beta}_j^{\text{lasso}} = \begin{cases} y_j - \lambda/2 & \text{if } y_j > \lambda/2; \\ y_j + \lambda/2 & \text{if } y_j < -\lambda/2; \\ 0 & \text{if } |y_j| < \lambda/2. \end{cases}$$

this is soft thresholding

Lasso and Ridge coefficients as a function of λ

there are hard thresholding and soft thresholding?



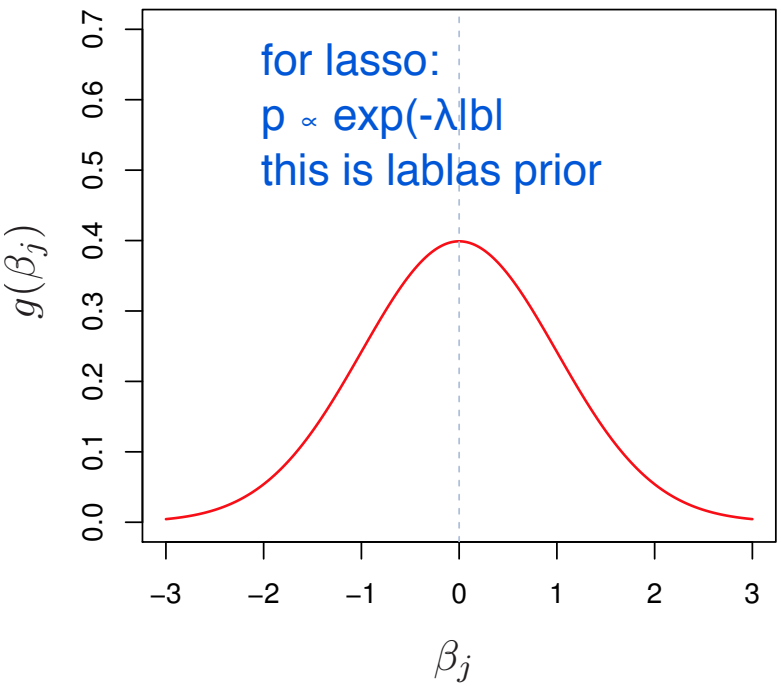


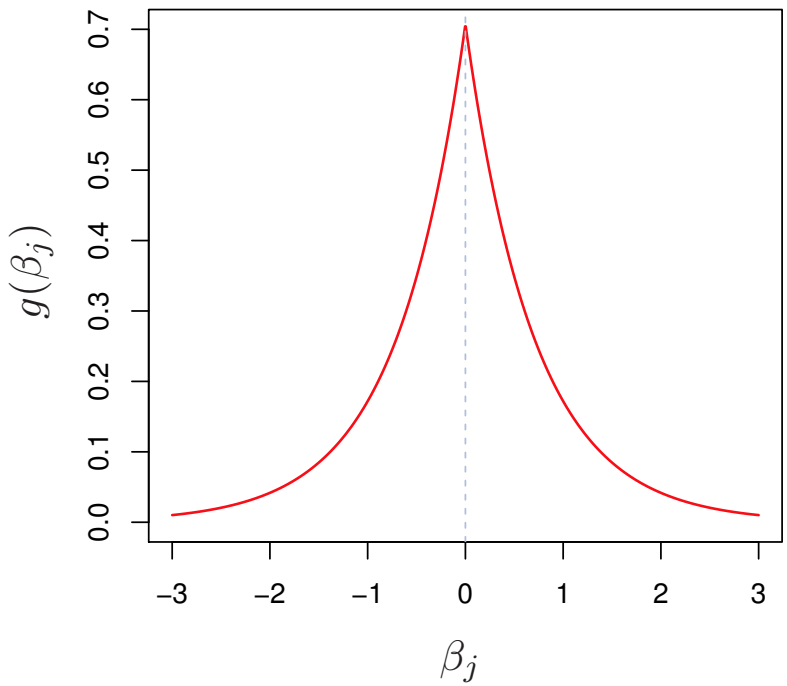
Bayesian interpretations

both method has bayesian interpretation, all the prior will shrink the model

Ridge: $\hat{\beta}^{\text{ridge}}$ is the posterior mean, with a Normal prior on β.

Lasso: $\hat{\beta}^{\text{lasso}}$ is the posterior mode, with a Laplace prior on β.





MAP will maximize the posterior and parameter

θ_hat(map) = argmax(∑logP(x|θ) + log q(θ))

RSS = ∑(yi - β1xi)^2 + λ|b1|

lasso (+penalty term)

Summary: Regression

Methods we have discussed:

- Linear regression with least squares
- Ridge regression, Lasso

Note: All of these are linear. The solutions are hyperplanes. The different methods differ only in how they *place* the hyperplane.

Summary: Regression

Ridge regression

Suppose we obtain two training samples $\mathcal{X}_1$ and $\mathcal{X}_2$ from the same distribution.

- Ideally, the linear regression solutions on both should be (nearly) identical.
- With standard linear regression, the problem may not be solvable (if $\mathbf{X}^T\mathbf{X}$ not invertible).
- Even if it is solvable, if the matrices $\mathbf{X}^T\mathbf{X}$ are close to singular (small spectral condition $c(\mathbf{X}^T\mathbf{X})$), then the two solutions can differ significantly.
- Ridge regression stabilizes the inversion of $\mathbf{X}^T\mathbf{X}$.
  Consequences:
  - Regression solutions for $\mathcal{X}_1$ and $\mathcal{X}_2$ will be almost identical if λ sufficiently large.
  - The price we pay is a bias that grows with λ.

Summary: Regression

Lasso

will directly shrink many coeff t0 0, do model selection automatically;
the solution are the singular

- The ℓ_1-costraint "switches off" dimensions; only some of the entries of the solution $\hat{\beta}^{\text{lasso}}$ are non-zero (sparse $\hat{\beta}^{\text{lasso}}$).
- This variable selection also stabilizes $\mathbf{X}^T\mathbf{X}$, since we are effectively inverting only along those dimensions which provide sufficient information.
- No closed-form solution; use numerical optimization.

Formulation as optimization problem

Method	$f(\beta)$	Penalty	Solution method
Least squares	$\|\mathbf{y} - \mathbf{X}\beta\|_2^2$	0	Analytic solution exists if $\mathbf{X}^T\mathbf{X}$ invertible
Ridge regression	$\|\mathbf{y} - \mathbf{X}\beta\|_2^2$	$\|\beta\|_2^2$	Analytic solution exists
Lasso	$\|\mathbf{y} - \mathbf{X}\beta\|_2^2$	$\|\beta\|_1$	Numerical optimization

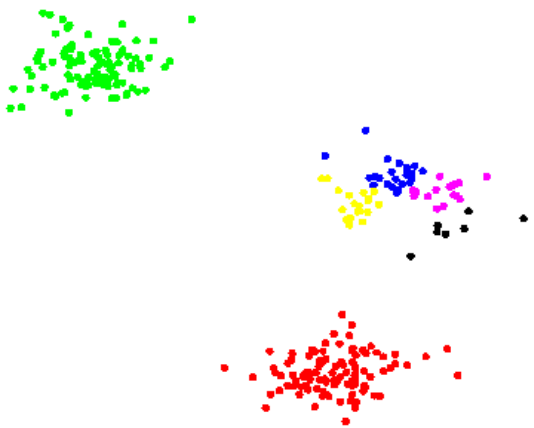
Model Selection for Clustering

The model selection problem

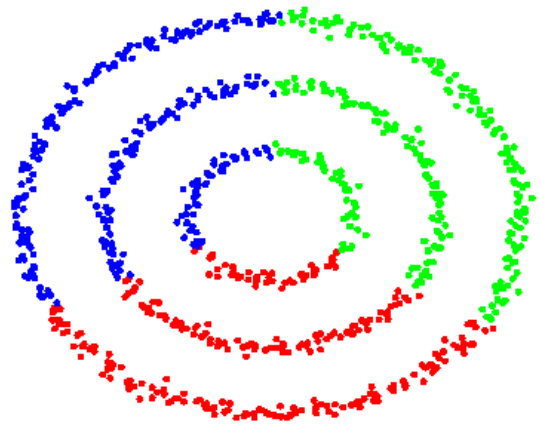
For mixture models $\pi(x) = \sum_{k=1}^{K} c_k p(x|\theta_k)$, we have so far assumed that the number K of clusters is known.

Model Order

Methods which automatically determine the complexity of a model are called **model selection** methods. The number of clusters in a mixture model is also called the **order** of the mixture model, and determining it is called **model order selection**.



(a) Inappropriate model order.



(b) Inappropriate model type.

Model Selection for Clustering

Notation

We write $\mathcal{L}$ for the log-likelihood of a parameter under a model $p(x|\theta)$:

$$\mathcal{L}(\mathbf{x}^n; \theta) := \log \prod_{i=1}^{n} p(x_i|\theta)$$

In particular, for a mixture model:

$$\mathcal{L}(\mathbf{x}^n; \mathbf{c}, \boldsymbol{\theta}) := \log \prod_{i=1}^{n} \Big(\sum_{k=1}^{K} c_k p(x_i|\theta_k) \Big)$$

Number of clusters: Naive solution (wrong!)

We could treat K as a parameter and use maximum likelihood, i.e. try to solve:

$$(K, c_1, \ldots, c_K, \theta_1, \ldots, \theta_K) := \arg \max_{K, \mathbf{c}', \boldsymbol{\theta}'} \mathcal{L}(\mathbf{x}^n; K, \mathbf{c}', \boldsymbol{\theta}')$$

Number of Clusters

Problem with naive solution: Example

Suppose we use a Gaussian mixture model.

- The optimization procedure can add additional components arbitrarily.
- It can achieve minimal fitting error by using a separate mixture component for each data point (ie $\mu_k = x_i$).
- By reducing the variance of each component, it can additionally increase the density value at $\mu_k = x_i$. That means we can achieve arbitrarily high log-likelihood.
- Note that such a model (with very high, narrow component densities at the data points) would achieve *low* log-likelihood on a new sample from the same source. In other words, it does not generalize well.

In short: The model overfits.

Number of Clusters

The general problem

- Recall our discussion of model complexity: Models with more degrees of freedom are more prone to overfitting.
- The number of degrees of freedom is roughly the number of scalar parameters.
- By increasing K, the clustering model can *add more degrees of freedom*.

Most common solutions

- **Penalization approaches**: A penalty term makes adding parameters expensive. Similar to shrinkage in regression.
- **Stability**: Perturb the distribution using resampling or subsampling. Idea: A choice of K for which solutions are stable under perturbation is a good explanation of the data.
- **Bayesian methods**: Each possible value of K is assigned a probability, which is combined with the likelihood given K to evaluate the plausibility of the solution. Somewhat related to penalization.

Penalization Strategies

General form

Penalization approaches define a *penalty function* ϕ, which is an increasing function of the number m of model parameters.
Instead of *maximizing* the log-likelihood, we *minimize* the *negative* log-likelihood and add ϕ:

$$(m, \theta_1, \ldots, \theta_m) = \arg \min_{m, \theta_1, \ldots, \theta_m} -\mathcal{L}(\mathbf{x}^n; \theta_1, \ldots, \theta_m) + \phi(m)$$

The most popular choices

The penalty function

$$\phi_{\mathsf{AIC}}(m) := m$$

is the **Akaike information criterion (AIC)**.

$$\phi_{\mathsf{BIC}}(m) := \frac{1}{2} m \log n$$

is the **Bayesian information criterion (BIC)**.

Clustering

Clustering with penalization

For clustering, AIC means:

$$(K, \mathbf{c}, \boldsymbol{\theta}) = \arg \min_{K, \mathbf{c}', \boldsymbol{\theta}'} -\mathcal{L}(\mathbf{x}^n; K, \mathbf{c}', \boldsymbol{\theta}') + K$$

Similarly, BIC solves:

$$(K, \mathbf{c}, \boldsymbol{\theta}) = \arg \min_{K, \mathbf{c}', \boldsymbol{\theta}'} -\mathcal{L}(\mathbf{x}^n; K, \mathbf{c}', \boldsymbol{\theta}') + \frac{1}{2} K \log n$$

Which criterion should we use?

- BIC penalizes additional parameters more heavily than AIC (i.e. tends to select fewer components).
- Various theoretical results provide conditions under which one of the criteria succeeds or fails, depending on:
  - Whether the sample is small or large.
  - Whether the individual components are mispecified or not.
- BIC is more common choice in practice.

Stability

Assumption

A value of K is plausible if it results in similar solutions on separate samples.

Strategy

As in cross validation and boostrap methods, we "simulate" different sample sets by perturbation or random splits of the input data.

Recall: Assignment in mixtures

Recall that, under a mixture model $\pi = \sum_{k=1}^{K} c_k p(x|\theta_k)$, we compute a "hard" assignment for a data point x_i as

$$m_i := \arg\max_k c_k p(x_i|\theta_k)$$

Stability

Computing the stability score for fixed K

1. Randomly split the data into two sets $\mathcal{X}'$ and $\mathcal{X}''$ of equal size.
2. Separately estimate mixture models π' on $\mathcal{X}'$ and π'' on $\mathcal{X}''$, using EM.
3. For each data point $x_i \in \mathcal{X}''$, compute assignments m_i' under π' and m_i'' under π''. (That is: π' is now used for prediction on $\mathcal{X}''$.)
4. Compute the score

$$\psi(K) := \min_{\sigma} \sum_{i=1}^{n} \mathbb{I}\{m_i' \neq \sigma(m_i'')\}$$

where the minimum is over all permutations σ which permute $\{1, \ldots, K\}$.

Stability

Explanation

- $\psi(K)$ measures: How many points are assigned to a different cluster under π' than under π''?
- The minimum over permutations is necessary because the numbering of clusters is not unique. (Cluster 1 in π' might correspond to cluster 5 in π'', etc.)

Stability

Selecting the number of clusters

1. Compute $\psi(K)$ for a range of values of K.
2. Select K for which $\psi(K)$ is minimial.

Improving the estimate of $\psi(K)$

For each K, we can perform multiple random splits and estimate $\psi(K)$ by averaging over these.

Performance

- Empirical studies show good results on a range of problems.
- Some basic theoretical results available, but not as detailed as for AIC or BIC.