Introduction to Machine Learning CS182

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Today:

- Linear Methods for Regression II
 - Ridge Regression
 - The Lasso
 - Discussion

Readings:

- The Elements of Statistical Learning (ESL), Chapter 3
- Pattern Recognition and Machine Learning (PRML), Chapter 3

Introduction

- · Subset selection为掉不必要的多集
 - retain a subset of the predictors, and discard the rest
 - accuracy and interpretation
 - discrete process
 - > variable are either retained or discarded
 - high variance
- Shrinkage methods
 continuous process 为美人心
 - - > don't suffer much from high variability
 - □ ridge regression, lasso, ...

Linear Methods for Regression

--- Ridge Regression

江城和、田为怨法员。无意义

またいとうない。 はまたがん いっちょう リラー Shrinkage Methods — Ridge Regression

- Shrink the regression coefficients
 - impose a penalty on the size

rinkage Methods — Ridge Regression

ink the regression coefficients impose a penalty on the size

$$\hat{\beta}^{\text{ridge}} = \underset{\beta}{\text{argmin}} \left\{ \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{i=1}^{p} x_{ij} \beta_j)^2 + \sum_{j=1}^{p} \beta_j^2 \right\}$$

- the larger the value of λ , the greater the amount of shrinkage
- the coefficients are shrunk toward zero
- An equivalent expression

P2

$$\hat{\beta}^{\text{ridge}} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j \right)^2$$

One-to-one correspondence between λ and t

• Squared
$$\ell_2$$
-norm on β

$$\|\beta\|_2^2 = \beta^T \beta = \sum_{i=1}^p \beta_i^2$$

Other possible constraints?

Shrinkage Methods – Ridge Regression *

• Equivalence between P1 and P2

P1:
$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \|\mathbf{y} - \mathbf{X}\beta\|_{2}^{2} + \lambda \|\beta\|_{2}^{2}$$

P2:
$$\tilde{\beta} = \underset{\beta}{\operatorname{argmin}} \|\mathbf{y} - \mathbf{X}\beta\|_{2}^{2}$$
, s.t. $\|\beta\|_{2}^{2} \le t$

- Goal: $\forall \lambda, \exists t \geq 0$: $\hat{\beta} = \tilde{\beta}$ (Step 1)
- $\forall t, \exists \lambda \geq 0 : \hat{\beta} = \tilde{\beta} \text{ (Step 2)}$

Proof:

- Step 1: assume that P1 is solved $-X^{T}(y X\hat{\beta}) + \lambda \hat{\beta} = 0$
- Lagrange form of P2

$$L(\beta, \mu) = \|\mathbf{y} - \mathbf{X}\beta\|_{2}^{2} + \mu(\|\beta\|_{2}^{2} - t)$$

- KKT conditions
 - 1. $\nabla_{\beta}L(\tilde{\beta},\tilde{\mu}) = 0$ \longrightarrow $-X^{T}(y X\hat{\beta}) + \tilde{\mu}\tilde{\beta} = 0$
 - $2. \quad \widetilde{\mu}\left(\left\|\widetilde{\beta}\right\|_{2}^{2}-t\right)=0$
 - $3. \quad \tilde{\mu} \geq 0$
 - 4. $\|\tilde{\beta}\|_2^2 \leq \epsilon$

- Thus,
 - □ if

$$t = \left\| \hat{\beta} \right\|_2^2$$

□ Then

$$\tilde{\mu} = \lambda, \qquad \tilde{\beta} = \hat{\beta}$$

- □ Satisfy the KKT conditions.
- Step 2: conversely, assume that P2 is solved
- The optimal solution $(\tilde{\beta}, \tilde{\mu})$ must satisfies KKT conditions. Therefore, let $\lambda = \tilde{\mu}$, we always have $\hat{\beta} = \tilde{\beta}$.

Strong duality holds for P2:

 $(\tilde{\beta}, \tilde{\mu})$ is the optimal solution of P2



 $(\beta, \tilde{\mu})$ satisfies KKT conditions

Shrinkage Methods – Ridge Regression

Important notes

- ridge solutions are not equivalent under scaling of inputs • standardize the inputs before solving it
- the intercept β_0 should be left out of the penalty term

$$x' = \frac{x - \bar{x}}{1 - \bar{x}}$$

Standardization

Ex. 3.5
$$\rightarrow$$
 once $x_{ij} - \bar{x}_j$, β_0 is estimated by $\bar{y} = \frac{1}{N} \sum_{i=1}^{N} y_i$ $\beta_0 = \bar{y}$ the rest parameters are estimated by the centered data $\beta_0 = \bar{y}$.

- Henceforth we assume the data has been standardized \mathbf{X} has p rather than p+1 columns
- Training: preprocess: X= X-X (对每例, 又是例 Prediction? Contering: Y-Y-Y (3-) Y

 Train: min(|| U-Xa||^2+) || (对每例, 又是例)

Test i preprocess : $x_0 = x_0 - \bar{x}$ predict : $\hat{y}_i = \hat{\beta}^{X} + \beta_0$ $x_i^T \beta$ Shrinkage Methods – Ridge Regression

Thouse with the Abit a Milbing 1

• Ridge regression in matrix form
$$\hat{\beta}^{\text{ridge}} = \underset{\beta}{\operatorname{argmin}} \left\{ \sum_{i=1}^{N} (y_i - \sum_{j=1}^{p} x_{ij} \beta_j)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 \right\}$$
• We can rewrite PRSS(λ, β) as follows

$$PRSS(\lambda, \beta) = (\mathbf{y} - \mathbf{X}\beta)^{T}(\mathbf{y} - \mathbf{X}\beta) + \lambda \beta^{T}\beta$$

$$T = \mathbf{A}^{T}\mathbf{Y}^{T} + \mathbf{A}^{T}\mathbf{Y}^{T}\mathbf{Y}^{T} + \mathbf{A}^{T}\mathbf{Y}^{T}\mathbf{Y}^{T}\mathbf{Y}^{T} + \mathbf{A}^{T}\mathbf{Y}$$

 $= \mathbf{y}^T \mathbf{y} - \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{y} - \mathbf{y}^T \mathbf{X} \boldsymbol{\beta} + \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{X} \boldsymbol{\beta} + \lambda \boldsymbol{\beta}^T \boldsymbol{\beta}$ • Differentiating PRSS(λ, β) w.r.t. β

一定大計会员

$$\frac{\partial PRSS(\lambda, \beta)}{\partial \beta} = -2\mathbf{X}^T \mathbf{y} + 2(\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_p)\beta = 0$$
• The closed form solution $\hat{\beta}^{ridge} = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_p)^{-1} \mathbf{X}^T \mathbf{y}$
• make the problem nonsingular, even if rank(\mathbf{X}) < p

-1-k-7+

SUD分解之后对一切此样为的况一定为非奇奇。

Shrinkage Methods – Ridge Regression

 $\chi^T\chi = (UDV^T)^T(UDV^T) = (VDU^T)(UDV^T) = VD^T \chi^T\chi + \lambda J_P$ Additional insight into ridge regression 対象矩阵、 $D^T = D$. = $VB^T + \lambda VV^T$

- $V \in \mathbb{R}^{p \times p}$: its columns span the row space (\mathbb{R}^p) of X
- $\mathbf{D} \in \mathbb{R}^{p \times p}$: diagonal matrix $(d_1 \ge d_2 \ge \cdots \ge d_n \ge 0)$

if $\exists d_i = 0, \mathbf{X}$ is singular

• Singular values of X

Least squares
$$\mathbf{X}\hat{\beta}^{\text{ls}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$$

$$\mathbf{X}\hat{\beta}^{\text{ls}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

$$= \mathbf{U}\mathbf{U}^T\mathbf{y},$$

$$= \sum_{j=1}^{p} \mathbf{u}_j \mathbf{u}_j^T\mathbf{y}$$
The *j*-th column of **U**

Ridge regression

$$\begin{split} \mathbf{X} \hat{\beta}^{\text{ridge}} &= \mathbf{X} (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y} \\ &= \mathbf{U} \mathbf{D} (\mathbf{D}^2 + \lambda \mathbf{I})^{-1} \mathbf{D} \mathbf{U}^T \mathbf{y} \\ &= \sum_{j=1}^p \mathbf{u}_j \underbrace{\frac{d_j^2}{d_j^2 + \lambda}}_{\mathbf{H}_j^T \mathbf{Y}, \mathbf{H}_j^T \mathbf{Y$$

Shrinkage Methods – Ridge Regression

- Prostate cancer example
 - \Box #training(N) = 67, #testing=30
 - wariables(p)=8 8412
 - ridge coefficient estimates
- Effective degree of freedom

$$df(\lambda) = \sum_{j=1}^{p} \frac{d_j^2}{d_j^2 + \lambda} \in (0, p]$$
有效自读 ⇒复杂度

$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^{T}, \mathbf{V}^{T}\mathbf{V} = \mathbf{I}_{p}$$

$$\mathbf{df}(\lambda) = \operatorname{Tr}\left(\mathbf{X}\left(\mathbf{X}^{T}\mathbf{X} + \lambda \mathbf{I}_{p}\right)^{-1}\mathbf{X}^{T}\right)$$

$$= \operatorname{Tr}\left(\mathbf{U}\mathbf{D}\left(\mathbf{D}^{2} + \lambda \mathbf{I}_{p}\right)^{-1}\mathbf{D}\mathbf{U}^{T}\right)$$

$$= \sum_{j=1}^{p} \frac{d_{j}^{2}}{d_{j}^{2} + \lambda}$$

Trace equals to sum of eigenvalues

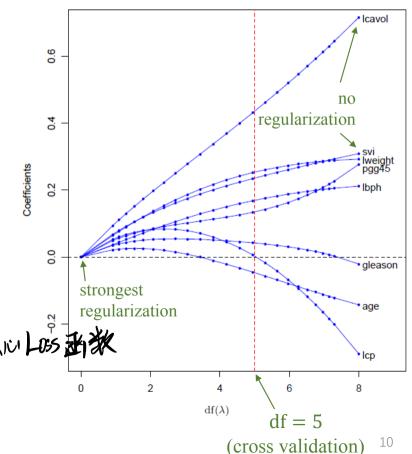
Shrinkage Methods – Ridge Regression

- Prostate cancer example
 - \Box #training(N) = 67, #testing=30
 - #variables(p)=8
 - ridge coefficient estimates
- Effective degree of freedom

$$df(\lambda) = \sum_{j=1}^{p} \frac{d_j^2}{d_j^2 + \lambda} \in (0, p]$$

- $\lambda \to 0$, df(λ) = $p \leftarrow$ no regularization

 $\lambda \to \infty$, $df(\lambda) \to 0$ で要認 しか起自由度 歌 没 う, 不再 先 い し の 数 数



Linear Methods for Regression

--- The Lasso



```
1.11, -范数 (convex)
(1.11, -范数 (convex) (距摩范徽最近面 convex是一范数)
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新聞化方法 Shrinkage Methods – The Lasso

• The lasso estimate:

Tage Methods – The Lasso model complexity
$$\beta$$
 is a serious of training error β is a serious β is a seri

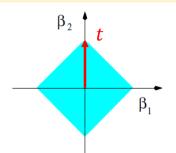
- the ℓ_2 ridge penalty is replaced by ℓ_1 lasso penalty.
- no closed-form solution (ℓ_1 penalty is nondifferentiable)
- · Or equivalently, 一方顶点处不可导, 动阴梯度下降逼近。

$$\hat{\beta}^{\text{lasso}} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j \right)^2 \quad \text{if } t = \frac{1}{2} \|\hat{\beta}^{ls}\|_1, \hat{\beta}^{ls} \text{ is shrunk about 50% on average}$$

subject to
$$\sum_{j=1}^{p} |\beta_j| \le t$$
.

 \square making t sufficiently small \rightarrow some coefficients equal to 0

if
$$t \ge \|\hat{\beta}^{ls}\|_1$$
, $\hat{\beta}^{lasso} = \hat{\beta}^{ls}$



Shrinkage Methods – The Lasso

• The lasso in matrix form

$$\hat{\beta}^{lasso} = \operatorname{argmin}_{\beta} \frac{1}{2} \|\mathbf{y} - \mathbf{X}\beta\|_{2}^{2} + \lambda \|\beta\|_{1}$$

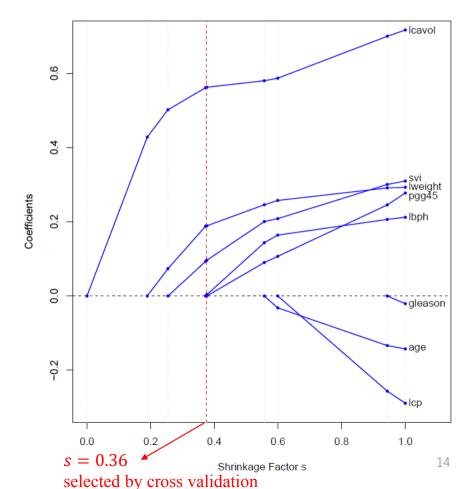
- Prostate cancer example
- The standardized parameter

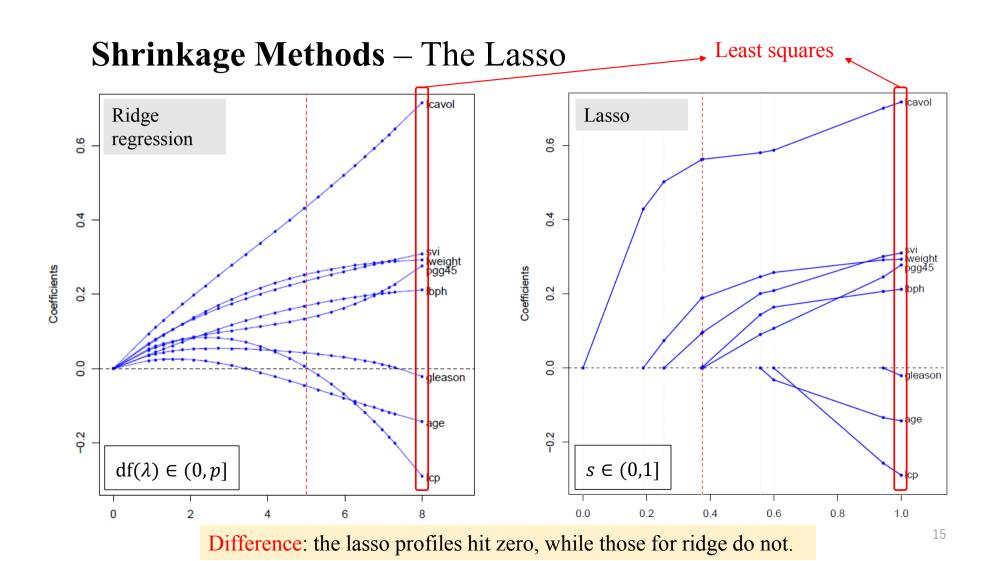
$$s = t / \|\hat{\beta}^{(s)}\|_1 \in (0,1]$$

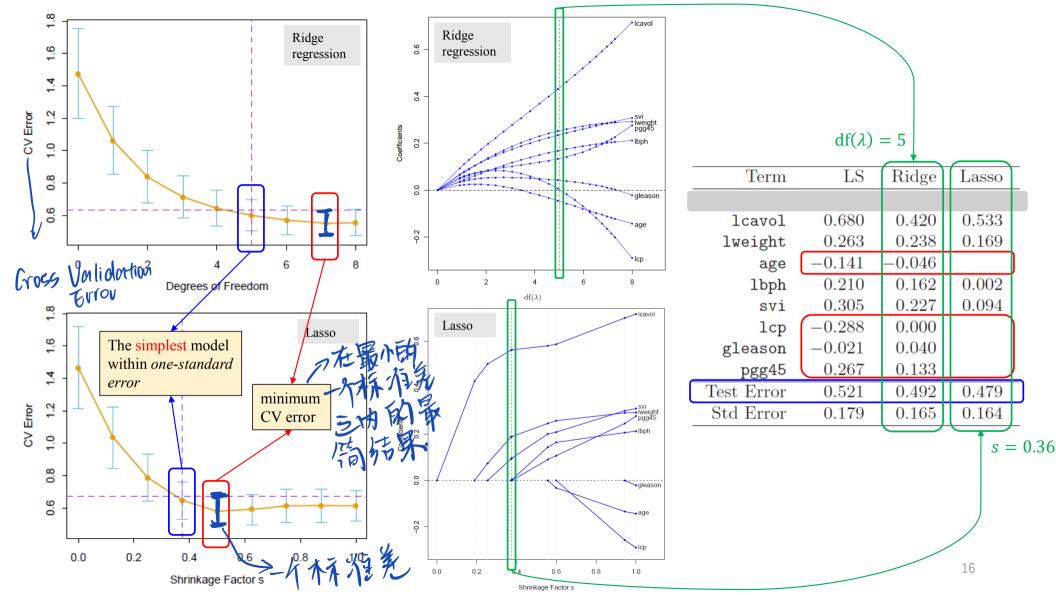
$$s = 1, \hat{\beta}^{lasso} = \hat{\beta}^{ls}$$

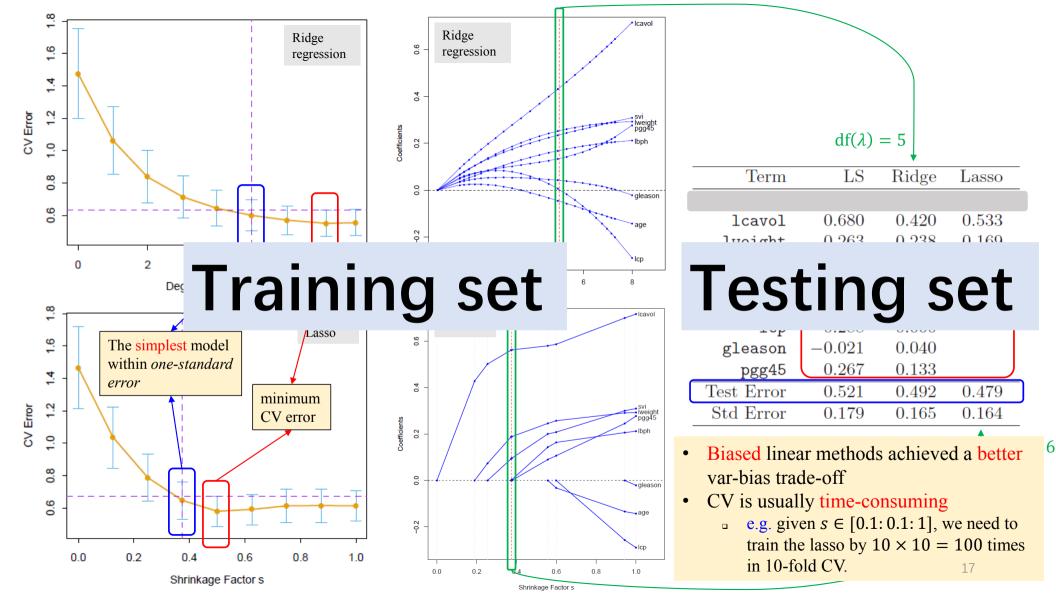
$$s \to 0, \hat{\beta}^{lasso} \to 0$$

$$\ \ \square \ \ s \in (0,1), \hat{\beta}_j^{lasso} \in \left(0,\hat{\beta}_j^{ls}\right), \forall j$$









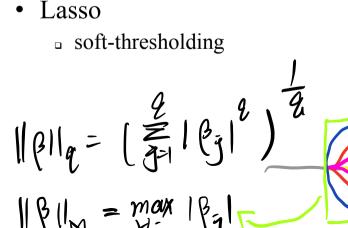
Linear Methods for Regression

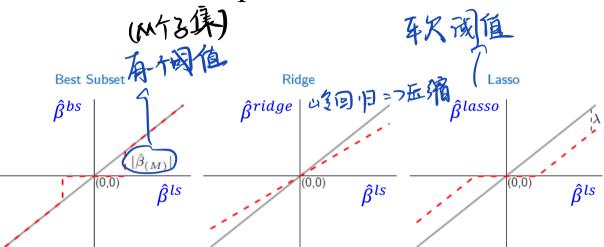
--- Discussion

Shrinkage Methods – Geometric Interpretation

Orthonormal case $(\mathbf{X}^T\mathbf{X} = \mathbf{I}_p)$

- Best-subset
 - hard-thresholding
 - discontinuity
- Ridge regression
 - proportional shrinkage





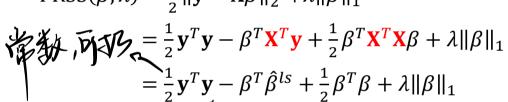
Estimator	Formula
Best subset (size M)	$\hat{\beta}_j \cdot I(\hat{\beta}_j \ge \hat{\beta}_{(M)})$
Ridge 取原的符号	$\hat{\beta}_j/(1+\lambda)$
Ridge 取 作的符号 Lasso	$(\operatorname{sign}(\hat{\beta}_j)(\hat{\beta}_j - \lambda)_+)$
In this table $\hat{\beta}_i$ represents $\hat{\beta}_i^{ls}$	

Shrinkage Methods – Geometric Interpretation

Orthonormal case $(\mathbf{X}^T\mathbf{X} = \mathbf{I}_p)$

- Least squares $\hat{\beta}^{ls} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{v} = \mathbf{X}^T \mathbf{v}$
- Ridge regression IPM $\hat{\beta}^{ridge} = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_p)^{-1} \mathbf{X}^T \mathbf{y}$ $=\frac{1}{1+1}\mathbf{X}^T\mathbf{y}=\frac{1}{1+1}\hat{\beta}^{ls}$

PRSS
$$(\beta, \lambda) = \frac{1}{2} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda \|\beta\|_1$$



• Minimizing PRSS(β , λ) is equivalent to

$$\min_{\beta_j} \frac{-\beta_j^{ls} \beta_j + \lambda |\beta_j|}{2}, \quad \forall j$$
Signs of $\hat{\rho}$ and $\hat{\rho}^{ls}$ must be the second

$$\hat{\beta}_j > 0 \rightarrow \hat{\beta}_j = \hat{\beta}_j^{ls} - \hat{\beta}_j^{ls} - \hat{\beta}_j^{ls} = \hat{\beta}_j^{ls} - \hat{\beta}_j^{ls} + \hat{\beta}_j^{ls} = \hat{\beta}_j^{ls} + \hat{\beta}_j^{ls} + \hat{\beta}_j^{ls} = \hat{\beta}_j^{ls} + \hat{\beta}_j$$

•
$$\hat{\beta}_j^{lasso} = \text{sign}(\hat{\beta}_j^{ls}) (|\hat{\beta}_j^{ls}| - \lambda)_+$$

Best subset
$$\hat{\beta}_{j}^{bs} = \mathbf{x}_{j}^{T}\mathbf{y}, \quad \forall j$$

$$\hat{\beta}_{j}^{bs} = \mathbf{x}_{j}^{bs} = \mathbf{x}_{j}^{bs} + \mathbf{x}_{j}^{bs}$$

Best subset (size
$$M$$
) $\hat{\beta}_j \cdot I(|\hat{\beta}_j| \ge |\hat{\beta}_{(M)}|)$
Ridge $\hat{\beta}_i/(1+\lambda)$

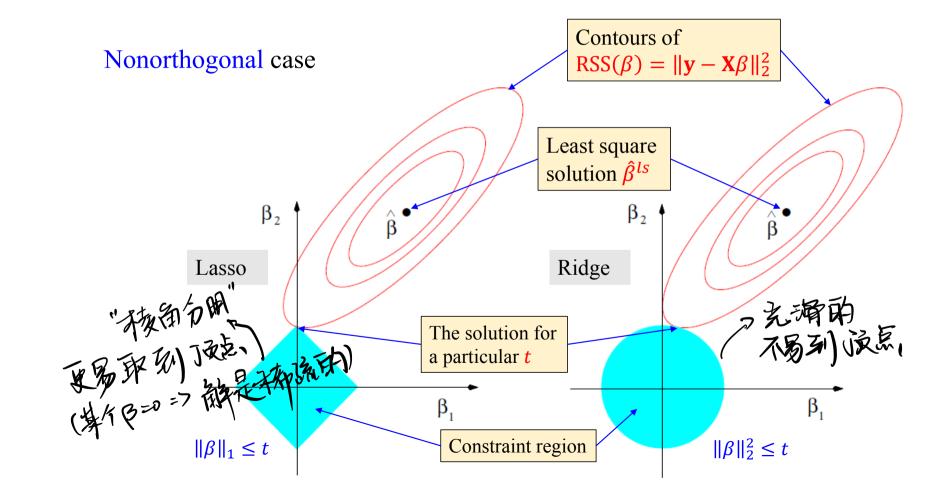
Lasso
$$\operatorname{sign}(\hat{\beta}_j)(|\hat{\beta}_j| - \lambda)_+$$
 for an dient.

Proximal operator: 4th 11 17-1811, + 11 1811,

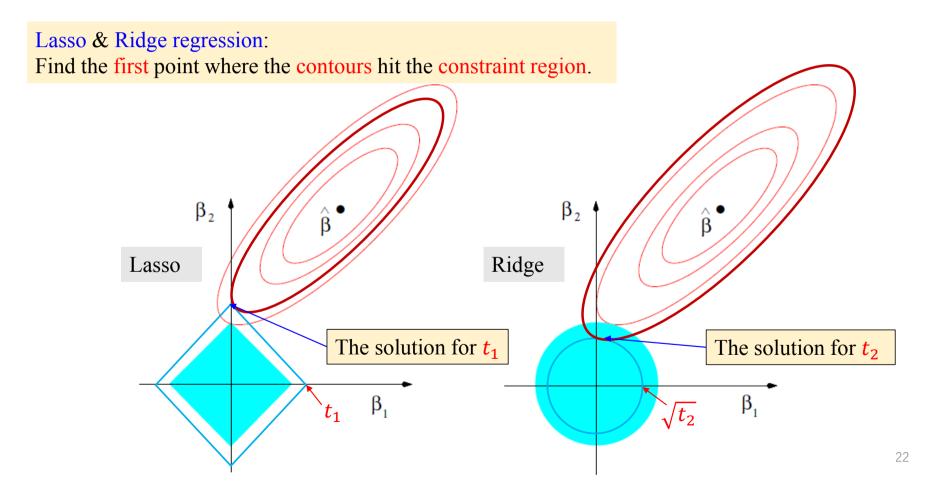
Proximal operator: 4th 12 mill 17-1811, + 11 1811.

Proximal operator: 4th 12 mill 17-1811, + 11 1811.

Shrinkage Methods – Geometric Interpretation



Shrinkage Methods – Geometric Interpretation



Shrinkage Methods – Probabilistic Interpretation

Ridge and Lasso in the Bayes framework

• Suppose a Gaussian conditional distribution

$$\Pr(Y|X,\beta) = \frac{1}{\sigma\sqrt{2\pi}} \exp(-\frac{1}{2}(\frac{Y - X^T\beta}{\sigma})^2)$$

MLE:

Log-likelihood

$$\ell(\beta) = \ln \Pr(\mathbf{y}|\mathbf{X}, \beta)$$

$$= \sum_{i=1}^{N} \ln \Pr(y_i|x_i, \beta)$$

 $\hat{\beta}^{ls} = \operatorname{argmax}_{\beta} \ell(\beta)$ = $\operatorname{argmin}_{\beta} ||\mathbf{y} - \mathbf{X}\beta||_{2}^{2}$ $= \left[-\frac{N}{2} \log(2\pi) - N \log \sigma \right] - \left[\frac{1}{2\sigma^2} \sum_{i=1}^{N} (y_i - x_i^T \beta)^2 \right]$

 $\Pr(Y|X,\beta) = \mathcal{N}(X^T\beta,\sigma^2)$

 Maximum a posterior (MAP) Posterior

$$\hat{\beta} = \operatorname{argmax}_{\beta} \Pr(\beta | \mathbf{X}, \mathbf{y}) = \operatorname{argmax}_{\beta} \frac{\Pr(\mathbf{y} | \mathbf{X}, \beta) \Pr(\beta)}{\Pr(\mathbf{X}, \mathbf{y})}$$

Likelihood

Posterior ∝ Likelihood × Prior

Irrelevant with β

Shrinkage Methods – Probabilistic Interpretation

Ridge and Lasso in the Bayes framework

MLE:
$$\hat{\beta}^{MLE} = \operatorname{argmax}_{\beta} \Pr(\mathbf{y}|\mathbf{X}, \beta)$$
 Least squares

MAP: $\hat{\beta}^{MAP} = \operatorname{argmax}_{\beta} \Pr(\mathbf{y}|\mathbf{X}, \beta) \Pr(\beta)$ Ridge & Lasso

- Ridge regression
 - MAP with a prior $Pr(\beta) = \mathcal{N}(\beta|0, \frac{1}{\lambda}\mathbf{I}_p)$ Gaussian distribution

$$\begin{split} \hat{\beta}^{ridge} &= \operatorname{argmax}_{\beta} \ln \left(\Pr(\mathbf{y} | \mathbf{X}, \beta) \Pr(\beta) \right) \\ &= \operatorname{argmax}_{\beta} \ln \left(\prod_{i=1}^{N} \mathcal{N}(y_i | x_i^T \beta, \sigma^2) \times \mathcal{N}(\beta | 0, \frac{1}{\lambda} \mathbf{I}_p) \right) \end{split}$$

- Lasso
 - MAP with a prior $Pr(\beta) = \frac{\lambda}{2} e^{-\lambda \|\beta\|_1}$ Laplacian distribution

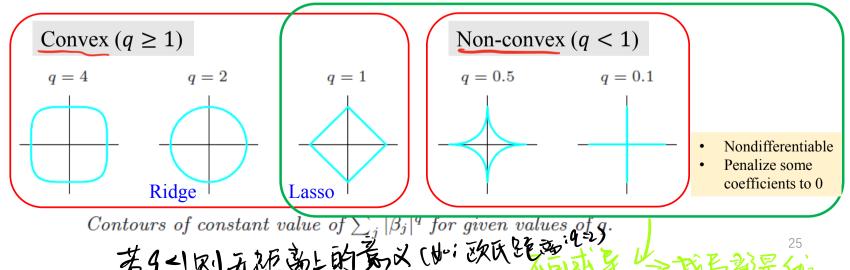
$$\hat{\beta}^{lasso} = \operatorname{argmax}_{\beta} \ln \left(\prod_{i=1}^{N} \mathcal{N}(y_i | x_i^T \beta, \sigma^2) \times \frac{\lambda}{2} e^{-\lambda \|\beta\|_1} \right)$$

Shrinkage Methods – Generalization

Generalization of Ridge and Lasso

• Consider the criterion $(q \ge 0)$

$$\tilde{\beta} = \underset{\beta}{\operatorname{argmin}} \left\{ \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^{p} |\beta_j|^q \right\}$$
• $q = 0$, best subset
• $q = 1$, lasso
• $q = 2$, ridge regression



国为不满展三角市多不多形儿林外儿《11111111111 这种人的。 Tethods - Generalization 超到了:若相为知识一个组,Lasso:我的智慧,相关的随机抽一个标识的形成。 到下的图 0.

Shrinkage Methods – Generalization

Generalization of Ridge and Lasso

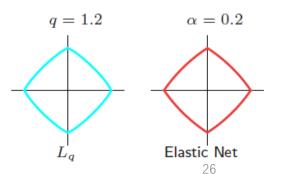
• Consider the criterion $(q \ge 0)$

$$\tilde{\beta} = \underset{\beta}{\operatorname{argmin}} \left\{ \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^{p} |\beta_j|^q \right\}$$
• $q = 0$, best subset
• $q = 1$, lasso
• $q = 2$, ridge regression

- $q \in (1,2)$: a compromise between lasso and ridge regression
 - $\mid \beta_i \mid^q$ is differentiable at $0 \to \text{hard to set } \beta_i = 0, \forall j$
- **Elastic-net**

$$\min_{\beta} \sum_{i=1}^{N} (y_i - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} (\alpha\beta_j^2 + (1-\alpha)|\beta_j|)$$

- □ ℓ₂ shrinks the coefficients of correlated predictors



Shrinkage Methods – Generalization

