

# UVA CS 6316: Machine Learning

## Lecture 6 Extra: Optimization for Linear Regression Model with Regularizations

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# EXTRA (Not required IN EXAMS)

# Extra Recap

- ❑ More about LR Model with Regularizations
  - ❑ Ridge Regression
  - ❑ Lasso Regression
    - ❑ Extra: how to perform training
  - ❑ Elastic net
    - ❑ Extra: how to perform training

# Why Invertible In Ridge Regression?

$$\beta^* = (X^T X + \lambda I)^{-1} X^T \bar{y}$$

(NOT AN EASY PROOF from SVD angle), many concepts, SVD, PCA, Eigenvalues, relation to singular

- NOT AN EASY PROOF If through SVD
  - <https://www.quora.com/When-is-the-matrix-frac-1-n-X-T-X+-lambda-I-d-times-d-invertible>
- The determinant of  $A$  is equal to the product of its eigenvalues,
$$|A| = \prod_{i=1}^n \lambda_i.$$
- The rank of  $A$  is equal to the number of non-zero eigenvalues of  $A$ .

# Why Invertible In Ridge Regression?

symmetric, positive semi-definite *square* Gram matrix  $K = A^T A$  — which can be naturally formed even when  $A$  is not square. Perhaps the eigenvalues of  $K$  might play a comparably important role for general matrices. Since they are not easily related to the eigenvalues of  $A$  — which, in the non-square case, don't even exist — we shall endow them with a new name.

**Definition 6.27.** The *singular values*  $\sigma_1, \dots, \sigma_r$  of an  $m \times n$  matrix  $A$  are the positive square roots,  $\sigma_i = \sqrt{\lambda_i} > 0$ , of the nonzero eigenvalues of the associated Gram matrix  $K = A^T A$ . The corresponding eigenvectors of  $K$  are known as the *singular vectors* of  $A$ .

Since  $K$  is necessarily positive semi-definite, its eigenvalues are always non-negative,  $\lambda_i \geq 0$ , which justifies the positivity of the singular values of  $A$  — independently of whether  $A$  itself has positive, negative, or even complex eigenvalues — or is rectangular and has no eigenvalues at all. The standard convention is to label the singular values in decreasing order, so that  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$ . Thus,  $\sigma_1$  will always denote the largest or

## Extra: two forms of Ridge Regression

- Totally equivalent

$$\left\{ \begin{array}{l} \text{(1) } \underset{\theta}{\operatorname{argmin}} J(\theta) + \lambda \beta^T \beta \\ \text{(2) } \underset{\theta}{\operatorname{argmin}} J(\theta), \text{ s.t. } \beta^T \beta \leq S \end{array} \right.$$

Optimal Solution  $\beta_{Rg}^*$  needs (necessary condition)  $\lambda > 0$

$$[\lambda \left( \sum_j (\beta_{Rg})_j^2 - S \right) = 0] \Rightarrow S = \sum_j (\beta_{Rg})_j^2$$

$$\text{When } X^T X = I, \quad S = \sum_j (\beta_{Rg})_j^2 = \frac{1}{(1+\lambda)^2} \sum_j (\beta_{OLS})_j^2$$

$$\lambda = \sqrt{\frac{\sum_j (\beta_{OLS})_j^2}{S}} - 1 \quad \Rightarrow S \propto \frac{1}{(1+\lambda)^2}$$

<http://stats.stackexchange.com/questions/190993/how-to-find-regression-coefficients-beta-in-ridge-regression>

# Extra: Intercept Term is usually not shrunked

- If the data is not centered, there exists bias term
  - <http://stats.stackexchange.com/questions/86991/reason-for-not-shrinking-the-bias-intercept-term-in-regression>
- We normally assume we centered x and y. If this is true, no ~~need to have bias~~ term, e.g. ~~for lasso~~

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

*just set the bias corresponding entry as 0 in the I-matrix*

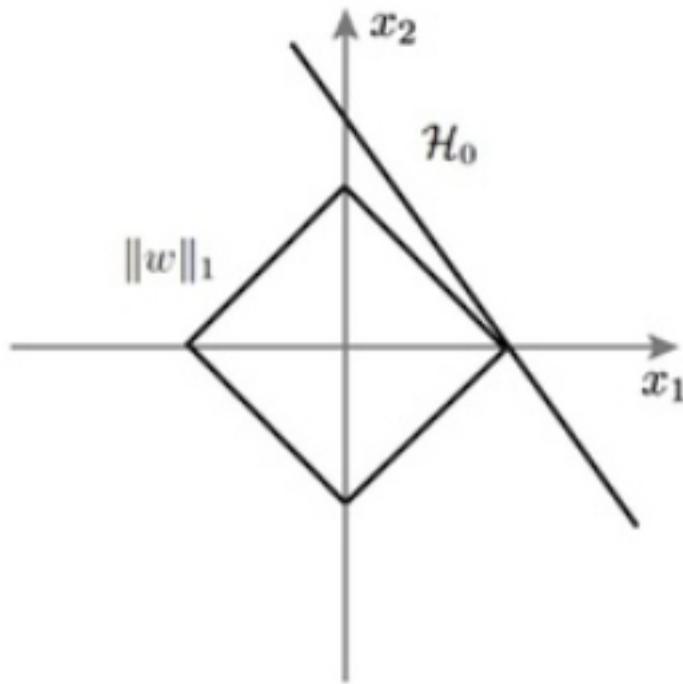
$$\hat{\beta} = \underset{\beta}{\operatorname{argmin}} \| \mathbf{y} - \mathbf{X}\beta \|^2 + \lambda_1 \|\beta\|_1$$

*for ridge  
+  $\lambda \|\beta\|^2$*

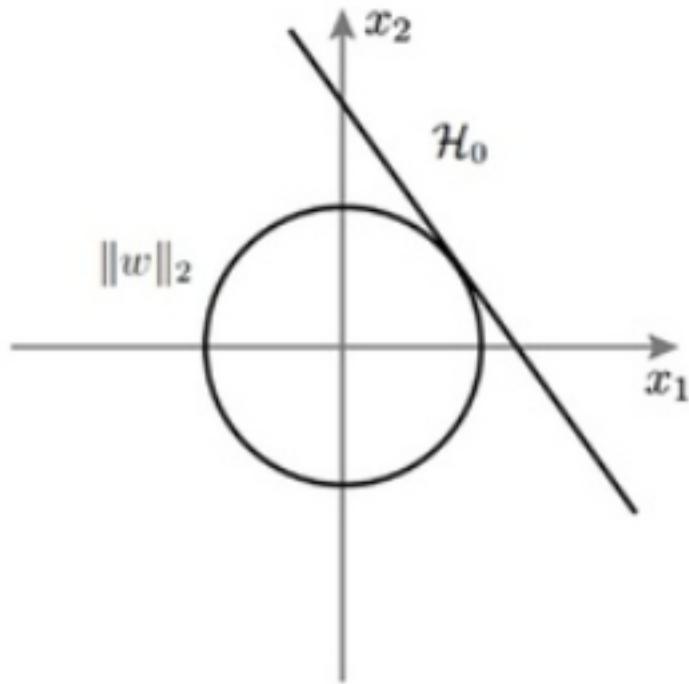
# Extra Recap

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**A** L1 regularization



**B** L2 regularization



due to the nature of L<sub>1</sub> norm, the viable solutions are limited to corners, which are on a few axis only  
- in the above case  $x_1$ . Value of  $x_2 = 0$ . This means that the solution has eliminated the role of  $x_2$ , leading to sparsity

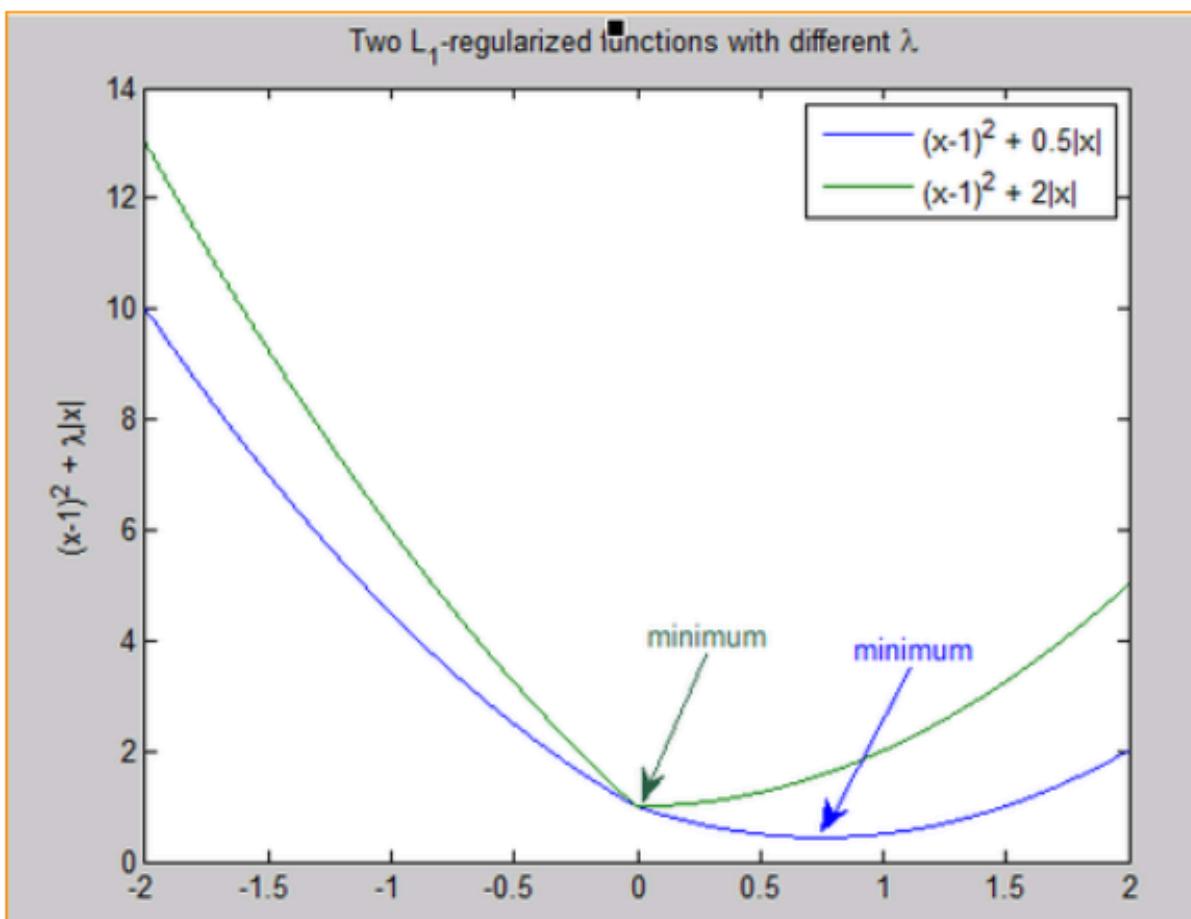
$L_2$ -regularized loss function  $F(x) = f(x) + \lambda \|x\|_2^2$  is smooth. This means that the optimum is the stationary point (o-derivative point). The stationary point of  $F$  can get very small when you increase  $\lambda$ , but still won't be o unless  $f'(0) = 0$ .

$L_1$ -regularized loss function  $F(x) = f(x) + \lambda \|x\|_1$  is non-smooth. It's not differentiable at o. Optimization theory says that the optimum of a function is either the point with o-derivative or one of the irregularities (corners, kinks, etc.). So, it's possible that the optimal point of  $F$  is o even if o isn't the stationary point of  $f$ . In fact, it would be o if  $\lambda$  is large enough (stronger regularization effect). Below is a graphical illustration.

In multi-dimensional settings: if a feature is not important, the loss contributed by it is small and hence the (non-differentiable) regularization effect would turn it off.

$L_1$ -regularized loss function  $F(x) = f(x) + \lambda\|x\|_1$  is non-smooth. It's not differentiable at 0. Optimization theory says that the optimum of a function is either the point with 0-derivative or one of the irregularities (corners, kinks, etc.). So, it's possible that the optimal point of  $F$  is 0 even if 0 isn't the stationary point of  $f$ . In fact, it would be 0 if  $\lambda$  is large enough (stronger regularization effect). Below is a graphical illustration.

<http://www.quora.com/What-is-the-difference-between-L1-and-L2-regularization>



In mathematics, particularly in calculus, a stationary point or critical point of a differentiable function of one variable is a point of the domain of the function where the derivative is zero (equivalently, the slope of the graph at that point is zero).

# How to train Parameter for Lasso

$$\hat{\beta}^{lasso} = \arg \min(y - X\beta)^T (y - X\beta)$$

$$\text{subject to } \sum |\beta_j| \leq s$$

- **$\ell_1$ -norm is non differentiable!**
  - cannot compute the gradient of the absolute value  
⇒ **Directional derivatives** (or subgradient)

Here assume x and y have been centered (normally), therefore no bias term needed in above !

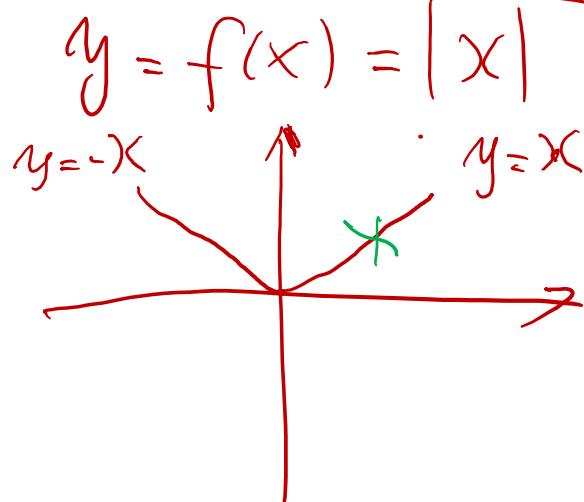
$$\begin{aligned}
 \text{RSS-Loss}(\lambda) &= (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) + \lambda \sum_{j=1}^p |\beta_j| \\
 &= \sum_{i=1}^n (y_i - \mathbf{x}_i^T \beta)^2 + \lambda \sum_{j=1}^p |\beta_j| \\
 &= \left[ \sum_{i=1}^n \underbrace{(y_i - \mathbf{x}_{ij} \beta_j - \mathbf{x}_{i\{-j\}} \beta_{-j})^2}_{(2)} \right] + \\
 &\quad \lambda \sum_{j=1}^p |\beta_j| \\
 \text{if } \beta &= (\beta_1, \beta_2, \beta_3) \\
 \Rightarrow \beta_{-2} &= (\beta_1, \beta_3) \\
 \Rightarrow \frac{\partial \ell}{\partial \beta_j} &= \sum_{i=1}^n \underbrace{2(y_i - \mathbf{x}_{ij} \beta_j - \mathbf{x}_{i\{-j\}} \beta_{-j}) (-\mathbf{x}_{ij})}_{\cdot} \\
 &\quad + \lambda \frac{\partial}{\partial \beta_j} |\beta_j|
 \end{aligned}$$

$$= \underbrace{2 \sum_{j=1}^h \gamma_{ij} \beta_j^2}_{a_j} - \underbrace{2 \sum_{j=1}^h (y_i - x_i \beta_j) \gamma_{ij}}_{c_j} + \lambda \frac{\partial}{\partial \beta_j} |\beta_j|$$

$$= a_j \beta_j - c_j + \lambda \frac{\partial}{\partial \beta_j} |\beta_j| \stackrel{\text{Set to 0}}{=} 0$$

convex  $\Rightarrow$  unique

⊕



$$\partial f(x) = \begin{cases} 1 & \text{if } x > 0 \\ -1 & \text{if } x < 0 \\ [-1, 1] & \text{if } x = 0 \end{cases}$$

$$\frac{\partial l}{\partial \beta_j} = \begin{cases} a_j \beta_j - c_j - \lambda & , \text{ if } \beta_j < 0 \\ a_j \beta_j - c_j + \lambda & , \text{ if } \beta_j > 0 \end{cases}$$

$[a_j \beta_j - c_j - \lambda, a_j \beta_j - c_j + \lambda]$ , if  $\beta_j = 0$

*Set  $\beta_0 = 0$*

$$\hat{\beta}_j = \begin{cases} \frac{c_j + \lambda}{a_j} & , \text{ if } c_j + \lambda < 0 \Rightarrow c_j < -\lambda \\ \frac{c_j - \lambda}{a_j} & , \text{ if } c_j > \lambda \\ 0 & , \text{ if } -\lambda \leq c_j \leq \lambda \end{cases}$$

*Soft thresholding*

We just need 0 in the region  $[-c_j - \lambda, -c_j + \lambda]$  (subgradient calculus)

$$\begin{aligned}
 RSS(\lambda) &= (y - x\beta)^T (y - x\beta) + \lambda \sum_{j=1}^P |\beta_j| \\
 &= \sum_{i=1}^n \left( y_i - \underbrace{x_i^T \beta}_g \right) + \lambda \sum_{j=1}^P |\beta_j| \\
 &= \left[ \sum_{i=1}^n (y_i - x_{ij}\beta_j - x_{i-j}^T \beta_j)^2 \right] + \left[ \lambda \sum_{j=1}^P |\beta_j| \right]
 \end{aligned}$$

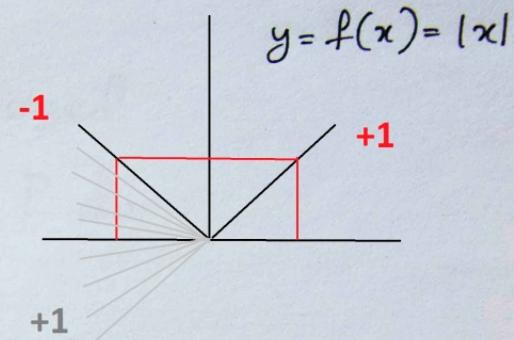
Here, if  $\beta = (\beta_1, \beta_2, \beta_3) \Rightarrow \beta_{-2} = (\beta_1, \beta_3)$

$$\begin{aligned}
 \frac{\partial}{\partial \beta_j} RSS(\lambda) &= \sum_{i=1}^n 2(y_i - x_{ij}\beta_j - x_{i-j}^T \beta_j)(-x_{ij}) \\
 &\quad + \lambda \frac{\partial}{\partial \beta_j} (|\beta_1| + |\beta_2| + \dots + |\beta_P|) \\
 &\doteq \boxed{2 \sum_{i=1}^n x_{ij}^2 \beta_j} - \boxed{2 \sum_{i=1}^n (y_i - x_{i-j}^T \beta_j) x_{ij}} \\
 &\quad + \lambda \frac{\partial}{\partial \beta_j} |\beta_j|
 \end{aligned}$$

## Sub differentials

$$f(x) = |x|$$

$$\partial f(x) = \begin{cases} \{-1\} & \text{if } x < 0 \\ \{-1, 1\} & \text{if } x = 0 \\ \{+1\} & \text{if } x > 0 \end{cases}$$



$$\begin{aligned} \frac{\partial}{\partial \beta_j} \text{RSS}(\alpha) &= \alpha_j \beta_j + c_j + \lambda \frac{\partial}{\partial \beta_j} |\beta_j| \\ &= \begin{cases} \{\alpha_j \beta_j - c_j - \lambda\} & \text{if } \beta_j < 0 \\ \{-c_j - \lambda, -c_j + \lambda\} & \text{if } \beta_j = 0 \\ \{\alpha_j \beta_j - c_j + \lambda\} & \text{if } \beta_j > 0 \end{cases} \end{aligned}$$

$$\hat{\beta}_j = \begin{cases} (c_j + \lambda)/\alpha_j & \text{if } c_j < -\lambda \\ 0 & \text{if } c_j \in [-\lambda, \lambda] \\ (c_j - \lambda)/\alpha_j & \text{if } c_j > \lambda \end{cases}$$

When,  $\beta_j < 0$   
 $\alpha_j \beta_j - c_j - \lambda = 0$   
 $\beta_j = \frac{c_j + \lambda}{\alpha_j}$   
 When,  $\beta_j > 0$   
 $\alpha_j \beta_j - c_j + \lambda = 0$   
 $\beta_j = \frac{c_j - \lambda}{\alpha_j}$

# Coordinate descent based Learning of Lasso

Coordinate descent  
(WIKI) → one does  
line search along one  
coordinate direction  
at the current point in  
each iteration.

One uses different  
coordinate directions  
cyclically throughout  
the procedure.

1. Initialize  $\beta$
2. Repeat until converged
3. For  $j = 1, 2, \dots, p$  do
$$\alpha_j = 2 \sum_{i=1}^n x_{ij}^2$$
$$c_j = 2 \sum_{i=1}^n x_{ij} (y_i - x_i^T \beta + x_{ij} \beta_j)$$

if  $c_j < -\lambda$

$$\beta_j = (c_j + \lambda) / \alpha_j$$

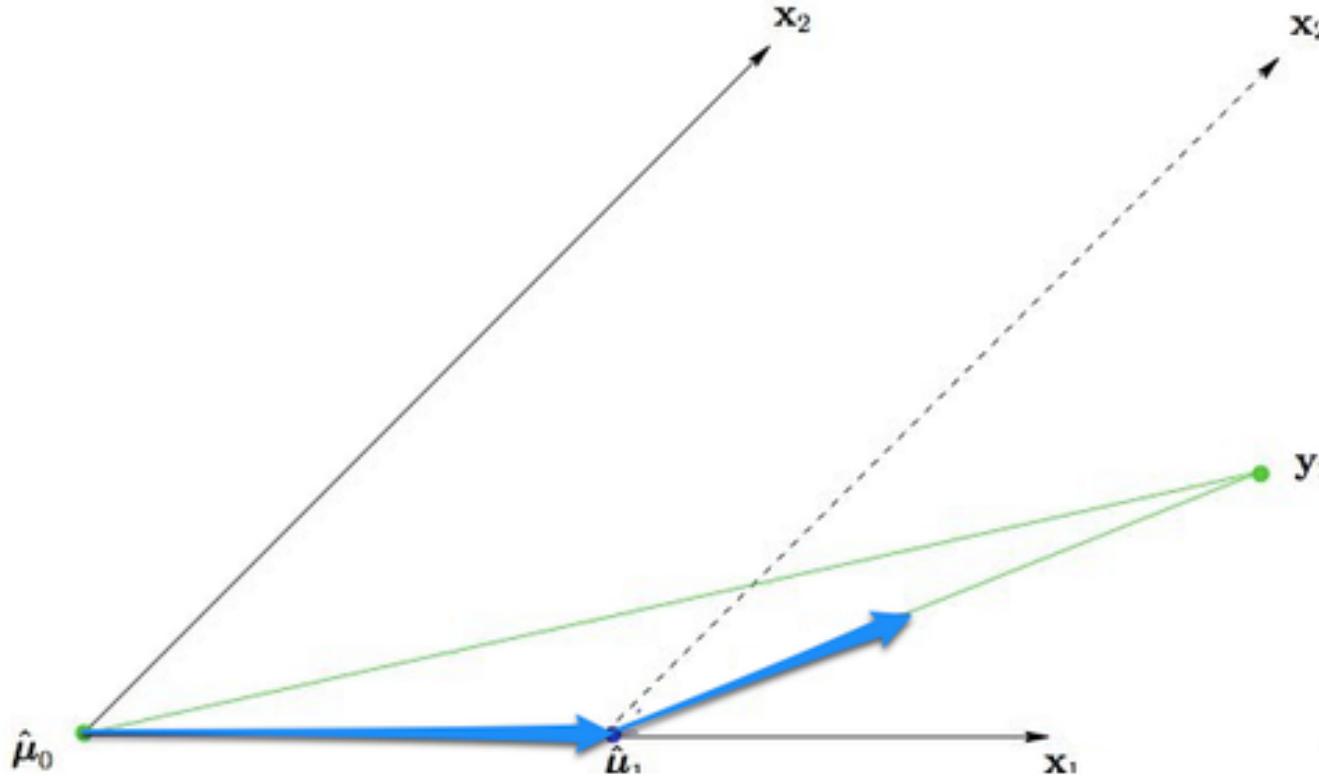
else if,  $c_j > \lambda$

$$\beta_j = (c_j - \lambda) / \alpha_j$$

else, soft-thresholding

$$\beta_j = 0$$

# Least Angle Regression (LARS) (State-of-the-art LASSO solver)



<http://statweb.stanford.edu/~tibs/ftp/lars.pdf>

# LARS: Least Angle Regression

- Starts like classic Forward Selection
  - Find predictor  $x_{j1}$  most correlated with the current residual
  - Make a step ( $\epsilon$ ) large enough until another predictor  $x_{j2}$  has as much correlation with the current residual
  - LARS – now step in the direction equiangular between two predictors until  $x_{j3}$  earns its way into the “correlated set”

Correlation:

$$c(\mu) = X'(y - \mu)$$

# Extra Recap

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# Naïve elastic net

- For any non negative fixed  $\lambda_1$  and  $\lambda_2$ , naive elastic net criterion:

$$L(\lambda_1, \lambda_2, \beta) = |\mathbf{y} - \mathbf{X}\beta|^2 + \lambda_2|\beta|^2 + \lambda_1|\beta|_1,$$

$$|\beta|^2 = \sum_{j=1}^p \beta_j^2, \quad |\beta|_1 = \sum_{j=1}^p |\beta_j|.$$

- The naive elastic net estimator is the minimizer of equation

$$\hat{\beta} = \arg \min_{\beta} \{L(\lambda_1, \lambda_2, \beta)\}.$$

- Let

$$\alpha = \lambda_2 / (\lambda_1 + \lambda_2)$$

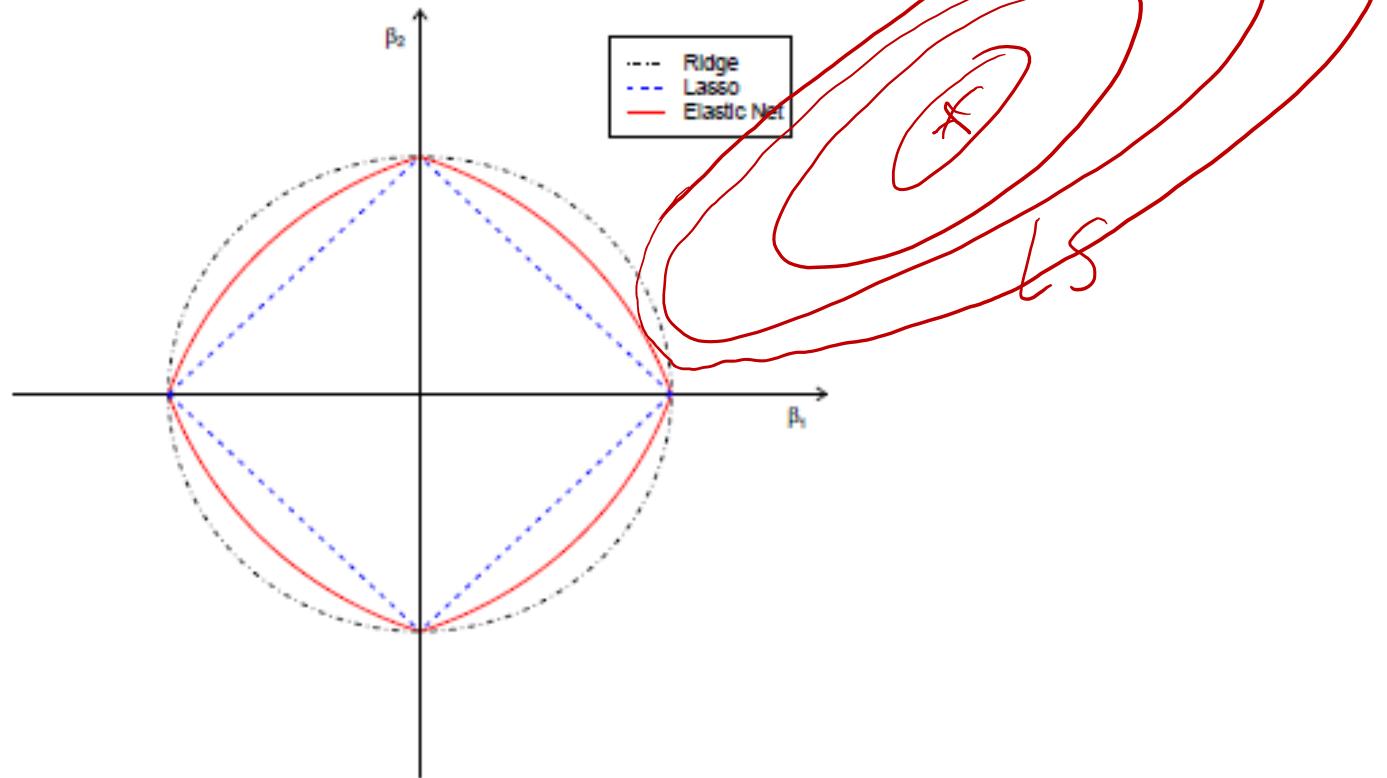
$$\frac{\lambda_2}{\lambda_1 + \lambda_2}$$

$$\hat{\beta} = \arg \min_{\beta} |\mathbf{y} - \mathbf{X}\beta|^2,$$

subject to  $(1 - \alpha)|\beta|_1 + \alpha|\beta|^2 \leq t$  for some  $t$ .

# Geometry of elastic net

2-dimensional illustration  $\alpha = 0.5$



# Connecting LASSO and Naïve Elastic net

- Lemma: Given  $\Omega \in \mathbb{R}^{n \times p}$  defines an  $(n+p) \times p$  artificial data set  $(\mathbf{x}^*, \mathbf{y}^*)$   $n \times 1$   
 $\mathbf{X}_{(n+p) \times p}^* = (1 + \lambda_2)^{-1/2} \begin{pmatrix} \mathbf{X} \\ \sqrt{\lambda_2} \mathbf{I} \end{pmatrix}$ ,  $\mathbf{y}_{(n+p)}^* = \begin{pmatrix} \mathbf{y} \\ 0 \end{pmatrix}$ .  $(n+p) \times 1$

Let  $\gamma = \lambda_1 / \sqrt{1 + \lambda_2}$  and  $\beta^* = \sqrt{1 + \lambda_2} \beta$ . Then the naïve elastic net criterion can be written as

$$L(\gamma, \beta) = L(\gamma, \beta^*) = \left[ |\mathbf{y}^* - \mathbf{X}^* \beta^*|^2 + \gamma |\beta^*|_1 \right] \Rightarrow \beta^*$$

- Let,  $\hat{\beta}^* = \arg \min_{\beta^*} L\{(\gamma, \beta^*)\}$ ;

$$\cancel{\sum} \beta = \vec{y}$$

- Then

elastic  $\hat{\beta} = \frac{1}{\sqrt{1 + \lambda_2}} \hat{\beta}^*$ .  $\cancel{\sum} \beta = \vec{y}$

LASSO augmented

$\hat{\beta} = \frac{1}{\sqrt{1 + \lambda_2}} \hat{\beta}^*$   $n \times p$   $p \times 1$   $(n+p) \times p$

$\vec{y}$   $n \times 1$   $(n+p) \times 1$

$$\text{Loss} = \left| y^* - \mathbb{E}^* \beta^* \right|^2 + r |\beta^*|_1$$

$$= \left| \begin{bmatrix} Y \\ 0 \end{bmatrix} - \begin{pmatrix} \mathbb{E} \\ \sqrt{\lambda_2} I \end{pmatrix} \beta^* \right|^2 + r |\beta^*|_1$$

$(n+p) \times p$

$$= \left| \begin{pmatrix} Y - \mathbb{E} \beta^* \\ -\sqrt{\lambda_2} \beta^* \end{pmatrix} \right|^2 + r |\beta^*|_1$$

$$= (Y - \mathbb{E} \beta)^2 + \lambda_2 \beta^* + r |\beta|_1$$

$$= (Y - \mathbb{E} \beta^*)^2 + \lambda_2 (1/\epsilon) \beta^2 + \frac{\lambda_1}{\sqrt{1+\lambda_2}} \left| \frac{\sqrt{1+\lambda_2}}{\lambda_2} \beta \right|_1$$

# Advantage of Elastic net

$P \gg h$

- Native Elastic set can be converted to lasso with augmented data

$\Rightarrow X_{n \times p} \quad (\text{when } n < p)$

- In the augmented formulation,
  - sample size  $n+p$  and  $X^*$  has rank  $p$
  - $\rightarrow$  can potentially select all the predictors
- Naïve elastic net can perform automatic variable selection like lasso

## Grouping Effect

Qualitatively speaking, a regression method exhibits the grouping effect if the regression coefficients of a group of highly correlated variables tend to be equal (up to a change of sign if negatively correlated). In particular, in the extreme situation where some variables are exactly identical, the regression method should assign identical coefficients to the identical variables.

If there is a group of variables among which the pairwise correlations are very high, then the lasso tends to select only one variable from the group and does not care which one is selected.

uations. We illustrate our points by considering the gene selection problem in microarray data analysis. A typical microarray data set has many thousands of predictors (genes) and often fewer than 100 samples. For those genes sharing the same biological ‘pathway’, the correlations between them can be high (Segal and Conklin, 2003). We think of those genes as forming a group. The ideal gene selection method should be able to do two things: eliminate the trivial genes and automatically include whole groups into the model once one gene among them is selected (‘grouped selection’). For this kind of  $p \gg n$  and grouped variables situation, the lasso is not the ideal method, because it can only select at most  $n$  variables out of  $p$  candidates (Efron *et al.*, 2004), and it lacks the ability to reveal the grouping information. As for prediction per-

# Grouping Effect of Naive Elastic net

- Consider the following equation where  $J(\cdot)$  positive for  $\beta \neq 0$ .
$$\hat{\beta} = \arg \min_{\beta} |\mathbf{y} - \mathbf{X}\beta|^2 + \lambda J(\beta)$$

*Lemma 2.* Assume that  $\mathbf{x}_i = \mathbf{x}_j$ ,  $i, j \in \{1, \dots, p\}$ .

- If  $J(\cdot)$  is strictly convex, then  $\hat{\beta}_i = \hat{\beta}_j$ ,  $\forall \lambda > 0$ .
- If  $J(\beta) = |\beta|_1$ , then  $\hat{\beta}_i \hat{\beta}_j \geq 0$  and  $\hat{\beta}^*$  is another minimizer of equation (7), where

$$\hat{\beta}_k^* = \begin{cases} \hat{\beta}_k & \text{if } k \neq i \text{ and } k \neq j, \\ (\hat{\beta}_i + \hat{\beta}_j) \cdot (s) & \text{if } k = i, \\ (\hat{\beta}_i + \hat{\beta}_j) \cdot (1 - s) & \text{if } k = j, \end{cases}$$

for any  $s \in [0, 1]$ .

Lemma 2 shows a clear distinction between *strictly convex* penalty functions and the lasso penalty. Strict convexity guarantees the grouping effect in the extreme situation with identical predictors. In contrast the lasso does not even have a unique solution. The elastic net penalty with  $\lambda_2 > 0$  is strictly convex, thus enjoying the property in assertion (1).

# Grouping Effect of Naive Elastic net

- Consider the follow for  $\beta \neq 0$ .

$$\hat{\beta} = \arg \min_{\beta} |\mathbf{y} - \mathbf{X}\beta|^2 + \lambda P(\beta) \quad \text{Where } J(\cdot) \text{ positive}$$

$P(\beta)$  data error Penalty

*elastic* Lemma 2. Assume that  $\mathbf{x}_i = \mathbf{x}_j, i, j \in \{1, \dots, p\}$ .

- (a) If  $P(\cdot)$  is strictly convex, then  $\hat{\beta}_i = \hat{\beta}_j, \forall \lambda > 0$ .
- (b) If  $P(\beta) = |\beta|_1$ , then  $\beta_i \hat{\beta}_j \geq 0$  and  $\hat{\beta}^*$  is another minimizer of equation (7), where

$$\hat{\beta}_k^* = \begin{cases} \hat{\beta}_k & \text{if } k \neq i \text{ and } k \neq j, \\ (\hat{\beta}_i + \hat{\beta}_j) \cdot (s) & \text{if } k = i, \\ (\hat{\beta}_i + \hat{\beta}_j) \cdot (1 - s) & \text{if } k = j, \end{cases}$$

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Lasso does not give a unique solution.

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# Grouping Effect of Naïve Elastic

## net

*Theorem 1.* Given data  $(\mathbf{y}, \mathbf{X})$  and parameters  $(\lambda_1, \lambda_2)$ , the response  $\mathbf{y}$  is centred and the predictors  $\mathbf{X}$  are standardized. Let  $\hat{\beta}(\lambda_1, \lambda_2)$  be the naïve elastic net estimate. Suppose that  $\hat{\beta}_i(\lambda_1, \lambda_2) \hat{\beta}_j(\lambda_1, \lambda_2) > 0$ . Define

$$D_{\lambda_1, \lambda_2}(i, j) = \frac{1}{|\mathbf{y}|_1} |\hat{\beta}_i(\lambda_1, \lambda_2) - \hat{\beta}_j(\lambda_1, \lambda_2)|;$$

then

$$D_{\lambda_1, \lambda_2}(i, j) \leq \frac{1}{\lambda_2} \sqrt{2(1 - \rho)},$$

where  $\rho = \mathbf{x}_i^T \mathbf{x}_j$ , the sample correlation.

□

- D is the difference between the coefficient paths of predictors i and j.
- If  $x_i$  and  $x_j$  are highly correlated ( $\rho=1$ ), this theorem provides a quantitative description for the grouping effect of Naive Elastic Net.

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then

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where  $\rho = \mathbf{x}_i^T \mathbf{x}_j$ , the sample correlation.

①

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- If  $x_i$  and  $x_j$  are highly correlated  $\rho=1$ , this theorem provides a quantitative description for the grouping effect of Naive Elastic Net.

$x_i \quad x_j$

# Elastic Net

In the regression prediction setting, an accurate penalization method achieves good prediction performance through the bias–variance trade-off. The naïve elastic net estimator is a two-stage procedure: for each fixed  $\lambda_2$  we first find the ridge regression coefficients, and then we do the lasso-type shrinkage along the lasso coefficient solution paths. It appears to incur a double amount of shrinkage. Double shrinkage does not help to reduce the variances much and introduces unnecessary extra bias, compared with pure lasso or ridge shrinkage. In the next section we improve the prediction performance of the naïve elastic net by correcting this double shrinkage.

- **Deficiency of the Naive Elastic Net:** Empirical evidence shows the Naive Elastic Net does not perform satisfactorily. The reason is that there are two shrinkage procedures (Ridge and LASSO) in it. Double shrinkage introduces unnecessary bias.
- Re-scaling of Naive Elastic Net gives better performance, yielding the Elastic Net solution:
- Reason: Undo shrinkage.

$$\hat{\beta}(\text{ENet}) = (1 + \lambda_2) \cdot \hat{\beta}(\text{Naive ENet})$$

# Elastic Net

## 3.2. The elastic net estimate

We follow the notation in Section 2.2. Given data  $(\mathbf{y}, \mathbf{X})$ , penalty parameter  $(\lambda_1, \lambda_2)$  and augmented data  $(\mathbf{y}^*, \mathbf{X}^*)$ , the naïve elastic net solves a lasso-type problem

$$\hat{\boldsymbol{\beta}}^* = \arg \min_{\boldsymbol{\beta}^*} |\mathbf{y}^* - \mathbf{X}^* \boldsymbol{\beta}^*|^2 + \frac{\lambda_1}{\sqrt{1 + \lambda_2}} |\boldsymbol{\beta}^*|_1. \quad (10)$$

The elastic net (corrected) estimates  $\hat{\boldsymbol{\beta}}$  are defined by

$$\hat{\boldsymbol{\beta}}(\text{elastic net}) = \sqrt{1 + \lambda_2} \hat{\boldsymbol{\beta}}^*. \quad (11)$$

Recall that  $\hat{\boldsymbol{\beta}}(\text{naïve elastic net}) = \{1/\sqrt{1 + \lambda_2}\} \hat{\boldsymbol{\beta}}^*$ ; thus

$$\hat{\boldsymbol{\beta}}(\text{elastic net}) = (1 + \lambda_2) \hat{\boldsymbol{\beta}}(\text{naïve elastic net}). \quad (12)$$

Hence the elastic net coefficient is a rescaled naïve elastic net coefficient.

Such a scaling transformation preserves the variable selection property of the naïve elastic net and is the simplest way to undo shrinkage. Hence all the good properties of the naïve elastic

# Computation of elastic net

- First solve the Naive Elastic Net problem, then rescale it.
- For fixed  $\lambda_2$ , the Naive Elastic Net problem is equivalent to a LASSO problem, with a huge data matrix if  $p \gg n$
- LASSO already has an efficient solver called LARS (Least Angle Regression).
- LARS-EN algorithm.

$$\begin{matrix} X^{*(n+p) \times p} \\ \downarrow \\ X_{n \times p} \end{matrix}$$

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# Elastic Net interpreted as a stabilized lasso

**Theorem 2.** Given data  $(\mathbf{y}, \mathbf{X})$  and  $(\lambda_1, \lambda_2)$ , then the elastic net estimates  $\hat{\boldsymbol{\beta}}$  are given by

$$\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta}} \boldsymbol{\beta}^T \left( \frac{\mathbf{X}^T \mathbf{X} + \lambda_2 \mathbf{I}}{1 + \lambda_2} \right) \boldsymbol{\beta} - 2\mathbf{y}^T \mathbf{X} \boldsymbol{\beta} + \lambda_1 |\boldsymbol{\beta}|_1. \quad (14)$$

It is easy to see that

$$\hat{\boldsymbol{\beta}}(\text{lasso}) = \arg \min_{\boldsymbol{\beta}} \boldsymbol{\beta}^T (\mathbf{X}^T \mathbf{X}) \boldsymbol{\beta} - 2\mathbf{y}^T \mathbf{X} \boldsymbol{\beta} + \lambda_1 |\boldsymbol{\beta}|_1. \quad (15)$$

Hence theorem 2 interprets the elastic net as a stabilized version of the lasso. Note that  $\hat{\Sigma} = \mathbf{X}^T \mathbf{X}$  is a sample version of the correlation matrix  $\Sigma$  and

$$\frac{\mathbf{X}^T \mathbf{X} + \lambda_2 \mathbf{I}}{1 + \lambda_2} = (1 - \gamma) \hat{\Sigma} + \gamma \mathbf{I}$$

with  $\gamma = \lambda_2 / (1 + \lambda_2)$  shrinks  $\hat{\Sigma}$  towards the identity matrix. Together equations (14) and (15) say that rescaling after the elastic net penalization is mathematically equivalent to replacing  $\hat{\Sigma}$  with its shrunken version in the lasso. In linear discriminant analysis, the prediction accuracy can often be improved by replacing  $\hat{\Sigma}$  by a shrunken estimate (Friedman, 1989; Hastie *et al.*, 2001). Likewise we improve the lasso by regularizing  $\hat{\Sigma}$  in equation (15).

# Extra Recap

- ❑ More about LR Model with Regularizations
  - ❑ Ridge Regression
  - ❑ Lasso Regression
    - ❑ Extra: how to perform training
  - ❑ Elastic net
    - ❑ Extra: how to perform training

# References

- Big thanks to Prof. Eric Xing @ CMU for allowing me to reuse some of his slides
- Prof. Nando de Freitas's tutorial slide
- **Regularization and variable selection via the elastic net**, Hui Zou and Trevor Hastie, *Stanford University, USA*