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Topic 11: Lasso And Beyond: Convex Learning

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Key points:

Disclaimer:

11.1 Lasso

Lasso (Least absolute Shrinkage and Selection Operator), proposed by Tibshirani (1996), aims to minimize the **SSR *(sum of residual squares)*** subject to the $L1-$**norm *(sum of the absolute value)*** of the coefficients being less than a constant.

11.1.1 Set up

For data $(\mathbf{x}_i, y_i)_{i=1}^n$, where

- y_i is the outcome for individual i
- $\mathbf{x}_i = (x_{i1}, \cdots, x_{ip})'$ is the $p \times 1$ vector of predictors

Then the Lasso estimator $\left(\hat{\alpha}, \hat{\boldsymbol{\beta}}\right)$ is defined as

$$\left(\hat{\alpha}, \hat{\boldsymbol{\beta}}\right) = \arg\min_{\alpha, \boldsymbol{\beta}} \left\{ \sum_{i=1}^{n} \left(y_i - \alpha - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \right\} \qquad \text{s.t. } \sum_{j=1}^{p} |\beta_j| \leq t$$

for the $n \times 1$ response vector $\mathbf{y} = (y_1, \cdots, y_n)'$, the $n \times p$ design matrix $\mathbf{X} = (\mathbf{x}_1, \cdots, \mathbf{x}_n)'$ where $\mathbf{x}_i = (x_{i1}, \cdots, x_{ip})'$ is a $p \times 1$ vector. Here $\hat{\alpha} = \overline{y}$, w.l.o.g., let $\overline{y} = 0$ and omit α for simplicity.

In matrix form, we have

- constrained form:

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta} \in \mathbb{R}^p} \left\{ \frac{1}{2n} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 \right\} \qquad \text{s.t. } \|\boldsymbol{\beta}\|_1 \leq t$$

- unconstrained form:

$$\hat{\boldsymbol{\beta}}(\lambda) = \arg\min_{\boldsymbol{\beta} \in \mathbb{R}^p} \left\{ \frac{1}{2n} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \lambda \|\boldsymbol{\beta}\|_1 \right\}$$

where the regularization parameter $\lambda \geq 0$:

- $\lambda \to \infty$: $\hat{\boldsymbol{\beta}}_{lasso} = \mathbf{0}$
- $\lambda = 0$: $\hat{\boldsymbol{\beta}}_{lasso} \to \hat{\boldsymbol{\beta}}_{OLS}$

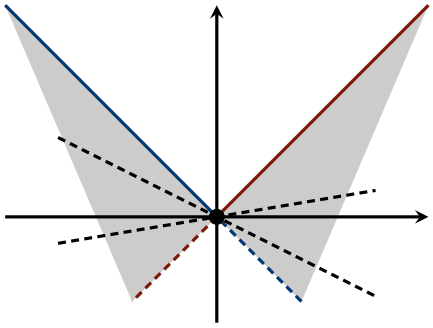
11.1.2 Solving Lasso

Lasso is essentially a quadratic optimization problem. Hence, the solution is given by taking the derivative (of the unconstrainted question) and set it equal to 0

$$\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\beta}}\left(\frac{1}{2n}\|\mathbf{y}-\mathbf{X}\boldsymbol{\beta}\|_2^2+\lambda\|\boldsymbol{\beta}\|_1\right)=0$$

$$\xrightarrow{\text{KKT condition}} \quad \frac{1}{n}\underbrace{\mathbf{X}'}_{p\times n}\underbrace{(\mathbf{y}-\mathbf{X}\boldsymbol{\beta})}_{=\boldsymbol{\epsilon},n\times 1}=\lambda\begin{cases}\text{sign}\left(\beta_j\right), & \beta_j\neq 0\\ [-1,1], & \beta_j=0\end{cases}$$

this result follows the fact the L-1 norm $\|\boldsymbol{\beta}\|$ is piecewise linear (convex)[1]:



L1-norm (1-dimension)

For each component of the vector of the L-1 norm $f(\beta_j)=|\beta_j|$, we have:
- $\beta_j>0$: $f'(\beta_j)=1$
- $\beta_j<0$: $f'(\beta_j)=-1$
- $\beta_j=0$: $\mathrm{d}f\in[-1,1]$ (shaded area)

which gives the results stated above.

Take another look at this result

Proposition 11.1.1: Lasso Parameter Selection Rule

$$\frac{1}{n}\mathbf{X}'\left(\mathbf{y}-\mathbf{X}\boldsymbol{\beta}\right)=\frac{1}{n}\mathbf{X}'\boldsymbol{\epsilon}=\lambda\begin{cases}\text{sign}\left(\beta_j\right), & \beta_j\neq 0\\ [-1,1], & \beta_j=0\end{cases}$$

which gives a parameter selection criterion: for $\beta_j\neq 0$, $\text{sign}(\beta_j)$ **must agree** with $\text{Corr}(\mathbf{x}_j,\boldsymbol{\epsilon})$, the correlation between the j-th variable $\mathbf{x}_j$ and (full-model) residuals $\boldsymbol{\epsilon}=\mathbf{y}-\mathbf{X}\boldsymbol{\beta}$.

11.1.3 Algorithm: LARS

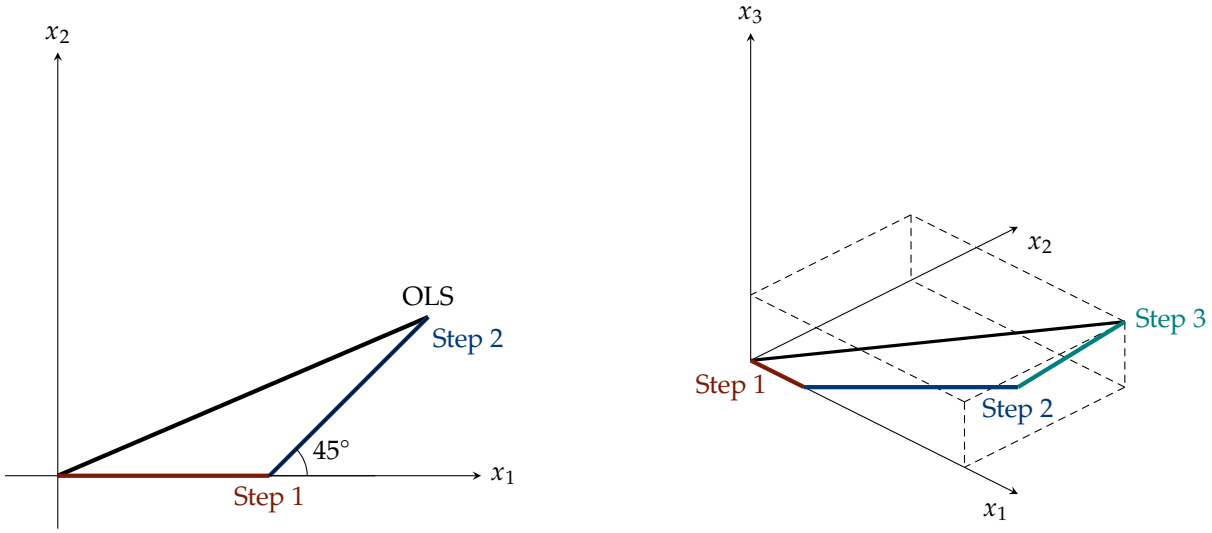
Mathematically, Lasso is quite intuitive, but computationally, it can be quite consuming. Efron et al. (2004) propose an algorithm that takes steps from a all-0 model to the biggest model (OLS), that is, **Least Angle Regression (LARS)**.

Intuition

The basic intuition of LARS is quite straight-forward: covariates are considered from the ***highest*** corerlation with $\mathbf{y}$ (*smallest* angle from $\mathbf{y}$) to the ***least*** correlated one (*largest* angle from $\mathbf{y}$) (illustrated below).

And the steps of the LARS algorithm are

[1] KKT condition gives the analytical optimization rule for **convex** function.



1 start with the null model $\hat{\boldsymbol{\beta}} = \mathbf{0}$: $\hat{\boldsymbol{\mu}} = \mathbf{X}'\mathbf{0} = \mathbf{0}$
2 calculate residual vector $\mathbf{r} = \mathbf{y} - \hat{\boldsymbol{\mu}}$
3 determine the correlation vector between $\mathbf{r}$ and each parameter $\mathbf{x}_j, \forall j = 1, \cdots, p$: $\mathbf{X}'\mathbf{r}$
4 pick the largest correlation $\mathbf{x}^*_{\text{step1,1}}$, increase its $\hat{\beta}$ to the point where its correlation with $\mathbf{r}$ will be **equal** with that of another parameter $\mathbf{x}^*_{\text{step1,2}}$
5 next, increase the $\hat{\beta}$ for both $\mathbf{x}^*_{\text{step1,1}}, \mathbf{x}^*_{\text{step1,2}}$ in an **equiangular** direction between these two, until a third parameter becomes equally important

And keep looping this way, until all the predictors enter the model and eventually $\mathbf{X}'\mathbf{r} = \mathbf{0}$

Properties of LARS

LARS has several properties:

- geometrically travels in the direction of **equal** angle to all active covariates
- assume all covariates are independent
- computationally quick: only take m steps, where m is the number of parameters being considered

And it is in between 2 classic model-selection methods: **Forward Selection** and **Stagewise Selection**:

- **Forward Selection**
  - for $\mathbf{y}$, select the most correlated $\mathbf{x}_{j_1}$
  - regress $\mathbf{x}_{j_1}$ on $\mathbf{y}$, get the residuals
  - select the most correlated $\mathbf{x}_{j_2}$ with the redisual of $\mathbf{y}$ net of $\mathbf{x}_{j_1}$

  looping this, for a $k-$parameter linear model, it takes k steps. Forward Selection is an aggressive fitting technique, can be overly greedy (some important predictors may be eliminated due to correlation with already selected variables).
- **Forward Stagewise**
  - also begin with $\hat{\boldsymbol{\mu}} = 0$
  - for a current Stagewise estimate $\hat{\boldsymbol{\mu}}$, the current residual vector is then $\mathbf{y} - \hat{\boldsymbol{\mu}}$, its correlation with $\mathbf{X}$ is then $\mathbf{X}'(\mathbf{y} - \hat{\boldsymbol{\mu}}) \equiv \hat{\mathbf{c}}$

– next, heavily computational, go in the direction of the greatest current correlation, but by only a **small** step

$$\hat{j} = \arg\max|\hat{c}_j|,\ \hat{\boldsymbol{\mu}} \to \hat{\boldsymbol{\mu}} + \epsilon \cdot \text{sign}(\hat{c}_{\hat{j}}) \cdot \mathbf{x}_{\hat{j}}$$

here, ϵ is a **small** constant, hence avoiding the greediness of Forward Selection, at a cost of computational efficiency[2].

LARS avoids the over-greediness of Forward Selection and computational heaviness of Forward Stagewise.

11.1.4 From LARS to Lasso

The Lasso algorithm is built upon LARS, with the constraint from the mathematical condition of Proposition 11.1.1: $\text{sign}(\beta_j)$ **must agree** with $\text{Corr}(\mathbf{x}_j, \boldsymbol{\epsilon})$.

Theorem 11.1.2: Lasso Modification Condition

If $\tilde{\gamma} < \hat{\gamma}$, stop the onging LARS step at $\gamma = \tilde{\gamma}$ and remove j from the calculation of the next equiangular direction, where

- the path at any LARS step is

$$\boldsymbol{\beta}(\gamma),\ \beta_j(\gamma) = \hat{\beta}_j + \gamma \hat{d}_j$$

  $\hat{d}_j$ specifies the **direction** to take the j-th component, γ is **how far** to travel in the direction of $\hat{d}_j$ before adding in a new covariate
- $\hat{\gamma}$ represents the smallest **positive** value of γ s.t. some new covariate joins the active set (the set of covariates used on path)
- $\tilde{\gamma}$ represents the first time $\beta_j(\gamma)$ **changes signs**.

The key point of 11.1.2 is that Lasso does **NOT** allow the $\hat{\beta}_j$ to change signs, if it changes sign, it will be substracted from the active set. Now, from this point of view, we can compare the 3 algorithms:

LARS	no sign restrictions
Lasso	$\hat{\beta}_j$ agrees in sign with $\hat{c}_j$
Stagewise	successive differences of $\hat{\beta}_j$ agree in sign with the current correlation $\hat{c} = \mathbf{x}_j'(\mathbf{y} - \hat{\boldsymbol{\mu}})$

Again, LARS requires the least steps but is most greedy, Stagewise is computationally consuming but robust. Lasso is in between.

11.2 Consistency of Lasso

Next, we want to establish the consistency of Lasso, by showing that Lasso selects exactly the relevant covariates asymptotically. We do this in 2 steps:

- show that Lasso at least captures all the relevant covariates
- asymptotically, under some conditions, Lasso selects exactly all the relevant covariates, not more

[2]Forward Selection is essentially choosing $\epsilon = |\hat{c}_{\hat{j}}|$

11.2.1 Overestimation

First, Lasso tends to select a superset of the relevant covariates.

Define the true relevant set Lasso selection estimation $\hat{S}_0$ aim to select as

$$S_0 = \left\{ j : \beta_j^0 \neq 0, j \neq 1, \cdots, p \right\}$$

and for some $C > 0$, define the relevant set w.r.t. C as

$$S_0^{\text{relevant}(C)} = \left\{ j : |\beta_j^0| \geq C, j = 1, \cdots, p \right\}$$

then we have

Theorem 11.2.1: Lasso Overestimation Condition

$\forall 0 < C < \infty$

$$\mathbb{P}\left[\hat{S}_0(\lambda) \supset S_0^{\text{relevant}(C)} \right] \xrightarrow{n \to \infty} 1$$

Consistency

The consistency of Lasso is established by Meinshausen and Bühlmann (2006) as

Theorem 11.2.2: Consistency of Lasso

For a suitable $\lambda = \lambda_n \gg \sqrt{s_0 \log(p)/n}$, Lasso is consistent, i.e.

$$\mathbb{P}\left[\hat{S}(\lambda) = S_0 \right] \xrightarrow{n \to \infty} 1$$

if and only if it satisfies the 2 properties:

- $\beta-$min condition (unselected coefficients non-trivial): $\inf_{j \in S_0^c} |\beta_j^0| \gg \sqrt{s_0 \log(p)/n}$
- **irrepresentable** condition: **X** should **NOT** exhibit too strong a degree of linear dependence w.r.t. the selected covariates

discussion on the irrepresentable condition denote $\hat{\Sigma} = n^{-1}\mathbf{X}\mathbf{X}'$, and let the active set $S_0 = \left\{ j : \beta_j^0 \neq 0 \right\} = \{1, \cdots, s_0\}$ consists of the first s_0 variables, let

$$\hat{\Sigma} = \begin{pmatrix} \hat{\Sigma}_{1,1} & \hat{\Sigma}_{1,2} \\ \hat{\Sigma}_{2,1} & \hat{\Sigma}_{2,2} \end{pmatrix}$$

where $\hat{\Sigma}_{1,1}$ is a $s_0 \times s_0$ var-cov matrix of the active variables, $\hat{\Sigma}_{2,2}$ is a $(p - s_0) \times (p - s_0)$ cov-var matrix of the other variables

11.2.2 Oracle

Next, we want show Lasso has the oracle procedure, which gives the consistency.

Definition 11.2.3: Oracle Property

For a fitting procedure δ, and the estimation $\hat{\beta}(\delta)$, then if δ is an oracle procedure if $\hat{\beta}(\delta)$ asymptotically has the following properties

- **consistency** (identifying right subset model): $\left\{j : \hat{\beta}_j \neq 0\right\} = S_0$
- **optimal estimation rate** (asymptotically normal): $\sqrt{n}\left(\beta(\delta)_{S_0} - \beta^0_{S_0}\right) \xrightarrow{d} \mathcal{N}(0, \Sigma_0)$, where Σ_0 is the *true* subset covariance matrix

11.3 Variants of Lasso

11.3.1 Other Variants

There are also some other useful variants of Lasso

- **Positive Lasso**: Constrains the $\hat{\beta}_j$ to enter the prediction equation in their **defined** directions, non-negative here

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}\in\mathbb{R}^p}\left\{\frac{1}{2n}\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2\right\} \qquad \text{s.t. } \|\boldsymbol{\beta}\|_1 \leq t \text{ and } \beta_j > 0, \forall j$$

- **LARS-OLS hybrid**: Use the covariates selected by LARS, but use $\hat{\boldsymbol{\beta}}$ from the OLS model
- **Main effects first**:
  - Step 1: run LARS for a model, considering **only** main effects
  - Step 2: run LARS again, with the chosen main effects, and **all possible interactions** between them
- **Backward Lasso**: start from the **full** OLS model, and eliminate covariates **backwards** (by the order of correlation going 0 the earliest)

11.4 Penalized Least Square Estimation

Lasso is one special class of Penalized Least Square (PLS) Estimation. For the linear regression model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$, if $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^2\mathbf{I}_n)$, we have PLS as

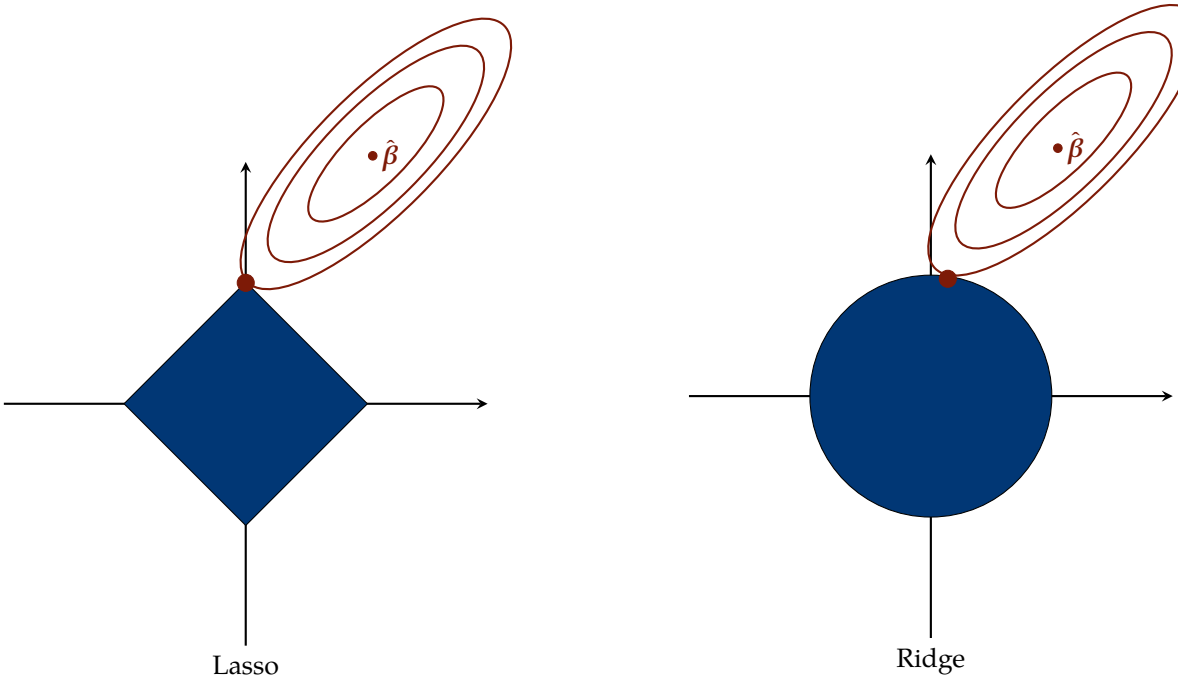
$$\min_{\boldsymbol{\beta}\in\mathbb{R}^p}\left\{\frac{1}{2n}\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \sum_{j=1}^{p} p_\lambda\left(|\beta_j|\right)\right\}$$

where $p_\lambda(\cdot)$ is a penalty function indexed by the regularization parameter $\lambda \geq 0$. Antoniadis and Fan (2001) showed that the PLS estimator $\hat{\boldsymbol{\beta}}$ has the following properties:

- **sparsity**: if $\min_{t\geq 0}\left\{t + p'_\lambda(t)\right\} > 0$
- **approximate unbiasedness**: if $p'_\lambda(t) = 0$ for t large enough
- **continuity**: iff $\arg\min_{t\geq 0}\left\{t + p'_\lambda(t)\right\} = 0$

In general

- the **sigularity** of penalty function at the origin, $p'_\lambda(0_+) > 0$ is needed for generating **sparsity** in variable selection
- the **concavity** is needed to reduce the bias



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