

The Geometry of Model Recovery by Penalized and Thresholded Estimators

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Uniqueness

Consider the optimization problem

$$S_{X, \lambda \text{pen}}(y) := \underset{b \in \mathbb{R}^p}{\text{Argmin}} \frac{1}{2} \|y - Xb\|_2^2 + \lambda \text{pen}(b).$$

Where $X \in \mathbb{R}^{n \times p}$, $y \in \mathbb{R}^n$, $\lambda > 0$ and

$\text{pen}(b) = \max\{u_0' b, u_1' b, \dots, u_l' b\}$, $u_0 = 0$ and $u_1, \dots, u_l \in \mathbb{R}^p$, is a polyhedral gauge.

Note: $S_{X, \lambda \text{pen}}(y) \neq \emptyset$.

- ▶ $\text{pen}(b) = \|b\|_1 \rightarrow$ LASSO.
- ▶ $\text{pen}(b) = \|b\|_\infty$.
- ▶ $\text{pen}(b) = \sum_{i=1}^p \lambda_i |b|_{\downarrow i}$ where $\lambda_1 > 0$, $\lambda_1 \geq \dots \geq \lambda_p \geq 0$ and $|b|_{\downarrow 1} \geq \dots \geq |b|_{\downarrow p} \rightarrow$ SLOPE.
- ▶ $\text{pen}(b) = \|Db\|_1$ for some $D \in \mathbb{R}^{m \times p} \rightarrow$ Generalized LASSO.

Theorem

Let $X \in \mathbb{R}^{n \times p}$, $\lambda > 0$ and pen be a polyhedral gauge where $\text{pen}(b) = \max\{u'_0 b, u'_1 b, \dots, u'_l b\}$. There exists $y \in \mathbb{R}^n$ for which the minimizer of

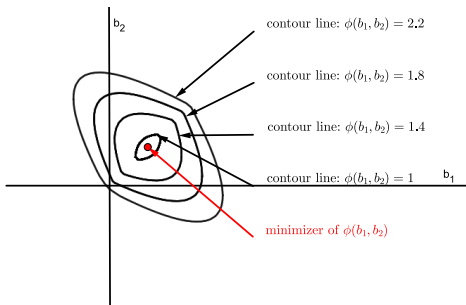
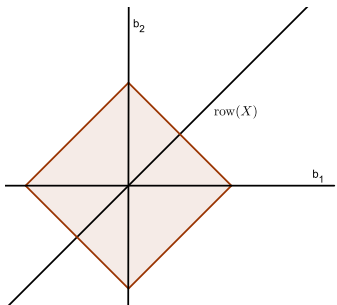
$$\underset{b \in \mathbb{R}^p}{\text{Argmin}} \frac{1}{2} \|y - Xb\|_2^2 + \lambda \text{pen}(b)$$

is not unique if and only if $\text{row}(X) := \{X'z : z \in \mathbb{R}^n\}$ intersects a face $B^* = \text{conv}\{u_0, u_1, \dots, u_l\}$ whose dimension is $< \dim(\ker(X))$.

- ▶ $\text{pen}(b) = \|b\|_1 \rightarrow B^* = [-1, 1]^p$.
- ▶ $\text{pen}(b) = \|b\|_\infty \rightarrow B^* = \{x \in \mathbb{R}^p : \|x\|_1 \leq 1\}$.
- ▶ $\text{pen}(b) = \|Db\|_1$ for some $D \in \mathbb{R}^{m \times p} \rightarrow B^* = D'[-1, 1]^m$.

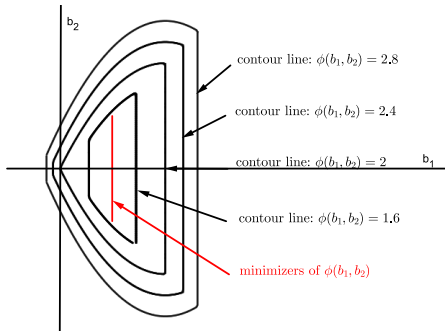
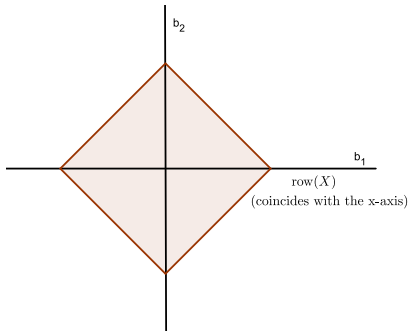
$$S_{X, \|\cdot\|_\infty}(y) := \underset{b \in \mathbb{R}^2}{\text{Argmin}} \underbrace{\frac{1}{2} \|y - Xb\|_2^2 + \max\{|b_1|, |b_2|\}}_{:= \phi(b)},$$

where $X = \begin{pmatrix} 1 & 1 \end{pmatrix}$ and $y = 2$.



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where $X = \begin{pmatrix} 1 & 0 \end{pmatrix}$ and $y = 2$.



Model pattern recovery

Consider the linear regression model $Y = X\beta + \varepsilon$ where $X \in \mathbb{R}^{n \times p}$, $\beta \in \mathbb{R}^p$ is an unknown parameter and $\varepsilon \in \mathbb{R}^n$ a random noise. Our goal is to recover $\partial_{\text{pen}}(\beta)$.

Let $f : \mathbb{R}^p \rightarrow \mathbb{R}$. $s \in \mathbb{R}^p$ is a subgradient of f at $x \in \mathbb{R}^p$ if

$$f(z) \geq f(x) + s'(z - x) \quad \forall z \in \mathbb{R}^p.$$

The subdifferential $\partial_f(x)$ at x is the set of all subgradients.

▶ $\partial_{\|\cdot\|_1}(x) = \partial_{\|\cdot\|_1}(z)$ iff $\text{sign}(x) = \text{sign}(z)$.



$$\partial_{\|\cdot\|_\infty}(x) = \partial_{\|\cdot\|_\infty}(z) \text{ iff } \begin{cases} \{i : x_i = \|x\|_\infty\} = \{i : z_i = \|z\|_\infty\} \\ \{i : x_i = -\|x\|_\infty\} = \{i : z_i = -\|z\|_\infty\} \end{cases}$$

▶ When $D^{\text{tv}}x = (x_2 - x_1, \dots, x_p - x_{p-1})$ and $\text{pen}(x) = \|D^{\text{tv}}x\|_1$

$$\partial_{\|D^{\text{tv}}\cdot\|_1}(x) = \partial_{\|D^{\text{tv}}\cdot\|_1}(z) \text{ iff } \begin{cases} \{i : x_{i+1} > x_i\} = \{i : z_{i+1} > z_i\} \\ \{i : x_{i+1} < x_i\} = \{i : z_{i+1} < z_i\} \end{cases}$$

▶ Let us assume that $\ker(D') = \{0\}$ then $\partial_{\|D\cdot\|_1}(x) = \partial_{\|D\cdot\|_1}(z)$ iff $\text{sign}(Dx) = \text{sign}(Dz)$.

Path Condition

$$S_{X, \lambda \text{pen}}(y) = \underset{b \in \mathbb{R}^p}{\text{Argmin}} \frac{1}{2} \|y - Xb\|_2^2 + \lambda \text{pen}(b).$$

Definition

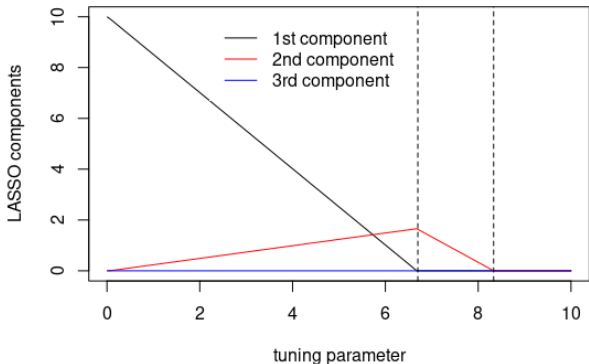
$\partial_{\text{pen}}(\beta)$ satisfies the path condition with respect to X and pen when

$$\exists \lambda > 0 \exists \hat{\beta} \in S_{X, \lambda \text{pen}}(X\beta) \text{ such that } \partial_{\text{pen}}(\hat{\beta}) = \partial_{\text{pen}}(\beta)$$

$$X = \begin{pmatrix} 5/6 & 1 & 0 \\ 1/3 & 0 & 1 \end{pmatrix}, \beta = (10, 0, 0).$$

$\text{sign}(\beta)$ does not satisfy the path condition wrt X and $\|\cdot\|_1$.

LASSO solution path



$$\|X_I' X_I (X_I' X_I)^{-1} \text{sign}(\beta_I)\|_\infty = 30/29 > 1$$

Necessary condition for model pattern recovery

Theorem

Let $Y = X\beta + \varepsilon$ where $X \in \mathbb{R}^{n \times p}$, $\beta \in \mathbb{R}^p$ is an unknown parameter and $\varepsilon \in \mathbb{R}^n$ has a symmetric distribution. If the subdifferential of β does not satisfies the path condition with respect to X and pen then

$$\mathbb{P}(\exists \lambda > 0 \exists \hat{\beta} \in \mathcal{S}_{X, \lambda \text{pen}}(Y) \text{ such that } \partial_{\text{pen}}(\hat{\beta}) = \partial_{\text{pen}}(\beta)) \leq 1/2.$$

Consequently, when $\|X_j' X_l (X_l' X_l)^{-1} \text{sign}(\beta_l)\|_\infty > 1$ then whatever $\lambda > 0$ we have

$$\mathbb{P}(\text{sign}(\hat{\beta}^{\text{lasso}}(\lambda)) = \text{sign}(\beta)) \leq 1/2.$$

Accessibility

Definition (Accessibility condition)

$\partial_{\text{pen}}(\beta)$ is accessible with respect to X and λ_{pen} when

$$\exists y \in \mathbb{R}^p \exists \hat{\beta} \in \mathcal{S}_{X, \lambda_{\text{pen}}}(y) \text{ such that } \partial_{\text{pen}}(\hat{\beta}) = \partial_{\text{pen}}(\beta)$$

Proposition

$\partial_{\text{pen}}(\beta)$ is accessible with respect to X and λ_{pen} iff for every $\gamma \in \mathbb{R}^p$ we have

$$X\beta = X\gamma \implies \text{pen}(\gamma) \geq \text{pen}(\beta).$$

Note that the accessibility condition does not depend on λ .

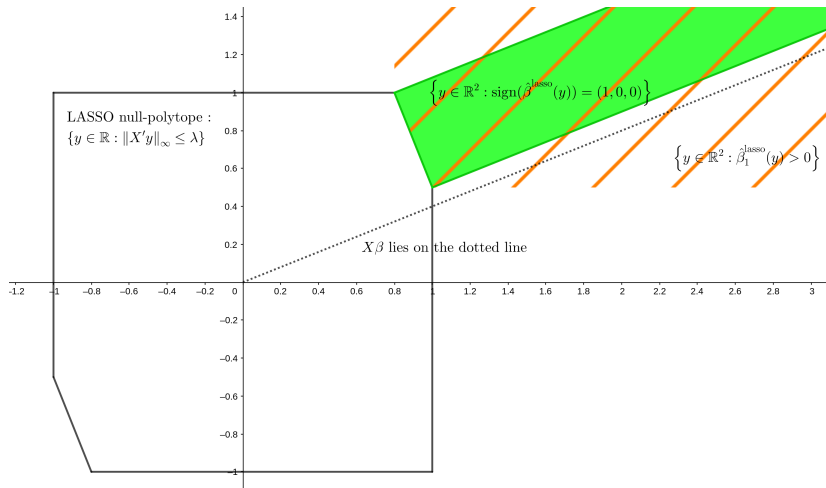
Proposition

The path condition implies the accessibility condition.

$$X = \begin{pmatrix} 5/6 & 1 & 0 \\ 1/3 & 0 & 1 \end{pmatrix}, \beta = (10, 0, 0).$$

The path condition does not occur but $\partial_{\text{pen}}(\beta)$ is accessible with respect to X and $\|\cdot\|_1$.

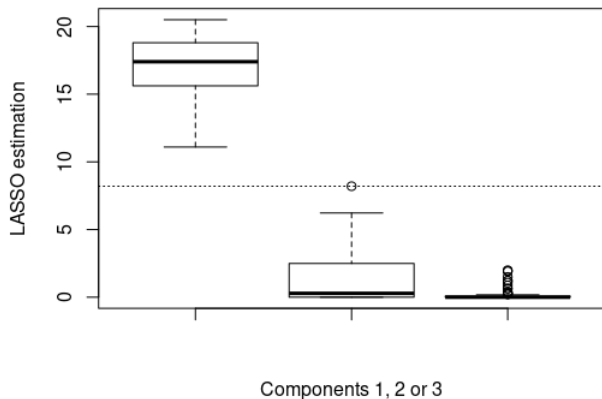
$$X = \begin{pmatrix} 5/6 & 1 & 0 \\ 1/3 & 0 & 1 \end{pmatrix}, \beta = (\beta_1, 0, 0) \text{ with } \beta_1 > 0.$$



For this figure, $\lambda = 1$.

$$X = \begin{pmatrix} 5/6 & 1 & 0 \\ 1/3 & 0 & 1 \end{pmatrix}, \beta = (20, 0, 0) \text{ et } \varepsilon \sim N(0, I)$$

Box plot for the LASSO estimator



For this figure, $\lambda = 1$.

NSC for sign recovery by generalized LASSO

- ▶ One may use the penalty $\text{pen}(b) = \|b\|_1$ in order to recover support: $\text{supp}(\beta) = \{i : \beta_i \neq 0\}$
- ▶ One may use the penalty $\text{pen}(b) = \|D^{\text{tv}} b\|_1$ in order to recover the jump set: $\{i : \beta_i \neq \beta_{i+1}\} = \text{supp}(D^{\text{tv}} \beta)$

$$D^{\text{tv}} = \begin{pmatrix} -1 & 1 & 0 & \dots & 0 \\ 0 & -1 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & -1 & 1 \end{pmatrix}.$$

- ▶ More generally base on the penalty term $\text{pen}(b) = \|Db\|_1$ we aim at recovering $\text{sign}(D\beta)$.

Let $\hat{\beta}$ be a generalized LASSO estimator. The path condition is necessary for recovering $\text{sign}(D\beta)$ via $\text{sign}(D\hat{\beta})$. One may relax the path condition using the estimator $(D\hat{\beta})^\tau$.

Theorem

Necessary condition) If $\partial_{\|D\|_1}(\beta)$ is not accessible with respect to X and $\|D\|_1$ then

$$\forall y \in \mathbb{R}^n \forall \lambda > 0 \forall \hat{\beta} \in S_{X, \lambda \|D\|_1}(y) \forall \tau \geq 0 \text{ we have} \\ \text{sign}((D\hat{\beta})^\tau) \neq \text{sign}(D\beta).$$

Sufficient condition) Given $\varepsilon \in \mathbb{R}^n$, let us set $y^k = X(k\beta) + \varepsilon$. We assume that $S_{X, \lambda \|D\|_1}(y^k)$ is a singleton and its unique element is $\hat{\beta}$. If $\partial_{\|D\|_1}(\beta)$ is accessible with respect to X and $\|D\|_1$ then

- ▶ $\exists k_0 \forall k \geq k_0 \exists \tau \geq 0$ such that $\text{sign}((D\hat{\beta})^\tau) = \text{sign}(D\beta)$
- ▶ $\exists k_0 \forall k \geq k_0$ we have $\text{supp}(D\beta) \in \{\emptyset, \{\pi(1)\}, \{\pi(1), \pi(2)\}, \dots, \text{supp}(D\hat{\beta})\}$. Where π is a permutation such that $|(D\hat{\beta})_{\pi(1)}| \geq \dots \geq |(D\hat{\beta})_{\pi(p)}|$.

PS: The article "The Geometry of Model Recovery by Penalized and Thresholded Estimators" provides a similar theorem for penalized least squares estimators (including SLOPE, OSCAR, ...).

Sign recovery by LASSO and thresholded LASSO (Tardivel and Bogdan)

To recover $\text{sign}(\beta)$ one needs the following conditions:

- ▶ **With the LASSO** one needs the irrepresentability condition (path condition in this presentation)

$$\|X_I' X_I (X_I' X_I)^{-1} \text{sign}(\beta_I)\|_\infty < 1.$$

- ▶ **With the thresholded LASSO/BP** one needs the identifiability condition (accessibility condition in this presentation)

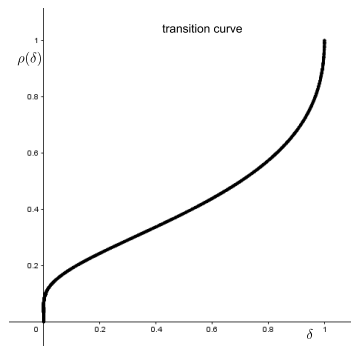
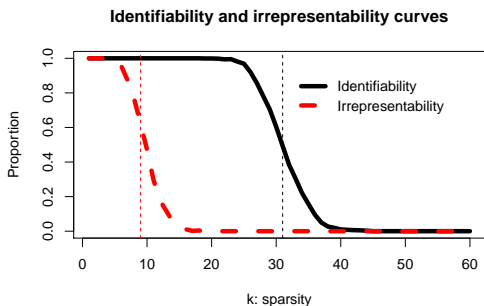
$$X\gamma = X\beta \Rightarrow \|\gamma\|_1 \geq \|\beta\|_1.$$

We remind that

$$\begin{array}{cc} \text{(Path condition)} & \text{(accessibility condition)} \\ \text{Irrepresentability condition} \Rightarrow & \text{Identifiability condition} \end{array}$$

Standard Gaussian design

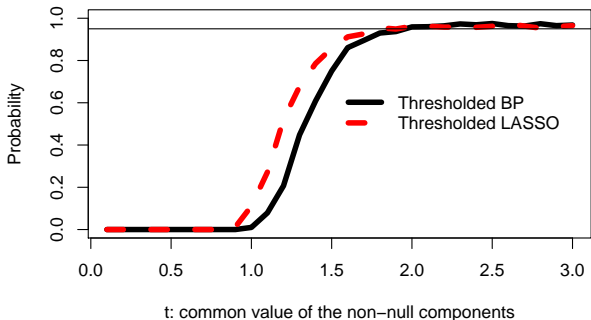
$X \in \mathbb{R}^{100 \times 300}$ standard Gaussian matrix



- ▶ black dotted line $k = \rho(100/300) \times 100 = 31$
- ▶ red dotted line $k = 100 / (2 \log(300)) = 9$

Let $Y = X\beta + \varepsilon$ where $X \in \mathbb{R}^{100 \times 300}$ is a standard Gaussian matrix, $\varepsilon \sim \mathcal{N}(0, I_n)$, $\|\beta\|_0 = 20$, non null components of β are all equal to $t > 0$.

Thresholded LASSO and BP sign estimators



Thank you!

- ▶ PJC. Tardivel, T. Skalski, P. Graczyk, U. Scheider. The Geometry of Model Recovery by Penalized and Thresholded Estimators.

Related articles

- ▶ PJC. Tardivel and M. Bogdan. On the sign recovery by LASSO, thresholded LASSO and thresholded Basis Pursuit Denoising
- ▶ U. Schneider, PJC. Tardivel. The Geometry of Uniqueness and Model Selection of Penalized Estimators including SLOPE, LASSO and Basis Pursuit.