Econometrics **March 19, 2023**

Topic 12: Non-convex Learning

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Key points: L-0 penalty is the best choice, but mostly computationally infeasible. Concave penalty (such as SCAD) works well with high dimensional problems.

Disclaimer: *The note is built on Prof. Jinchi Lv's lectures of the course at USC, DSO 607, High-Dimensional Statistics and Big Data Problems.*

12.1 L0 Penalized Likelihood

Consider the model selection problem of choosing a parameter vector $\boldsymbol{\theta}$ that maximizes the penalized likelihood

$$\mathcal{L}_n(\boldsymbol{\theta}) - \lambda\|\boldsymbol{\theta}\|_0 \tag{12.1}$$

where the L_0-norm $\|c\|_0$ denotes the **the number of nonzero components**, and $\lambda \geq 0$ is still the regularization parameter.

The L_0−penalized likelihood method is equivalent to **the best subset selection**

- given $\|\boldsymbol{\theta}_0\|_0 = m$, the solution to Problem 12.1 is the **best subset** that has the **largest** maximum likelihood among all subsets of size m
- then, choose the model size m among the p size-m best subsets ($1 \leq m \leq p$) by maximizing 12.1

hence it's a combinatorial problem, computationally complex.

L_0-Penalized Empirical Risk Minimization More generally, consider a unified approach of L_0−penalized empirical risk minimization for variable selection:

$$\min_{\boldsymbol{\theta}\in\mathbb{R}^p} \left\{\hat{R}(\boldsymbol{\theta}) + \lambda\|\boldsymbol{\theta}\|_0\right\} \tag{12.2}$$

where $\hat{R}(\boldsymbol{\theta})$ is the empirical risk function, which could be of different forms

- **negative log-likelihood loss**: equivalent t L_0-penalized likelihood
- **squared error (quadratic) loss**: L_0-penalized least squares
- selection via **RSS** (residual sum of squares): for the adjusted R^2

$$R^2_{\text{adj}} = 1 - \frac{n-1}{n-d}\frac{RSS_d}{TSS}$$

it's clear that $\max R^2_{\text{adj}} \Leftrightarrow \min \log\left(\frac{RSS_d}{n-d}\right)$, and since $\frac{RSS_d}{n} \simeq \sigma^2$, then

$$n\log\frac{RSS_d}{n-d} \simeq \frac{RSS_d}{\sigma^2} + d + n(\log\sigma^2 - 1)$$

which shows that adjusted R^2 method is approximately equivalent to 12.2 with $\lambda = 1/2$

- **generalized corss-validation** (GCV), **corss-validation** (CV)
- **risk inflation factor** (RIC): use $\lambda = \log p$, adjusting for the inflation of prediction risk caused by searching p variables[1]
- **AIC** ($\lambda = 1$), **BIC** ($\lambda = \frac{\log n}{2}$)

12.1.1 Properties of L0-Regularization Methods

risk bounds for model selection (Barron et al., 1999): for a family of models $\{S_m : m \in \mathcal{M}_p\}$, The penalty term generally takes the form of

$$\frac{\kappa L_m D_m}{n}$$

where

- κ: a positive constant
- $D_m = |S_m|$: the model dimension, account for the difficulty to estimate **within** the model S_m
- $L_m \geq 1$: a weight that satisfies: $\sum_{m \in \mathcal{M}_p} \exp(-L_m D_m) \leq 1$, accounting for the noise due to **the size** of the list of models

hence, in the linear model, the L_0-regularized estimator $\hat{\boldsymbol{\beta}}$ satisfies that

$$\mathbb{E}\left[n^{-1}\|\mathbf{X}\hat{\boldsymbol{\beta}} - \mathbf{X}\boldsymbol{\beta}_0\|_2^2\right] \leq C \inf_{m \in \mathcal{M}_p} \left\{\min_{\boldsymbol{\beta} \in \text{model } S_m} \left[n^{-1}\|\mathbf{X}\boldsymbol{\beta} - \mathbf{X}\boldsymbol{\beta}_0\|_2^2\right] + \frac{\kappa L_m D_m}{n}\right\}$$

where ***the tradeoff***: approximation error $n^{-1}\|\mathbf{X}\hat{\boldsymbol{\beta}} - \mathbf{X}\boldsymbol{\beta}_0\|_2^2$, and the cost of searching $\frac{\kappa L_m D_m}{n}$

computational complexity L_0−regularization methods are appealing w.r.t. risk properties, but in high-dimensional settings, the computation is infeasible (combinatorial), and discontinuous, non-convex penalty function $\lambda\|\boldsymbol{\beta}\|_0$

12.1.2 Generalizations of L0-Regularization Methods

Consider continuous or convex relaxation of the L_0-regularization method

$$\min_{\boldsymbol{\beta} \in \mathbb{R}^p} \left\{\hat{R}(\boldsymbol{\beta}) + \sum_{j=1}^{p} p_\lambda\left(|\beta_j|\right)\right\} \tag{12.3}$$

where, as in Problem 12.2

- $\hat{R}(\boldsymbol{\beta})$: the empirical risk function
- $p_\lambda(t), t \geq 0$: the nonnegative penalty function indexed by the regularization parameter $\lambda \geq 0$ with $p_\lambda(0) = 0$

[1]The $\log p$ is, once again, from the fact that for Gaussian random variables

$$\max_{1 \leq j \leq p} |Z_i| \simeq \sqrt{2 \log p}$$

for $(Z_1, \cdots, Z_p)' \sim \mathcal{N}(0, \mathbf{I}_p)$

Choices of penalty function In general, the choices of penalty function can be up for the researchers to decide. Fan and Li (2001) proposed 3 criteria for the selection of penalty function $p_\lambda(t)$

- **Sparsity**: $p'_\lambda(0+) > 0$, sets small coefficients to 0, for *variable selection* and *reducing model complexity*
- **Approximate unbiasedness**: nearly unbiased, especially when the true coefficient β_j is large
- **Continuity**: continuous in data to reduce instability in model selection

To elaborate the 3 criterion, consider a class of penalty function, L_q-penalty

$$p_\lambda(t) = \lambda t^q, t \geq 0 \Rightarrow p'_\lambda(t) = \lambda q t^{q-1}$$

then we can compare

	Sparsity	Approx. unbiasedness	Continuity
$0 < q < 1$	Y	Y	N
$q = 1$	Y	N	Y
$1 < q \leq 2$	N	N	Y

this class of penalty functions includes:

- $q = 0$: L_0- regression (best subset selection)
- $q = 1$: Lasso
- $q = 2$: Ridge
- $0 < q < 2$: Bridge estimator

12.2 High Dimensional Variable Selection

For a generalized linear model

$$f_n(\mathbf{y}; \mathbf{X}, \boldsymbol{\beta}) = \prod_{i=1}^{n} \left\{ c(y_i) \exp\left(\frac{y_i \theta_i - b(\theta_i)}{\phi} \right) \right\}$$

where $\boldsymbol{\theta} = (\theta_1, \cdots, \theta_n)' = \mathbf{X}\boldsymbol{\beta}$ is the **natural parameter vector**, which can a very challenging problem. Instead of the penalized least squares, now we examine **penalized likelihood**

$$\max_{\boldsymbol{\beta} \in \mathbb{R}^p} \mathcal{L}_n(\boldsymbol{\beta}) - \sum_{j=1}^{p} p_{\lambda_n}\left(|\beta_j|\right) \tag{12.4}$$

where $\mathcal{L}_n(\boldsymbol{\beta}) = n^{-1}\left[\mathbf{y}'\mathbf{X}\boldsymbol{\beta} - \mathbf{1}'\mathbf{b}(\mathbf{X}\boldsymbol{\beta})\right]$ is the *affine transformation* of log-likelihood,

$$\mathbf{b}(\boldsymbol{\theta}) = \mathbf{b}(\mathbf{X}\boldsymbol{\beta}) = (b(\theta_1), \cdots, b(\theta_n))'$$

So the natural question is, when can we find the solution to Problem 12.4, s.t. $\text{supp}(\hat{\boldsymbol{\beta}}) = \text{supp}(\boldsymbol{\beta}_0)$, that is, covering exactly the ture underlying sparse model?

12.3 Penalized Likelihood with Concave Penalties

$$\max_{\beta\in\mathbb{R}^p} \mathcal{L}_n(\boldsymbol{\beta}) - \sum_{j=1}^{p} p_{\lambda_n}\left(|\beta_j|\right)$$

where $\mathcal{L}_n(\boldsymbol{\beta}) = n^{-1}\left[\mathbf{y}'\mathbf{X}\boldsymbol{\beta} - \mathbf{1}'\mathbf{b}(\mathbf{X}\boldsymbol{\beta})\right]$, and $p_\lambda(\cdot)$ is a concave penalty function. Let $\rho(t;\lambda) = \lambda^{-1}p_\lambda(t), t \geq 0$, we aim for penalty functions that satisfy

- $\rho(t)$ is **increasing and concave** in t
- $\rho'(t)$ is **continuous** with $\rho'(0+) > 0$
- if $\rho(t)$ depends on λ, $\rho'(t;\lambda)$ is **increasing** in λ and $\rho'(0_+;\lambda)$ is **independent** of λ

Here are some notations

- Moment property: $k-$th component-wise derivative corresponds to $k-$th moment
  - $\boldsymbol{\mu}(\boldsymbol{\theta}) = (b'(\theta_1), \cdots, b'(\theta_n))'$: $\mathbb{E}(\mathbf{y})$
  - $\boldsymbol{\Sigma}(\boldsymbol{\theta}) = \operatorname{diag}\{b''(\theta_1), \cdots, b''(\theta_n)\}$
- local concavity of ρ at $\mathbf{v} = (v_1, \cdots, v_q)' \in \mathbb{R}^q$, with $\|\mathbf{v}\|_0 = q$, that is

$$\kappa(\rho;\mathbf{v}) = \lim_{\epsilon\to 0_+} \max_{1\leq j\leq q} \sup_{t_1<t_2\in(|v_j|-\epsilon,|v_j|+\epsilon)} -\frac{\rho'(t_2)-\rho'(t_1)}{t_2-t_1}$$

  if $\rho''(t)$ is continuous, this becomes

$$\max_{1\leq j\leq q} -\rho''(|v_j|)$$

And the solution is given by the following theorem

Theorem 12.3.1: Penalized Likelihood estimator

$\hat{\boldsymbol{\beta}}$ is **strict** **local** maximizer of penalized likelihood if

$$\mathbf{X}_1'\mathbf{y} - \mathbf{X}_1'\boldsymbol{\mu}(\hat{\boldsymbol{\theta}}) - n\lambda_n \operatorname{sign}(\hat{\boldsymbol{\beta}}_1) \circ \rho'(|\hat{\boldsymbol{\beta}}_1|) = \mathbf{0}$$
$$\|(n\lambda_n)^{-1}\mathbf{X}_2'[\mathbf{y} - \boldsymbol{\mu}(\hat{\boldsymbol{\theta}})]\|_\infty < \rho'(0_+)$$
$$\lambda_{\min}\left[\mathbf{X}_1'\boldsymbol{\Sigma}(\hat{\boldsymbol{\theta}})\mathbf{X}_1\right] > n\lambda_n\kappa(\rho;\hat{\boldsymbol{\beta}}_1)$$

where $\circ$ is the component-wise multiplication, $\lambda_{\min}(\cdot)$ is the smallest eigenvalue.

12.3.1 Global Optimality

Theorem 12.3.1 gives the rule to find local maximizers, but what about global optimality?

Proposition 12.3.2: Global Optimality of Penalized Likelihood Estimator

Assume that $\mathbf{X}$ has rank p, and satisfies

$$\min_{\beta\in\mathcal{L}_c} \lambda_{\min}\left[n^{-1}\mathbf{X}'\boldsymbol{\Sigma}(\mathbf{X}\boldsymbol{\beta})\mathbf{X}\right] \geq \kappa(p_{\lambda_n})$$

where

- NOT high-dimensional: $p \le n$
- for some $c < \mathcal{L}_n(\mathbf{0})$,
$$\mathcal{L}_c = \left\{\boldsymbol{\beta} \in \mathbb{R}^p : \mathcal{L}_n(\boldsymbol{\beta}) \ge c\right\}$$
is a sublevel set of $-\mathcal{L}_n(\boldsymbol{\beta})$
- maximum concavity
$$\kappa(p_\lambda) = \sup_{t_1<t_2\in(0,\infty)} -\frac{p'_\lambda(t_2) - p'_\lambda(t_1)}{t_2 - t_1}$$

12.3.2 SCAD penalty

Now, consider a penalized likelihood model: **SCAD** (Fan and Li, 2001, smoothly clipped absolute deviation)

$$\min_{\boldsymbol{\beta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + p(\boldsymbol{\beta})$$

where the derivative of the penalty function

$$p_\lambda^{\mathrm{SCAD}}(\beta_j) = \begin{cases} \lambda|\beta_j| & |\beta_j| \le \lambda \\ -\left(\frac{|\beta_j|^2 - 2a\lambda|\beta_j| + \lambda^2}{2(a-1)}\right) & \lambda < |\beta_j| \le a\lambda \\ \frac{(a+1)\lambda^2}{2} & |\beta_j| > a\lambda \end{cases}$$

and its derivative

$$p'(\boldsymbol{\beta}) = \lambda\left[I(\boldsymbol{\beta} \le \lambda) + \frac{(a\lambda - \boldsymbol{\beta})_+}{(a-1)\lambda} I(\boldsymbol{\beta} > \lambda)\right]$$

the solution to SCAD penalty model is

$$\hat{\beta}_j^{\mathrm{SCAD}} = \begin{cases} (|\hat{\beta}_j|)_+ \mathrm{sign}(\hat{\beta}_j) & |\hat{\beta}_j| < 2\lambda \\ \frac{(a-1)\hat{\beta}_j - \mathrm{sign}(\hat{\beta}_j)a\lambda}{a-2} & 2\lambda < |\hat{\beta}_j| \le a\lambda \\ \hat{\beta}_j & |\hat{\beta}_j| > a\lambda \end{cases}$$

the SCAD penalty is continuously differentiable on $(-\infty, 0) \cup (0, \infty)$, singular at 0. SCAD has some great properties, one of them is robustness.

Proposition 12.3.3: Robustness of SCAD

Assume that $\mathbf{X}$ has rank $p = s$, and $\exists c < \mathcal{L}_n(\mathbf{0})$ s.t. for some $c_0 > 0$

$$\min_{\boldsymbol{\beta}\in\mathcal{L}_c} \lambda_{\min}\left[n^{-1}\mathbf{X}'\boldsymbol{\Sigma}(\mathbf{X}\boldsymbol{\beta})\mathbf{X}\right] \ge c_0$$

then the SCAD penalized likelihood estimator $\hat{\boldsymbol{\beta}}^{\mathrm{SCAD}}$ is the **global** maximizer and equals the oracle MLE $\boldsymbol{\beta}^*$, if $\hat{\boldsymbol{\beta}}^{\mathrm{SCAD}}$ and

$$\min_{j=1}^{p} |\hat{\beta}_j^{\mathrm{SCAD}}| > \left(a + \frac{1}{2c_0}\right)\lambda_n$$

Next, we extend this global optimality result to high-dimensional cases, where $p > n$

Proposition 12.3.4: Global Optimality, $p > n$

On the union of all $s-$dimensional coordinate subspaces of $\mathbb{R}^p$

- Under Proposition 12.3.2 for each $n \times 2s$ submatrix of $\mathbf{X}$, then the NCPMLE $\hat{\boldsymbol{\beta}}$ is a global maximizer on $\mathbb{S}_s$
- Under Proposition 12.3.3 for $n \times s$ submatrix of $\mathbf{X}$ formed by columns in $\text{supp}(\boldsymbol{\beta}_0)$, the true model is δ-identifiable for some $\delta > \frac{(a+1)s\lambda_n^2}{2}$, and $\text{supp}(\hat{\boldsymbol{\beta}}) = \text{supp}(\boldsymbol{\beta}_0)$. Then the SCAD penalized likelihood estimator $\hat{\boldsymbol{\beta}}$ is the global maximizer on $\mathbb{S}_s$ and **equals** to the oracle MLE $\boldsymbol{\beta}^*$

12.3.3 Regularity Conditions for Concave Penalties

The regularity conditions for concave penalty are

- the true sub design matrix $\mathbf{X}_1$ should be well conditioned

$$\left\| \left[\mathbf{X}_1' \boldsymbol{\Sigma}(\boldsymbol{\theta}_0) \mathbf{X}_1\right]^{-1} \right\|_\infty = O(b_s n^{-1})$$

- A generalized version of the irrepresentable condition

$$\left\| \mathbf{X}_2' \boldsymbol{\Sigma}(\boldsymbol{\theta}_0) \mathbf{X}_1 \left[\mathbf{X}_1' \boldsymbol{\Sigma}(\boldsymbol{\theta}_0) \mathbf{X}_1\right]^{-1} \right\|_\infty \leq \min\left\{ C \frac{\rho'(0+)}{\rho'(d_n)}, O(n^{\alpha_1}) \right\} \tag{12.5}$$

- also

$$\max_{\boldsymbol{\delta} \in \mathcal{N}_0} \max_{j=1}^{p} \lambda_{\max} \left[\mathbf{X}_1' \text{diag}\left\{ |\mathbf{x}_j| \circ |\boldsymbol{\mu}''(\mathbf{X}_1 \boldsymbol{\delta})| \right\} \mathbf{X}_1\right] = O(n)$$

Here, $b_s \to \infty$ with $s = \|\boldsymbol{\beta}_0\|_0 = O(n^{\alpha_0})$, $\alpha_1 \in [0, 1/2]$, $C \in (0,1)$, $\mathcal{N}_0 = \left\{ \boldsymbol{\delta} \in \mathbb{R}^s : \|\boldsymbol{\delta} - \boldsymbol{\beta}_1\|_\infty \leq d_n \right\}$; $\alpha = \min(\frac{1}{2}, 2\gamma - \alpha_0) - \alpha_1$, $d_n \geq n^{-\gamma} \log n$ for some $\gamma \in (0, 1/2]$.

Notice that in a linear model, Condition 12.5 becomes

$$\left\| \mathbf{X}_2' \mathbf{X}_1 \left(\mathbf{X}_1' \mathbf{X}_1\right)^{-1} \right\|_\infty \leq \min\left\{ C \frac{\rho'(0+)}{\rho'(d_n)}, O(n^{\alpha_1}) \right\}$$

- For L_1 penalty, this becomes ($\rho'(0+) = \rho'(d_n) = 1$) a **stronger** form of the irrepresentable condition

$$\left\| \mathbf{X}_2' \mathbf{X}_1 \left(\mathbf{X}_1' \mathbf{X}_1\right)^{-1} \right\|_\infty \leq C < 1$$

  , this speaks about the restrictive nature of L_1 penalty in higher dimensions
- For concave penalty, $\frac{\rho'(0+)}{\rho'(d_n)}$ **can grow** to ∞, hence, it is a much weaker condition: **the flexibility** of concave penalty.

12.3.4 Properties of Concave Penalty

Next, we establish the nonasymptotic weak oracle property for estimator with concave penalties.

Theorem 12.3.5: Nonasymptotic Weak Oracle Property

Under some regularity conditions, $s = o(n)$ and $\log p = O(n^{1-2\alpha})$, there exists a penalized likelihood estimator $\boldsymbol{\beta}$ s.t. for sufficiently large n, with probability of at least

$$1 - 2\left[sn^{-1} + (p-s)e^{-n^{1-2\alpha}\log n}\right]$$

$\hat{\boldsymbol{\beta}}$ satisfies
- Sparsity: $\hat{\boldsymbol{\beta}}_2 = \mathbf{0}$
- L_∞ loss: $\|\hat{\boldsymbol{\beta}}_1 - \boldsymbol{\beta}_1\|_\infty = O(n^{-\gamma} logn)$

This theorem shows that concave penalties can reduce biases of estimates. The L_∞ estimation loss can de decomposed into $L_\infty \leq h_1 + h_2 + h_3$, $h_2 \sim b_s \lambda_s \frac{\rho'(d_n)}{\rho'(0+)}$. Theorem 12.3.5 establishes nonasymptotic weak oracle property of penalized likelihood estimator with penalties, where dimensionality p can grow non-polynomially with sample size n.

Theorem 12.3.6: Non-Concave Penalized Likelihood Estimator

Under some regularity conditions, $s \ll n$ and $\log p = O(n^{\alpha})$ for some $\alpha \in (0, 1/2)$, there exists a strict local maximizer $\hat{\boldsymbol{\beta}}$ of penalized likelihood such that $that \boldsymbol{\beta}_2 = \mathbf{0}$ with probability tending to 1 as $n \to \infty$ and $\|\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0\|_2 = O_P(\sqrt{s}n^{-1/2})$.

These conditions are incompatible for L_1 penalty, suggesting that L_1 penalized likelihood estimator generally **cannot** achieve consistency rate $O_P(\sqrt{s}n^{-1/2})$ and **does not** have oracle property, when dimensionality p is diverging with sample size n.

Theorem 12.3.7: Oracle Property of Non-Concave Penalty

Under some regularity conditions and $s = o(n^{1/3})$, then with probability tending to 1 as $n \to \infty$, then non-concave penalized likelihood estimator $\hat{\boldsymbol{\beta}}$ in Theorem 12.3.6 must satisfies
- **Sparsity**

$$\hat{\boldsymbol{\beta}}_2 = \mathbf{0}$$

- **Asymptotic normality**

$$\mathbf{A}_n \left[\mathbf{X}_1' \boldsymbol{\Sigma}(\boldsymbol{\theta}_0) \mathbf{X}_1\right]^{1/2} (\hat{\boldsymbol{\beta}}_1, \boldsymbol{\beta}_1) \xrightarrow{d} \mathcal{N}(\mathbf{0}, \phi \mathbf{G})$$

  where $\mathbf{A}_n$ is a $q \times s$ matrix s.t. $\mathbf{A}_n \mathbf{A}_n' \to \mathbf{G}$, and $\mathbf{G}$ is a $q \times q$ symmetric positive definite matrix.

A simulation of SCAD versus Lasso is presented in Figure 12.1. It's clear that SCAD gives a more consistent estimation of the model. In this simulation, the

References

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Figure 12.1: Numercial Comparison: SCAD vs Lasso