

Topic 12: Non-convex Learning

by Sai Zhang

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 L_0 Penalized Likelihood

Consider the model selection problem of choosing a parameter vector θ that maximizes the penalized likelihood

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

where the L_0 -norm $\|\theta\|_0$ 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 $\|\theta\|_0 = m$, 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:

$$\min_{\theta \in \mathbb{R}^p} \{ \hat{R}(\theta) + \lambda \|\theta\|_0 \} \quad (12.2)$$

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

- **negative log-likelihood loss:** equivalent to 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

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

it's clear that $\max R_{\text{adj}}^2 \Leftrightarrow \min \log \left(\frac{RSS_d}{n-d} \right)$, 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 variables¹
- **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 $\hat{\beta}$ satisfies that

$$\mathbb{E} \left[n^{-1} \|\mathbf{X}\hat{\beta} - \mathbf{X}\beta_0\|_2^2 \right] \leq C \inf_{m \in \mathcal{M}_p} \left\{ \min_{\beta \in \text{model } S_m} \left[n^{-1} \|\mathbf{X}\beta - \mathbf{X}\beta_0\|_2^2 \right] + \frac{\kappa L_m D_m}{n} \right\}$$

where **the tradeoff**: approximation error $n^{-1} \|\mathbf{X}\hat{\beta} - \mathbf{X}\beta_0\|_2^2$, 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 $\lambda \|\beta\|_0$

12.1.2 Generalizations of L0-Regularization Methods

Consider continuous or convex relaxation of the L_0 -regularization method

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

where, as in Problem 12.2

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

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

$$\max_{1 \leq j \leq p} |Z_j| \approx \sqrt{2 \log p}$$

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

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

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

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

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

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

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

where $\mathcal{L}_n(\beta) = n^{-1} [\mathbf{y}'\mathbf{X}\beta - \mathbf{1}'\mathbf{b}(\mathbf{X}\beta)]$, 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
 - $\mu(\theta) = (b'(\theta_1), \dots, b'(\theta_n))': \mathbb{E}(\mathbf{y})$
 - $\Sigma(\theta) = \text{diag}\{b''(\theta_1), \dots, b''(\theta_n)\}$
- local concavity of ρ at $\mathbf{v} = (v_1, \dots, v_q)' \in \mathbb{R}^q$, with $\|\mathbf{v}\|_0 = q$, that is

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

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

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

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

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

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

where

- NOT high-dimensional: $p \leq n$
- for some $c < \mathcal{L}_n(\mathbf{0})$,

$$\mathcal{L}_c = \{\boldsymbol{\beta} \in \mathbb{R}^p : \mathcal{L}_n(\boldsymbol{\beta}) \geq c\}$$

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

$$p'_\lambda(\beta_j) = \begin{cases} \lambda |\beta_j| & |\beta_j| \leq \lambda \\ -\left(\frac{|\beta_j|^2 - 2a\lambda|\beta_j| + \lambda^2}{2(a-1)}\right) & \lambda < |\beta_j| \leq a\lambda \\ \frac{(a+1)\lambda^2}{2} & |\beta_j| > a\lambda \end{cases}$$

and its derivative

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

the solution to SCAD penalty model is

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

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 $c_0 > 0$

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

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

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

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 $\hat{\beta}$ 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 $\text{supp}(\beta_0)$, the true model is δ -identifiable for some $\delta > \frac{(a+1)s\lambda_n^2}{2}$, and $\text{supp}(\hat{\beta}) = \text{supp}(\beta_0)$. Then the SCAD penalized likelihood estimator $\hat{\beta}$ is the global maximizer on \mathbb{S}_s and **equals** to the oracle MLE β^*

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

$$\left\| [\mathbf{X}_1' \Sigma(\theta_0) \mathbf{X}_1]^{-1} \right\|_{\infty} = O(b_s n^{-1})$$

- A generalized version of the irrepresentable condition

$$\left\| \mathbf{X}_2' \Sigma(\theta_0) \mathbf{X}_1 [\mathbf{X}_1' \Sigma(\theta_0) \mathbf{X}_1]^{-1} \right\|_{\infty} \leq \min \left\{ C \frac{\rho'(0+)}{\rho'(d_n)}, O(n^{\alpha_1}) \right\} \quad (12.5)$$

- also

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

Here, $b_s \rightarrow \infty$ with $s = \|\beta_0\|_0 = O(n^{\alpha_0})$, $\alpha_1 \in [0, 1/2]$, $C \in (0, 1)$, $\mathcal{N}_0 = \{ \delta \in \mathbb{R}^s : \|\delta - \beta_1\|_{\infty} \leq d_n \}$; $\alpha = \min(\frac{1}{2}, 2\gamma - \alpha_0) - \alpha_1$, $d_n \geq n^{-\gamma} \log n$ for some $\gamma \in (0, 1/2]$.

Notice that in a linear model, Condition 12.5 becomes

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

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

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

, 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 $\hat{\beta}$ s.t. for sufficiently large n , with probability of at least

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

$\hat{\beta}$ satisfies

- Sparsity: $\hat{\beta}_2 = \mathbf{0}$
- L_∞ loss: $\|\hat{\beta}_1 - \beta_1\|_\infty = O(n^{-\gamma} \log n)$

This theorem shows that concave penalties can reduce biases of estimates. The L_∞ estimation loss can be 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 $\hat{\beta}$ of penalized likelihood such that $\hat{\beta}_2 = \mathbf{0}$ with probability tending to 1 as $n \rightarrow \infty$ and $\|\hat{\beta} - \beta_0\|_2 = O_P(\sqrt{s}n^{-1/2})$.

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 $n \rightarrow \infty$, then non-concave penalized likelihood estimator $\hat{\beta}$ in Theorem 12.3.6 must satisfy

- **Sparsity**

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

- **Asymptotic normality**

$$\mathbf{A}_n \left[\mathbf{X}_1' \boldsymbol{\Sigma}(\theta_0) \mathbf{X}_1 \right]^{1/2} (\hat{\beta}_1, \beta_1) \xrightarrow{d} \mathcal{N}(\mathbf{0}, \phi \mathbf{G})$$

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

A simulation of SCAD versus Lasso is presented in Figure 12.1

References

- Andrew Barron, Birgé Lucien, and Massart Pascal. Risk bounds for model selection via penalization. *Probability theory and related fields*, 113(3):301–413, 1999.
- Jianqing Fan and Runze Li. Variable selection via nonconcave penalized likelihood and its oracle properties. *Journal of the American statistical Association*, 96(456):1348–1360, 2001.

Figure 12.1: Numerical Comparison: SCAD vs Lasso

