

## Topic 12: Non-convex Learning

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**Key points:**

**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  $\theta$  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  $p$  variables<sup>1</sup>
- **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

- $\kappa$ : 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  $p_\lambda(0) = 0$

<sup>1</sup>The 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  $\beta_j$  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  $\lambda$ ,  $\rho'(t; \lambda)$  is **increasing in  $\lambda$**  and  $\rho'(0+; \lambda)$  is **independent** of  $\lambda$

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  $\rho$  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  $\delta$ -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  $\beta^*$

### 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

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

- A generalized version of the irrepresentable condition

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

- also

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

## 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.