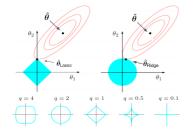
Introduction to Machine Learning

Regularization Other Regularizers





Learning goals

- L1/L2 regularization induces bias
- Lq (quasi-)norm regularization
- L0 regularization
- SCAD and MCP

RIDGE AND LASSO ARE BIASED ESTIMATORS I

Although ridge and lasso have many nice properties, they are biased estimators and the bias does not (necessarily) vanish as $n \to \infty$.

For example, in the orthonormal case $(\mathbf{X}^{\top}\mathbf{X} = \mathbf{I})$ the bias of the lasso is

$$\begin{cases} \mathbb{E} \left| \widehat{\theta}_j - \theta_j \right| = 0 & \text{if } \theta_j = 0 \\ \mathbb{E} \left| \widehat{\theta}_j - \theta_j \right| \approx \theta_j & \text{if } |\theta_j| \in [0, \lambda] \\ \mathbb{E} \left| \widehat{\theta}_j - \theta_j \right| \approx \lambda & \text{if } |\theta_j| > \lambda \end{cases}$$

To reduce the bias/shrinkage of regularized estimators various penalties were proposed, a few of which we briefly introduce now.



LQ REGULARIZATION ► Fu and Knight 2000

Besides L1/L2 we could use any Lq (quasi-)norm penalty $\lambda \|\theta\|_q^q$

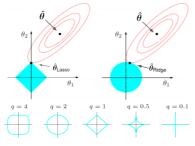


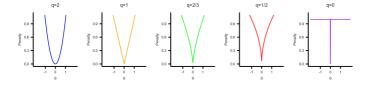


Figure: *Top:* loss contours and *L*1/*L*2 constraints. *Bottom:* Constraints for *Lq* norms $\sum_i |\theta_i|^q$.

- For q < 1 penalty becomes non-convex but for q > 1 no sparsity is achieved
- Non-convex Lq has nice properties like oracle property Zou and Hastie 2005 : consistent (+ asy. unbiased) param estimation and var selection
- Downside: non-convexity makes optimization even harder than L1 (no unique global minimum but multiple local minima)

LO REGULARIZATION I

$$\mathcal{R}_{\text{reg}}(oldsymbol{ heta}) = \mathcal{R}_{\text{emp}}(oldsymbol{ heta}) + \lambda \|oldsymbol{ heta}\|_0 := \mathcal{R}_{\text{emp}}(oldsymbol{ heta}) + \lambda \sum_{i} | heta_i|^0.$$





- L0 "norm" simply counts the nr of non-zero params
- Induces sparsity more aggressively than L1, but does not shrink
- AIC and BIC are special cases of L0
- L0-regularized risk is not continuous or convex
- NP-hard to optimize; for smaller n and p somewhat tractable, efficient approximations are still current research

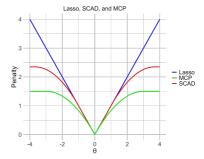


Smoothly Clipped Absolute Deviations: non-convex, $\gamma >$ 2 controlls how fast penalty "tapers off"

$$\mathrm{SCAD}(\theta \mid \lambda, \gamma) = \begin{cases} \lambda |\theta| & \text{if } |\theta| \leq \lambda \\ \frac{2\gamma\lambda |\theta| - \theta^2 - \lambda^2}{2(\gamma - 1)} & \text{if } \lambda < |\theta| < \gamma\lambda \\ \frac{\lambda^2(\gamma + 1)}{2} & \text{if } |\theta| \geq \gamma\lambda \end{cases}$$



- Smooth
- Contrary to lasso/ridge, SCAD continuously relaxes penalization rate as $|\theta|$ increases above λ



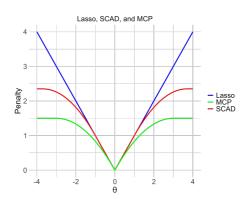




Minimax Concave Penalty: also non-convex; similar idea as SCAD with $\gamma >$ 1

$$\mathit{MCP}(\theta|\lambda,\gamma) = \begin{cases} \lambda|\theta| - \frac{\theta^2}{2\gamma}, & \text{if } |\theta| \leq \gamma\lambda\\ \frac{1}{2}\gamma\lambda^2, & \text{if } |\theta| > \gamma\lambda \end{cases}$$

- As with SCAD, MCP starts by applying same penalization rate as lasso, then smoothly reduces rate to zero as |θ| ↑
- Different from SCAD, MCP immediately starts relaxing the penalization rate, while for SCAD rate remains flat until $|\theta| > \lambda$
- Both SCAD and MCP possess oracle property: they can consistently select true model as n → ∞ while lasso may fail



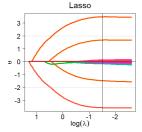


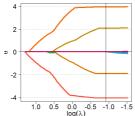
EXAMPLE: COMPARING REGULARIZERS I

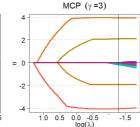
Let's compare coeff paths for lasso, SCAD, and MCP.

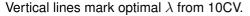
We simulate n = 100 samples from the following DGP:

$$y = \mathbf{x}^{\top} \boldsymbol{\theta} + \varepsilon, \quad \boldsymbol{\theta} = (4, -4, -2, 2, 0, \dots, 0)^{\top} \in \mathbb{R}^{1500}, \quad x_j, \varepsilon \sim \mathcal{N}(0, 1)$$
Lasso SCAD $(\gamma = 3.7)$ MCP $(\gamma = 3)$









Conclusion: Lasso underestimates true coeffs while SCAD/MCP achieve unbiased estimation and better variable selection

