High-dimensional Linear Discriminant Analysis with Moderately Clipped LASSO [1]

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Overview

1. Introduction
   - Linear discriminant analysis
   - Literature review
2. Main Results
   - Clipped LASSO
   - Theory
   - Simulation studies
   - Real Data Analysis
3. Concluding remarks

LDA: Bayes discriminant rule

- Bayes classifier

$$\phi^{\text{Bayes}}(\mathbf{x}) = \arg\max_{c\in\{1,2\}} \mathbf{P}(C = c|\mathbf{X} = \mathbf{x})$$

  - $\mathbf{X} \in \mathbb{R}^p$, $C \in \{1, 2\}$ are random
- The linear discriminant analysis (LDA) (Fisher, 1936)

$$\left(\mathbf{x} - (\boldsymbol{\mu}_1 + \boldsymbol{\mu}_2)/2\right)^T \boldsymbol{\beta}^{\text{Bayes}} + \log(\pi_2/\pi_1) > 0,$$

  - $\mathbf{X}|C = c \sim \mathcal{N}_p(\boldsymbol{\mu}_c, \boldsymbol{\Sigma}),\ c \in \{1, 2\}$
  - $\boldsymbol{\mu}_c$ and $\boldsymbol{\Sigma}$ are mean and covariance
  - $\pi_1 + \pi_2 = 1$; fixed class probabilities
  - $\boldsymbol{\beta}^{\text{Bayes}} = \boldsymbol{\Sigma}^{-1}\boldsymbol{\theta}$ ($\boldsymbol{\theta} := \boldsymbol{\mu}_2 - \boldsymbol{\mu}_1$) is the Bayes direction vector

LDA: Estimation

- LDA direction vector

$$\hat{\beta}^{\mathrm{LDA}} = \hat{\mathbf{\Sigma}}^{-1}\hat{\boldsymbol{\theta}}, \tag{1}$$

  - $\hat{\mathbf{\Sigma}}$ is the pooled sample covariance matrix and
  - $\hat{\boldsymbol{\theta}} = \hat{\boldsymbol{\mu}}_2 - \hat{\boldsymbol{\mu}}_1$

Linear discriminant rule: assign $C|\mathbf{X} = \mathbf{x}$ to the class 2 if $\mathbf{x}$ satisfies

$$\left(\mathbf{x} - \frac{\hat{\boldsymbol{\mu}}_1 + \hat{\boldsymbol{\mu}}_2}{2}\right)^T \hat{\beta}^{\mathrm{LDA}} + \log(n_2/n_1) > 0, \tag{2}$$

where $n_1 = |\{c_i; c_i = 1\}|$ and $n_2 = |\{c_i; c_i = 2\}|$ for $i = 1, \cdots, n$

What if $p > n$?

- Direct modification of the covariance (Krzanowski et al., 1995), (Bickel et al., 2004)
- Constructing relevant shrunken centroid means Guo et al. (2006); Fan and Fan (2008); Wu et al. (2009); Cai and Liu (2011); Witten and Tibshirani (2011); Clemmensen et al. (2011); Shao et al. (2011)
- Penalized LSE (Mai et al., 2012; Tibshirani, 1996) motivated by Hastie et al. (2009)

Connection between LS and LDA

- LSE for the LDA problem (Hastie et al., 2009)

$$(\hat{\alpha}^{\mathrm{LSE}}, \hat{\boldsymbol{\beta}}^{\mathrm{LSE}}) = \underset{\alpha,\boldsymbol{\beta}}{\arg\min} \sum_{i=1}^{n} (y_i - \alpha - \mathbf{x}_i^T \boldsymbol{\beta})^2 / 2n \qquad (3)$$

  - $\hat{\beta}^{\mathrm{LSE}} = (\mathbf{Z}^T \mathbf{Z}/n)^{-1} \hat{\boldsymbol{\theta}}$ for the centered desgin matrix $\mathbf{Z}$
  - $y_i = (-1)^{c_i} n/n_{c_i}, i \leqslant n$.
- relation

$$\hat{\boldsymbol{\beta}}^{\mathrm{LSE}} = c \hat{\boldsymbol{\beta}}^{\mathrm{LDA}} \qquad (4)$$

- ... and the discriminant rule becomes

$$\left(\mathbf{x} - \frac{\hat{\boldsymbol{\mu}}_1 + \hat{\boldsymbol{\mu}}_2}{2} \right)^T \hat{\boldsymbol{\beta}}^{\mathrm{LSE}} + c \log(n_2/n_1) > 0 \qquad (5)$$

Penalized LSE

(1) and (4) fail to hold when $p > n$ and $\nexists \hat{\Sigma}^{-1}$

Q. How to estimate β^{Bayes}?

Mai et al. (2012) used the least absolute shrinkage and selection operator (LASSO):

$$(\hat{\alpha}^{\lambda}, \hat{\boldsymbol{\beta}}^{\lambda}) = \arg\min_{\alpha, \boldsymbol{\beta}} \left\{ \sum_{i=1}^{n} (y_i - \alpha - \mathbf{x}_i^T \boldsymbol{\beta})^2 / 2n + \lambda \sum_{j=1}^{p} |\beta_j| \right\},$$

for some $\lambda > 0$, where the solution can be well defined even when $p > n$.

Moderately Clipped LASSO

- Clipped LASSO (Kwon et al., 2015)

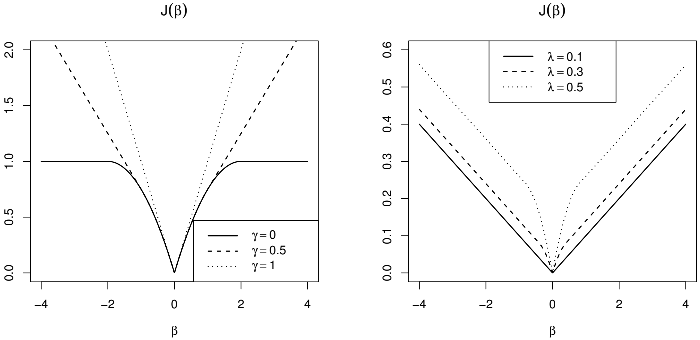
$$\begin{cases} J_{\gamma,\lambda}(0) = 0 \\ \nabla J_{\gamma,\lambda}(t) = \lambda - t/a, & t < a(\lambda - \gamma) \\ \nabla J_{\gamma,\lambda}(t) = \gamma, & o.w. \end{cases}$$

for $0 \leqslant \gamma \leqslant \lambda$

- property
  1. $J_{\lambda,\lambda}$ attains LASSO & $J_{0,\lambda}$ attains MCP
  2. λ mainly controls the concavity of the penalty near the origin for like the MCP
  3. γ regularizes the amount of shrinkage non-zero regression coefficients like the LASSO

Behavior

Figure: Various shapes of the MCL with $a = 2$: $\lambda = 1$ for the left panel and $\gamma = 0.1$ for the right panel.



What can we expect from the MCL?

- Kwon et al. (2015)
- Correct model selection + good prediction accuracy
- Does not perfectly outperform LASSO or MCP
  BUT enjoys the advantages of the both
- The MCL estimator for β^{Bayes}=oracle[2] LASSO estimator with probability tending to one

[2] a theoretically optimal estimator obtained by using the signal variables only

Oracle Property I

$Q_{\gamma,\lambda}(\beta)$: LS-type loss penalized with $J_{\gamma,\lambda}$
$\Xi^{\kappa}_{\gamma,\lambda} := \{\beta \in \{\text{all local minimizers of } Q_{\gamma,\lambda}\}; |\mathrm{supp}(\beta)| \leqslant \kappa\}.$

Theorem

Under some conditions,

$$\lim_{n\to\infty} \mathbf{P}\left(\{\hat{\beta}^{\text{Oracle LASSO},\gamma}\} = \Xi^{\kappa}_{\gamma,\lambda}\right) = 1.$$

That is, the oracle LASSO estimator is the unique minimizer of $Q_{\gamma,\lambda}$ with probability tending to one.

Oracle Property II

- This also holds for $J_{0,\lambda}$ (MCP)
  So the oracle LSE becomes the unique minimizer of $Q_{\gamma,\lambda}$
- linear regression

$$m_{\mathcal{A}} \gg \lambda \gg \sqrt{\log p/n}$$
$$for \;\; m_{\mathcal{A}} := \min_{j\in\mathcal{A}} |\beta_j^{\text{Bayes}}|,$$

- LDA

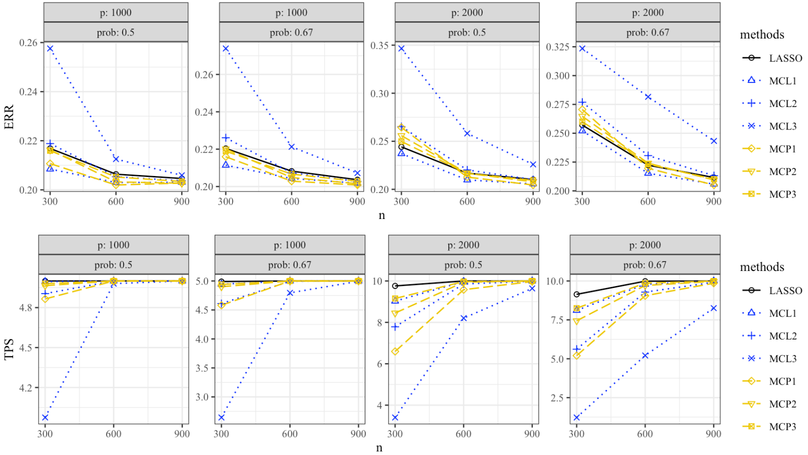
$$m_{\mathcal{A}} \gg \lambda \gg q\sqrt{\log p/n}$$

if $n \gg \kappa^3 \log p$, where $a \gg b$ implies $a/b \to \infty$ as $n \to \infty$.

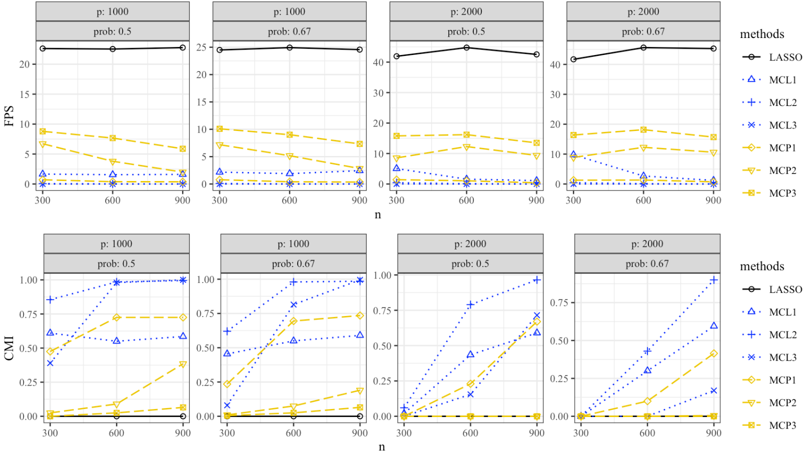
Simulations

- simulation design
  - $\pi_1 = 0.5$ and $\pi_1 = 0.67$
  - $\mathbf{\Sigma} = \mathbf{\Sigma}^{(i)}, i \leqslant 2$:
    1. $\mathbf{\Sigma}^{(1)} = \mathbf{I}_p$ (independent)
    2. $\Sigma^{(2)}_{jk} = 0.5^{|j-k|}$ for $j, k \leqslant p$ (power decaying correlation)
  - $\beta_j^{\text{Bayes}} = \alpha(-1)^j I(j \leqslant q), j \leqslant p$
    α is calculated so that all Bayes error rates to be 0.2
    $\boldsymbol{\mu}_1 = \mathbf{0}_p$ and $\boldsymbol{\mu}_2 = \mathbf{\Sigma}\boldsymbol{\beta}^{\text{Bayes}}$
  - $n \in \{300, 600, 900\}$, $(p, q) \in \{(1000, 5), (2000, 10)\}$
- estimators: for $k \in \{1, 2, 3\}$,
  - MCL_k with $a = 2.1$ and $\gamma = k\hat{\lambda}^{\text{LASSO}}$ (Kwon et al., 2015)
  - MCP_k with $a = k + 0.1$, and $\gamma = 0$.
  - LASSO

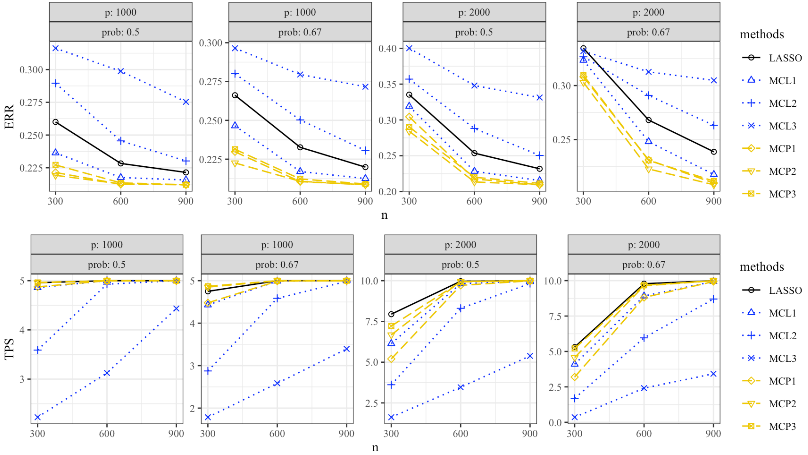
$\boldsymbol{\Sigma} = \boldsymbol{\Sigma}^{(1)}$: ERR, TPS



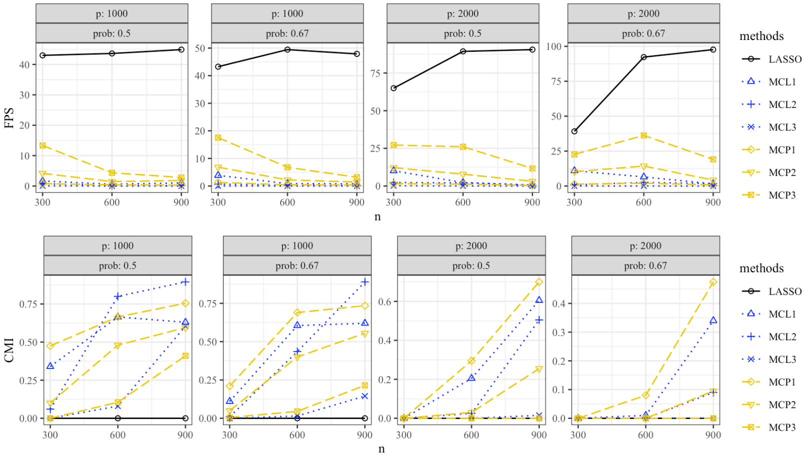
$\boldsymbol{\Sigma} = \boldsymbol{\Sigma}^{(1)}$: FPS, CMI



$\boldsymbol{\Sigma} = \boldsymbol{\Sigma}^{(2)}$: ERR, TPS



$\mathbf{\Sigma} = \mathbf{\Sigma}^{(2)}$: FPS, CMI



Summary

The MCL can be a nice alternative to the LASSO for the high-dimensional penalized LDA

- can correctly identify the sparse Bayes direction vector
- keeps almost the same prediction accuracy as the LASSO

Remark

MCL_1 performed quite well regardless of the simulation designs considered; this aligns with the recommendation by Kwon et al. (2015)

Analysis of micro-array samples I

HD microarray data sets in R (John, 2016): Burczynski et al. (2006); Chin et al. (2006); Chowdary et al. (2006); Gordon et al. (2002)

Sure independence screening procedure (Fan et al., 2010): used first top d predictive variables with the largest marginal regression coefficients

For comparison,

- tuning via the 10-fold CV & prediction via the leave-one-out CV
- counted the number of incorrectly classified samples (error)
- calculated the average of fit sizes (sizes)

Analysis of micro-array samples II

	d	LASSO	MCL_1	MCL_2	MCL_3	MCP_1	MCP_2	MCP_3
				Chowdary et al. (2006), $n = 104$, $p = 22283$				
errors	400	1	1	2	2	4	4	5
sizes	400	36.28	28.50	24.78	21.84	11.44	11.60	12.33
				Gordon et al. (2002), $n = 181$, $p = 12533$				
errors	400	2	2	2	1	3	3	3
sizes	400	41.28	37.33	24.41	16.71	7.17	6.79	7.03
				Burczynski et al. (2006), $n = 127$, $p = 22283$				
errors	400	6	6	7	9	15	13	15
sizes	400	47.67	41.50	26.19	24.06	13.70	13.81	13.13
				Chin et al. (2006), $n = 118$, $p = 22215$				
errors	400	12	11	13	15	21	22	22
sizes	400	33.62	27.28	21.53	15.16	9.74	9.69	9.61

Analysis of micro-array samples III

- LASSO: highest prediction accuracy BUT largest fit sizes
- MCPs: lowest prediction accuracy BUT smallest fit sizes
- $d = 400$: MCL_1 was similar to LASSO in terms of the prediction accuracy while having small fit sizes
- MCL_2: much smaller fit sizes than the LASSO + similar prediction accuracy

Conclusion

High-dimensional LDA with MCL:

- predicts similarly or better than the LASSO while recovering the sparsity of the direction vector
- get the variable selection consistency under reasonable regularity conditions as supported by numerical studies
- An additional tuning parameter γ seems inattractive; however, the heuristic choice of $\gamma = \hat{\gamma}^{\text{opt}}$ or $\gamma = 2\hat{\gamma}^{\text{opt}}$ worked practically
- Further research may focus on the choice of γ

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