High Dimensional Classification in the Presence of Correlation: A Factor Model Approach

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Overview

- 1. A Factor-model linear classification rule for High-Dimensional correlated data
- 2. Asymptotic properties with $p \rightarrow \infty$
- 3. Variable selection for problems with "rare" and "mostly weak" group differences
- 4. Performance in Micro-Array problems
- 5. Conclusions and Perspectives

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Problem Statment:

$$(Y; X) \quad Y \in \{0,1\} \qquad X \in \mathfrak{R}^p$$

We want to find a rule that predicts Y given X

Bayes rule: $\hat{\mathbf{Y}} = \operatorname{argmax}_{g} \pi_{g} \mathbf{f}_{g}(\mathbf{X})$

Assuming $X \mid Y \sim N_p(\mu_{(Y)}, \Sigma)$

 \Rightarrow Bayes rule:

$$\hat{\mathbf{Y}} = \mathbf{1} \left\{ \Delta^{\mathrm{T}} \Sigma^{-1} \left(\mathbf{X}_{\mathrm{i}} - \frac{1}{2} (\mu_{0} + \mu_{1}) \right) > \log \frac{\pi_{0}}{\pi_{1}} \right\} \qquad \Delta = \mu_{(1)} - \mu_{(0)}$$

How to estimate Σ^{-1} when p > n and the X correlations are important ?

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<u>A Factor-Model Approach</u>

$$\begin{split} \mathbf{X}_{i} &= \mu_{(\mathbf{Y}i)} + \mathbf{B} \ \mathbf{f}_{i} + \epsilon_{i} \qquad \mathbf{f}_{i} \in \Re^{\mathbf{q}} \qquad \epsilon_{i} \in \Re^{\mathbf{p}} \qquad \mathbf{q} << \mathbf{p} \\ & \mathbf{f}_{i} \sim \mathbf{N}_{q}(\mathbf{0}, \mathbf{I}_{q}) \qquad \epsilon_{i} \sim \mathbf{N}_{p}(\mathbf{0}, \mathbf{D}_{\epsilon}) \qquad \forall \mathbf{j} \ \mathbf{D}_{\epsilon}(\mathbf{j}) > \mathbf{k}_{0} \in \Re_{0} \\ \Rightarrow \\ \Sigma &= \mathbf{B} \ \mathbf{B}^{\mathsf{T}} + \mathbf{D}_{\epsilon} \\ \Sigma^{-1} &= \mathbf{D}_{\epsilon}^{-1} - \mathbf{D}_{\epsilon}^{-1} \ \mathbf{B} \ [\mathbf{I}_{\mathbf{q}} + \mathbf{B}^{\mathsf{T}} \ \mathbf{D}_{\epsilon}^{-1} \ \mathbf{B}]^{-1} \ \mathbf{B}^{\mathsf{T}} \mathbf{D}_{\epsilon}^{-1} \\ \hat{\Sigma}_{\mathsf{RFctq}} &= \ \hat{\mathbf{B}} \ \hat{\mathbf{B}}^{\mathsf{T}} + \hat{\mathbf{D}}_{\epsilon} \\ \hat{\mathbf{B}}, \hat{\mathbf{D}}_{\epsilon} &= \arg \min_{\hat{\mathbf{B}}, \hat{\mathbf{D}}_{\epsilon}} || \ \hat{\mathbf{V}}^{-1/2} \hat{\Sigma}_{\mathsf{RFctq}} \ \hat{\mathbf{V}}^{-1/2} - \ \hat{\mathbf{V}}^{-1/2} \mathbf{S} \ \hat{\mathbf{V}}^{-1/2} ||_{\mathsf{F}}^{2} \end{split}$$

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Asymptotic Properties

We will compare empirical linear rules

$$\delta_{\mathrm{L}} = 1\left\{\hat{\Delta}^{\mathrm{T}}\hat{\Sigma}_{\delta_{\mathrm{L}}}^{-1}\left(\mathrm{X}_{\mathrm{i}} - \frac{1}{2}(\overline{\mathrm{X}}_{0} + \overline{\mathrm{X}}_{1})\right) > \log\frac{n_{0}}{n_{1}}\right\}$$

For some parameter space $\Gamma_{\delta_{II}}$ and Δ estimator $\hat{\Delta}$ satisfying

$$\max_{\Gamma_{\delta_{L}}} \mathbf{E}_{\theta} \| \hat{\Delta} - \Delta \|^{2} = \mathbf{o}(1)$$
 (C1)

based on the criterion

$$\overline{W}_{\Gamma_{\delta_{L}}}(\delta_{L}) = \max_{\Gamma_{\delta_{L}}} P_{\theta}(\delta_{L}(Y_{i}) = 1 \mid Y_{i} = 0) = \max_{\Gamma_{\delta_{L}}} \left(1 - \Phi\left(\frac{\hat{\Delta}^{T} \hat{\Sigma}_{\delta_{L}}^{-1} \hat{\Delta}}{2\sqrt{\hat{\Delta}^{T} \hat{\Sigma}_{\delta_{L}}^{-1} \Sigma \hat{\Sigma}_{\delta_{L}}^{-1} \hat{\Delta}}}\right)\right)$$

when
$$p \to \infty$$
; $\frac{n(p)}{p} \to d < \infty$

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Asymptotic Properties

Main Result

 $\begin{array}{l} \textbf{Result} \\ \theta : \ \Delta^{\mathrm{T}} \ \Sigma^{-1} \ \Delta \ge c^{2} \ , \\ k_{1} \le \ \lambda_{\min}(\Sigma) \le \ \lambda_{\max}(\Sigma) \ \le k_{2} \\ \Delta \in B \end{array} \end{array}$ when $\pi_{0} = \pi_{1} = 1/2 \qquad \qquad \forall \mathbf{j}, \mathbf{a} \sum_{\mathbf{j}', \mathbf{l}'} \left| \frac{\partial \beta(\mathbf{j}, \mathbf{a})}{\partial \mathbf{R}(\mathbf{j}', \mathbf{l}')} \right| < \infty$ (C1) is satisfied $\forall \mathbf{j} \sum_{\mathbf{j}', \mathbf{l}'} \left| \frac{\partial \mathbf{D}_{\varepsilon}(\mathbf{j})}{\partial \mathbf{R}(\mathbf{j}', \mathbf{l}')} \right| < \infty$

 $\Sigma_{\text{RFctq}} = \mathbf{B} \mathbf{B}^{\text{T}} + \mathbf{D}_{\varepsilon}^{2} = \operatorname{arg\ min}_{\text{B},\text{D}_{\varepsilon}} \|\mathbf{R}_{\text{RFctq}} - \mathbf{V}^{-1/2} \Sigma \mathbf{V}^{-1/2} \|_{\text{F}}^{2} \qquad \mathbf{R}_{\text{RFctq}} = \mathbf{V}^{-1/2} \Sigma_{\text{RFct}_{\sigma}} \mathbf{V}^{-1/2}$

It follows that: when $p \to \infty$; $\frac{n(p)}{\log n} \to \infty$

$$\overline{W}_{\Gamma_{\delta_{F_{q}}}}(\delta_{F_{q}}) \rightarrow 1 - \Phi\left(\frac{\sqrt{K_{0F_{q}}}}{1 + K_{0F_{q}}} c\right) \qquad K_{0F_{q}} = \max_{\Gamma_{F_{q}}} \frac{\lambda_{\max}(\Sigma_{0F_{q}})}{\lambda_{\min}(\Sigma_{0F_{q}})} \qquad \Sigma_{0F_{q}} = \sum_{RFct_{q}}^{-\frac{1}{2}} \sum_{RFct_{q}} \sum_{RFct_{q}}$$

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Selecting Predictors

- 1 Rank variables acording to two-sample t-scores
- 2 Choose a selection cut-off for the score values

Higher Criticism

(Donoho e Jin 2004)

Given p ordered p-values: π_1, \ldots, π_p

HC(j;
$$\pi_{j}$$
) = $\sqrt{p} \frac{(j/p) - \pi_{j}}{\sqrt{(j/p)(1 - (j/p))}}$

$$HC*=max_{j\leq \alpha_0} HC(j;\pi_j)$$

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Selecting Predictors

Higher Criticism

In a two-group homokedastic model, with :

- Diagonal classification rules
- p-values derived from two-group t-scores
- Independent variables
- Rare "effects" (mean group diferences)
- Weak effects

when $p \rightarrow \infty$

HC* is asymptotically equivalent to the optimal selection threshold

(Donoho e Jin 2009)

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Selecting Predictors

Control of false discovery rates

Given a sequence of p <u>independent</u> tests with ordered p-values: $\pi_1, ..., \pi_p$

Reject the null hypothesis (H_{0i}) where $j \le k$, with

$$\mathbf{k} = \max\left\{\mathbf{j}: \boldsymbol{\pi}_{\mathbf{j}} \leq \frac{\mathbf{j}}{\mathbf{p}} \boldsymbol{\alpha}\right\}$$

(Benjamini e Hochberg 1995)

Given a sequence of p <u>dependent</u> tests with ordered p-values: π_1, \ldots, π_p

Reject the null hypothesis (H_{0j}) where $j \le k$, with $k = max \begin{cases} j : \pi_j \le \frac{j}{p\sum_{i=1}^p \frac{1}{i}} \alpha \end{cases}$ (Benjar)

(Benjamini e Yekutieli 2001)

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Selecting Predictors

Expanded Higher Criticism

A selection scheme for problems where effects are rare and **most** (but not necessarly all) effects are weak

- Include all variables that satisfy Benjamini and Yekutieli's criterion
- 2 Estimate an "empirical null distributiuon"
- Compute p-values for the effects of non-selected variables, based on the null estimated in step 2
- 4 Find the HC* threshold from the p-values computed in step 3

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Error Estimate Rule **# Variables kept** (std error) (min – median - max) 0.2146 Fisher's LDA* 58 **- 134.5 -** 421 (0.0101)0.0670 **Naive Bayes*** 58 **- 134.5 -** 421 (0.0052)0.0642 **Support Vector Machines*** 58 - 134.5 - 421 (0.0052)0.0838 Nearest Shruken Centroids 108 - 356 - 1771 (0.0063)0.0741 **Regularized DA** 82 - **390** - 1201 (0.0053)0.0650 Shrunken DA* 58 **- 134.5 -** 421 (0.0051)0.0641 Factor-based LDA* (q=1) 58 - 134.5 - 421 (0.0052)0.0720 NLDA* 58 **- 134.5 -** 421 (0.0052)

Singh's Prostate Cancer Data -p=6033; n=50+52

 * After variable selection by the maximum of FDR (False Discovery Rates) and HC (Higher Criticism), both derived from Independence based T-scores. The p-values used in the HC computations are derived from empirical Null distributions



Golubs's Leukemia Data -- p = 7 129; n = 47+25

Rule	Error Estimate	# Variables kept
	(std error)	(min – median - max)
Fisher's LDA*	0.2558	326 - 478 - 712
	(0.0109)	
Naive Bayes*	0.480	326 - 478 - 712
	(0.0085)	
Support Vector Machines*	0.0405	326 - 478 - 712
	(0.0049)	
Nearest Shruken Centroids	0.0201	703 - 3166 - 7129
	(0.0039)	
Regularized DA	0.0491	12 – 1934 – 7124
	(0.0062)	
Shrunken DA*	0.0276	326 – 478 – 712
	(0.0044)	
Factor-based LDA* (q=1)	0.0174	326 - 478 - 712
	(0.0034)	
	0.1510	
NLDA*	0.1510	326 - 478 - 712
	(0.0085)	

 * After variable selection by the maximum of FDR (False Discovery Rates) and HC (Higher Criticism), both derived from Independence based T-scores. The p-values used in the HC computations are derived from empirical Null distributions



Rule **Error Estimate # Variables kept** (std error) (min – median - max) 0.3285 Fisher's LDA* 3 - 71.5 - 200(0.0143)0.2275 3 - 71.5 - 200Naive Bayes* (0.0133)0.1576 **Support Vector Machines*** 3 - 71.5 - 200(0.0095)0.1563 **Nearest Shruken Centroids** 7 - 39 - 527 (0.0098)0.2174 Regularized DA 14 - 425 - 2000(0.0126)0.1865 Shrunken DA* 3 - 71.5 - 200 (0.0100)0.1746 3 - 71.5 - 200Factor-based LDA* (q=1) (0.0098)0.2614 NLDA* 3 -71.5 - 200 (0.0114)

Alon's Colon Data $-p = 2\ 000$; n = 40+22

 * After variable selection by the maximum of FDR (False Discovery Rates) and HC (Higher Criticism), both derived from Independence based T-scores. The p-values used in the HC computations are derived from empirical Null distributions

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Conclusions

✓ A factor-model classification rule, designed for highdimensional correlated data, was proposed

Asymptotic Analysis show that

As $p \rightarrow \infty$ the new rule can approach a low expected error rate

Often, much lower than

unrestricted covariance rules

independence-based rules

Empirical comparisons sugest that

when combined with sensible variable selection schemes

the new rule is highly competitive in MicroArray Applications

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High Dimensional Correlation Adjusted Classification Open Questions

Should correlations also be incorporated the selection scheme ?

When and How ?

- How do factor-based rules perform in problems with more than two groups ?
- Do differences in misclassification costs affect the relative standing of different classification rules ?

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References

* Ahdesmaki, P. and Strimmer, K. (2009). Feature selection in "omics" prediction problems using cat scores and non-discovery rate control. *rXiv,stat.AP:0903.2003v1*.

* Benjamini, Y. and Hochberg, Y. (1995). Controlling the false discovery rate: a practical and powerful approach to multiple testing. *Journal of the Royal Statistical Society* B 57, 289-300.

* Benjamini, Y. and Yekutileli, D. (2001). The control of the false discovery rate in multiple testing under dependency. *Annals of Statistics* 29, 1165-1188.

* Donoho, D. and Jin, J. (2004). Higher criticism for detecting sparse heterogeneous mixtures. *Annals of Statistics*, 32, 962-944.

* Donoho, D. and Jin, J. (2008). Higher criticism thresholding: Optimal feature selection when useful features are rare and weak. *Proc. Natl. Acad. Sci*, USA 105, 14790-14795.

* Donoho, D. and Jin, J. (2009). Feature selection by higher criticism thresholding: Optimal phase diagram. *Philosophical Transactions of the Royal Society A*, 367, 4449-4470.

* Duarte Silva, A.P. (2009). Linear Discriminant Analysis with more Variables than Observations. A not so Naïve Approach. In: *Classification as a Tool for Research. Proceedings of the 11th IFCS Biennial Conference and 33rd Annual Conference of the Gesellschaft für Klassifikation*. Dresden, Germany, 227-234.

* Efron, B. (2008). Microarrays, empirical Bayes and the two-groups model. *Statistical Science* 1, 1-22. * Guo, Y., Hastie, T. and Tibshirani, T. (2007). Regularized discriminant analysis and its application in microarrays. *Biostatistics* 8, 86-100.

* Tibshirani, R., Hastie, B., Narismhan, B. and Chu, G. (2003). Class prediction by nearest shrunken centroids with applications to DNA microarrays. *Statistical Science*, 18, 104-117.

* Thomaz, C.E. and Gillies, D.F. (2005). A maximum uncertainty lda-based approach for limited sample size problems with application to face recognition. In: 18th Brazilian Symposium on computer Graphics and Image Processing. SIBGRAPI 2005, 89-96.