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# Discriminant Analysis in High-Dimensional Gaussian Latent Mixtures

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Joint work with Xin (Mike) Bing, University of Toronto 
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#### References

#### Based on

• Xin Bing and Marten Wegkamp. Interpolating Discriminant Functions in High-Dimensional Gaussian Latent Mixtures. Biometrika (2023)

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• Xin Bing and Marten Wegkamp. Optimal Discriminant Analysis in High-Dimensional Latent Factor Models. Annals of Statistics (2023)

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#### Introduction

### Latent Factor Model

We observe independent copies of the pair (X, Y) with features  $X \in \mathbb{R}^p$  according to

$$X = AZ + W$$

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and labels  $Y \in \{0, 1\}$ .

- Only X is observed
- A is a deterministic, unknown  $p \times K$  loading matrix
- $Z \in \mathbb{R}^{K}$  are unobserved, latent factors
- W is unobserved, random noise

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#### Assumptions

(i) W is independent of both Z and Y  
(ii) 
$$\mathbb{E}[Z] = \mathbf{0}_K$$
,  $\mathbb{E}[W] = \mathbf{0}_p$   
(iii) A has rank K  
(iv)  $Z \mid Y = k \sim N_K(\alpha_k, \Sigma_{Z|Y})$  with  $\alpha_k := \mathbb{E}[Z|Y = k]$  and  
 $\Sigma_{Z|Y} := \operatorname{Cov}(Z|Y = 0) = \operatorname{Cov}(Z|Y = 1) > 0$   
(v)  $W = \Sigma_W^{1/2} V$  with  $\mathbb{E}[V] = \mathbf{0}_p$ ,  $\mathbb{E}[VV^\top] = \mathbf{I}_p$  and  
 $\sup_{\|u\|_2 = 1} \mathbb{E}[\exp(u^\top V)] \le \exp(\gamma^2/2)$ 

(vi) For some absolute constant  $c \in (0, 1)$ ,  $\min\{\pi_0, \pi_1\} \ge c$  with  $\pi_k := \mathbb{P}\{Y = k\}, k = 0, 1$ 

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### Basic inequality

#### Lemma

Under (i), (ii), (iii), we have

$$R_x^* := \inf_g \mathbb{P}\{g(X) \neq Y\} \geq R_z^* := \inf_h \mathbb{P}\{h(Z) \neq Y\}$$

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### Oracle Benchmark

We have the explicit expression

$$R_z^* = 1 - \pi_1 \Phi\left(\frac{\Delta}{2} + \frac{\log \frac{\pi_1}{\pi_0}}{\Delta}\right) - \pi_0 \Phi\left(\frac{\Delta}{2} - \frac{\log \frac{\pi_1}{\pi_0}}{\Delta}\right).$$

Here

$$\Delta^2 := (\alpha_0 - \alpha_1)^\top \Sigma_{Z|Y}^{-1} (\alpha_0 - \alpha_1)$$

is the Mahalanobis distance between the conditional means  $\alpha_0 = \mathbb{E}[Z \mid Y = 0]$  and  $\alpha_1 = \mathbb{E}[Z \mid Y = 1]$ .

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### Oracle Benchmark

- If  $\Delta \to \infty$ , then  $R_z^* \to 0$ . Trivial asymptotic Bayes error -Expect fast rates
- If  $\Delta \rightarrow 0$  and  $\pi_0 > \pi_1$ , then  $R_z^* \rightarrow \pi_1$ . Trivial asymptotic Bayes rule votes 0 all the time Expect fast rates

• If  $\Delta \rightarrow 0$  and  $\pi_0 = \pi_1 = 1/2$ , then  $R_z^* \rightarrow 1/2$ . Asymptotic random guessing - Expect slow rates

#### Conclusion:

In a way, the most interesting case is  $\Delta \simeq 1$ .

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### Oracle Benchmark

$$\Sigma_{X|Y} = A \Sigma_{Z|Y} A^{\top} + \Sigma_W$$

If the signal-to-noise ratio

$$\xi := \frac{\lambda_{\mathcal{K}}(A\Sigma_{Z|Y}A^{\top})}{\lambda_1(\Sigma_W)}$$

for predicting Z from X given Y is large, the gap between  $R_x^*$  and  $R_z^*$  is small.

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Minimax Lower Bounds



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### Minimax Lower Bound

We establish minimax-optimal rates of convergence of the excess risk

$$R_{x}(\widehat{g}) - R_{z}^{*} := \mathbb{P}\{\widehat{g}(X) \neq Y\} - \inf_{h} \mathbb{P}\{h(Z) \neq Y\}$$

for any classification rule  $\widehat{g} : \mathbb{R}^p \to \{0,1\}$  based on independent pairs  $(X_1, Y_1), \ldots, (X_n, Y_n)$  from our factor model (i)–(iv).

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### Minimax Lower Bound

• Define the parameter space of  $\theta := (A, \Sigma_{Z|Y}, \Sigma_W, \alpha)$  as

$$\begin{aligned} \pi_0 &= \pi_1 = 1/2 \\ \lambda_1(\Sigma_W) &\asymp \lambda_p(\Sigma_W) \asymp \sigma^2 \\ \lambda_1(A\Sigma_{Z|Y}A^\top) &\asymp \lambda_K(A\Sigma_{Z|Y}A^\top) \asymp \lambda \end{aligned}$$

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Set

$$\omega^2 := \frac{\kappa}{n} + \frac{\sigma^2}{\lambda} \Delta + \frac{\sigma^2 p}{\lambda n} \frac{\sigma^2}{\lambda} \Delta.$$

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#### Theorem

Assume (i) – (vi), 
$$K \ge 2$$
,  $K/(n \land p) \le c_1$ ,  $\sigma^2/\lambda \le c_2$  and  $\sigma^2 p/(\lambda n) \le c_3$  for some small constants  $c_1, c_2, c_3 > 0$ .

 $\textbf{0} \ \ \text{If} \ \Delta \asymp 1, \ \text{then there exists some constants} \ c_0 \in (0,1) \ \text{and} \ C > 0 \\ \text{such that}$ 

$$\inf_{\widehat{g}} \sup_{\theta} \mathbb{P}_{\theta} \left\{ R_{x}(\widehat{g}) - R_{z}^{*} \geq C\omega^{2} \right\} \geq c_{0}.$$

② If  $\Delta \to \infty$  and  $\sigma^2 / \lambda \to 0$ , as  $n \to \infty$ , then there exists some constants  $c_0 \in (0, 1)$  and C > 0 such that

$$\inf_{\widehat{g}} \sup_{\theta} \mathbb{P}_{\theta} \left\{ R_{x}(\widehat{g}) - R_{z}^{*} \geq C \omega^{2} e^{-\frac{1}{8}\Delta^{2} + o(\Delta^{2})} \right\} \geq c_{0}.$$

If  $\Delta \rightarrow 0$ , as *n* → ∞, then there exists some constants *c*<sub>0</sub> ∈ (0, 1) and *C* > 0 such that

$$\inf_{\widehat{g}} \sup_{\theta} \mathbb{P}_{\theta} \left\{ R_{x}(\widehat{g}) - R_{z}^{*} \geq C\omega \min\left(\frac{\omega}{\Delta}, 1\right) \right\} \geq c_{0}$$

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### Minimax lower bound

$$\omega^2 := \frac{K}{n} + \frac{\sigma^2}{\lambda} \Delta + \frac{\sigma^2 p}{\lambda n} \frac{\sigma^2}{\lambda} \Delta.$$

The lower bounds consist of three terms:

- the one related with K/n is the optimal rate of the excess risk even when Z were observable;
- the second one related with σ<sup>2</sup>/λ is the irreducible error for not observing Z;
- the last one involving  $\sigma^2 p/(\lambda n) \times (\sigma^2/\lambda)$  is the price to pay for estimating the column space of A.

- The third term can be absorbed by the second term as  $\sigma^2 p/(\lambda n) \leq c_3$ .
- The lower bounds are tight (later).

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#### Methodology

### Methodology

To motivate our approach, suppose that we observe Z. The optimal Bayes rule to classify a new point  $z \in \mathbb{R}^{K}$  is

$$g_z^*(z) = \mathbb{1}\{z^\top \eta + \eta_0 \ge 0\}$$

where

$$\eta = \Sigma_{Z|Y}^{-1}(\alpha_1 - \alpha_0), \qquad \eta_0 = -\frac{1}{2}(\alpha_0 + \alpha_1)^\top \eta + \log \frac{\pi_1}{\pi_0}.$$

This rule is optimal in the sense that it has the smallest possible misclassification error  $\mathbb{P}\{Y \neq g(Z)\}$ .

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- Modern efficient empirical LDA in the high-dimensional setting exploit potential sparsity of  $\sum_{X|Y}^{-1}(\mu_1 \mu_0)$ . See, e.g., Tibshirani et al (2002), Fan and Fan (2008), Witten and Tibshirani (2011), Shao, Wang, Deng, Wang (2011), Cai and Liu (2011), Mai, Zou, Yuan (2012), Cai and Zhang (2019ab).
- In the high-dimensional regime, many features are highly correlated and any sparsity assumption becomes questionable.

• Instead: assume low-dimensional structure and "classify projections".

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### Connection between LDA and Regression

Let  $\Sigma_Z = \mathbb{E}[ZZ^\top]$  be the unconditional covariance matrix of Z. Define

$$\beta = \pi_0 \pi_1 \Sigma_Z^{-1} (\alpha_1 - \alpha_0),$$
  
$$\beta_0 = -\frac{1}{2} (\alpha_0 + \alpha_1)^\top \beta + \pi_0 \pi_1 \left[ 1 - (\alpha_1 - \alpha_0)^\top \beta \right] \log \frac{\pi_1}{\pi_0}.$$

#### Proposition

Under Assumptions (ii) and (iv), we have

$$z^{\top}\eta + \eta_0 \ge 0 \quad \iff \quad z^{\top}\beta + \beta_0 \ge 0.$$

Furthermore,

$$\beta = \Sigma_Z^{-1} \mathbb{E}[ZY].$$

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# Methodology

- The key difference is the use of the unconditional Σ<sub>Z</sub>, as opposed to the conditional Σ<sub>Z|Y</sub>.
- We can interpret β as the regression coefficient of Y on Z. This suggests to estimate β via least squares.
- We only have access to  $x \in \mathbb{R}^p$ ,  $\boldsymbol{X} = [X_1 \cdots X_n]^\top \in \mathbb{R}^{n \times p}$ , and  $\boldsymbol{y} = (Y_1, \dots, Y_n)^\top \in \{0, 1\}^n$ .
- Since X = ZA<sup>T</sup> + W, we need to find some appropriate matrix B ≈ A(A<sup>T</sup>A)<sup>-1</sup> so that XB ≈ Z + WA(A<sup>T</sup>A)<sup>-1</sup>.

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### Methodology

Estimate the inner-product  $z^{\top}\beta$  by

$$x^{ op} \widehat{\theta} := x^{ op} B(\boldsymbol{X}B)^{+} \boldsymbol{y} = x^{ op} B(B^{ op} \boldsymbol{X}^{ op} \boldsymbol{X}B)^{+} B^{ op} \boldsymbol{X}^{ op} \boldsymbol{y}$$

for some appropriate matrix B.

#### Estimate $\beta_0$ by

$$\widehat{eta}_0 := -rac{1}{2}(\widehat{\mu}_0 + \widehat{\mu}_1)^ op \widehat{ heta} + \widehat{\pi}_0 \widehat{\pi}_1 \left[1 - (\widehat{\mu}_1 - \widehat{\mu}_0)^ op \widehat{ heta} \ 
ight] \log rac{\widehat{\pi}_1}{\widehat{\pi}_0}$$

based on standard non-parametric estimates

$$n_k = \sum_{i=1}^n \mathbb{1}\{Y_i = k\}, \quad \widehat{\pi}_k = \frac{n_k}{n}, \quad \widehat{\mu}_k = \frac{1}{n_k} \sum_{i=1}^n X_i \mathbb{1}\{Y_i = k\}.$$

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Our proposed classifier (Bing and W. 2023) is

$$\widehat{g}_x(x) := \mathbb{1}\{x^{\top}\widehat{\theta} + \widehat{\beta}_0 \ge 0\}.$$

The estimates  $\widehat{\theta}$  and  $\widehat{\beta}_0$  depend on *B*.

- We investigate  $B = U_r \in \mathbb{R}^{p \times r}$ , where  $U_r$  consists of the first r right-singular vectors of  $\widetilde{X}$ .
- X is an auxiliary n × p data matrix (unlabelled observations only), independent of the training data (X, y). If not available, split the data in two equal parts.

• What if we use **X** instead?

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### PCR-based LDA

Bing and W. (2019, 2023) propose to use  $r = \widehat{K}$  with

$$\widehat{K} := \arg\min_{0 \le k \le \bar{K}} \frac{\sum_{j > k} \sigma_j^2}{np - 2.1(n+p)k}$$

based on the singular-values  $\sigma_j$  of  $\widetilde{\boldsymbol{X}}$ , with  $\overline{K} < \lfloor \frac{1}{4.2}(n \wedge p) \rfloor$ .

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### Real data analysis

- We analyze three popular gene expression datasets (leukemia data, colon data and lung cancer data).
- For all three data sets, the features are standardized to zero mean and unit standard deviations.
- For each dataset, we randomly split the data, within each category, into 70% training set and 30% test set.
- We compare our proposed algorithm, PCLDA- $\widehat{K}$ , with the
  - Nearest Shrunken Centroids classifier (PAMR) of Tibshirani, Hastie, Narasimhan, Chu (2002),
  - *l*<sub>1</sub>-Penalized Linear Discriminant (PenalizedLDA) of Witten and Tibshirani (2011),
  - Direct Sparse Discriminant (DSDA) of Mai, Zou, Yuan (2012).

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Data name	р	n	n <sub>0</sub> (category)	n1 (category)
Leukemia	7129	72	47 (acute lymphoblastic leukemia)	25 (acute myeloid leukemia)
Colon	2000	62	22 (normal)	40 (tumor)
Lung cancer	12533	181	150 (adenocarcinoma)	31 (malignant pleural mesothelioma)

#### Summary of three data sets.

	PCLDA- $\widehat{K}$	DSDA	PenalizedLDA	PAMR
Leukemia	<b>3.57</b> (0.036)	5.52 (0.044)	3.91 (0.043)	4.61 (0.039)
Colon	16.37 (0.077)	18.11 (0.07)	33.95 (0.086)	19.00 (0.089)
Lung cancer	<b>0.55</b> (0.008)	1.69 ( 0.017)	1.80 (0.026)	0.91 (0.011)

The averaged misclassification errors (in percentage). The numbers in parentheses are the standard deviations over 100 repetitions.

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Rates of convergence for the excess risk



## General method for deriving upper bounds

We view  $R_z^*$  as an oracle risk since the  $Z_i$  aren't observed. Our proposed classifier is designed to estimate the Bayes classifier  $g_z^*$  in  $\mathbb{R}^K$  and to adapt to the underlying low-dimensional structure.

#### We define

$$\widehat{G}_x(x) := x^\top \widehat{\theta} + \widehat{\beta}_0, \qquad G_z(z) := z^\top \beta + \beta_0$$

so that  $\widehat{g}_x(x) = \mathbb{1}\{\widehat{G}_x(x) \ge 0\}$  and  $g_z^*(z) = \mathbb{1}\{G_z(z) \ge 0\}$ .

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#### Theorem

Set 
$$c_* = (1 + \pi_0 \pi_1 \Delta^2)/(\pi_0 \pi_1)$$
. For all  $t > 0$ ,  
 $R_x(\widehat{g}_x) - R_z^* \leq \mathbb{P}\{|\widehat{G}_x(X) - G_z(Z)| > t\} + c_* t P(t),$ 
with

$$egin{aligned} & P(t) := & \pi_0 \mathbb{P}\{-c_* t < G_z(Z) < 0 \mid Y = 0\} + \ & \pi_1 \mathbb{P}\{0 < G_z(Z) < c_* t \mid Y = 1\}. \end{aligned}$$

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Rate depends on

- estimate of optimal half space
- behavior around the decision boundary

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## Explicit expression for P(t)

#### Since Z is Gaussian, P(t) can be simplified.

Proposition

Assume (i) – (iv). For all  $\omega_n 
ightarrow$  0, the exists 0 < c < 1/8,

$$P(\omega_n) \lesssim \begin{cases} \omega_n & \text{if } \Delta \asymp 1\\ \omega_n \exp(-c\Delta^2) & \text{if } \Delta \to \infty\\ \omega_n \exp(-c/\Delta^2) & \text{if } \Delta \to 0 \text{ and } \pi_0 \neq \pi_1\\ \min(1, \omega_n/\Delta) & \text{if } \Delta \to 0 \text{ and } \pi_0 = \pi_1 = 1/2 \end{cases}$$

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### Estimation of optimal boundary

Since

$$\widehat{G}_{x}(\boldsymbol{X}) - G_{z}(\boldsymbol{Z}) = \boldsymbol{Z}^{\top}(\boldsymbol{A}^{\top}\widehat{\theta} - \beta) + \boldsymbol{W}^{\top}\widehat{\theta} + \widehat{\beta}_{0} - \beta_{0}$$

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the key quantities to bound are

• 
$$\|\widehat{\theta}\|_2$$
  
•  $\|\Sigma_Z^{1/2}(A^{\top}\widehat{\theta} - \beta)\|_2$ .

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### Rates of Convergence

#### Theorem - simplified case

Let  $\theta \in \Theta(\lambda, \sigma, \Delta)$  with  $\Delta \simeq 1$  and  $\kappa(A\Sigma_Z A^\top) \simeq 1$ . With probability  $1 - \mathcal{O}(n^{-1})$ ,

$$R_{x}(\widehat{g}_{x}) - R_{z}^{*} \lesssim \left[\frac{K \log n}{n} + \frac{\sigma^{2}}{\lambda} + \left(\frac{p}{n}\frac{\sigma^{2}}{\lambda}\right)^{2}\right] \log n, \quad \text{if } B = U_{K};$$
  
$$R_{x}(\widehat{g}_{x}) - R_{z}^{*} \lesssim \left[\frac{K \log n}{n} + \frac{\sigma^{2}}{\lambda}\right] \log n, \quad \text{if } B = \widetilde{U}_{K}.$$

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### Rates of Convergence

- (1) If p < n, the two rates coincide and consistency of both PC-based classifiers requires that  $K \log^2 n/n \rightarrow 0$  and  $\sigma^2 \log n/\lambda \rightarrow 0$ .
- (2) If p > n, and

$$\frac{\lambda}{\sigma^2} \gtrsim \min\left\{\left(\frac{p}{n}\right)^2, \frac{p}{\sqrt{nK\log n}}\right\}$$

the two rates coincide.

(3) If p > n and  $\lambda/\sigma^2$  is relatively small, the effect of using  $B = \tilde{U}_K$  based on an independent data set  $\tilde{X}$  is real as evidenced on the next slide where we keep  $\lambda/\sigma^2$ , n and K fixed but let p grow.

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Illustration of the advantage of constructing  $\tilde{U}_K$  from an independent dataset: PCLDA represents the PC-based classifier based on  $B = U_K$  while PCLDA-split uses  $B = \tilde{U}_K$  that is constructed from an independent  $\tilde{X}$ . Oracle-LS is the oracle benchmark that uses both Z and Z while Bayes represents the risk of using the oracle Bayes rule. We fix n = 100 and K = 5 and keep  $\lambda/\sigma^2$  fixed, while we let p grow.

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#### Simulations

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• We set 
$$\pi_0 = \pi_1 = 1/2$$
,  $\alpha_0 = -\alpha_1 = -(\frac{1}{2}\sqrt{\eta/K}) \mathbf{1}_K$ .

- The parameter  $\eta$  controls the signal strength  $\Delta$ .
- We generate  $\Sigma_{Z|Y}$  as follows:

• 
$$[\Sigma_{Z|Y}]_{ii}$$
 are iid Unif(1,3)  
•  $[\Sigma_{Z|Y}]_{ij} = \sqrt{[\Sigma_{Z|Y}]_{ii}[\Sigma_{Z|Y}]_{jj}}(-1)^{i+j}(0.5)^{|i-j|}$  for each  $i \neq j$ 

- We generate  $\Sigma_W$  in the same way, except  $\operatorname{diag}(\Sigma_W) = \mathbf{1}_p$ .
- Rows of  $\mathbf{W} \in \mathbb{R}^{n \times p}$  are iid  $N_p(0, \Sigma_W)$ .
- Entries of A are iid  $N(0, 0.3^2)$ .



#### $\eta = 5, K = 10, p = 300 \text{ and } n \in \{50, 100, 300, 500, 700\}$

#### $K = 5, n = 100, p = 300 \text{ and } \eta \in \{2, 4, 6, 8, 10\} \Longrightarrow \Delta^2 \in \{3.1, 6.3, 9.4, 12.6, 15.7\}$



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 $K = 5, \eta = 5, n = 100 \text{ and } p \in \{100, 300, 500, 700, 900\}.$ 



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#### Interpolation

### Question:

What happens if 
$$B = I_p$$
, hence  $\hat{\theta} = X^+ y$  (generalized least squares)?

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### Interpolation

#### Phenomenon: deep neural networks

It is possible to achieve good generalization error despite zero training error (overfitting)!

- In regression context: Bartlett et al (2020), Belkin et al (2018), Hastie et al (2022)
   For this model: Bing, Bunea, Strimas-Mackey, W (2021), Bunea, Strimas-Mackey, W (2022)
- For binary classification: Cao et al (2021), Chatterji and Long (2021), Hsu et al (2021), Minsker et al (2021), Muthukumar et al (2019), Wang and Thrampoulidis (2021)

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- Current literature on classification considers
  - Decision boundaries are hyperplanes through origin
  - Misclassification risk, not excess risk, is bounded.
- These interpolation methods without intercept actually fail when the mixture probabilities are asymmetric and the Bayes error does not vanish.

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#### Our results:

- We will show that  $\widehat{g}(x) = x^{\top}\widehat{\theta} + \widehat{\beta}_0$  has zero training error, but is inconsistent due to plug-in estimate  $\widehat{\beta}_0$ .
- We need to use an independent hold-out sample to estimate intercept  $\beta_0$  to obtain consistency and sometimes even minimax optimality.
- The interpolation property may be destroyed. However, if we encode the labels differently, e.g., via ±1, interpolation is preserved (if one cares).
- We provide a concrete instance of the interesting phenomenon that overfitting and minimax-optimal generalization performance can coexist in a latent low-dimensional statistical model, against traditional statistical belief.

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### Interpolation

#### Proposition (Bunea, Strimas-Mackey, W 2022)

Assume  $n \ge K$ . Then, there exist finite, positive constants C, c depending on  $\sigma$  only, such that, provided  $r_e(\Sigma_W) = tr(\Sigma_W)/||\Sigma_W||_{op} \ge Cn,$ 

$$\mathbb{P}\left\{\sigma_n^2(\boldsymbol{X}) \geq \frac{1}{8} \mathrm{tr}(\boldsymbol{\Sigma}_W)\right\} \geq 1 - 3\exp(-c \ n)$$

#### Corollary: interpolation is common

Assume  $p \ge n \ge K$ ,  $\|\Sigma_W\|_{op} \asymp 1$  and  $tr(\Sigma_W) \asymp p$ . Then the GLS  $\widehat{\theta} = \mathbf{X}^+ \mathbf{y}$  interpolates the data

$$\lim_{n\to\infty} \mathbb{P}\{\boldsymbol{X}\widehat{\theta} = \boldsymbol{y}\} = 1.$$

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### Interpolation

Observation: zero training error if intercept in (-1, 0]

If  $\widehat{\theta} = \mathbf{X}^+ \mathbf{y}$  interpolates, then the classifier

$$\mathbb{1}\{x^{\top}\widehat{\theta} + \overline{\beta}_0 > 0\}$$

perfectly classifies the training data for any  $\bar{\beta}_0 \in (-1, 0]$  (including zero intercept).

Simply note that, as long as  $\bar{\beta}_0 \in (-1, 0]$ ,

$$X_i^{\top} \widehat{\theta} + \overline{\beta}_0 = Y_i + \overline{\beta}_0 > 0 \iff Y_i = 1$$
, for all  $i \in [n]$ 

We will argue that interpolation depends on how we encode labels

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### Interpolation

#### Question:

Does the classifier  $\mathbb{1}\{x^{\top}\widehat{\theta} + \beta_0 > 0\}$  that uses the true intercept  $\beta_0$  yield zero training error ?

This is equivalent with verifying if  $\beta_0 \in (-1, 0]$ .

#### Answer:

It depends! Only if we encode the majority class as 0.

#### Lemma

The true intercept  $\beta_0$  satisfies

$$\operatorname{sgn}(eta_0) = \operatorname{sgn}\left(rac{1}{2} - \pi_0
ight), \qquad |eta_0| \leq \left|rac{1}{2} - \pi_0
ight|.$$

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#### Observation

- The optimal decision boundary in the latent space is independent of the particular encoding.
- Interpolation property crucially depends on the way we encode the labels.
- For instance, if we encode Y as  $\{-1,1\}$ , the classifier

$$2\mathbb{1}\{x^{\top}\widehat{\theta}+2\beta_0>0\}-1$$

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always has zero training error (as  $|\beta_0| \leq 1/2$ ).

### Interpolation leads to inconsistency

The following lemma shows that  $\hat{\beta}_0 = -1/2$ , irrespective of the true value of  $\beta_0$ , whenever  $\hat{\theta}$  interpolates.

#### Proposition

Let  $\hat{\beta}_0$  be the plug-in estimate. On the event  $\{\mathbf{X}\hat{\theta} = \mathbf{y}\}$  where  $\hat{\theta}$  interpolates, we have  $\hat{\beta}_0 = -1/2$ .

•  $\widehat{g}(x) = \mathbb{1}\{x^{\top}\widehat{\theta} + \widehat{\beta}_0 > 0\}$  always interpolates as  $\widehat{\beta}_0 \in (-1, 0]$ .

- $\hat{\beta}_0$  is an inconsistent estimate of  $\beta_0$  in general.
- Confirmed in simulations: classifier is inconsistent.

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### What can we do?

π<sub>0</sub> = π<sub>1</sub> = 1/2. In this case β<sub>0</sub> = 0, no need to estimate β<sub>0</sub> (current literature).

2) 
$$\pi_0 
eq \pi_1$$
. Estimate  $\beta_0$  by

$$\widehat{eta}_0 := -rac{1}{2} (\widetilde{\mu}_0 + \widetilde{\mu}_1)^ op \widehat{ heta} + \left[ 1 - (\widetilde{\mu}_1 - \widetilde{\mu}_0)^ op \widehat{ heta} \ 
ight] \widehat{\pi}_0 \widehat{\pi}_1 \log rac{\widehat{\pi}_1}{\widehat{\pi}_0}$$

with  $\widehat{ heta}$  and  $\widehat{\pi}_k$  as before, but

$$\widetilde{\mu}_k = \frac{1}{\widetilde{n}_k} \sum_{i=1}^{n'} X_i' \mathbb{1}\{Y_i' = k\}, \quad \widetilde{n}_k = \sum_{i=1}^{n'} \mathbb{1}\{Y_i' = k\}$$

are based on an independent hold-out sample of size  $n' \simeq n$ .

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### Modified classifier

#### Theorem: Simplified rates of convergence

#### Suppose

$$\theta \in \Theta(\lambda, \sigma, A), \ p \gg n \gg K, \ \Delta \asymp 1, \ n \asymp n', \ \kappa \asymp 1$$

Then  $\widetilde{g}(x) = \mathbb{1}\{x^{\top}\widehat{\theta} + \widetilde{\beta}_0 > 0\}$  satisfies

$$R_x(\widetilde{g}) - R_z^* \lesssim \left[ rac{K \log(n)}{n} + rac{n}{p} + \left(rac{p}{n \ \xi}
ight)^2 + rac{1}{\xi} 
ight] \log(n).$$

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## Simplified rates of convergence

#### Summary

- If  $\xi \gg p/n$ , then  $\widetilde{g}$  is consistent
- If, furthermore,  $\xi\gtrsim (p/n)\cdot (n/{\cal K})^{1/2}$ , then

$$\mathbb{P}\{\widetilde{g}(X) \neq Y\} - R_z^* \lesssim \frac{K}{n}\log^2(n) + \frac{n}{p}\log(n).$$

• If, in addition,  $p \gtrsim n^2/K$ , then  $\tilde{g}$  is minimax-optimal.

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#### Simulations

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We generated the data as follows:

• 
$$\pi_0 = \pi_1 = 0.5$$

• 
$$\alpha_0 = -\alpha_1, \ \alpha_1 = \mathbf{1}_K \sqrt{2/K}$$

• 
$$\Sigma_{Z|Y} = I_K$$
 (This implies  $\Delta^2 = 8$ ).

 Entries of W and A are independent realizations of N(0, 1) and N(0, 0.3<sup>2</sup>), respectively.

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We first verify the inconsistency of the naive classifier that uses the naive plug-in estimator of  $\beta_0$  and contrast with other consistent classifiers.

- GLS-Naive: classifier  $\widehat{g}(x) = \mathbb{1}\{x^{\top}\widehat{\theta} + \widehat{\beta}_0 > 0\}$  with  $\widehat{\beta}_0$  being the naive plug-in estimator
- GLS-Oracle, GLS-Plugin and GLS-ERM represent  $\mathbb{1}\{x^{\top}\widehat{\theta} + \overline{\beta}_0 > 0\}$  with  $\overline{\beta}_0$  chosen as the true  $\beta_0$ , the plug-in estimate based on data splitting, and the estimate based on empirical risk minimization, respectively.
- Besides the optimal Bayes classifier (Bayes), we also choose the oracle procedure (Oracle-LS) that uses both **Z** and *Z* as our benchmark.



The performance of all classifiers on 200 test data points, averaged over 100 simulations, for K = 5 and n = 100, and  $p \in \{300, 600, 1000, 2000, 4000, 6000\}$ .



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- We evaluate the performance of our proposed classifier and examine its dependence on *p*, *K* and ξ.
- We consider the misclassification error on 200 test data points, the estimation error  $\|\beta A^{\top}\widehat{\theta}\|_{\Sigma_{Z}}$  of  $\beta$ , and the estimation error  $|\widetilde{\beta}_{0} \beta_{0}|$  of  $\beta_{0}$ .
- The sample size is fixed as n = 100 and we use a validation set with 100 data points to compute β
  <sub>0</sub>.

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Setting	Misclassification errors	Errors of estimating $\beta$	Errors of estimating $\beta_0$
$K = 5, \sigma_A = 0.3$			
<i>p</i> = 300	0.256 (0.046)	0.144 (0.052)	0.040 (0.031)
p = 600	0.198 (0.037)	0.127 (0.046)	0.034 (0.023)
p = 1000	0.156 (0.032)	0.117 (0.041)	0.029 (0.021)
<i>p</i> = 2000	0.132 (0.034)	0.115 (0.039)	0.029 (0.024)
<i>p</i> = 4000	0.116 (0.027)	0.112 (0.032)	0.027 (0.020)
$p = 1000, \sigma_A = 0.3$	}		
K = 3	0.152 (0.033)	0.091 (0.039)	0.028 (0.020)
K = 5	0.161 (0.029)	0.117 (0.039)	0.032 (0.022)
K = 10	0.178 (0.036)	0.180 (0.036)	0.033 (0.027)
K = 15	0.186 (0.038)	0.219 (0.040)	0.030 (0.022)
p = 1000, K = 5			
$\sigma_A = 0.01$	0.479 (0.038)	0.397 (0.004)	0.048 (0.039)
$\sigma_A = 0.05$	0.282 (0.039)	0.239 (0.024)	0.034 (0.026)
$\sigma_A = 0.1$	0.187 (0.035)	0.124 (0.037)	0.029 (0.019)
$\sigma_A = 0.24$	0.161 (0.033)	0.109 (0.034)	0.029 (0.022)

Introduction	Minimax Lower Bounds	Methodology	Rates of convergence	Simulation study	Interpolation	Simulation study
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#### Thank you!