



Bended discriminant analysis:

a Bayesian nonparametric approach to discriminant analysis

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- ▶ Joint project with Laura D'Angelo and Tommaso Rigon
- ▶ Preliminary results in this presentation



Discriminant analysis

- ▶ Classical approach to supervised classification
- ▶ Very popular thanks to its simplicity

Variants:

- ▶ Linear discriminant analysis (**LDA**) [Fisher, 1936]
- ▶ Quadratic discriminant analysis (**QDA**)
- ▶ Various generalizations [see EOSL, Hastie et al, 2009]

*“Both **LDA** and **QDA** perform well on an amazingly large and diverse set of classification tasks. [...] It seems that whatever exotic tools are the rage of the day, we should always have available these two simple tools.”* [Hastie et al, 2009]

Setup and notation

- ▶ Data: $(\mathbf{x}, \mathbf{y}) = \{(x_i, y_i) : i = 1, \dots, n\}$, where:
predictors: $x_i \in \mathbb{R}^d$
categorical response: $y_i \in \mathcal{G} = \{1, \dots, G\}$
- ▶ Assumption on the distribution of the predictors x_i :

$$x_i \mid y_i = g, \boldsymbol{\mu}, \boldsymbol{\Sigma} \stackrel{\text{ind}}{\sim} \text{N}_d(\mu_g, \Sigma_g),$$

where $\boldsymbol{\mu} = (\mu_1, \dots, \mu_G)$ and $\boldsymbol{\Sigma} = (\Sigma_1, \dots, \Sigma_G)$

- ▶ Bayes classifier: given a predictor x_* , a prediction $\hat{y}(x_*)$ is made based on the posterior probability of the response y_* :

$$\hat{y}(x_*) = \underset{g \in \mathcal{G}}{\operatorname{argmax}} \Pr(y_* = g \mid x_*)$$

Discriminant functions

$$\begin{aligned}\Pr(y_* = g \mid x_*) &\stackrel{\text{Bayes}}{\propto} \Pr(y_* = g)p(x_* \mid y_* = g) \\ &= \pi_g f_{\mathbf{N}_d}(x_*; \mu_g, \Sigma_g)\end{aligned}$$

π_g : prior probability for category g

$f_{\mathbf{N}_d}$: pdf of a d -dimensional normal

- ▶ E.g., two categories (g_1, g_2) with $\pi_1 = \pi_2$: $\hat{y}(x_*) = g_1$ if

$$\log \Pr(y_* = g_1 \mid x_*) > \log \Pr(y_* = g_2 \mid x_*)$$

- ▶ The assumption of normality of the predictors leads to a discriminant inequality *quadratic* in x_* (QDA)
- ▶ Further assuming that $\Sigma_g = \Sigma$ for every $g \in \mathcal{G}$ leads to a discriminant inequality *linear* in x_* (LDA)

Parameters

The discriminant inequalities involve parameters to be estimated:

LDA: $\boldsymbol{\pi} = (\pi_1, \dots, \pi_G)$, $\boldsymbol{\mu} = (\mu_1, \dots, \mu_G)$, $\boldsymbol{\Sigma}$

QDA: $\boldsymbol{\pi} = (\pi_1, \dots, \pi_G)$, $\boldsymbol{\mu} = (\mu_1, \dots, \mu_G)$, $\boldsymbol{\Sigma} = (\boldsymbol{\Sigma}_1, \dots, \boldsymbol{\Sigma}_G)$

Approach is flexible in the choice of the estimation method:

- ▶ Maximum likelihood estimators
- ▶ Bayesian posterior estimators
- ▶ Other estimators, depending on the focus

LDA, QDA or other variants?

- ▶ QDA makes less assumptions than LDA but requires estimating a larger number of parameters
- ▶ Issue when the class-specific sizes n_g are small and d is large

Compromises studied in the literature, e.g.:

- ▶ Regularized discriminant analysis (RDA) [Friedman, 1989]

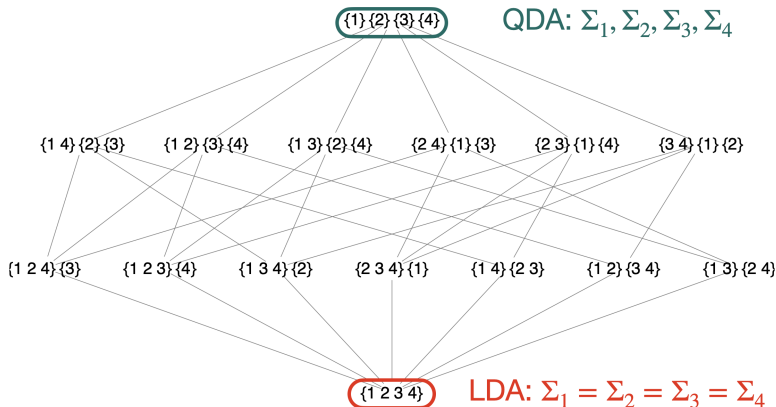
$$\hat{\Sigma}_g(\alpha) = \alpha \hat{\Sigma}_g + (1 - \alpha) \hat{\Sigma}$$

$\hat{\Sigma}_g(\alpha)$ combines the assumptions of LDA and QDA

We instead explore methods that lie in between LDA and QDA

Between LDA and QDA

Example with $G = 4$. Hasse diagram:



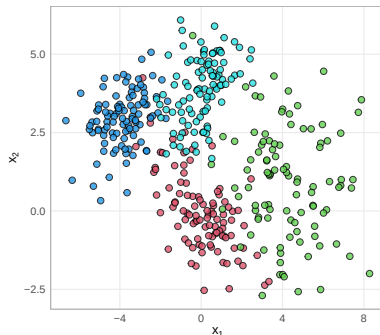
► LDA and QDA extreme cases of a rich collection of models

Bended discriminant analysis

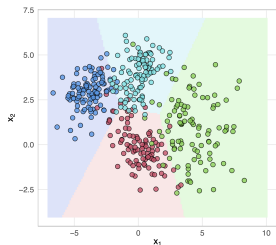
- ▶ Problem of selecting among B_G (Bell number) models
- ▶ $B_G = 15$ when $G = 4$ as in the example
- ▶ $\{\text{models}\} \longleftrightarrow \{\text{partitions of } \mathcal{G} = \{1, \dots, G\}\}$
e.g. $\{1, 2\}, \{3, 4\}$ corresponds to model $\Sigma_1 = \Sigma_2, \Sigma_3 = \Sigma_4$
- ▶ Idea: assigning positive prior probability to all possible partitions of $\mathcal{G}$
- ▶ Our proposal: bended discriminant analysis (BDA)
- ▶ LDA and QDA are special cases of BDA

Toy example with $G = 4$ classes

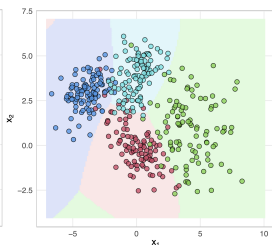
- ▶ Simulate $n_g = 100$ points per class from a normal distribution
- ▶ Means: $\mu_1 = (0, 0)$, $\mu_2 = (4, 1)$, $\mu_3 = (-4, 3)$, $\mu_4 = (0, 4)$
- ▶ Covariances: $\Sigma_1, \Sigma_2, \Sigma_3 = \Sigma_4$ (i.e. $\{1\}, \{2\}, \{3, 4\}$)



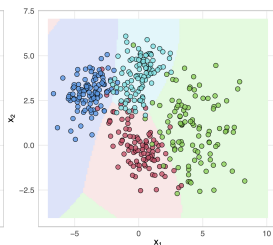
Toy example: classification regions



LDA



QDA



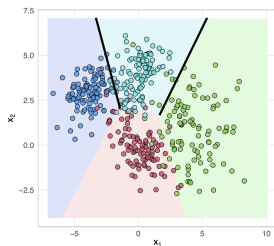
BDA

LDA: $\Sigma_1 = \Sigma_2 = \Sigma_3 = \Sigma_4$

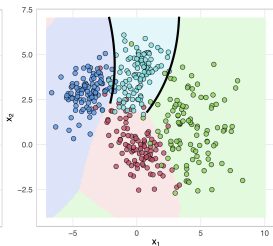
QDA: $\Sigma_1, \Sigma_2, \Sigma_3, \Sigma_4$

BDA: selected model: $\{1\}, \{2\}, \{3, 4\}$, i.e. $\Sigma_1, \Sigma_2, \Sigma_3 = \Sigma_4$

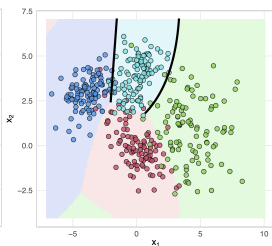
Toy example: classification regions



LDA



QDA



BDA

LDA: $\Sigma_1 = \Sigma_2 = \Sigma_3 = \Sigma_4$

QDA: $\Sigma_1, \Sigma_2, \Sigma_3, \Sigma_4$

BDA: selected model: $\{1\}, \{2\}, \{3, 4\}$, i.e. $\Sigma_1, \Sigma_2, \Sigma_3 = \Sigma_4$

Latent partition model

- ▶ BDA exploits a latent partition model over $\mathcal{G} = \{1, \dots, G\}$
- ▶ A random partition $\mathcal{S}$ of $\mathcal{G}$ is implied by a nonparametric mixture with only $\{\Sigma_1, \dots, \Sigma_G\}$ modeled nonparametrically

Hierarchical model on $\{(\mu_g, \Sigma_g) : g = 1, \dots, G\}$:

$$\mu_g \mid \Sigma_g \stackrel{\text{iid}}{\sim} \text{N}_d \left(\mu_{0,g}, \frac{\Sigma_g}{\tau_{0,g}} \right)$$

$$\Sigma_g \mid P \stackrel{\text{iid}}{\sim} P$$

$$P \sim Q$$

- ▶ Q : distribution of discrete nonparametric random measure (e.g. DP, Gibbs) on the space of positive-definite matrices
- ▶ Inverse-Wishart(Λ_0, ν_0) as base measure of Q

Complete Bayesian model for BDA

$$\Pr(y_* = g \mid x_*) \propto \pi_g f_{N_d}(x_*; \mu_g, \Sigma_g)$$

We define a Bayesian model with two components:

1. Scale-only mixture model for $\{(\mu_g, \Sigma_g) : g = 1, \dots, G\}$
2. Prior for prior probabilities

$$(\pi_1, \dots, \pi_G) \sim \text{Dirichlet}(\beta_1, \dots, \beta_G)$$

Recall: the EPPF of a Gibbs-type prior Q [De Blasi et al., 2013] with $\sigma \leq 1$ and weights $\{V_{n,k} : n \geq 1, 1 \leq k \leq n\}$ is given by

$$p(\mathcal{S}) = \Pi_k^{(G)}(\tilde{n}_1, \dots, \tilde{n}_k) = V_{n,k} \prod_{j=1}^k (1 - \sigma)^{\tilde{n}_j - 1}$$

with $\mathcal{S}$ partition of $\mathcal{G} = \{1, \dots, G\}$ with k blocks of size $\tilde{n}_1, \dots, \tilde{n}_k$

Posterior over the space of partitions (I)

Key for model selection is the posterior distribution of $\mathcal{S}$:

$$p(\mathcal{S} \mid \mathbf{x}, \mathbf{y}) \propto V_{n,k} \frac{|\Lambda_0|^{k\nu_0/2}}{\Gamma_d(\nu_0/2)^k} \prod_{j=1}^k \left\{ (1 - \sigma)^{\tilde{n}_j - 1} \frac{\Gamma_d(\nu_{n,j}/2)}{|\Lambda_{n,j}|^{\nu_{n,j}/2}} \right\},$$

obtained after *marginalizing* with respect to parameters $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$

- ▶ In classification problems, G is typically of moderate size
- ▶ $p(\mathcal{S} \mid \mathbf{x}, \mathbf{y})$ can be evaluated over the whole space of models

How many evaluations?

G	2	3	4	5	6	7	8	9	10
B_G	2	5	15	52	203	877	4140	21147	115975

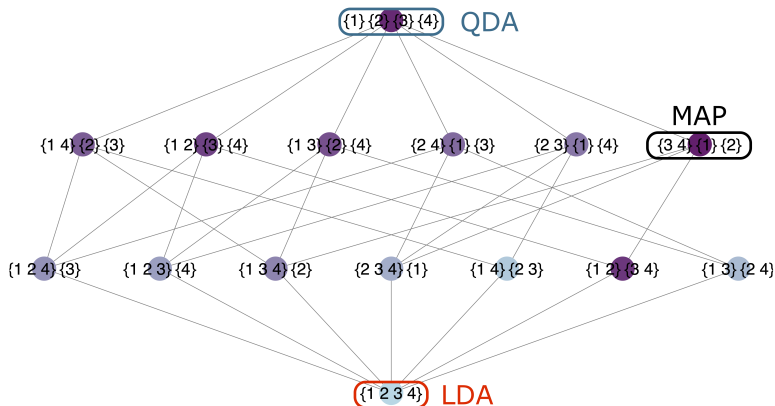
Posterior over the space of partitions (II)

The evaluation of $p(\mathcal{S} \mid \mathbf{x}, \mathbf{y})$ allows us to:

- ▶ Compute the normalizing constant
- ▶ Identify the MAP $\hat{\mathcal{S}}$
- ▶ Identify a set of likely partitions/models
[Wade & Ghahramani, 2018; Balocchi & Wade, 2025]
- ▶ Sample exactly from $p(\mathcal{S} \mid \mathbf{x}, \mathbf{y})$
- ▶ Evaluate functionals of interest, e.g. the posterior distribution of the number of blocks $|\mathcal{S}|$:

$$\Pr(|\mathcal{S}| = k \mid \mathbf{X}, \mathbf{y}) \propto V_{n,k} \frac{|\Lambda_0|^{k\nu_0/2}}{\Gamma_d(\nu_0/2)^k} \sum_{\mathcal{S}: |\mathcal{S}|=k} \left\{ \prod_{j=1}^k (1 - \sigma) \tilde{n}_j - 1 \frac{\Gamma_d(\nu_{n,j}/2)}{|\Lambda_{n,j}|^{\nu_{n,j}/2}} \right\}$$

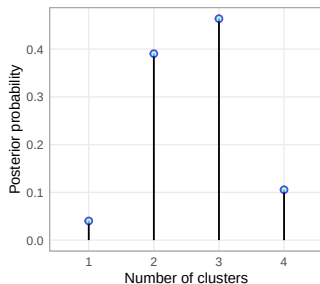
Back to toy example with $G = 4$ classes



purple: high posterior; light blue: low posterior.

Toy example: posterior inference on $\mathcal{S}$

- ▶ MAP: $\hat{\mathcal{S}} = \{\{1\}, \{2\}, \{3, 4\}\}$
- ▶ Posterior distribution of number of blocks in $\mathcal{S}$:



Classification via conditional posterior predictive

We want to classify a new statistical unit with predictors x_* :

- Conditionally on an estimated partition/model $\hat{\mathcal{S}}$:

$$\Pr(y_* = g \mid x_*, \mathbf{x}, \mathbf{y}, \hat{\mathcal{S}}) \propto \frac{\beta_g + n_g}{\sum_{h=1}^G (\beta_h + n_h)} t_{\nu_{n,j} - d + 1} \left(x_*; \mu_{j,n}, \frac{\Lambda_{n,j}(\tau_{n,g} + 1)}{\tau_{n,g}(\nu_{n,j} - d + 1)} \right)$$

- Bayes classifier:

$$\hat{y}(x_*) = \operatorname{argmax}_{g \in \mathcal{G}} \Pr(y_* = g \mid x_*, \mathbf{x}, \mathbf{y}, \hat{\mathcal{S}})$$

Classification via marginal posterior predictive

We want to classify a new statistical unit with predictors x_* :

- By marginalizing with respect to $\mathcal{S}$:

$$\Pr(y_* = g \mid x_*, X, y) = \sum_{\mathcal{S} \in \mathcal{P}_{\mathcal{G}}} \Pr(y_* = g \mid x_*, \mathbf{x}, \mathbf{y}, \mathcal{S}) p(\mathcal{S} \mid x_*, \mathbf{x}, \mathbf{y})$$

whose evaluation is possible but computationally intensive

- If G is not small, via Monte Carlo:

$$\mathbb{E}_{\mathcal{S} \mid x_*, \mathbf{x}, \mathbf{y}} [\Pr(y_* = g \mid x_*, \mathbf{x}, \mathbf{y}, \mathcal{S})]$$

- Bayes classifier:

$$\hat{y}(x_*) = \operatorname{argmax}_{g \in \mathcal{G}} \mathbb{E}_{\mathcal{S} \mid x_*, \mathbf{x}, \mathbf{y}} [\Pr(y_* = g \mid x_*, \mathbf{x}, \mathbf{y}, \mathcal{S})]$$

Simulation experiment

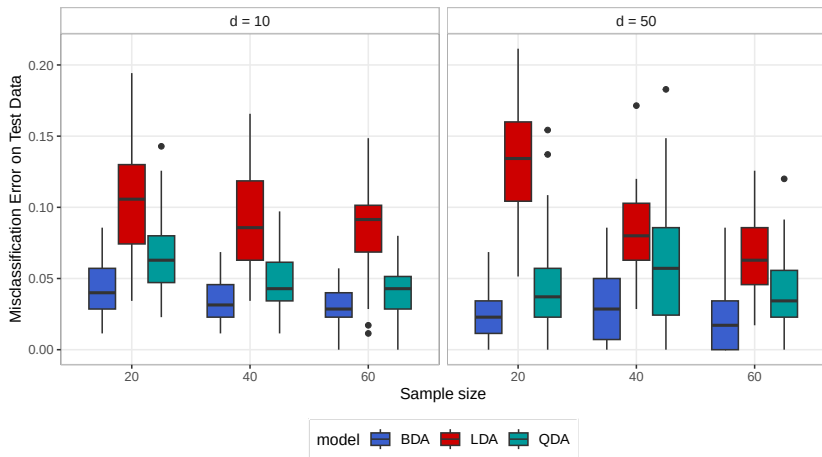
Synthetic data:

- ▶ $d \in \{10, 50\}$
- ▶ $G = 7$, with $n_g \in \{20, 40, 60\}$
- ▶ $\mathcal{S} = \{\{1, 2, 3\}, \{4, 5, 6\}, \{7\}\}$
i.e. $\Sigma_1 = \Sigma_2 = \Sigma_3$; $\Sigma_4 = \Sigma_5 = \Sigma_6$; Σ_7
- ▶ 50 replicated datasets per scenario

Data analyzed with:

- ▶ LDA
- ▶ QDA
- ▶ BDA (via conditional posterior predictive)

Simulation experiment



What's next?

- ▶ Algorithmic approach to find the MAP $\hat{\mathcal{S}}$ when $G > 10$
- ▶ BDA's performance on challenging scenarios
- ▶ Study the impact of the choice nonparametric prior for P
- ▶ Incorporate class-specific covariates by modeling P with a PPMx (product partition model with regression on covariates)
[Müller et al., 2011]
- ▶ Comments and suggestions are welcome!

Some references

- ▶ Balocchi, C., & Wade, S. (2025). Understanding uncertainty in Bayesian cluster analysis. *arXiv preprint*.
- ▶ De Blasi, P., Favaro, S., Lijoi, A., Mena, R. H., Prünster, I., & Ruggiero, M. (2013). Are Gibbs-type priors the most natural generalization of the Dirichlet process?. *IEEE transactions on pattern analysis and machine intelligence*.
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