Variational Nonparametric Discriminant Analysis

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Abstract

Variable selection and classification methods are common objectives in the analysis of high-dimensional data. Most of these methods make distributional assumptions that may not be compatible with the diverse families of distributions in the data. In this paper, we propose a novel Bayesian nonparametric discriminant analysis model that performs both variable selection and classification in a seamless framework. Pólya tree priors are assigned to the unknown group-conditional distributions to account for their uncertainty and allow prior beliefs about the distributions to be incorporated simply as hyperparameters. The computational cost of the algorithm is kept within an acceptable range by collapsed variational Bayes inference and a chain of functional approximations. The resultant decision rules carry heuristic interpretations and are related to the existing two-sample Bayesian nonparametric hypothesis test. By an application to some simulated and publicly available real datasets, we showed that our method performs well in comparison to current state-of-art approaches.

1 Introduction

Discriminant analysis (DA) is a classification model that has seen several recent applications in high dimensional data analysis. In the context of two response groups, DA classifies a new observation to group 1 if the joint likelihood of the variables and response evaluated at group 1 is greater than the joint likelihood evaluated at group 0. To facilitate the computation of the joint likelihood, the group-conditional distribution (the conditional distribution given the response) of the predictor-variables is commonly assumed to be Gaussian as with the popular variants such as linear discriminant analysis and quadratic discriminant analysis (Fisher, 1936; McLachlan, 1992). However, the usefulness of DA in high-dimensional data analysis is limited by its inability to perform variable selection and its restrictive distributional assumptions. In particular, the analysis of large datasets often involves the identification of discriminative variables among a huge set of variables that do not follow the same distributional family. While extensions that perform variable selection are available (see for example: Friedman, 1989; Ahdès-mäki and Strimmer, 2010; Witten and Tibshirani, 2011; Yu and Ormerod, 2018), most of them rely on the Gaussian distributional assumption that is unlikely to be a good fit for all available variables.

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While solutions such as monotonic transformations (see for example Box and Cox 1964; Benjamini and Speed 2012) and finite mixture modelling for the group-conditional distributions (Hastie and Tibshirani 1993; Celeux 2006) can improve the fit of the data to the distributional assumptions in DA, problems may still arise. In particular, finite mixture modelling is still subject to model misspecification if the number of mixture components and/or the mixture densities are incorrectly specified (Fraley and Raftery 2002).

These problems can be avoided by adopting nonparametric approaches as they do not confine the model space to a particular parametric family. An example of the nonparametric approach is to estimate the unknown group-conditional distributions with kernel density estimators (see Hall and Wand 1988; Ghosh and Chaudhuri 2004; Ghosh et al. 2006). However, the density may be undersmoothed in regions of the domain space where there are few observations. This risk is mitigated in Bayesian nonparametrics where the data can be down-weighted with a prior distribution in the posterior inference. In Bayesian nonparametrics, the unknown group-conditional distributions are regarded as random measures and assigned a prior on the space of possible distributions. A popular option is the Dirichlet process mixture that has been incorporated into several DA models (see for example Fuentes-García et al. 2010; Ouyang and Liang 2017). An alternative prior is the Pólya tree (Mauldin et al. 1992). Unlike the Dirichlet process mixture, it allows us to incorporate our prior “guess” of the unknown distribution as the prior expectation. While the Pólya tree has been applied to density estimation and Bayesian nonparametric hypothesis testing problems (Hanson and Johnson 2002; Berger and Guglielmi 2001; Holmes et al. 2015; Filippi and Holmes 2017), it has not been used in the context of classification models to our knowledge.

In this paper, we propose a novel dual-objective Bayesian nonparametric DA model that makes inference for variable selection and classification with a single model. This is achieved by introducing a set of variable selection parameters into the hierarchical framework of the Bayesian DA model. We assign a Pólya tree prior to the unknown group-conditionals as a representation of our uncertainty. To obtain posterior estimates, we used a collapsed variational Bayes inference. This leads to a classification rule that carries a heuristic interpretation. The heavy computational burden that is typical of fitting a nonparametric model is reduced to an acceptable range through several computational short cuts that follow from functional approximations. This makes our proposed model appealing for analysing high dimensional data.

In Section 2, we will provide a description of our proposed classification model and justify the choice of priors. This will also include a brief description of the Pólya tree construction scheme. In Section 3, we will elaborate on the posterior inference of our model and the heuristic interpretation of our resultant classification rule. This will be followed by a short Section 4 that discusses the setting of a hyperparameter in our model. In Section 5, we compare our proposed model with existing options in simulated and gene expression datasets. Circumstances that lead to good performance of the model will also be discussed. Finally, we will conclude in Section 6.

2 Discriminant analysis with variable selection

Consider a data set consisting of n observations \{ (y_i, x_i), i = 1, \ldots, n \}, where \( x_i = (x_{i1}, \ldots, x_{ip})^T \in \mathbb{R}^p \) are the \( p \) variables and \( y_i \) is the binary response of the \( i \)-th observation respectively. By conditioning on the responses \( (y_1, \ldots, y_n)^T \), we assume independence between observations, i.e., \( x_u \perp x_v \) where \( u \neq v \), and between variables, i.e., \( x_{ih} \perp x_{ig} \) where \( h \neq g \). Here, we describe a modification that allows for variable selection to the usual
discriminant analysis model described in [McLachlan (1992)] in the context of pairwise independent variables. Given two distributions $F_{j1}$ and $F_{j0}$, the group-conditional distributions of the usual discriminant analysis are

$$x_{ij} \mid y_i \overset{iid}{\sim} \begin{cases} F_{j1}, & \text{if } y_i = 1; \\ F_{j0}, & \text{if } y_i = 0. \end{cases}$$

To extend this model to select discriminative variables, we shall introduce a set of binary variable selection parameters

$$\gamma = (\gamma_1, \ldots, \gamma_p)^T.$$ 

Given three distributions $F_j$, $F_{j1}$ and $F_{j0}$, each $\gamma_j$ controls the sampling scheme of $X_{ij}$ for $1 \leq i \leq n$ as follows:

If $\gamma_j = 1$, then $x_{ij} \mid y_i \overset{iid}{\sim} \begin{cases} F_{j1}, & \text{if } y_i = 1; \\ F_{j0}, & \text{if } y_i = 0; \end{cases}$ and if $\gamma_j = 0$, then $x_{ij} \overset{iid}{\sim} F_j.$ (1)

Note that $\gamma_j = 1$ corresponds to a case in which variable $j$ is discriminative while $\gamma_j = 0$ corresponds to a non-discriminative case.

The binary responses are distributed as

$$y_i \mid \rho_y \overset{iid}{\sim} \text{Bernoulli}(\rho_y),$$

where the parameter $\rho_y$ may be interpreted as the probability of sampling an observation from response group 1 from the population.

### 2.1 Priors for $\rho_y$ and $\gamma$

In most applications, the population proportion $\rho_y$ is unknown and this has also been the case with the data which we have analysed in Section 5. A Bayesian solution is to assign a hyper prior distribution for $\rho_y$, and a natural choice of prior would be the Beta distribution, i.e.,

$$\rho_y \sim \text{Beta}(a_y, b_y).$$

Due to the Beta-binomial conjugacy, this choice leads us to a closed form expression for the joint density of the model marginalised over $\rho_y$ which is useful for posterior inference.

A natural choice of prior for the binary variable selection parameter is also the Bernoulli distribution, i.e.,

$$\gamma_j \mid \rho_\gamma \overset{iid}{\sim} \text{Bernoulli}(\rho_\gamma).$$

The parameter $\rho_\gamma$ may be interpreted as the proportion of “discriminative” variables in the dataset. Following the class of complexity priors ([Castillo et al., 2015](#)) that has demonstrated the ability to down-weight high-dimension models while allocating sufficient prior probability to the true model in several problems, we have chosen the hyper prior

$$\rho_\gamma \sim \text{Beta}(1, p^u), \text{ for some } u > 1.$$ 

The choice of constant $u$ affects the penalty on the resultant variable selection as described later in Section 5.
Table 1  Pólya tree construction scheme

1. Construct the dyadic tree in Figure 1 by specifying recursive partitions of the domain $B$. Note that each tree layer is a partition of $B$ and the recursive relationship between successive layers is: $B = B_0 \cup B_1$, $B_0 = B_{00} \cup B_{01}$, $B_1 = B_{10} \cup B_{11}$ and so on.

2. Set $\Pi = \{B, B_0, B_1, B_{00}, B_{01}, \ldots\}$ as the collection of partition-subsets obtained by taking the union of the partitions in step 1.

Remark: Notice that the partition-subsets are enumerated with binary representations. These representations carry information about the path down the tree which is taken to reach the subset from the start point at $B$. In particular, a ‘0’ indicates branching in the leftward direction, whereas ‘1’ denotes branching rightwards. For example, the subset $B_{100}$ denotes branching right from $B \to B_1$ followed by branching left from $B_1$ to $B_{10}$ and finally branching left again from $B_{10}$ to $B_{100}$.

3. Specify an infinite set of non-negative numbers $A = \{\alpha_0, \alpha_1, \alpha_{00}, \alpha_{01}, \alpha_{10}, \alpha_{11}, \ldots\}$.

4. Attach random probabilities at all edges on the tree. For every binary representation $\epsilon$, draw independently $\theta_{\epsilon} \sim \text{Beta}(\alpha_{\epsilon0}, \alpha_{\epsilon1})$.

5. Set the probability of each partition-subset as the product of the probabilities along the path taken. For example,

$$ p(B_{01}) = \theta(1 - \theta_0). $$

2.2 Priors for unknown distributions

Yu and Ormerod (2018) modelled the distributions $F_{j1}$, $F_{j0}$ and $F_j$, $1 \leq j \leq p$ described in (1) as Gaussian. As discussed in the introduction this is restrictive. Instead we will treat them in this paper as unknown probability measures and assign them a Pólya tree prior (Lavine, 1992). This prior is a distribution defined on a family of distributions on a domain $B$, hence one draw from a Pólya tree is a probability distribution. A draw from the Pólya tree may be obtained as described in Table 1.

Following the Pólya tree prior construction scheme described above, we specify our priors for the unknown
denote the set of all binary representations. For any $\epsilon \in \text{bin}$, set

$$\alpha_{j,\epsilon 1} = \alpha_{j,\epsilon 0} = \begin{cases} 1, & \text{if } l = 0; \\
\epsilon_j \times l^2, & \text{if } l \geq 1,
\end{cases}$$

where $l$ is the length of $\epsilon$.

The partitions $\Pi$ may be specified such that the Pólya tree prior is centred about a (fixed) “centering” distribution $G$, i.e., $\mathbb{E}\{F(B_j)\} = G(B_j)$ for all sets $B_j$. This is implemented through the following scheme - for any binary representation $\epsilon$,

$$B_{\epsilon} = \left( G^{-1} \left\{ \frac{1}{2} \sum_{h=1}^{\ell} \epsilon_h 2^{\ell-h} \right\}, G^{-1} \left\{ \frac{1}{2} \left( 1 + \sum_{h=1}^{\ell} \epsilon_h 2^{\ell-h} \right) \right\} \right),$$

where $\ell$ is the length of $\epsilon$, the binary digit $\epsilon_h = 1$ if the path involves branching left at layer $h$ of the tree; and $\epsilon_h = 0$ otherwise. We denote a Pólya tree prior centred about $G$ by $PT(\Pi(G), A)$. In our model, we set $\Pi_j = \Pi(G_j)$, where $G_j$ is the Gaussian distribution parametrised by sample moments. This choice of $G_j$ is in line with other DA models that outrightly assume a Gaussian distribution for the variables. However, unlike these Gaussian DA models, the choice of $G_j$ has little influence on the posterior inference as it will be overruled by a sufficient amount of data.

### 3 Model inference

The objective of our model is to identify the discriminative variables and classify new observations. Suppose we have observed $Y = \{(y_i, x_i)\}, 1 \leq i \leq n$ as realisations of the model in Section 2. Let $\{(y_{n+r}, x_{n+r})\}, 1 \leq r \leq m$ denote $m$ new observations to be classified. The required posterior is

$$p(\gamma, y^{(\text{new})} \mid x, y, x^{(\text{new})}) = \frac{p(x, y, x^{(\text{new})}, y^{(\text{new})}, \gamma)}{p(x, y^{(\text{new})}, y)},$$

where $y^{(\text{new})} = (y_{n+1}, \ldots, y_{n+m})$ and $x^{(\text{new})} = [x_{n+1}, \ldots, x_{n+m}]^T$ are the responses and variables of the new observations respectively. Clearly, this posterior is intractable as it requires a sum of $p(x, y, x^{(\text{new})}, y^{(\text{new})}, \gamma)$ over $2^{p+m}$ combinations of $(\gamma, y^{(\text{new})})$.

We will utilise the collapsed variational Bayes (CVB) as described in Teh et al. (2007) to approximate the required posterior. This choice of posterior inference stems from the scalability of CVB to high dimension problems. Since we have performed posterior inference with variational inference, we shall name our model the variational nonparametric discriminant analysis (VNPDA).

The CVB approach approximates the actual posterior in (4) with a product of densities of the form

$$q(\gamma, y^{(\text{new})}) = \prod_{r=1}^{m} q(y_{n+r}) \prod_{j=1}^{p} q(\gamma_j)$$
that minimises the KL-divergence
\[ \mathbb{E}_q \left[ \log \frac{q(\gamma, y^{(new)})}{p(x, y, x^{(new)}, y^{(new)}, \gamma)} \right], \]

where \( \mathbb{E}_q \) is an expectation with respect to \( q(\gamma, y^{(new)}) \). The product components of this optimal \( q \)-density may be obtained via the iterative equation:

\[ q(\gamma_j) \propto \exp \left[ \mathbb{E}_{-q_j} \left\{ \log p(x, y, x^{(new)}, y^{(new)}, \gamma) \right\} \right], \]  

(5)

and

\[ q(y_{n+r}) \propto \exp \left[ \mathbb{E}_{-q(y_{n+r})} \left\{ \log p(x, y, x^{(new)}, y^{(new)}, \gamma) \right\} \right], \]  

(6)

where the expectations are taken with respect to \( \prod_{s \neq j} q(\gamma_s) \prod_{r=1}^{n} q(y_{n+r}) \) and \( \prod_{j=1}^{p} q(\gamma_j) \prod_{h \neq r} q(y_{n+h}) \) respectively.

Since \( \gamma_j \) and \( y_{n+r} \) are binary random variables, their respective \( q \)-densities are Bernoulli probability mass functions and hence we need only to compute their probabilities \( \omega_j = q(\gamma_j = 1) \) for \( 1 \leq j \leq p \), and \( \psi_r = q(y_{n+r} = 1) \) for \( 1 \leq r \leq m \). These values are computed with a coordinate ascent algorithm (Blei et al., 2017) as described in Table 2. Details on the derivations of the algorithm may be found in the Appendix A.

The update equations are as follows.

- **Update for \( \omega_j \).** Following equation (5), the resultant update equation for \( \omega_j \) is approximately

\[ \omega_j \approx \expit \left\{ \log(1 + 1^T \omega_{-j}) - \log(p^u + p - 1^T \omega_{-j} - 1) + \log \text{BF}_j \right\}, \]  

(7)

where \( \omega_{-j} = E_{-q_j}(\gamma_{-j}) \), the column vector \( \gamma_{-j} \) is the result of removing the \( j \)-th entry from \( \gamma \), the function \( \expit(z) = (1 + e^{-z})^{-1} \) and the term \( \log \text{BF}_j \) (refer to equation 10 for explicit expression) is the log Bayes factor of a two-sample Bayesian nonparametric test between the hypotheses \( \{H_{1j} : \gamma_j = 1\} \) against \( \{H_{0j} : \gamma_j = 0\} \) (Holmes et al., 2015). Consequently, \( \omega_j \) is an increasing function of a penalised log Bayes factor.

To keep the computational cost of the CVB algorithm within an acceptable range, we used the following approximations: (i) Taylor’s expansion on nonlinear functions of \( 1^T \gamma_{-j} \), e.g. \( \log(1 + 1^T \gamma_{-j}) \); (ii) Stirling’s
approximation (Abramowitz and Stegun [2002]) on beta functions involving \( y_{n+r} \) (under assumption that \( 1/n \) is small). The reader may refer to Appendix A for details on how we have applied the approximations.

Observe that the penalty term \( \log(1 + 1^T \omega - j) - \log(p^u + p - 1^T \omega - j - 1) \) is decreasing in \( u \). Therefore, the setting of \( u \) should be considered carefully as it controls the trade-off between errors of type I (selecting truly non-discriminative variables as discriminative) and type II (missing out on truly discriminative variables).

- **Update for \( \psi_r \).** The update equation for \( \psi_r \) is approximately
  \[
  \psi_r \approx \exp \left[ \log \left( \frac{a_y + n_1}{b_y + n_0} \right) + \omega^T \log \left\{ \pi_r^{(1)} \right\} - \omega^T \log \left\{ \pi_r^{(0)} \right\} \right],
  \]
  where \( \psi_r = q(y_{n+r} = 1) \), the number of observations from response group \( k \) is \( n_k \), the column vector \( \pi_r^{(k)} \) of size \( p \) is such that the \( j \)-th element is
  \[
  \pi_r^{(k)} \approx \exp \left[ \sum_{\ell \leq N_j} \left\{ \log \left( \alpha_{j,\epsilon_r}^{(\ell+1)} + n_{j,\epsilon_r}^{(k)}(\ell+1) \right) - \log \left( 2\alpha_{j,\epsilon_r}^{(\ell+1)} + n_{j,\epsilon_r}^{(k)}(\ell) \right) \right\} \right],
  \]
  the binary representation \( \epsilon_r^{(\ell)} \) denotes the first \( \ell \) branching directions of the path of \( x_{n+r,j} \) through the Pólya tree \( PT(\Pi(G_j), A_j) \), the number of observations from response group \( k \) that fall in the partition-subset \( B_{j,r} \) is \( n_{j,r}^{(k)} \), and \( N_j \) is a constant.

Both Taylor’s and Stirling’s approximations are also used to obtain (8). This allows us to update \( \omega \) in isolation before using their converged value to calculate each \( \psi_r \) individually, thus reducing the computational cost.

The final classification rule may be heuristically interpreted as a function of pseudo-proportion ratios. Observe that the term
  \[
  \omega^T \log \left\{ \pi_r^{(1)} \right\} - \omega^T \log \left\{ \pi_r^{(0)} \right\} = \sum_{j=1}^{p} \omega_j \left\{ \log(\pi_r^{(1)}/\pi_r^{(0)}) \right\},
  \]
  is a weighted sum of log proportion ratios. Briefly, the proportion \( \pi_r^{(1)} \) is large if a large proportion of observations from group 1 have similar branching directions as \( x_{n+r,j} \). In other words, the classification rule classifies a new observation as group 1 if its path is more similar to paths taken by group 1 observations than those from group 0.

### 4 The smoothing parameter \( c_j \)

The choice of the \( c_j \)'s are crucial as it affects both the variable selection and classification rules. Hanson and Johnson (2002) assigned a hyper prior for \( c_j \). Alternatively, empirical estimates have been used in Holmes et al. (2015) and Berger and Guglielmi (2001), whereas Holmes et al. (2015) has also found that any value of \( c_j \) between 1 to 10 works well in practice though their generalisation has not been discussed. These strategies have been proposed in the context of low dimension problems only. However, when scaled up to high dimensionality settings, both the hyper prior and empirical estimation options prove to be too computationally burdensome.

Since our context is the analysis of high dimensional data, we suggest an approach of choosing \( c_j \) based on an *a priori* analysis that can be executed efficiently. More specifically, we “infer” a likely value of \( c_j \) from a list of candidate values that has generated our observed data under each of the two possible hypotheses \( \{ H_{0j} : \gamma_j = 0 \} \) and \( \{ H_{1j} : \gamma_j = 1 \} \). Under \( H_{0j} \), the value of \( c_j \) that generated our data is likely to be large if the empirical
Table 3 Method for choosing $c_1, \ldots, c_p$

1. Under $H_{0j}$, we assess the goodness of fit $F_j$ to $G_j$ for each $j$ by the p-value of an appropriate hypothesis test, eg. the Shapiro-wilk’s test. Here, a large p-value favours a large $c_j$.

2. Under $H_{1j}$, we assess the distance between $F_{j1}$ and $F_{j0}$ by computing the p-value of a Kolmogorov-Smirnov test. Here, a large p-value favours a large $c_j$.

3. Denote the p-values computed in steps 1 and 2 by $\{v_{j0}\}_{j=1}^p$ and $\{v_{j1}\}_{j=1}^p$ respectively. Let $\tilde{v}_j$ be the p-value of whichever $H_{0j}$ or $H_{1j}$ that is true, i.e. $\tilde{v}_j = v_{j0}$ if $H_{0j}$ is true; $\tilde{v}_j = v_{j1}$ otherwise. Calculate the prior expected value of $\tilde{v}_j$:

$$E_j = E(\tilde{v}_j) = (v_{j1} + p^n \times v_{j0})/(1 + p^n).$$

4. Rank the expected values in ascending order: $E(1), \ldots, E(p)$.

5. Assign

$$c_j = \begin{cases} 
  a_1, & \text{if } E_j < E(\lfloor p/4 \rfloor); \\
  a_2, & \text{if } E(\lfloor p/4 \rfloor) \leq E_j < E(\lfloor p/2 \rfloor); \\
  a_3, & \text{if } E(\lfloor p/2 \rfloor) \leq E_j < E(\lfloor 3p/4 \rfloor); \\
  a_4, & \text{if } E_j \geq E(\lfloor 3p/4 \rfloor), 
\end{cases}$$

where $a_1 \leq a_2 \leq a_3 \leq a_4$ are constants that may be chosen from the range $(0, 100]$ to minimise resubstitution error in the training data.

distribution of $F_j$ is close to $G_j$, whereas under $H_{1j}$, the value of $c_j$ that generated our data is likely to be large if the Euclidean distance between the empirical distributions of $F_{j1}$ and $F_{j0}$ is small. To make the implementation more computationally feasible, the variables are grouped into clusters such that variables within each cluster are assumed to have equal values of $c_j$. Detailed steps of this a priori analysis can be found in Table 3.

5 Numerical

In this section, we examine the performance of our proposed classifier in 6 simulation settings and 2 publicly-available gene expression datasets. Specifically, our proposed VNPDA model is compared with the classifiers - variational linear discriminant analysis (VLDA, [Yu and Ormerod, 2018]), variational quadratic discriminant analysis (VQDA, [Yu and Ormerod, 2018]), penalised-LDA (penLDA, [Witten and Tibshirani, 2011]), nearest shrunken centroid (NSC, [Tibshirani et al., 2003]) (NSC) and naïve Bayes kernel discriminant analysis (naiveBayesKernel, [Strbenac et al., 2015]). Both VLDA and VQDA are Bayesian analogues of diagonal discriminant analysis that have exhibited competitive classification errors. The penLDA classifier is a penalised version of Fisher’s discriminant analysis that performs well when the true signal (difference in true group-conditional means divided by standard deviation) is sparse, whereas the NSC classifier has been chosen as a competing classifier due to its popularity in bioinformatics literature. Lastly, the naiveBayesKernel is a two-stage nonparametric classifier from the ClassifyR package. It performs variable selection with the Kolmogorov-Smirnov test before fitting the selected variables into a diagonal discriminant analysis model that estimates the group-conditional distributions with kernel density estimates.
5.1 Simulation Study

The models are trained with \( n = 100 \) observations and used to classify \( m = 1000 \) new observations in each simulation setting for 50 repetitions. At each repetition, the simulated dataset consists of 50 truly discriminative variables that follow various non-Gaussian distributions (simulation 2 as an exception), and 450 non-discriminative variables. Details of their distribution are provided below and in Figure 2.

**Simulation 1**
We compare the models’ performance in discriminating a trimodal distribution from a kurtotic unimodal distribution. The distributions have equal means. These two distributions are mentioned in [Marron and Wand (1992)](#).

**Group 1:** \( \frac{9}{20} \mathcal{N}(-\frac{6}{5}, (\frac{3}{5})^2) + \frac{9}{20} \mathcal{N}(\frac{6}{5}, (\frac{3}{5})^2) + 0.1 \mathcal{N}(0, (0.25)^2) \).

**Group 0:** \( \frac{2}{5} \mathcal{N}(0,1) + \frac{1}{5} \mathcal{N}(0,0.1^2) \).

**Simulation 2**
Here, we assess the loss incurred by nonparametric classification when the Gaussian assumption holds.

**Group 1:** \( \mathcal{N}(0.7,1) \).

**Group 0:** \( \mathcal{N}(0,1) \).

**Simulation 3**
We examine the models’ ability to discriminate distributions that differ by a density spike at \( x = 0.5 \).

**Group 1:** \( 0.5 \mathcal{N}(0,1) + 0.5 \mathcal{N}(0.5,0.001^2) \).

**Group 0:** \( \mathcal{N}(0,1) \).

**Simulation 4**
We assess the models’ performance when the group-conditional distributions differ largely by tail thickness.

**Group 1:** \( \mathcal{N}(0,1) \).

**Group 0:** Cauchy distribution with location 0 and scale 3.

**Simulation 5**
Here, we compare the models’ performance in a challenging classification scenario when the group-conditional distributions differ by an additional minor mode between two major modes. These two distributions are mentioned in [Marron and Wand (1992)](#).

**Group 1:** \( \frac{9}{20} \mathcal{N}(-\frac{6}{5}, (\frac{3}{5})^2) + \frac{9}{20} \mathcal{N}(\frac{6}{5}, (\frac{3}{5})^2) + 0.1 \mathcal{N}(0, (0.25)^2) \).

**Group 0:** \( 0.5 \mathcal{N}(-1,(\frac{3}{5})^2) + 0.5 \mathcal{N}(1, (\frac{3}{5})^2) \).

**Simulation 6**
We assess the models’ performance when discriminating two Exponential distributions of different rates.

**Group 1:** \( \text{Exp}(6) \).

**Group 0:** \( \text{Exp}(2) \).

The non-discriminative variables are partitioned into 9 groups of 50 variables. Within each group, variables are independent, identically distributed. The distributions of each group are: \( t_1 \), \( \text{Cauchy}(0,1) \), \( \text{Ga}(2,2) \), \( \text{Exp}(1) \), \( \mathcal{N}(0,0.5^2), \mathcal{N}(0,1), 0.1 \mathcal{N}(0,1) + 0.9 \mathcal{N}(0,0.1^2) \) (zero-inflated model), \( \sum_{\ell=0}^{7} \frac{1}{8} \mathcal{N}(3\{(\frac{3}{5})^\ell - 1\}, (\frac{3}{5})^{2\ell}) \) (multiple modes) and \( 0.5 \mathcal{N}(-1.5,0.5^2) + 0.5 \mathcal{N}(1.5,0.5^2) \) (bi-normal).
Figure 2: Distribution of discriminative variables.

Results of the simulation study is summarised in Figures 3 and 4. The median computation time of VNPDA for one repetition is approximately 55s (within an acceptable range).

In simulations 1 and 4, three models VNPDA, naiveBayesKernel and VQDA have high selection rates among the discriminative variables. In simulation 1, the group-conditional distributions have well-separated major modes (0 vs. ±6/5), while the two distributions have differing tail thickness in simulation 4. However, VQDA did not perform as well in classification as it is unable to distinguish noise generated by non-discriminative variables with thick-tailed distributions such as $t_1$ and Cauchy(0, 2). VNPDA also performed excellently in simulation 3 and is evidence of its superiority in detecting density spikes. However, it did not exhibit any edge in simulations 2 and 6. In simulation 2, we expected the nonparametric classifiers naiveBayesKernel and VNPDA to exhibit poorer performance than the other models as the Gaussian assumption holds. In simulation 6, VLDA and penLDA exhibited a slight edge over VNPDA as the nonparametric option did not perform as well in the variable selection. This is due to the lack of separation between the modes of the group-conditional distributions.

Overall, the conditions which are favourable to VNPDA are: (i) differing tail thickness; (ii) well-separated major modes.

5.2 Application to gene expression datasets

Melanoma dataset

The Melanoma dataset has been analysed by Mann et al. (2013). The data underwent pre-processing to remove under-expressed genes, i.e. median ≤ 7. Patients whose survival time are lesser than 1 year and died due to the disease are labelled as poor prognosis; patients who are still alive and free from Melanoma after 4 years are labelled as good prognosis. Finally, we standardise the dataset to obtain $z_{ij} = (x_{ij} - \overline{x}_j)/s_j$, where $x_{ij}$ is the gene $j$ reading for observation $i$. The processed dataset that has been analysed consists of $n = 47$ observations by $p = 12881$ DNA microarray readings.
Figure 3: Classification errors of simulation study for \( n = 100 \) training and \( m = 1000 \) new observations.

Figure 4: Variable selection rates by simulation setting.
Sarcoma dataset

The Sarcoma dataset is uploaded by Colaprico et al. (2016) and is made publicly available on bioconductor. The data underwent pre-processing to retain only variables with variance > 0.1. Patients whose survival time are lesser than the 20th percentile are labelled as poor prognosis; patients whose survival time are greater than 80th percentile are labelled as good prognosis.

The dataset is standardised in a similar manner to the Melanoma dataset. A further log$_2(1 + \text{FPKM})$ is applied to the dataset before fitting the DA models that make Gaussian assumptions. The processed dataset that has been analysed consists of $n = 74$ observations by $p = 20449$ RNA readings.

![Figure 5: 5-fold cross validation classification errors of gene expression datasets.](image)

The classification errors are summarised in Figure 5. The median computation time for one CV iteration are approximately 80s and 200s for the melanoma and sarcoma dataset respectively. This is slower than other methods but still within an acceptable range to most users. In terms of classification errors, VNPDA outperformed the Gaussian DA models, including VLDA, in the melanoma dataset but there is no significant difference in performance in the Sarcoma dataset. This warrants a more detailed investigation into the reasons that led to this disparity. For simplicity, we shall focus on the performances of VLDA and VNPDA as these classifiers exhibited the greatest contrast in performance between the two gene expression datasets. A visualisation of genes selected by each classifiers has been provided in Appendix B.

![Figure 6: Venn diagrams showing the number of frequently selected genes.](image)

Based on the venn diagrams in Figure 6 it is clear that the disparity is due to the number of frequently selected genes. In particular, we found that VNPDA has more frequently selected genes than VLDA in the melanoma dataset, whereas VLDA has more frequently selected genes than VNPDA in the sarcoma dataset.

Next, we shall identify the reason that led to this difference in number of frequently selected genes. In the melanoma dataset, there are 925 genes selected by VNPDA but not VLDA. Among these genes, a substantial proportion (18.8%) are not selected because their group-conditional distributions exhibited a strong departure from normality assumptions (Shapiro-Wilk’s $p$-value < 0.05). Figure 7 presents the Pólya predictive density plot (see Hanson and Johnson, 2002 for definition) of 9 of these genes which shows that their group-conditional distributions are favourable for VNPDA to perform well, i.e. they either differ in tail thickness or have well-separated major modes. For example, the group-conditional of the poor prognosis group (red) for the C1ORF53
gene looks like a kurtotic unimodal distribution.

In contrast, more genes are selected by VLDA than VNPDA in the sarcoma dataset. By plotting the Pólya predictive density of genes that are selected by VLDA but not VNPDA, we observed that many of these genes have unimodal, right skewed group-conditional distributions (see Figure 8). We notice that the positions of their group-conditional major modes nearly coincide with one another. Such conditions lead to a smaller Bayes factor for the VNPDA variable selection rule and hence weaker evidence for the variable to be discriminative. On the other hand, the VLDA variable selection rule performed better as they depend only on the separation between the group-conditional means, and these are indeed well-separated among most of the genes.

Figure 6: Number of frequently selected genes (selection rate > 20%).

Figure 7: Pólya tree predictive density (c=1) of 9 frequently select genes by VNPDA but not VLDA for melanoma dataset.
Figure 8: Pólya tree predictive density (c=1) of 9 frequently select genes by VLDA but not VNPDA for sarcoma dataset.

6 Conclusion

In this paper, we presented a novel Bayesian discriminant analysis model that performs both variable selection and classification without making assumptions about the parametric form of the unknown distributions. To deal with our uncertainty about these distributions, we assigned them with Pólya tree priors. Since the results using the Pólya tree prior is sensitive to the choice of the smoothing parameter, we suggested a feasible approach based on an a priori inference that helps with the choice of this parameter. By adopting a collapsed variational Bayes approximation for posterior inference, we arrive at a classification rule that carries a heuristic interpretation.

As Bayesian nonparametric methods are unpopular for analysing high-dimensional data due to the computational cost, we applied computational shortcuts to the CVB update equations. The approximations effectively isolate the updates of the variable selection probabilities from the classification probabilities. Thus, we compute the variable selection probabilities in an iterative loop before using their converged value for calculating the classification probabilities. This, in combination with an implementation in C++, led to a computation cost that is within an acceptable range in both simulated and publicly available datasets we have examined.

The numerical results indicate that our proposed model performs reasonably well in most cases and is superior when the group-conditional distribution have either well-separated major modes or differing tail thickness. The findings are validated when we examine the group-conditional distributions of the variables in the publicly-available datasets. By taking these into account, we believe that VNPDA has great potentials in analysing most datasets when the normality assumption is questionable.

A Derivation for algorithm in Table 2

We shall present the derivation in the case where we have a single new observation \((x_{n+1}, y_{n+1})\) and describe the generalisation to multiple new observations towards the end. Following [5], the updates for the parameter
\[ \omega_j = q(\gamma_j = 1) = \exp \left[ \mathbb{E}_{-q_j} \left\{ \log(1 + 1^T \gamma_{-j}) - \log(p^u + p - 1^T \gamma_{-j} - 1) + \log BF_j \right\} \right]. \]  

(9)

The expression involves an expectation of the log Bayes factor

\[
\log BF_j \\
= \sum_{\ell=0}^{\infty} \sum_{c \in \text{bin}(\ell)} \left[ \log B \left\{ \alpha_{j,0} + n_{j,0}^{(1)} + I(y_{n+1} = 1, x_{n+1,j} \in B_{j,0}), \alpha_{j,c} + n_{j,c}^{(1)} + I(y_{n+1} = 1, x_{n+1,j} \in B_{j,c}) \right\} \\
+ \log B \left\{ \alpha_{j,0} + n_{j,0}^{(0)} + I(y_{n+1} = 0, x_{n+1,j} \in B_{j,0}), \alpha_{j,c} + n_{j,c}^{(0)} + I(y_{n+1} = 0, x_{n+1,j} \in B_{j,c}) \right\} \\
- \log B \left\{ \alpha_{j,0} + n_{j,0} + I(x_{n+1,j} \in B_{j,0}), \alpha_{j,c} + n_{j,c} + I(x_{n+1,j} \in B_{j,c}) \right\} - \log B(\alpha_{j,0}, \alpha_{j,c}) \right],
\]

where \( \text{bin}(\ell) \) is the set of all binary representations of length \( \ell \), \( I(\cdot) \) is the indicator function, \( B(a,b) = \Gamma(a)\Gamma(b)/\Gamma(a+b) \) is the beta function, \( n_{j,k}^{(k)} \) is the number of group \( k \) observations in the partition-subset \( B_{j,k} \) and \( n_{j,c} = n_{j,0} + n_{j,c}^{(0)} \).

Clearly, the expectation in equation (9) involves nonlinear functions of \( \gamma_{-j} \) and \( y_{n+1} \). Therefore, we shall utilise some approximations to get around this. We may use Taylor's expansion about \( 1^T \omega_{-j} \) to approximate

\[
\mathbb{E}_{-q_j} \log(1 + 1^T \gamma_{-j}) \approx \log(1 + 1^T \omega_{-j}),
\]

\[
\mathbb{E}_{-q_j} \log(p^u + p - 1^T \gamma_{-j} - 1) \approx \log(p^u + p - 1^T \omega_{-j} - 1),
\]

and, for small \( 1/n \), a Stirling's approximation to approximate the beta functions

\[
\log B(\alpha_{j,0} + n_{j,0}^{(1)} + I(y_{n+1} = 1, x_{n+1,j} \in B_{j,0}), \alpha_{j,c} + n_{j,c}^{(1)} + I(y_{n+1} = 1, x_{n+1,j} \in B_{j,c})) \\
\approx \log B(\alpha_{j,0} + n_{j,0}^{(1)}, \alpha_{j,c} + n_{j,c}^{(1)}).
\]

Hence, the update equation for \( \omega_j \) may be approximated as

\[
\omega_j \approx \exp \left[ \log(1 + 1^T \omega_{-j}) - \log(p^u + p - 1^T \omega_{-j} - 1) + \log BF_j \right].
\]

where

\[
\log BF_j \approx \sum_{\ell=0}^{\infty} \sum_{c \in \text{bin}(\ell)} \left\{ \log B(\alpha_{j,0} + n_{j,0}, \alpha_{j,c} + n_{j,c}) + \log B(\alpha_{j,0} + n_{j,0}, \alpha_{j,c} + n_{j,c}) \\
- \log B(\alpha_{j,0} + n_{j,0}, \alpha_{j,c} + n_{j,c}) - \log B(\alpha_{j,0}, \alpha_{j,c}) \right\}.
\]

The sum to infinity in the above expression is computationally tractable as the subset counts decrease as we go further down the layers of the tree. In particular, there exists a constant \( M_j \) such that either \( n_{j,c}^{(1)} = 0 \) or \( n_{j,c}^{(0)} = 0 \) for all \( c \in \bigcup_{\ell>M_j} \text{bin}(\ell) \) and \( k \in \{0,1\} \). Hence, we may rewrite the log Bayes factor as

\[
\log BF_j \approx \sum_{\ell=0}^{M_j} \sum_{c \in \text{bin}(\ell)} \left\{ \log B(\alpha_{j,0} + n_{j,0}, \alpha_{j,c} + n_{j,c}) + \log B(\alpha_{j,0} + n_{j,0}, \alpha_{j,c} + n_{j,c}) \\
- \log B(\alpha_{j,0} + n_{j,0}, \alpha_{j,c} + n_{j,c}) - \log B(\alpha_{j,0}, \alpha_{j,c}) \right\}.
\]

(10)

Similarly, we use \( \psi \) to derive the update for \( y_{n+1} \) as

\[
\psi = q(y_{n+1} = 1),
\]

\[
= \exp \left[ \mathbb{E}_{q(y_{n+1})} \left\{ \log \left( \frac{a_y + n_1 + I(y_{n+1} = 1)}{b_y + n_0 + I(y_{n+1} = 0)} \right) + \gamma^T \log \left( \pi^{(1)} \right) - \gamma^T \log \left( \pi^{(0)} \right) \right\} \right],
\]

\[
\approx \exp \left[ \log \left( \frac{a_y + n_1}{b_y + n_0} \right) + \omega^T \log \left( \pi^{(1)} \right) - \omega^T \log \left( \pi^{(0)} \right) \right], \text{ if } n \text{ is large},
\]

(11)
where the number of observations in groups 1 and 0 are \(n_1\) and \(n_0\) respectively, the vector \(\pi^{(k)}\) of size \(p\) is such that the \(j\)-th element is

\[
\pi^{(k)}_j = \exp \left[ \sum_{\ell=0}^{N_j} \log \mathbb{P}_k \{ B_{j,\epsilon_j(\ell)} \to B_{j,\epsilon_j(\ell+1)} \} \right],
\]

\[
= \exp \left[ \sum_{\ell=0}^{N_j} \left\{ \log \left( \alpha_{j,\epsilon_j(\ell+1)} + n^{(k)}_{j,\epsilon_j(\ell+1)} + I(y_{n+1} = k, x^* \in B_{\epsilon_j(\ell+1)}) \right) \right. \\
- \left. \log \left( 2\alpha_{j,\epsilon_j(\ell+1)} + n^{(k)}_{j,\epsilon_j(\ell+1)} + I(y_{n+1} = k, x^* \in B_{\epsilon_j(\ell)}) \right) \right\} \right],
\]

\[
\approx \exp \left[ \sum_{\ell=0}^{N_j} \left\{ \log \left( \alpha_{j,\epsilon_j(\ell+1)} + n^{(k)}_{j,\epsilon_j(\ell+1)} \right) - \log \left( 2\alpha_{j,\epsilon_j(\ell+1)} + n^{(k)}_{j,\epsilon_j(\ell+1)} \right) \right\} \right],
\]

the log prefix of a vector denotes element-wise log, the binary representation \(\epsilon_j(\ell)\) denotes the first \(\ell\) branching directions taken by \(x_{n+1,j}\) and the number \(N_j\) is such that \(n^{(k)}_{j,\epsilon_j(\ell)} = 0\) for all \(\ell > N_j\) and \(k \in \{0,1\}\). Note that the approximation in equation (11) follows from Taylor’s approximation.

We may extend the classification rule in equation (11) to \(m > 1\) new observations by simply replacing each \(\pi^{(k)}\) with \(\pi^{(k)}_{r\ell}\), where the \(j\)-th element of \(\pi^{(k)}_{r\ell}\) is

\[
\pi^{(k)}_{r\ell}_j = \exp \left[ \sum_{\ell=0}^{N_j} \log \mathbb{P}_k \{ B_{j,\epsilon_j(\ell)} \to B_{j,\epsilon_j(\ell+1)} \} \right],
\]

\[
= \exp \left[ \sum_{\ell=0}^{N_j} \left\{ \log \left( \alpha_{j,\epsilon_j(\ell+1)} + n^{(k)}_{j,\epsilon_j(\ell+1)} + I(y_{n+r} = k, x_{n+r,j} \in B_{\epsilon_j(\ell+1)}) \right) \right. \\
- \left. \log \left( 2\alpha_{j,\epsilon_j(\ell+1)} + n^{(k)}_{j,\epsilon_j(\ell+1)} + I(y_{n+r} = k, x_{n+r,j} \in B_{\epsilon_j(\ell)}) \right) \right\} \right],
\]

\[
\approx \exp \left[ \sum_{\ell=0}^{N_j} \left\{ \log \left( \alpha_{j,\epsilon_j(\ell+1)} + n^{(k)}_{j,\epsilon_j(\ell+1)} \right) - \log \left( 2\alpha_{j,\epsilon_j(\ell+1)} + n^{(k)}_{j,\epsilon_j(\ell+1)} \right) \right\} \right],
\]

the number \(N_j\) is such that \(n^{(k)}_{j,\epsilon_j(\ell)} = 0\) for all \(\ell > N_j\) and \(1 \leq r \leq m\) and the rest of the notations used have been explained in Section 3.

Remark: In our numerical examples, we set \(N_j = M_j = \log_2(n)\) for all \(1 \leq j \leq p\). This allows us to account for the details at higher resolution of the group-conditional distributions as \(n\) increases (Hanson and Johnson, 2002).

B Instructions for visualising selected genes

1. Access the page http://vcg.github.io/upset/.
2. Click on “Load Data”.
3. Enter the following url into the query box and then click on “submit”.

https://raw.githubusercontent.com/weichangyu10/VaDA/master/SelectMelanomaMeta.json

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