Nearest Neighbor Classifier based on Generalized Inter-point

DISTANCES FOR HDLSS DATA

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Abstract

In high dimension, low sample size (HDLSS) settings, Euclidean distance based classifiers suffer from curse of dimensionality if the competing populations are similar in terms of their location and scale parameters. In this article, we propose a classifier which can discriminate between populations having different marginal distributions. A generalization of the proposed classifier has been developed to differentiate between populations having different joint distributions for the component variables. Performance of the proposed classifiers are demonstrated using a variety of simulated data sets.

1 Introduction

Nearest neighbor (NN) classification is among the most popular supervised classification methods because of its simplicity and computational speed. For an appropriate choice of $k \in \mathbb{N}$, the misclassification probability of the kNN classifier converges to the Bayes risk as the size of the training sample (say, n) grows to infinity keeping the dimensionality of data (say, D) to be fixed (see, e.g., Devroye et al. (2013)). In this article, we assume n to be fixed and allow D to grow to infinity.

Consider a classification problem involving F_1 and F_2 , two unknown probability distribution functions on \mathbb{R}^D . Assuming appropriate moments exist, let $\boldsymbol{\mu}_D^{(j)}$ and $\boldsymbol{\Sigma}_D^{(j)}$ denote the mean vector and the dispersion matrix corresponding to F_j , respectively, for j=1,2. Define the following constants:

$$\nu_{12}^2 = \lim_{D \to \infty} D^{-1} \|\boldsymbol{\mu}_D^{(1)} - \boldsymbol{\mu}_D^{(2)}\|^2 \text{ and } \sigma_j^2 = \lim_{D \to \infty} D^{-1} trace(\Sigma_D^{(j)}) \text{ for } j = 1, 2.$$

Here, $\|\cdot\|$ denotes the Euclidean norm on \mathbb{R}^D and $trace(A) = \sum_{i=1}^D a_{ii}$ (sum of the diagonal elements) for a $D \times D$ matrix A. Let us denote the kNN classifier on \mathbb{R}^D by δ_D^k , and its misclassification probability by Δ_D^k for a fixed $k \in \mathbb{N}$. Under appropriate distributional assumptions, Hall et al. (2005) showed that Δ_D^k converges to zero as $D \to \infty$ if we have $\nu_{12}^2 > |\sigma_1^2 - \sigma_2^2|$. Intuitively, this means that the competing populations have their difference in scales dominated by the differences in their locations. Some methods exist in the literature that improve the performance of the kNN classifier in HDLSS settings. Chan and Hall (2009) developed some scale adjustments to the usual 1NN classifier (referred to as kNN-scl.adj), and this method performs well under the weaker condition that $\nu_{12}^2 > 0$. A non-linear transformation of covariate space followed by the 1NN classification was proposed by Dutta and Ghosh (2016) (referred to as kNN-TRIPD). Recently, Pal et al. (2016) used a new dissimilarity index instead of the usual Euclidean distance for 1NN classification (referred to as kNN-MADD). However, all these methods require either of the conditions $\nu_{12}^2 > 0$ or $\sigma_1^2 \neq \sigma_2^2$ to yield good results for high-dimensional data. So, they can deal with distributions that differ either in their locations or scales.

Consider a two class classification problem (say, **Example 1**) with the competing distributions as $F_1 \equiv N_D(\mathbf{0}_D, \Sigma_D^{(1)})$ and $F_2 \equiv N_D(\mathbf{0}_D, \Sigma_D^{(2)})$. Here, N_D denotes the *D*-dimensional Gaussian distribution, $\mathbf{0}_D$ is the *D*-dimensional vector of zeros, and $\Sigma_D^{(1)}$ and $\Sigma_D^{(2)}$ are described below:

$$\Sigma_D^{(1)} = \begin{bmatrix} \mathbf{I}_{[\frac{D}{2}]} & \mathbf{0}_{[\frac{D}{2}] \times (D - [\frac{D}{2}])} \\ \mathbf{0}_{(D - [\frac{D}{2}]) \times [\frac{D}{2}]} & 0.5 \mathbf{I}_{D - [\frac{D}{2}]} \end{bmatrix} \text{ and } \Sigma_D^{(2)} = \begin{bmatrix} 0.5 \mathbf{I}_{D - [\frac{D}{2}]} & \mathbf{0}_{(D - [\frac{D}{2}]) \times [\frac{D}{2}]} \\ \mathbf{0}_{[\frac{D}{2}] \times (D - [\frac{D}{2}])} & \mathbf{I}_{[\frac{D}{2}]} \end{bmatrix},$$

with \mathbf{I}_d being the $d \times d$ identity matrix and $\mathbf{0}_{l \times m}$ being the $l \times m$ matrix of zeros. As **Example 2**, we consider $F_1 \equiv N_D(\mathbf{0}_D, \frac{5}{3}\mathbf{I}_D)$ and $F_2 \equiv \prod_{d=1}^D F_{2d}$ with $F_{2d} = t_5(0,1)$ for each $1 \leq d \leq D$. It is easy to check that $\nu_{12}^2 = 0$ and $\sigma_1^2 = \sigma_2^2 = 0.75$ for **Example 1**. For **Example 2**, the parameters are $\boldsymbol{\mu}_D^{(1)} = \boldsymbol{\mu}_D^{(2)} = \mathbf{0}_D$ and $\boldsymbol{\Sigma}_D^{(1)} = \boldsymbol{\Sigma}_D^{(2)} = \frac{5}{3}\mathbf{I}_D$, hence we obtain $\nu_{12}^2 = 0$ and $\sigma_1^2 = \sigma_2^2 = \frac{5}{3}$. Hence, the existing classifiers fail to yield promising results in high-dimensional spaces. In Figure 1, we report the empirical misclassification probabilities of the Bayes classifier, the usual 1NN, 1NN-MADD, 1NN-scl.adj and 1NN-TRIPD classifiers. It is clear that none of them perform satisfactorily.

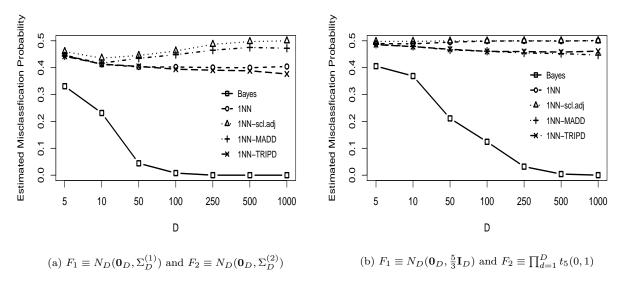


Figure 1: Misclassification rates of classifiers in Examples 1 and 2.

In this article, we focus on the kNN classifier based on Mean Absolute Differences of Distances (MADD) proposed by Pal et al. (2016) and make appropriate adjustments to the Euclidean distance function to discriminate among populations under more general settings. A transformation of the usual MADD is proposed in Section 2. Section 3 further generalizes the proposed classifier to address cases where discriminative information comes from the joint distribution of groups of components. Empirical performance of the proposed classifiers on simulated datasets is evaluated in Section 4.

2 Transformation of MADD

Let us denote the training data set $\{(\mathbf{X}_1, Y_1), (\mathbf{X}_2, Y_2), \dots, (\mathbf{X}_n, Y_n)\}$ by \mathcal{X}_n (a random sample of size n). Here, \mathbf{X}_i s are D-dimensional random vectors and $Y_i \in \{1, \dots, J\}$ denotes the class label associated with \mathbf{X}_i for $1 \leq i \leq n$. Let n_j be the number of observations from the j-th class for $1 \leq j \leq J$ and $n = \sum_{j=1}^{J} n_j$. For a fixed i, suppose that $P[Y_i = j] = \pi_j$ with $0 < \pi_j < 1$, $\mathbf{X}_i | Y_i = j \sim F_j$ for $1 \leq j \leq J$ and $\sum_{j=1}^{J} \pi_j = 1$. Our objective is to predict the class label $Y_{\mathbf{Z}}$ of a new observation $\mathbf{Z} \in \mathbb{R}^D$.

For a given training sample χ_n and test point $\mathbf{Z} \in \mathbb{R}^D$, Pal et al. (2016) defined the dissimilarity index MADD between \mathbf{Z} and \mathbf{X}_{i_0} for a fixed index $1 \le i_0 \le n$ as follows:

$$\psi_{1,D}(\mathbf{Z}, \mathbf{X}_{i_0}) = \frac{1}{n-1} \sum_{1 \le i \ne i_0 \le n} \left| D^{-\frac{1}{2}} \| \mathbf{Z} - \mathbf{X}_i \| - D^{-\frac{1}{2}} \| \mathbf{X}_{i_0} - \mathbf{X}_i \| \right|.$$
(1)

MADD uses the usual Euclidean (also known as l_2) distance to compute dissimilarity between two vectors. However, one may use any other distance function instead of the l_2 -distance to define a measure of dissimilarity like $\psi_{1,D}$. Observe that the limiting values $\nu_{jj'}^2$, σ_j^2 and $\sigma_{j'}^2$ come into the picture as a consequence of using the Euclidean distance in $\psi_{1,D}$. It is established that MADD performs well when $\nu_{jj'}^2 > 0$ or $\sigma_j^2 \neq \sigma_{j'}^2$ for $1 \leq j \neq j' \leq J$ (see Pal et al. (2016)), but fails

under more general conditions (see. e.g., Figure 1). We propose some adjustments to the Euclidean norm that will lead to better performance compared to usual MADD (denoted by $\psi_{1,D}$ in equation (1)) under more general situations. Let $\gamma:[0,\infty)\longmapsto[0,\infty)$ and $\phi:[0,\infty)\longmapsto[0,\infty)$ be two continuous, monotonically increasing functions with $\gamma(0)=\phi(0)=0$. For $\mathbf{u},\mathbf{v}\in\mathbb{R}^D$, we define

$$\beta_D(\mathbf{u}, \mathbf{v}) = \phi \left[D^{-1} \sum_{d=1}^D \gamma(|u_d - v_d|^2) \right]. \tag{2}$$

It is clear that by considering $\gamma(t) = t^{\frac{p}{2}}$ and $\phi(t) = t^{\frac{1}{p}}$ for $p \ge 1$, we get $\beta_D(\mathbf{u}, \mathbf{v}) = \frac{1}{\sqrt[p]{D}} ||\mathbf{u} - \mathbf{v}||_p$, i.e., the l_p distance between \mathbf{u} and \mathbf{v} scaled by $\sqrt[p]{D}$. For given choices of γ and ϕ , we define the dissimilarity between a test point \mathbf{Z} and an observation \mathbf{X}_{i_0} for a fixed $1 \le i_0 \le n$ as follows:

$$\psi_{2,D}(\mathbf{Z}, \mathbf{X}_{i_0}) = \frac{1}{n-1} \sum_{1 \le i \ne i_0 \le n} \left| \beta_D(\mathbf{Z}, \mathbf{X}_i) - \beta_D(\mathbf{X}_{i_0}, \mathbf{X}_i) \right|.$$
(3)

Instead of looking at the Euclidean distance, which is the case for MADD, we now consider Mean Absolute Difference of Generalized Distances (gMADD) based on the general distance function defined in equation (2). Clearly, one can see that we get back $\psi_{1,D}$ (stated in equation (1)) by choosing $\gamma(t) = t$ and $\phi(t) = t^{\frac{1}{2}}$.

We denote the kNN classifier based on the transformations $\psi_{1,D}$ and $\psi_{2,D}$ by $\delta_{1,D}^k$ and $\delta_{2,D}^k$, respectively. The misclassification probabilities of the classifier $\delta_{i,D}^k$ is defined as follows:

$$\Delta_{i,D}^k = P[\delta_{i,D}^k(\mathbf{Z}) \neq Y_{\mathbf{Z}}] \text{ for } i = 1, 2.$$

Recall **Examples 1** and **2** discussed in Section 1. Consider $\pi_1 = \pi_2 = 1/2$ and generate 100 (50+50) training and 500 (250+250) test observations. In Figure 2, we plot the estimated values of the Bayes risk, and the misclassification rates Δ_D^k , $\Delta_{1,D}^k$ and $\Delta_{2,D}^k$ based on 100 replications for D = 5, 10, 50, 100, 250, 500, 1000 and k = 1. For the rest of this article, we consider $\phi(t) = t$ and three choices of the function $\gamma(t)$, namely, $\gamma_1(t) = 1 - e^{-t/2}$, $\gamma_2(t) = \sqrt{t}/2$ and $\gamma_3(t) = \log(t/(1+t))$ for $t \geq 0$. Throughout this article, we report misclassification rates of the classifier NN-gMADD $(\delta_{2,D}^1)$ based on γ_1 since it outperformed γ_2 and γ_3 .

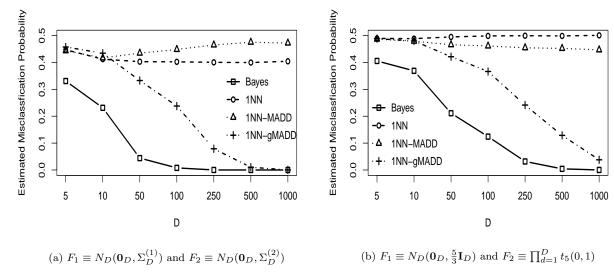


Figure 2: Misclassification rates of classifiers in Examples 1 and 2.

In Figure 2, the estimated misclassification probability of the classifiers $\delta_{1,D}^1$ and $\delta_{2,D}^1$ are shown. It is clear that $\delta_{1,D}^1$ misclassifies almost 50% of the test observations when the dimension is large. On the other hand, the classifier $\delta_{2,D}^1$ yields good performance. In fact, when the populations have different marginal distributions, we proved that $\Delta_{2,D}^1$ converges to zero as $D \to \infty$.

3 Identifying Joint Structures

In Section 2, we observed that the kNN classifier based on $\psi_{2,D}$ (namely, $\delta_{2,D}^k$) can discriminate between populations that have difference in their one-dimensional marginal distributions. But, if the one-dimensional marginals are same, gMADD will fail to differentiate between populations. Such scenarios impose further challenges on the proposed classifier $\delta_{2,D}^1$. Consider the classification problem described below. Let $\Sigma_D^{(1)}$ and $\Sigma_D^{(2)}$ denote the $D \times D$ dispersion matrices of the first and second populations F_1 and F_2 , respectively, as follows:

$$\Sigma_D^{(j)} = \begin{bmatrix} \mathbf{H}_j & & & \\ & \mathbf{H}_j & & \\ & & \ddots & \\ & & & \mathbf{H}_j \end{bmatrix} \text{ and } \mathbf{H}_j = \begin{bmatrix} 1 & \rho_j \cdots \rho_j \\ \rho_j & 1 \cdots \rho_j \\ \vdots & \ddots & \\ \rho_j & \rho_j \cdots 1 \end{bmatrix} \text{ for } j = 1, 2.$$

Here, \mathbf{H}_1 and \mathbf{H}_2 are $r \times r$ positive definite matrices. In other words, $\Sigma_D^{(1)}$ and $\Sigma_D^{(2)}$ are block diagonal positive definite matrices with block size r (a fixed positive integer). The number of blocks, denoted by B, satisfies D = rB. We consider $\rho_1 = 0.3$ and $\rho_2 = 0.7$ as particular choices. Take $F_1 \equiv N_D(\mathbf{0}_D, \Sigma_D^{(1)})$ and $F_2 \equiv N_D(\mathbf{0}_D, \Sigma_D^{(2)})$, respectively and consider this as **Example 3**. Note that $\boldsymbol{\mu}_D^{(1)} = \boldsymbol{\mu}_D^{(2)} = \mathbf{0}_D$ and $trace(\Sigma_D^{(1)}) = trace(\Sigma_D^{(2)}) = D$, i.e., $\nu_{12}^2 = 0$ and $\sigma_1^2 = \sigma_2^2$. The usual kNN classifier (namely, δ_D^k) and the MADD based kNN classifier (namely, $\delta_{1,D}^k$) fail to work in this example (see Figure 3). Moreover, there is no difference between the marginal distributions of these two populations as the component variables are all standard normal and $\delta_{2,D}^k$ will fail too.

3.1 Improvements to gMADD

In **Examples 3**, we can observe that the competing populations have same one-dimensional marginal distributions, and $\psi_{2,D}$ does not contain any discriminatory information between the distributions F_1 and F_2 . But, the joint distribution of the individual groups of component variables are clearly different for these two populations. This motivates the idea of capturing differences between the population distributions through appropriate joint distributions of the groups of components. We formalize this idea as follows.

Let us write any $D \times 1$ vector \mathbf{U} as $(\mathbf{U}_1^{\top}, \dots, \mathbf{U}_B^{\top})^{\top}$, where \mathbf{U}_b is a $D_b \times 1$ vector for $1 \leq b \leq B$, and $\sum_{b=1}^B D_b = D$. Here, the D-dimensional vector \mathbf{U} has been partitioned into smaller groups \mathbf{U}_b for $1 \leq b \leq B$. For a random vector $\mathbf{U} = (\mathbf{U}_1^{\top}, \dots, \mathbf{U}_B^{\top})^{\top} \sim F_j$, we denote the distribution of $\mathbf{U}_b/\sqrt{D_b}$ by $F_{j,b}$ for $1 \leq b \leq B$ and $1 \leq j \leq J$. Analogous to the quantities $\beta_D(\mathbf{Z}, \mathbf{X}_{i_0})$ and $\psi_{2,D}(\mathbf{Z}, \mathbf{X}_{i_0})$ for $\mathbf{Z}, \mathbf{X}_{i_0} \in \mathbb{R}^D$ with a fixed $1 \leq i_0 \leq n$ (see equations 2 and 3 in Section 2), we now define the following two transformations:

$$\beta_B(\mathbf{Z}, \mathbf{X}_{i_0}) = \phi \left[B^{-1} \sum_{b=1}^B \gamma \left(D_b^{-1} || \mathbf{Z}_b - \mathbf{X}_{i_0 b} ||^2 \right) \right], \text{ and}$$
 (4)

$$\psi_{3,B}(\mathbf{Z}, \mathbf{X}_{i_0}) = \frac{1}{n-1} \sum_{1 \le i \ne i_0 \le n} \left| \beta_B(\mathbf{Z}, \mathbf{X}_i) - \beta_B(\mathbf{X}_{i_0}, \mathbf{X}_i) \right|.$$
 (5)

This transformation $\psi_{3,B}$ is the Mean Absolute Difference of the generalized group based Distances (ggMADD). We denote the kNN classifier based on ggMADD as $\delta_{3,B}^k$. When the populations have different joint distributions of groups of components, we proved that the misclassification probability of $\delta_{3,B}^k$ converges to zero as $B \to \infty$.

4 Results from the Analysis of Simulated Data Sets

We analyze several high-dimensional simulated data sets to compare the performance of the proposed classifiers. Recall the examples introduced in Section 1 (**Examples 1, 2**) and also the example introduced later in Section 3 (**Example 3**). Along with these three, we now consider one more example in this section.

Recall the two scale matrices \mathbf{H}_1 and \mathbf{H}_2 defined in **Example 3**. Let $\mathbf{U}_1, \ldots, \mathbf{U}_B$ be independent $r \times 1$ random vectors, identically distributed as the multivariate Cauchy distribution with location parameter $\mathbf{0}_r$ and scale matrix \mathbf{H}_1 (say, $Mt_1(\mathbf{0}_r, \mathbf{H}_1)$). Consider a $D \times 1$ random vector from the first population $\mathbf{U} = (\mathbf{U}_1^\top, \ldots, \mathbf{U}_B^\top)^\top$. The distribution function of \mathbf{U} is $F_1(\mathbf{u}) = \prod_{b=1}^B F_{1,b}(\mathbf{u}_b)$, where $F_{1,b} \equiv Mt_1(\mathbf{0}_r, \mathbf{H}_1)$. Similarly, a $D \times 1$ random vector \mathbf{V} from the second population follows $F_2(\mathbf{v}) = \prod_{b=1}^B F_{2,b}(\mathbf{v}_b)$, where $F_{2,b} \equiv Mt_1(\mathbf{0}_r, \mathbf{H}_2)$. We consider this as **Example 4**. Since moments do not exist for the multivariate Cauchy distribution, the constants ν_{12}^2 , σ_1^2 and σ_2^2 do not exist in this examples. So, we cannot comment on the performances of the usual NN or NN-MADD as $D \to \infty$. But, the proposed classifier can deal with such heavy-tailed distributions if we choose the γ function to be bounded. However, in **Example 4**, the one-dimensional marginals for both F_1 and F_2 are all Cauchy distribution with location zero and scale one (i.e., C(0,1)). Therefore, gMADD cannot differentiate between F_1 and F_2 . This motivates us to capture the differences between F_1 and F_2 through the joint distributions of the groups.

In each example, we generated 50 observations from each of the two classes to form the training sample, while a test set of size 500 (250 from each class) was used. This procedure was repeated 100 times to compute the estimated misclassification probabilities of the different classifiers. The misclassification probabilities were computed for a set of increasing values of D, namely, 5, 10, 50, 100, 250, 500 and 1000 for **Examples 1** and **2**; and 50, 100, 250, 500 and 1000 for **Examples 3** and **4**.

In the last two cases, i.e., **Examples 3** and **4**, the distribution functions F_1 and F_2 have differences through the joint distributions of the groups of components. We have carried out the analysis for these two examples with r = 5, 10 and 25, and observed improvement in the performance of NN-ggMADD as r decreases. As we had discussed earlier, in **Example 4** we need the function γ to be a bounded and one such choice of γ is $\gamma_1(t) = 1 - e^{-t/2}$. For the other three examples, we have carried out analysis with two more choices, namely, $\gamma_2(t) = \sqrt{t}/2$ and $\gamma_3(t) = \log(t/(1+t))$. But, the results are reported only for γ_1 since it outperformed the other two choices.

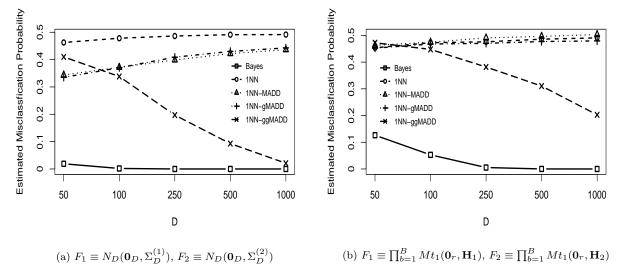


Figure 3: Misclassification rates of classifiers in Examples 3 and 4.

4.1 Comparison with Other Popular Classifiers

We also compare the performance of NN-ggMADD with some well known classifiers available in the literature. The performance of different classifiers for **Examples 1-4** with D = 1000 have been studied. The training and test sets remain the same as before with sizes 50 (25 + 25) and 500 (250 + 250), respectively. We have iterated the procedure 100 times. The average misclassification rates along with the corresponding standard errors for the usual NN and NN-ggMADD are reported in Table 1. Misclassification rates of the linear and non-linear support vector machines (SVM) are also reported. We use the radial basis function (RBF), i.e., $K_{\theta}(\mathbf{x}, \mathbf{y}) = \exp\{-\theta ||\mathbf{x} - \mathbf{y}||^2\}$ as our non-linear kernel in SVM. The results are reported for the default value of regularization parameter $\theta = 1/D$. Performance of GLMNET, random forest (referred to as RF) and NN classifiers based on random projection (referred to as NN-RAND) methods have also been studied, and the respective misclassification rates are reported as well.

Table 1: Misclassification rates of different classifiers for D = 1000.

Example	Bayes	NN-gMADD	NN-ggMADD	GLMNET	RF	NN-RAND	SVM-LIN	SVM-RBF
1	0.00(0.00)	0.00 (0.00)	-	0.47(0.02)	0.01 (0.01)	0.40(0.02)	0.37(0.02)	0.36(0.02)
2	0.00(0.00)	0.04 (0.01)	-	0.47(0.02)	0.35(0.02)	0.50(0.02)	0.37(0.02)	0.38(0.02)
3	0.00(0.00)	0.44(0.02)	0.02 (0.01)	0.48(0.02)	0.49(0.02)	0.50(0.02)	0.51(0.00)	0.47(0.00)
4	0.00(0.00)	0.48(0.02)	0.20 (0.03)	0.47(0.01)	0.49(0.02)	0.49(0.02)	0.50(0.02)	0.49(0.02)

Clearly, one can observe that our proposed classifiers outperform the rest for all the examples, and the misclassification rates quite close to the respective Bayes risks. Except RF (in **Example 1**), performance of none of the other methods are even close to the proposed classifiers. In some examples, the average misclassification rates of the other classifiers are almost as bad as that of a classifier which assigns an observation randomly to any one of the two classes.

5 Concluding Remarks

In this article, we considered the nearest neighbor (NN) classifier in HDLSS settings. We overcame the difficulty this classifier faces due to the use of the Euclidean norm as a distance between two points. The Euclidean distance was replaced with other appropriately constructed dissimilarity indices. We showed that even when the underlying populations are same in terms of their location and scale parameters, the proposed classifier showcases perfect classification as long as the components (or, groups of component variables) have different one-dimensional marginal (or, joint) distributions across the competing populations.

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