On Perfect Clustering for Gaussian Processes

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Abstract

In this paper, we propose a data based transformation for infinite-dimensional Gaussian processes and derive its limit theorem. In a clustering problem using mixture models, an appropriate modification of this transformation asymptotically leads to perfect separation of the populations. Theoretical properties related to label consistency are studied for the k-means clustering algorithm when used on this transformed data. Good empirical performance of the proposed methodology is demonstrated using simulated as well as benchmark data sets, when compared with some popular parametric and nonparametric methods for such functional data.

Keywords: Consistency in probability, Difference in covariance operators, Hajek and Feldman property, J class problem, Location and scale differences, Mahalanobis' distances.

1 Introduction

Suppose that we are given two Gaussian distributions (say, GDs) $\mathbb{P}_1$ and $\mathbb{P}_2$. The Hajek and Feldman property (established independently by Hajek (1958) and Feldman (1958)) states that $\mathbb{P}_1$ and $\mathbb{P}_2$ are either equivalent, or else mutually singular. In other words, for every measurable set A, $\mathbb{P}_1(A) = 0$ if and only if $\mathbb{P}_2(A) = 0$, or else there exist two disjoint measurable sets S_1 and S_2 such that

$$\mathbb{P}_1(S_1) = 1, \mathbb{P}_2(S_1) = 0 \text{ and } \mathbb{P}_1(S_2) = 0, \mathbb{P}_2(S_2) = 1.$$

Mutual singularity is not very interesting in finite dimensions because it happens only when at least one of the covariance matrices is singular. However, in the functional setting, this singularity appears in non-trivial situations. To mention an example, it was shown by Rao and Varadarajan (1963) that if the covariance operators of $\mathbb{P}_1$ and $\mathbb{P}_2$, namely, Σ_1 and Σ_2 satisfy $\Sigma_2 = a\Sigma_1$ for some $a \neq 1$, then $\mathbb{P}_1$ and $\mathbb{P}_2$ are mutually singular.

It is clear that the mutually singular case of the Hajek and Feldman property (say, HFp) looks very promising for classification as well as clustering (in the mixture setting) of data points. Recently, some results have appeared taking advantage of this property to propose *perfect classifiers* (see the references given below). However, the clustering problem seems to be harder, and as far as we know, Delaigle et al (2019) is the only available paper with results in this area. The main drawbacks of the paper by Delaigle et al (2019) are that it deals mainly with location problems (see Section M of Appendix II for a detailed discussion). In this paper, we present a family of transformations on functional data which allows one to identify some mutually singular situations. The transformed data are then used to obtain *perfect clustering* in the mixture setting.

To give an overview of our main contributions, let us consider a Gaussian process (say, $\mathbf{Z}$) defined on a bounded real interval, which without loss of generality, we identify with the unit interval $[0, 1]$. Further, assume that its trajectories belong to the Hilbert space of square integrable functions $\mathbb{H}$, which is defined as follows:

$$\mathbb{H} : \text{ set of real functions } f(t) \text{ with } t \in [0, 1] \text{ such that } \int_0^1 f^2(t)dt < \infty.$$

The inner product in $\mathbb{H}$ is $\langle f, g\rangle = \int_0^1 f(t)g(t)dt$. The keystone of this paper is Theorem 2.1. It states that under appropriate assumptions, if $b \in \mathbb{H}$, then the limit of a sequence of scaled Mahalanobis distances between some finite-dimensional projections of $\mathbf{Z}$ and b converges in probability to a non-random limit. Scaling is done using the dimension of the projection, and this convergence holds as the dimension goes to infinity. Practical interest of this result lies in the fact that the limit depends only on the distribution of $\mathbf{Z}$ (say, $\mathbb{P}_{\mathbf{Z}}$). Therefore, Theorem 2.1 allows one to identify some cases in which GDs are *mutually singular*. In such scenarios, this result allows one to obtain *perfect classification* as well as *perfect clustering*. Let us explain this point a bit more precisely.

Consider a probability distribution $\mathbb{P}$ such that $\mathbb{P} = \sum_{h=1}^{J} \pi_h \mathbb{P}_h$, where $0 < \pi_h < 1$ with $\sum_{h=1}^{J} \pi_h = 1$ and $\mathbb{P}_h$ are GDs on $\mathbb{H}$ for $1 \leq h \leq J$. Additionally, assume $\mathbb{P}$ to be *known*, but the precise values of J, π_h and $\mathbb{P}_h$ for $1 \leq h \leq J$ are *unknown*. According to this mixture model, every function $\mathbf{z}$ produced by $\mathbb{P}$ was in fact generated from one of the $\mathbb{P}_h$'s. Consequently, under appropriate conditions, the proposed transformation leads to different limits (depending on the $\mathbb{P}_h$ which generated $\mathbf{z}$) in Theorem 2.1. Now, if we have a set of observations (with at least one observation from each $\mathbb{P}_h$), we can identify the value of J as well as the subsets of observations produced by each $\mathbb{P}_h$ with high probability using a large value of the dimension.

We believe that the HFp should have attracted the attention of researchers in classification and clustering for functional data, the 'orthogonality case' apparently being more attractive because it would allow one to obtain *perfect classification* and *perfect clustering*. It took 50 years before the HFp was formally used in classification. To the best of our knowledge, the first paper using HFp in classification was Baillo et al (2011), where the authors derived a classification procedure using likelihood ratios. They focused on the 'equivalence case' and hence, did not obtain perfect classification. Optimal classification of Gaussian processes (say, GPs) was analyzed in Torrecilla et al (2020) from the HFp viewpoint. Further, the optimal (Bayes') classifier of equivalent GPs was derived and a procedure to obtain asymptotically perfect classification of mutually singular GPs was described as well. The results covered both homoscedastic and heteroscedastic cases. Additionally, Delaigle and Hall (2012) and Delaigle and Hall (2013) investigated conditions under which a perfect classification procedure for GPs was possible and developed related classifiers. The paper by Dai et al (2017) proposed a functional classifier based on ratio of density functions, which also leads to perfect classification. These papers contain no reference of the HFp. In fact, the relationship between Delaigle and Hall (2012) and the HFp was analyzed in Berrendero et al (2018), where the authors presented an expression of the optimal Bayes' rule in some classification problems for functional data. As mentioned earlier, perfect clustering has been studied by Delaigle et al (2019) only.

In Rao and Varadarajan (1963) and Shepp (1966b), the authors obtained characterizations of the singularity or equivalence of Gaussian measures in functional spaces. Their results involve increasing sequences of subspaces. For equivalent GDs, the limit obtained in Rao and Varadarajan (1963) includes a term which is the exponential of an expression involving the difference of the means of $\mathbb{P}_1$ and $\mathbb{P}_2$. Curiously, the logarithm of this term is related with the expressions of our limits. Similarities between our proposal and those in Rao and Varadarajan (1963) and Shepp (1966b) end here because the other involved terms are different. Moreover, we handle Mahalanobis distances *between data points*, while these papers use Hellinger and Jeffreys functionals to measure discrepancy *between distributions*. As a consequence, the characterizations they obtain are not applicable in practice to classify or cluster data points because they depend on the full distribution. It is not straight forward to compute such functionals using data points.

In this paper, we first analyze the limit of the above mentioned scaled Mahalanobis' distances by assuming the underlying parameters of the GPs to be *known* in Section 2. We begin with a general concentration result in Theorem 2.1. Then, we propose a transformation for clustering that asymptotically yield *perfect separation* among the clusters (see Theorem 2.5). Further, this transformation can be used to find the unknown number of clusters (see Proposition 2.3). In Section 3, we *estimate* the covariance operator of the mixture distribution from data and state related asymptotic results for the proposed transformation. In Theorem 3.2, we prove uniform (on the sample points) consistency of the empirical version for the transformation associated with GP clustering. It is surprising that our GP clustering method fails to discriminate 'location only' scenarios, but yields perfect clustering for 'differences in scales' (see Remark 2.2.2). We have also compared our work both theoretically (see Section M of Appendix II) as well as numerically (see Sections 4, 5 and Section N in

Appendix II) with the existing literature on perfect clustering for functional data. All proofs are deferred to Appendix I. Some additional material is presented in Appendix II, which includes a possible extension to non-Gaussian distributions (Section K), discussion on a clustering procedure in the 'location only' case (Section L) and theoretical comparisons of our results with those obtained in the paper by Delaigle et al (2019) (Section M).

In this paper, we will use the following notations. The distribution of the random process $\mathbf{Z}$ will be denoted as $\mathbb{P}_{\mathbf{Z}}$, its mean function by $\mu^{\mathbf{Z}}$ and its covariance operator (referred to simply as covariance) by $\Sigma^{\mathbf{Z}}$. We use $\Sigma^{\mathbf{Z}}(s,t)$ to denote the covariance between $\mathbf{Z}(s)$ and $\mathbf{Z}(t)$ for $s,t \in [0,1]$. Further, we will assume that all involved random quantities are defined on a common probability space $(\Omega, \mathcal{A}, \mathbb{P})$. Given a square matrix A, $trace(A)$ denotes its trace. The usual Euclidean norm on $\mathbb{R}^d$ is denoted by $\|\cdot\|$. To simplify notation, we do not explicitly state the dependence of the norm on the dimension d.

2 Transformation with Known Gaussian Distributions

Let $\{V_d\}_{d\in\mathbb{N}}$ be an increasing sequence of subspaces of $\mathbb{H}$. Here, the dimension of V_d is d. This restriction is not necessary for the development which follows as long as the dimension of V_d goes to infinity with increasing d, but it simplifies the notation. Given the subspace V_d, let $\mu_d^{\mathbf{Z}}$ and $\Sigma_d^{\mathbf{Z}}$ represent the d-dimensional mean and the $d \times d$ covariance matrix of the projection of $\mathbf{Z}$ on V_d. If $\mathbf{u} \in \mathbb{H}$, we denote $\mathbf{u}_d$ to be its projection on V_d.

Fix $b \in \mathbb{H}$. Theorem 2.1 analyses the behaviour of the limit of squared Mahalanobis norm of the d-dimensional random vector $(\mathbf{Z}-b)_d$ for $d \in \mathbb{N}$. For every positive definite $d \times d$ matrix A_d, we define the map

$$D_d^{A_d}(\mathbf{u},\mathbf{v}) = \frac{1}{d}\left\|A_d^{-1/2}(\mathbf{u}-\mathbf{v})_d\right\|^2, \text{ for } \mathbf{u},\mathbf{v} \in \mathbb{H}. \tag{1}$$

In this section, the underlying distributions are assumed to be *known*. After stating Theorem 2.1 and some remarks related to it, we will look into an application to cluster analysis inspired from this result. We will take advantage of the fact that the limit in this theorem is not random, but it may depend on the underlying probability distribution $\mathbb{P}_{\mathbf{Z}}$.

Theorem 2.1 *Let $\{A_d\}$ be a sequence of $d \times d$ symmetric, positive definite matrices and $\alpha_1^d, \ldots, \alpha_d^d$ be the eigenvalues of the matrix $S_d = (A_d)^{-1/2}\Sigma_d^{\mathbf{Z}}(A_d)^{-1/2}$ for $d \in \mathbb{N}$. We define $\alpha_d = (\alpha_1^d, \ldots, \alpha_d^d)^T$ and $\|\alpha_d\|_\infty = \max(\alpha_1^d, \ldots, \alpha_d^d)$ is the supremum norm. Let $b \in \mathbb{H}$ such that there exist constants L_μ and L_S (finite, or not) with*

$$\begin{aligned} L_\mu &= \lim_{d\to\infty} D_d^{A_d}(\mu^{\mathbf{Z}}, b), && (2)\\ L_S &= \lim_{d\to\infty} \frac{1}{d}\, trace(S_d) \text{ and} && (3)\\ 0 &= \lim_{d\to\infty} \frac{\|\alpha_d\|_\infty}{d}. && (4)\end{aligned}$$

Then, $D_d^{A_d}(\mathbf{Z}, b) \xrightarrow{P} L := L_\mu + L_S$ as $d \to \infty$.

Remark 2.1.1 A condition in Theorem 2.1 is required to ensure that no single component is extremely influential. For instance, it may happen that we take a sequence such that $\alpha_1^d = d$ and $\alpha_i^d = o(d^{-1})$ for every $2 \le i \le d$. Under this condition, no limit is possible in Theorem 2.1. However, this possibility is excluded by assumption (4).

Remark 2.1.2 We allow both the constants in Theorem 2.1 to be infinite. When L_S is finite, Lemma B.1 (see Appendix I) shows that assumption (4) follows from assumption (3).

Remark 2.1.3 Let $\mathbf{Z}_1$ and $\mathbf{Z}_2$ be independent observations generated from the GDs $\mathbb{P}_1$ and $\mathbb{P}_2$. Thus, $\mathbf{Z}_1 - \mathbf{Z}_2$ is a GP with mean $\mu_1 - \mu_2$ and covariance $\Sigma^{\mathbf{Z}_1} + \Sigma^{\mathbf{Z}_2}$. Consider the matrix $S_d = (A_d)^{-1/2}(\Sigma_d^{\mathbf{Z}_1} +$

$\Sigma_d^{\mathbf{Z_2}})(A_d)^{-1/2}$ with $d \in \mathbb{N}$. Take $\mathbf{Z} = \mathbf{Z}_1 - \mathbf{Z}_2$ and $b = 0$ in Theorem 2.1. Then, the following convergence result holds:

$$D_d^{A_d}(\mathbf{Z}_1, \mathbf{Z}_2) = D_d^{A_d}(\mathbf{Z}_1 - \mathbf{Z}_2, 0) \xrightarrow{P} L := L_\mu + L_S \text{ as } d \to \infty.$$

Here, $L_\mu = \lim_{d\to\infty} D_d^{A_d}(\mu_1, \mu_2)$ and L_S is as defined in (3) of Theorem 2.1.

Remark 2.1.4 In general, the fact that $V_d \subset V_{d+1}$ does not guarantee the existence of any relationship between the sets $\{\alpha_1^d, \dots, \alpha_d^d\}$ and $\{\alpha_1^{d+1}, \dots, \alpha_{d+1}^{d+1}\}$. However, in some cases $\{\alpha_1^d, \dots, \alpha_d^d\} \subset \{\alpha_1^{d+1}, \dots, \alpha_{d+1}^{d+1}\}$ (see, for instance, Section 2.1, where V_d is generated by the first d eigenfunctions of $\Sigma^{\mathbf{Z}}$).

2.1 Application: Cluster Analysis

In this subsection, we deal with a random function $\mathbf{Z}$ whose distribution is a two component mixture distribution of the form: $\mathbb{P}_{\mathbf{Z}} = \pi_1\mathbb{P}_1 + \pi_2\mathbb{P}_2$, where $0 < \pi_1 < 1$ and $\pi_1 + \pi_2 = 1$. Here, $\mathbb{P}_h$ denotes the GD on $\mathbb{H}$ with mean function μ_h and covariance Σ_h for $h = 1, 2$. The mean function and the covariance of the mixture satisfy $\mu^{\mathbf{Z}}(t) = \pi_1\mu_1(t) + \pi_2\mu_2(t)$ with $t \in [0, 1]$ and

$$\Sigma^{\mathbf{Z}}(s, t) = \pi_1\Sigma_1(s, t) + \pi_2\Sigma_2(s, t) + \pi_1\pi_2[\mu_1(s) - \mu_2(s)][\mu_1(t) - \mu_2(t)] \text{ for } s, t \in [0, 1]. \tag{5}$$

Given a random sample $\mathbf{Z}_1, \dots, \mathbf{Z}_N$ from $\mathbb{P}_{\mathbf{Z}}$, consider the following set:

$$\mathcal{C}_h = \{j : \mathbf{Z}_j \text{ was obtained from } \mathbb{P}_h \text{ for } 1 \leq j \leq N\} \tag{6}$$

with $h \in \{1, 2\}$. Clearly, the set $\mathcal{C}_h$ depends on the sample size N. The components of the mixture distribution $\mathbb{P}_{\mathbf{Z}}$ and the sets $\mathcal{C}_h$ for $h = 1, 2$ are *unknown*, and the problem we are dealing with is the estimation of these sets. However, we assume $\mathbb{P}_{\mathbf{Z}}$ and the sets $\mathcal{C}_1$ and $\mathcal{C}_2$ to be *known* in this section to build the fundamental idea behind using the proposed transformation for GP clustering.

Let V_d with $d \in \mathbb{N}$ denote the sequence of d-dimensional subspaces generated by the d eigenfunctions associated with the d largest eigenvalues of $\Sigma^{\mathbf{Z}}$ (recall the discussion in Remark 2.1.4). In the following result, $\mathbf{Z}_1$ and $\mathbf{Z}_2$ are assumed to be independent and $\mathbb{P}_{\mathbf{Z}_1} = \mathbb{P}_h$ and $\mathbb{P}_{\mathbf{Z}_2} = \mathbb{P}_k$ with $h, k \in \{1, 2\}$. The clustering procedure that we propose is based on the behavior of the transformation $D_d^{\Sigma_d^{\mathbf{Z}}}(\mathbf{Z}_1, \mathbf{Z}_2)$, which is stated below in Theorem 2.2.

Theorem 2.2 *(a) Assume that $h = k \in \{1, 2\}$. Define $S_d^h := (\Sigma_d)^{-1/2}(2\Sigma_{hd})(\Sigma_d)^{-1/2}$ for $d \in \mathbb{N}$, and assume that $L_S^h = \lim_d \frac{1}{d} trace(S_d^h)$ exists. Then,*

$$D_d^{\Sigma_d^{\mathbf{Z}}}(\mathbf{Z}_1, \mathbf{Z}_2) \xrightarrow{P} L_S^h \text{ as } d \to \infty. \tag{7}$$

(b) Assume that $h \neq k \in \{1, 2\}$. Define $S_d^{hk} := (\Sigma_d)^{-1/2}(\Sigma_{hd} + \Sigma_{kd})(\Sigma_d)^{-1/2}$ for $d \in \mathbb{N}$, and assume that $L_S^{hk} = \lim_d \frac{1}{d} trace(S_d^{hk})$ exists. Then,

$$D_d^{\Sigma_d^{\mathbf{Z}}}(\mathbf{Z}_1, \mathbf{Z}_2) \xrightarrow{P} L^{hk} := L_S^{hk} \text{ as } d \to \infty. \tag{8}$$

(c) If $h \neq k \in \{1, 2\}$, then $L_\mu^{hk} = \lim_d D_d^{\Sigma_d^{\mathbf{Z}}}(\mu_h, \mu_k) = 0$ and both L_S^h and L_S^{hk} are finite.

Remark 2.2.1 The structure of the covariance $\Sigma^{\mathbf{Z}}$ stated in equation (5) imposes some restrictions on the associated constants as stated in part (c) of Theorem 2.2. In particular, the fact that L_S^h and L_S^{hk} are finite implies that assumption (4) in Theorem 2.1 always holds for the sequence of matrices $\{S_d^h\}_{d\in\mathbb{N}}$ and $\{S_d^{hk}\}_{d\in\mathbb{N}}$ with $h, k \in \{1, 2\}$.

Remark 2.2.2 It follows from part (c) in Theorem 2.2 that the statistic we propose is useless for cluster analysis in the homoscedastic case (independently of the difference between μ_1 and μ_2) because if $\Sigma_1 = \Sigma_2$, then $L^{12} = L_S^1 = L_S^2$. A possibility is to modify the statistic $D_d^{\Sigma_d^{\mathbf{Z}}}(\mathbf{z}_1, \mathbf{z}_2)$ so that the value of the transformation $D_d^{\Sigma_d^{\mathbf{Z}}}(\mu_1, \mu_2)$ increases with $d \in \mathbb{N}$. Our proposal is to use

$$D_d^{\Sigma_d, r}(\mathbf{u}, \mathbf{v}) := \frac{1}{d}\left\|(\Sigma_d^{-1/2})^r(\mathbf{u} - \mathbf{v})_d\right\|^2 = \frac{1}{d}\sum_{i=1}^{d}\frac{(u_i - v_i)^2}{\lambda_i^r}, \text{ with } r \in \mathbb{N}.$$

Discussion of this transformation, and some numerical results are included in Appendix II.

To simplify notation and avoid technicalities with empty classes, we additionally assume that the observations whose indices belong to the sets $\mathcal{C}_1 = \{1, \ldots, N_1\}$ and $\mathcal{C}_2 = \{N_1 + 1, \ldots, N\}$ with $N = N_1 + N_2$ and $N_1, N_2 > 0$, were generated by $\mathbb{P}_1$ and $\mathbb{P}_2$, respectively. In practice, these sets are *unknown* and in fact our aim is their estimation. We begin with this simplifying assumption for ease of notation, and to obtain a clear exposition of the proposed methodology.

Define the $N \times N$ matrix Γ_d whose (i, j)-th element is

$$\Gamma_d(\mathbf{Z}_i, \mathbf{Z}_j) = \gamma_{ij}^d = \frac{1}{N-2} \sum_{t=1,\ t \neq i,j}^{N} \left[D_d^{\Sigma_d^{\mathbf{Z}}}(\mathbf{Z}_t, \mathbf{Z}_i) - D_d^{\Sigma_d^{\mathbf{Z}}}(\mathbf{Z}_t, \mathbf{Z}_j) \right]^2 \tag{9}$$

for $1 \leq i, j \leq N$. Theorem 2.2 and the fact that $t \neq i, j$ in (9) give us the following:

$$\gamma_{ij}^d \xrightarrow{P} \begin{cases} 0, & \text{if } i, j \in \mathcal{C}_h \text{ for } h = 1, 2, \\ \gamma_{hk}, & \text{if } i \in \mathcal{C}_h \text{ and } j \in \mathcal{C}_k, \text{ with } h \neq k \in \{1, 2\}, \end{cases} \tag{10}$$

as $d \to \infty$. Here,

$$\gamma_{hk} = \frac{N_h - 1}{N-2}(L_S^h - L_S^{hk})^2 + \frac{N_k - 1}{N-2}(L_S^k - L_S^{kh})^2.$$

Combining the fact stated above in (10), as $d \to \infty$, we obtain (remember that N, N_1, N_2 are fixed now)

$$\Gamma_d \xrightarrow{P} \Gamma := \begin{bmatrix} \mathbf{0}_{N_1}\mathbf{0}_{N_1}^T & \gamma_{12}\mathbf{1}_{N_1}\mathbf{1}_{N_2}^T \\ \gamma_{21}\mathbf{1}_{N_2}\mathbf{1}_{N_1}^T & \mathbf{0}_{N_2}\mathbf{0}_{N_2}^T \end{bmatrix}. \tag{11}$$

Let β_i^d and β_i (for $1 \leq i \leq N$) denote the eigenvalues corresponding to the matrices Γ_d and Γ, respectively. Define the following quantities

$$K_d = \sum_{i=1}^{N} I(|\beta_i^d| > a_d) \text{ and } K_0 = \sum_{i=1}^{N} I(|\beta_i| > 0), \tag{12}$$

with $\{a_d\}_{d \in \mathbb{N}}$ decreasing to 0 as $d \to \infty$ at an appropriate rate, and I is the indicator function. The constant K_0 clearly equals 2 for the limiting $N \times N$ matrix Γ stated in (11), and hence, correctly identifies the true underlying number of clusters.

Proposition 2.3 *Assume $N_1, N_2 \geq 1$ are fixed. Under the assumptions of Theorem 2.2, if $L_S^{12} \neq L_S^1$ and $L_S^{21} \neq L_S^2$, then there exists a sequence $\{a_d\}_{d \in \mathbb{N}} \subset \mathbb{R}^+$ such that $a_d \to 0$ and $K_d \xrightarrow{P} 2$ as $d \to \infty$.*

This now implies that we can correctly identify the true number of clusters asymptotically, as $d \to \infty$. The structure of the matrix Γ in (11) is straight forward because of the simplifying assumption on the sets $\mathcal{C}_1$ and $\mathcal{C}_2$. However, this is not a requirement and we will drop it. Proposition 2.3 holds more generally for *any permutation* of the data points $\mathbf{Z}_1, \ldots, \mathbf{Z}_N$. In fact, if the sets $\mathcal{C}_1$ and $\mathcal{C}_2$ are *unknown*, then the rows/columns of the Γ matrix will be permuted accordingly. But, the underlying structure remains the same and Proposition 2.3 continues to hold. As a followup of our previous result, we now prove that if any standard clustering method is used on the Γ_d matrix, then we can *perfectly cluster* all the observations asymptotically (as $d \to \infty$) because of the structure of the Γ matrix stated in (11).

Definition 2.4 *A clustering method can be defined as a map from $\mathbb{H}$ to the set $\{1, \ldots, J\}$. Consider the sequence of maps $\{\psi_d : d \in \mathbb{N}\}$ and a second map ϕ. A measure of distance between two clusterings based on the Rand index (see p. 847 of Rand (1971)) is defined as follows:*

$$\mathbb{R}_{d,N} = \frac{1}{\binom{N}{2}} \sum_{1 \leq i < j \leq N} I\big[I[\psi_d(\mathbf{z}_i) = \psi_d(\mathbf{z}_j)] + I[\phi(\mathbf{z}_i) = \phi(\mathbf{z}_j)] = 1\big],$$

for a fixed $N \geq 2$.

Let ϕ be the map which gives the true labels, i.e., $\phi(\mathbf{x}_j) = h$ for $j \in \mathcal{C}_h$ with $h \in \{1, 2\}$. We can construct a data based ψ_d by directly applying any clustering technique on the rows or columns of the matrix Γ_d. Here, we use the k-means algorithm on the rows of Γ_d.

Mathematically, the k-means algorithm finds J groups (say, $\mathcal{G}_1, \ldots, \mathcal{G}_J$) with centers $\mathbf{c}_1, \ldots, \mathbf{c}_J$ such that $\phi(\mathcal{G}_1, \ldots, \mathcal{G}_J) = \sum_{h=1}^{J} \sum_{\{i:\mathbf{x}_i \in \mathcal{G}_h\}} \|\mathbf{x}_i - \mathbf{c}_h\|^2$ is minimized. The asymptotic properties of the matrix Γ_d as $d \to \infty$ (stated above in (11)) imply that differences in the limiting constants should yield *perfect clustering*. Our next result proves label consistency for this k-means algorithm when $J = 2$.

Theorem 2.5 *Assume $J = 2$ and $\gamma_{12} > 0$. Further, assume that the conditions in Theorem 2.2 and Proposition 2.3 hold. Then, the clusters will be perfectly identifiable, i.e., $\mathbb{R}_{d,N} \xrightarrow{P} 0$ as $d \to \infty$.*

Remark 2.5.1 The well-known Rand index (*a measure of similarity*) is usually defined as $1 - \mathbb{R}_{d,N}$. As a consequence, Theorem 2.5 implies that the Rand index goes to one as $d \to \infty$.

Remark 2.5.2 The structure of the $N \times N$ symmetric matrix Γ stated in (11) continues to hold, and will lead us to *perfect clustering* for every value of $J \geq 2$. Moreover, the procedure described in Proposition 2.3 also works fine, with the limit equal to the rank of Γ. However, generalizing this idea to $J (> 2)$ clusters is not trivial.

The quantity K_0 in (12) is the rank of Γ, and one may be tempted to think that it generally coincides with J. But, this is true only for $J \leq 3$ and may be different for $J \geq 4$ (as shown in Lemma F.1 of Appendix F). The proof of Lemma F.1 further shows that the condition under which $\text{Rank}(\Gamma) < J$ is quite restrictive. Thus, in practice, our proposal is to estimate the number of clusters J using K_d.

2.1.1 Example with GPs

If we assume that $\Sigma_2 = a\Sigma_1$ with $a > 0$, then we have the following expressions for the scale constants stated in Theorem 2.2:

$$L_S^1 = \frac{2}{\pi_1 + \pi_2 a}, \; L_S^2 = \frac{2a}{\pi_1 + \pi_2 a} \text{ and } L_S^{12} = \frac{1 + a}{\pi_1 + a\pi_2}.$$

Thus, it is possible to identify perfectly the clusters as long as $a \neq 1$, since this implies that γ_{12} and γ_{21} both are positive quantities.

2.1.2 Uniform Convergence

In Theorem 2.2, we have proved consistency for finite sets of data points for the transformation $D_d^{\Sigma_d}(\mathbf{Z}_1, \mathbf{Z}_2)$ defined in (1). We now prove the uniform (on the random sample) convergence of this function as $N \to \infty$. This result will be useful in establishing a second result on uniform convergence, which we state in the next section.

Theorem 2.6 *Assume the conditions in Theorem 2.2, and let $\{d_N\} \subset \mathbb{N}$ be such that $d_N \to \infty$, as $N \to \infty$. Then,*

a) For $h \in \{1, 2\}$, let $\alpha_{d_N} = (\alpha_1^{d_N}, \ldots, \alpha_{d_N}^{d_N})^T$ be the eigenvalues of $S_{d_N}^h$ with $d_N \in \mathbb{N}$. If

$$\log N = o\left(\frac{d_N}{\|\alpha_{d_N}\|_\infty}\right), \tag{13}$$

then it happens that

$$\sup_{\mathbf{Z}_1, \mathbf{Z}_2 \in \mathcal{C}_h^N} \left| D_{d_N}^{\Sigma_{d_N}}(\mathbf{Z}_1, \mathbf{Z}_2) - L_S^h \right| \xrightarrow{P} 0 \text{ as } N \to \infty. \tag{14}$$

b) For any $h \neq k \in \{1, 2\}$, let $\alpha_{d_N} = (\alpha_1^{d_N}, \ldots, \alpha_{d_N}^{d_N})^T$ be the eigenvalues of $S_{d_N}^{hk}$ with $d_N \in \mathbb{N}$. If

$$\log N = o\left(\frac{d_N}{\|\alpha_{d_N}\|_\infty}\right), \tag{15}$$

then it happens that

$$\sup_{\mathbf{Z}_1 \in \mathcal{C}_h^N, \mathbf{Z}_2 \in \mathcal{C}_k^N} \left| D_{d_N}^{\Sigma_{d_N}}(\mathbf{Z}_1, \mathbf{Z}_2) - L^{hk} \right| \xrightarrow{P} 0 \text{ as } N \to \infty. \tag{16}$$

Remark 2.6.1 Assumption (4) holds here, so $\dfrac{\|\alpha_{d_N}\|_\infty}{d_N} = \dfrac{1}{d_N} \max_{1 \le i \le d_N} \alpha_i^{d_N} \to 0$. Thus, if we take d_N growing fast enough, then it is assured that assumptions (13) and (15) hold. The structure of the matrices S_d^h and S_d^{hk} for $d \in \mathbb{N}$ with $h \neq k \in \{1, 2\}$ implies that a sufficient condition is $\log N = o(d_N)$ (see Proposition H.1 in Appendix H).

3 Transformations with Estimated Gaussian Distributions

In this section, we will discuss the steps to implement the procedure described in Section 2. In practice, the involved distributions and all the associated quantities need to be estimated from the data. Here, $\mathbf{Z}$ will denote a random element with distribution the mixture $\pi_1 \mathbb{P}_1 + \pi_2 \mathbb{P}_2$.

For $j \in \mathbb{N}$, let $\phi_j^{\mathbf{Z}}(t)$ with $t \in [0, 1]$ and $\lambda_j^{\mathbf{Z}}$ denote the eigenfunctions and eigenvalues of $\Sigma^{\mathbf{Z}}$, respectively. We will now make the following assumptions:

A.1 $\sup_{t \in [0,1]} E[(\mathbf{Z}(t))^4] < \infty$.

A.2 It happens that $\lambda_1^{\mathbf{Z}} > \lambda_2^{\mathbf{Z}} > \cdots > 0$ satisfying $\sum_{j=1}^{\infty} \lambda_j^{\mathbf{Z}} < \infty$.

It is well-known that assumption *A.2* implies $\{\phi_j^{\mathbf{Z}}\}_{j \in \mathbb{N}}$ forms an orthonormal basis of $\mathbb{H}$.

To estimate $\Sigma^{\mathbf{Z}}$ and its eigenvalues and eigenfunctions, we will use the corresponding empirical quantities. Suppose that we have a simple random sample $\mathbf{Z}_1, \ldots, \mathbf{Z}_N$ taken from $\mathbb{P}_{\mathbf{Z}}$. Given $s, t \in [0, 1]$, we define

$$\hat{\Sigma}^{\mathbf{Z}}(s, t) = \frac{1}{N} \sum_{i=1}^{N} [\mathbf{Z}_i(s) - \overline{\mathbf{Z}}_N(s)][\mathbf{Z}_i(t) - \overline{\mathbf{Z}}_N(t)],$$

where $\bar{\mathbf{Z}}_N(t) = \frac{1}{N} \sum_{i=1}^{N} \mathbf{Z}_i(t)$. Consider the corresponding families $\hat{\lambda}_1^{\mathbf{Z}} \ge \hat{\lambda}_2^{\mathbf{Z}} \ge \cdots$ and $\hat{\phi}_1^{\mathbf{Z}}, \hat{\phi}_2^{\mathbf{Z}}, \ldots$ of its eigenvalues and eigenvectors, respectively. Note that $\hat{\Sigma}^{\mathbf{Z}}$ as well as all the $\hat{\lambda}_j^{\mathbf{Z}}$'s and $\hat{\phi}_j^{\mathbf{Z}}$'s depend on N. Given $\mathbf{u} \in \mathbb{H}$, we denote

$$\hat{u}_j^{\mathbf{Z}} = \langle \mathbf{u}, \hat{\phi}_j^{\mathbf{Z}} \rangle = \int_0^1 \mathbf{u}(t) \hat{\phi}_j^{\mathbf{Z}}(t) dt \text{ for } \ j \in \mathbb{N}.$$

With a finite sample, we cannot estimate all the infinite eigenvalues and eigenvectors. Thus, we follow the work of Delaigle and Hall (2012) and Hall and Hosseini-Nasab (2006), and select a non-random decreasing sequence η_N going to zero slowly enough as to satisfy $\lim_N N^{1/5} \eta_N = \infty$. We take

$$\hat{R}_N^{\mathbf{Z}} = \inf\{j : \hat{\lambda}_j^{\mathbf{Z}} - \hat{\lambda}_{j+1}^{\mathbf{Z}} < \eta_N\} - 1. \tag{17}$$

This definition implies that $\hat{\lambda}_j^{\mathbf{Z}} \ge \eta_N$ for every $j \le \hat{R}_N^{\mathbf{Z}}$. Moreover, we will also need that the theoretical eigenvalues are reasonably well separated. To obtain this, given $\delta > 0$, we also define

$$R_N^{\mathbf{Z}} = \inf\{j : \lambda_j^{\mathbf{Z}} - \lambda_{j+1}^{\mathbf{Z}} < (1 + \delta)\eta_N\} - 1. \tag{18}$$

We now state empirical analogues of the results stated in Section 2.1.

3.1 Consistency of Clustering

Let $\mathbf{Z}_1, \ldots, \mathbf{Z}_N$ be a simple random sample taken from $\mathbb{P}_{\mathbf{Z}}$. Now, $\mathbb{P}_{\mathbf{Z}}$ and the sets $\mathcal{C}_1$ and $\mathcal{C}_2$ (containing information on the class labels and defined in (6)) are unknown. Extension of Theorems 2.2 and 2.6 to Theorems 3.1 and 3.2 is presented below. The following results will be based on the analysis of the map $\hat{D}_{\hat{R}_N}(\mathbf{u}, \mathbf{v})$, which is the transformation $D_d^{\Sigma}(\mathbf{u}, \mathbf{v})$ defined in (1) with $d = \hat{R}_N$ (defined in (17)), and the pooled covariance matrix $\Sigma_{\hat{R}_N}$ which is estimated by $\hat{\Sigma}_{\hat{R}_N}$ (sample covariance of the full sample). The first result is related to the consistency of the transformation on finite sets.

Theorem 3.1 *Let assumptions A.1 and A.2 and those in Theorem 2.2 hold.*

(a) If $h = k \in \{1, 2\}$, then

$$\hat{D}_{\hat{R}_N}(\mathbf{Z}_1, \mathbf{Z}_2) \xrightarrow{P} L_S^h \text{ as } N \to \infty. \tag{19}$$

(b) If $h \neq k \in \{1, 2\}$, then

$$\hat{D}_{\hat{R}_N}(\mathbf{Z}_1, \mathbf{Z}_2) \xrightarrow{P} L_S^{hk} \text{ as } N \to \infty. \tag{20}$$

We need an increasing sample size in order to estimate the parameters consistently. Thus, it is desirable to be able to cluster the increasing number of data points, asymptotically without error. The only way to achieve this is to get some kind of uniform convergence in (19) and (20) when the sample size increases. This is the purpose of Theorem 3.2, which gives us clear evidence that using this transformation would lead to asymptotic perfect separation in the empirical case as well.

Theorem 3.2 *Let us assume all the conditions in Theorem 2.6 with $\log N = o(R_N^{\mathbf{Z}})$ in (18).*

(a) For $h \in \{1, 2\}$, it happens that

$$\sup_{\mathbf{Z}_1, \mathbf{Z}_2 \in \mathcal{C}_h^N} \left| \hat{D}_{\hat{R}_N}(\mathbf{Z}_1, \mathbf{Z}_2) - L_S^h \right| \xrightarrow{P} 0 \text{ as } N \to \infty.$$

(b) For any $h, k \in \{1, 2\}$ with $h \neq k$, we have that

$$\sup_{\mathbf{Z}_1 \in \mathcal{C}_h^N, \mathbf{Z}_2 \in \mathcal{C}_k^N} \left| \hat{D}_{\hat{R}_N}(\mathbf{Z}_1, \mathbf{Z}_2) - L_S^{hk} \right| \xrightarrow{P} 0 \text{ as } N \to \infty.$$

Remark 3.2.1 Clearly, Theorem 3.1 follows from Theorem 3.2. But, the conditions required for proving the former are weaker and hence, we state it as a separate result.

Remark 3.2.2 (*Asymptotic perfect identification of clusters*) Recall the matrix Γ_d from (9) with $d \in \mathbb{N}$. Now, consider the matrix $\hat{\Gamma}_{\hat{R}_N}$, which is obtained by replacing γ_{ij}^ds in the matrix $\Gamma_{\hat{R}_N}$ with their estimated values $\hat{\gamma}_{ij}^{\hat{R}_N}$ (I.e. $\hat{\gamma}_{ij}^{\hat{R}_N} = \hat{D}_{\hat{R}_N}(\mathbf{Z}_i, \mathbf{Z}_j)$ with $1 \leq i \neq j \leq N$). Define $\upsilon_{12} = \pi_1 \left| L_S^1 - L_S^{12} \right|^2 + \pi_2 \left| L_S^2 - L_S^{21} \right|^2$. Fix $\epsilon > 0$. Theorem 3.2 implies that with probability converging to one as $N \to \infty$, we have

- if $\mathbf{Z}_i, \mathbf{Z}_j \in \mathcal{C}_h$ for $h \in \{1, 2\}$, then $\left| \hat{\gamma}_{ij}^d \right| \leq 4\epsilon^2$,
- if $\mathbf{Z}_i \in \mathcal{C}_h, \mathbf{Z}_j \in \mathcal{C}_k$ for $h \neq k \in \{1, 2\}$, then $\left| \hat{\gamma}_{ij}^d - \upsilon_{12} \right| \leq H\epsilon$,

for some $H > 0$. Consequently, if $\upsilon_{12} > 0$, then the elements in $\hat{\Gamma}_d$ will be clustered into two well-separated clusters: one around 0 and another one around υ_{12} with probability converging to one.

Similarly, let $\mathbb{P}_{\mathbf{Z}}$ be a mixture of $J(> 2)$ components and denote

$$\upsilon_{hk} := \pi_h \left| L_S^h - L_S^{hk} \right|^2 + \pi_k \left| L_S^k - L_S^{kh} \right|^2$$

with $1 \leq h \neq k \leq J$. For positive and distinct v_{hk}s, the elements in the matrix $\hat{\Gamma}_d$ will be perfectly clustered into $1 + \binom{J}{2}$ well-separated clusters: one of them around the point 0 and the remaining around the values v_{hk} (for $h < k$) with probability converging to one as $N \to \infty$. Therefore, asymptotically, the sequence of matrices $\{\hat{\Gamma}_{\hat{R}_N}\}_{N \in \mathbb{N}}$ will contain enough information to perfectly cluster all the data points.

3.2 Implementation in Practice

We are given a sample of functional data points without the labels. Here, we consider the $N \times N$ estimated matrix $\hat{\Gamma}_N$ with the (i,j)-th element as $\hat{D}_{\hat{R}_N}(\mathbf{Z}_i, \mathbf{Z}_j)$ (which is just the empirical version of $D_d^{\Sigma_d^{\mathbf{Z}}}(\mathbf{Z}_i, \mathbf{Z}_j)$ based on the pooled sample covariance) for $1 \leq i, j \leq N$ and apply any clustering procedure on its rows (or, columns). Note again that we *do not need to estimate* the unknown constants L_S^h and L_S^{hk} for $h, k \in \{1, 2\}$ (stated in Theorem 3.1) for the implementation of our clustering procedure. The expression related with $\hat{R}_N$ is not used in practice as well (see Section 4.2 for the details of our implementation).

4 Analysis of Simulated Datasets

For our simulation study, we consider two class problems ($J = 2$). We generated data on a discrete grid of 100 equi-spaced points in the unit interval $[0, 1]$ from four different simulation models, which are described below. Let us fix $s > 0$.

I. Define $X_h(t) = \sum_{j=1}^{40} (\lambda_{hj}^{1/2} Z_{hj} + \mu_{hj}) \phi_j(t)$ with $t \in [0, 1]$ and $h = 1, 2$. Here, the Z_{hj}s are independent standard normal (i.e., $N(0, 1)$) random variables, $\phi_j(t) = \sqrt{2} \sin(\pi j t)$ with $t \in [0, 1]$ and $1 \leq j \leq 40$. Also, $\mu_{hj} = 0$ for $j > 6$, and we set the other components equal to $(0, -0.5, 1, -0.5, 1, -0.5)^T$ and $(0, -0.75, 0.75, -0.15, 1.4, 0.1)^T$ for $k = 1, 2$, and $\lambda_{1j} = 1/j^2$ and $\lambda_{2j} = s/j^2$ for $1 \leq j \leq 40$.
This model is from the paper Delaigle and Hall (2012).

II. In this example, $X_1 \sim B$ and $X_2 \sim \mu + sB$ with $\mu(t) = Gt$ for $t \in [0, 1]$ and $G \sim N(0, 4)$ independent of B. Here, B is the standard Brownian bridge, i.e., a centered Gaussian process with $\sigma_{ij} = \min(t_i, t_j) - t_i t_j$ with $t_i, t_j \in [0, 1]$ for $i, j \in \mathbb{N}$.

Since $E[X_2(t)] = E[Gt] = 0$ for $t \in [0, 1]$, the *differences in mean never appear* in this setting. In fact, the inclusion of μ modifies the covariances because if $0 < t_i < t_j < 1$, then the independence between G and the B yields the following:

$$E[X_2(t_i) X_2(t_j)] = 4 t_i t_j + s^2 t_i (1 - t_j).$$

This model is from the paper Berrendero et al (2018).

III. Let $X_h = \mu_h + \sum_{j=1}^{50} \xi_{hj} {\lambda_{hj}}^{1/2} \phi_j$ for $h = 1, 2$. Here, ξ_{hj}s are i.i.d. $N(0, 1)$, $\mu_1 = 0$ and $\mu_2(t) = t$ with $t \in [0, 1]$, $\lambda_{1j} = e^{-j/3}$ and $\lambda_{2j} = \sqrt{s} e^{-j/3}$ for $1 \leq j \leq 50$, and $\phi_{2i-1} = \sqrt{2} \sin(2 i \pi t)$ and $\phi_{2i} = \sqrt{2} \cos(2 i \pi t)$ for $1 \leq i \leq 25$ with $t \in [0, 1]$.
This model is from the paper Dai et al (2017).

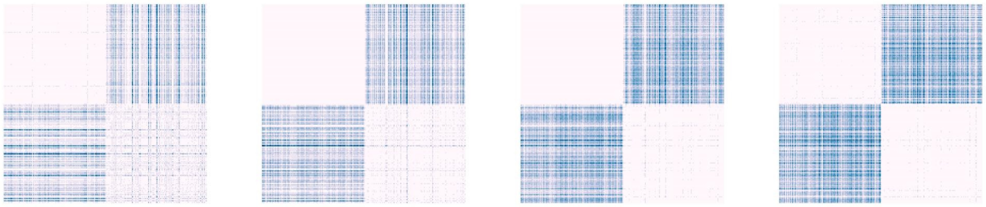
IV. This problem consists of two Brownian motions defined in the closed interval $[0, 1]$ with means $\mu_1(t) = 20 t^{1.1} (1 - t)$ and $\mu_2(t) = 20 t (1 - t)^{1.1}$, respectively, for $t \in [0, 1]$. For the first class, the eigenfunctions are $\phi_j(t) = \sqrt{2} \sin((j - 0.5) \pi t)$ and associated eigenvalues are $\lambda_{1j} = 1/(\pi(j - 0.5))^2$ for $1 \leq j \leq 15$. The second class is similar to the first one, but the eigenvalues are multiplied by $\sqrt{s}$ (i.e., $\lambda_{2j} = \sqrt{s} \lambda_{1j} = \sqrt{s}/(\pi(j - 0.5))^2$) for $1 \leq j \leq 15$.
This model is from the paper Galeano et al (2015).

We set $s = 1$ for `location only` problems. In `location and scale` problems, we fixed $s = 3$, while for `scale only` problems the mean functions μ_1 and μ_2 were set to be the constant function 0 and $s = 3$ was retained.

4.1 Choice of d

A critical issue is selection of the optimal dimension of the projected space for a given a set of data points (i.e., a fixed value of (N_1, N_2) or N). Let us recall Theorem 3.1; according to this result we expect the rows of the matrix $\hat{\Gamma}_d$ to form two clearly separated clusters depending on the class label of the observation for large values of d. To demonstrate this, we construct a sequence of images and show how this separation varies with increasing values of d.

We generated samples of size 250 from each of the two classes for the 'scale case' of Example II. For the purpose of demonstration, the first 250 observations correspond to the first GD, while the next 250 observations to the second. Figure 1 below shows the heatmap for increasing values of d, and we observe the best concentration at $d = 80$. However, some noise in the off-diagonal submatrices for $d = 80$ (compared to $d = 60$) makes us to consider that the optimum could be somewhere between the values 60 and 80.



(a) $d = 20$ (b) $d = 40$ (c) $d = 60$ (d) $d = 80$

Figure 1: Heatmap of $\hat{\Gamma}_d$ for varying values of d.

Clearly, the choice of d is quite important as d is the dimension of the subspace where we project our observations (for a fixed sample size). We observe from Figure 1 that its estimation is quite crucial. Subsection 4.2 contains further details on the choice of d.

4.2 Clustering Procedure

To implement the clustering method, one needs to choose the dimension d suitably, and we use cross-validation (CV) to do the job. We use the idea developed by Wang (2010), which we state briefly here: given $B \in \mathbb{N}$, split the data into three random subsets (say, S_{1b}, S_{2b} and S_{3b}) each of equal size for $1 \leq b \leq B$. For each value of b, treat the points in S_{1b} and S_{2b} as the training sets, and S_{3b} as the validation set. For a fixed value of d and given a clustering algorithm, the two training sets S_{1b} and S_{2b} are used to construct two cluster assignments. An appropriate distance between these two cluster assigments (say, $\mathbb{D}$) is computed based on the validation set S_{3b} (see Section 2 of Wang (2010) for more details). We repeat this partition $B = 50$ times and average it over these B samples to get $\hat{\mathbb{D}}_d^{CV}$. Define $\hat{d}_{CV} = \arg\min_{2 \leq d \leq N} \hat{\mathbb{D}}_d^{CV}$.

Recall the structure of the Γ matrix stated in (11), and also see Figure 1. As mentioned in Section 3.2, the number of clusters were estimated using the method described in Section 2.1 (see (12)). To implement the procedure in practice, one needs to estimate the sequence $\{a_d\}_{d \in \mathbb{N}}$. We have used the function `optishrink` available in the `R` package `denoiseR`. This function extracts a *low-rank signal from Gaussian noisy data using the optimal shrinker of singular values.* The low rank structure of the Γ matrix motivates us to directly apply this function on $\hat{\Gamma}_d$. The overall implementation yielded quite desirable results in our numerical study (see Tables 4.1 and 4.2 below). We can apply any clustering method on the transformed data $\hat{\Gamma}_d$. In addition to the k-means algorithm (CD-k-means) discussed in Theorem 2.5, we considered spectral clustering (CD-Spectral) and Gaussian mixture models (CD-mclust). One may refer to the book by Hastie et al (2009) for details on these three popular clustering methods. The `R` codes for our methods are available here: GP clustering. As we do with the other methods we are comparing with, we only report here the better obtained result. Complete results are reported in Appendix N.

We considered several methods for comparison. The first method is the classical k-means algorithm for functional data. Several competent methods for functional clustering using functional mixed mixture models are implemented in the function `funcit` from the `R` package `funcy`. We report this method as funclust. The methodology developed by Chiou and Li (2007) is available in the function `FClust` from the `R` package `fdaspace` using two clustering techniques 'EMcluster' (CL1) and 'kCFC' (CL2). We have reported the minimum result, and stated it as CL. In Delaigle et al (2019), the authors developed functional clustering based on the k-means using basis functions. We implemented this method for two choices of the basis functions, namely, Haar and PC, and reported the best result among these two (we call it DHP). We have not used the DB2 basis for our comparisons because it requires the grid points to be of a power of 2. The DHP method is available from the journal website, and we used those `Matlab` codes for our comparisons.

We conducted simulations based on models I to IV, which were introduced in the beginning of Section 4. We did not consider the `location only` scenario as our proposed method is useless in such cases (recall part (c) of Theorem 2.2). However, we have some discussion and additional results in Section L in Appendix II for this scenario. The sample size of each class was set to be 250. Our experiment was replicated 100 times, and the results are reported in Tables 4.1 and 4.2 below. To measure the similarity between two cluster assignments, we computed the adjusted Rand index using the function `RRand` in the `R` package `phyclust`. One minus the adjusted Rand index (we call it *adjusted Rand distance*) is reported in tables below, where the minimum is marked in **bold** and the second lowest is in *italics*.

It is worth noting that all the competing methods require the number of clusters as an input variable, and we have run these methods with $k = 2$ (the true number of clusters). However, when applying the CD procedure we have estimated the number of clusters following the procedure described above. We obtained the correct value in more than 99% of the cases (across all four examples for both scenarios) in our simulation study.

Table 4.1: Adjusted Rand distances for different GPs with difference in location and scales (with standard error in brackets).

Ex.	k-means	funclust	CL	DHP	CD
I	0.0632	0.1541	*0.0239*	0.0818	**0.0001**
	(0.0007)	(0.0017)	(0.0007)	(0.0025)	(0.0001)
II	0.9445	0.8222	*0.5767*	0.5149	**0.4240**
	(0.0036)	(0.0027)	(0.0045)	(0.0049)	(0.0030)
III	0.4250	0.3858	*0.2891*	0.4137	**0.0625**
	(0.0017)	(0.0003)	(0.0000)	(0.0054)	(0.0006)
IV	0.4945	0.3975	0.1833	*0.1379*	**0.0000**
	(0.0005)	(0.0011)	(0.0000)	(0.0033)	(0.0000)

In the first setting, we considered clustering problems with differences in their `location and scale` parameters. Usefulness of the proposed transformation is clear from Table 4.1. Our method attains the first position across all examples, while in Example IV we obtain perfect clustering. Although there is no location difference in Example II, sub-optimal performance of our method is probably due to low signal from the difference between the two covariance structures. CL attains the second best performance in the first three examples among the competing methods, while DHP performs better than CL in Example IV.

In the next setting, we dealt with differences only in `scale` parameters. It is clear from Table 4.2 that the separation in scatters is captured very well by the proposed transformation $\hat{\Gamma}_d$. Moreover, our method again leads to perfect clustering (with a significant improvement in Example II compared to Table 4.1). The method funclust (respectively, CL) attains the second position in Examples II and III (respectively, Examples I and IV). The performances of k-means and DHP are similar, and quite bad in this scenario. Generally, the results in Table 4.2 suggest that all existing methods fail to judiciously capture information if it is present only in the scale parameters.

After applying the transformation $\hat{\Gamma}_d$, we had used three methods for clustering the transformed observations. Overall, it seems that the Gaussian mixture model (i.e., mclust) achieves better results than the other two procedures (see the complete numerical results in Section N of Appendix II).

Table 4.2: Adjusted Rand distances for different GPs with difference only in scales (with standard error in brackets).

Ex.	k-means	funclust	CL	DHP	CD
I	1.0019	0.9776	*0.8269*	0.9966	**0.0000**
	(0.0000)	(0.0006)	(0.0000)	(0.0005)	(0.0000)
II	1.0006	*0.5004*	0.9065	0.9999	**0.0084**
	(0.0001)	(0.0049)	(0.0007)	(0.0003)	(0.0003)
III	0.9990	*0.9956*	0.9994	0.9967	**0.0856**
	(0.0002)	(0.0000)	(0.0000)	(0.0007)	(0.0006)
IV	0.968	1.0006	*0.8464*	0.9980	**0.0005**
	(0.0001)	(0.0000)	(0.0000)	(0.0006)	(0.0004)

5 Analysis of Benchmark Datasets

We have applied our proposed methods to some benchmark data sets, `Wheat` (from the `R` package `fds`), `Satellite` (available at `https://www.math.univ-toulouse.fr/∼ferraty/SOFTWARES/NPFDA/index.html`), and `Cars` (kindly provided by the first author of Torrecilla et al (2020)).

To evaluate the clustering algorithms, we ran a single execution (without splitting). Class assigments are already available for the `Wheat` dataset. The `Satellite` data has been analyzed in detail in the paper Dabo-Niang et al (2007), where the authors split the curves into two clusters 'unimodal' and 'multimodal'. The authors of this paper kindly shared the exact cluster assignments for this data set with us. The `Cars` data contains asset log-returns of the car companies Tesla, General Motors and BMW (see Torrecilla et al (2020) for more details). However, the rank of the estimated $\hat{\Gamma}_d$ matrix was two for this data set, and our method detected only two distinct clusters. This is coherent with Torrecilla et al (2020), where the authors had noted that assets of General Motors and BMW were very similar and quite difficult to distinguish. So, we merged General Motors with BMW while assigning the class labels for this data set. Consequently, the number of clusters was set to be two for all competing methods. We report the adjusted Rand distance for these three data sets in Table 5.1. Superiority of our proposed methodology w.r.t. the competing methods is clear from the results given below.

Table 5.1: Adjusted Rand distances for different clustering methods.

Data	M	k-means	funclust	CL	DHP	CD
Wheat	100	0.6960	0.6960	0.8058	*0.5730*	**0.3644**
Satellite	472	0.6072	0.6072	*0.6060*	0.7253	**0.4448**
Cars	90	*0.8856*	*0.8856*	0.9650	0.9088	**0.4680**

To get a better understanding of the performance of our proposed method, we further computed the well-known average purity function. A value of average purity function close to one indicates good performance of a method. We obtained the values as 0.90, 0.8622 and 0.8666 for the `Wheat` data, the `Satellite` data and the `Cars` data, respectively. Overall, our proposed method CD yields quite promising results in all three benchmark data sets.

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Appendix I: Proofs and Mathematical Details

A Proof of Theorem 2.1

Fix $d \in \mathbb{N}$. The d-dimensional random vector $(\mathbf{Z} - b)_d$ has a Gaussian distribution with mean equal to $(\mu - b)_d$ and covariance matrix equal to Σ_d. Now, $\|(A_d)^{-1/2}(\mathbf{Z} - b)_d\|^2$ is equal to the square of the norm of a d-dimensional normal variable with mean $\mathbf{m}_d = (A_d)^{-1/2}(\mu - b)_d$ and covariance matrix $S_d = (A_d)^{-1/2}\Sigma_d(A_d)^{-1/2}$. Therefore, if $\mathbf{u}_d$ is a d-dimensional vector with centered normal distribution and covariance matrix equal to S_d, then

$$D_d^{A_d}(\mathbf{Z}, b) \sim \frac{1}{d}\langle \mathbf{m}_d + \mathbf{u}_d, \mathbf{m}_d + \mathbf{u}_d\rangle = \frac{1}{d}\left(\|\mathbf{m}_d\|^2 + \|\mathbf{u}_d\|^2 + 2\langle \mathbf{m}_d, \mathbf{u}_d\rangle\right). \tag{21}$$

By assumption (2), we have

$$\lim_{d\to\infty} \frac{1}{d}\|\mathbf{m}_d\|^2 = L_\mu.$$

Let us consider the *second term* in (21). Fix a basis in V_d spanned by the eigenvectors of S_d. Note that this term is not dependent on L_μ. Denote $\mathbf{u}_d = (u_{d,1}, \ldots, u_{d,d})^T$ and $\mathbf{m}_d = (m_{d,1}, \ldots, m_{d,d})^T$ in this basis. Therefore, the random variables $(u_{d,i})^2$ with $1 \le i \le d$ are independent with means equal to α_i^d for $1 \le i \le d$ and $\sum_{i=1}^d (u_{d,i})^2 \sim \sum_{i=1}^d \alpha_i^d (u_i)^2$. Here, $\{u_i\}_{1\le i\le d}$ is a sequence of independent and identically distributed (i.i.d.) real variables with the standard normal distribution. We split the proof into two cases.

A.0.1 L_S is finite

Fix $\epsilon > 0$. Taking into account that the variance of a χ^2 distribution with one degree of freedom is two and using Tchebychev's inequality, we have that

$$\begin{aligned}
\mathbb{P}\left[\frac{1}{d}\left|\|\mathbf{u}_d\|^2 - \mathrm{trace}(S_d)\right| \ge \epsilon\right] &= \mathbb{P}\left[\frac{1}{d}\left|\sum_{i=1}^d \left((u_{d,i})^2 - \alpha_i^d\right)\right| \ge \epsilon\right] \\
&\le \frac{2}{\epsilon^2 d^2}\sum_{i=1}^d (\alpha_i^d)^2 \\
&\le \frac{2}{\epsilon^2 d^2}\|\alpha^d\|_\infty \sum_{i=1}^d \alpha_i^d,
\end{aligned}$$

which converges to zero by assumptions (3) and (4). Consequently, we have shown that

$$\frac{1}{d}\|\mathbf{u}_d\|^2 - \frac{1}{d}\mathrm{trace}(S_d) \xrightarrow{P} 0 \text{ as } d \to \infty,$$

and assumption (3) gives

$$\frac{1}{d}\|\mathbf{u}_d\|^2 \xrightarrow{P} L_S \text{ as } d \to \infty.$$

A.0.2 L_S is infinite

We have that

$$\begin{aligned}
\mathbb{P}\left[\frac{1}{\sum_{i=1}^d \alpha_i^d}\left|\sum_{i=1}^d \left((u_{d,i})^2 - \alpha_i^d\right)\right| \ge \epsilon\right] &= \mathbb{P}\left[\left|\sum_{i=1}^d \frac{\alpha_i^d}{\sum_{i=1}^d \alpha_i^d}\left((u_i)^2 - 1\right)\right| \ge \epsilon\right] \\
&\le \frac{2}{\epsilon^2}\sum_{i=1}^d \left(\frac{\alpha_i^d}{\sum_{i=1}^d \alpha_i^d}\right)^2 \\
&\le \frac{2}{\epsilon^2}\frac{\|\alpha^d\|_\infty}{\sum_{i=1}^d \alpha_i^d},
\end{aligned}$$

which converges to zero because $L_S = \infty$ and assumption (4). Thus, we have shown that

$$\frac{1}{\frac{1}{d}\sum_{i=1}^{d} \alpha_i^d} \left(\frac{1}{d} \|\mathbf{u}_d\|^2 - \frac{1}{d} \operatorname{trace}(S_d) \right) \xrightarrow{P} 0. \tag{22}$$

Consequently, $\frac{1}{d}\|\mathbf{u}_d\|^2$ converges to ∞ at the same rate as $\frac{1}{d}$ trace(S_d).

Concerning the *last term* in (21), we have $\langle \mathbf{m}_d, \mathbf{u}_d \rangle = \sum_{i=1}^{d} m_{d,i} u_{d,i}$. We split the proof into cases.

A.0.3 L_μ is finite

Fix $\epsilon > 0$, and define $\alpha^d = (\alpha_1^d, \ldots, \alpha_d^d)^T$. Using Tchebychev's inequality again, we get

$$\mathbb{P}\left[\frac{1}{d} |\langle \mathbf{m}_d, \mathbf{u}_d \rangle| > \epsilon \right] \leq \frac{1}{\epsilon^2 d^2} \sum_{i=1}^{d} (m_{d,i})^2 \alpha_i^d \leq \frac{1}{\epsilon^2 d^2} \|\alpha^d\|_\infty \|\mathbf{m}_d\|^2,$$

which converges to zero by assumptions (2) and (4), and the proposition is proved in this case.

A.0.4 L_μ is infinite

The result follows from equation (21) and the previous results, if we are able to show that the sequence of real valued random variables

$$w_d = \frac{\langle \mathbf{m}_d, \mathbf{u}_d \rangle}{\max(\|\mathbf{m}_d\|^2, \|\mathbf{u}_d\|^2)}$$

converges to zero in probability as $d \to \infty$. In turn, this will be fixed if we show that every subsequence of $\{w_d\}$ contains a new subsequence which satisfies this property. Thus, let $\{w_{d_k}\}$ be a subsequence of $\{w_d\}$ and let us consider the associated subsequences $\{\|\mathbf{m}_{d_k}\|\}$ and $\{\|\mathbf{u}_{d_k}\|\}$. Obviously, there exists a further subsequence $\{d_{k^*}\}$ such that one of the following holds:

(i) $\lim_{d_{k^*}} \frac{\|\mathbf{m}_{d_{k^*}}\|^2}{\operatorname{trace}(S_{d_{k^*}})} = 0.$

(ii) $\lim_{d_{k^*}} \frac{\|\mathbf{m}_{d_k}\|^2}{\operatorname{trace}(S_{d_{k^*}})} = \infty.$

(iii) There exists a finite $C > 0$ such that $\lim_{d_{k^*}} \frac{\|\mathbf{m}_{d_{k^*}}\|^2}{\operatorname{trace}(S_{d_{k^*}})} = C.$

Notice that in cases (i) and (iii), we have $L_S = \infty$. To simplify notation, we denote the sequence $\{S_{d_{k^*}}\}$ by $\{S_h\}$, and similarly for the remaining ones. In case (i), since equation (22) shows that

$$\frac{\|\mathbf{u}_h\|^2}{\operatorname{trace}(S_h)} \xrightarrow{P} 1 \text{ as } h \to \infty, \tag{23}$$

we have $\frac{\|\mathbf{m}_h\|}{\|\mathbf{u}_h\|} \xrightarrow{P} 0$ as $h \to \infty$. Consequently,

$$\lim_h |w_h| = \lim_h \frac{|\langle \mathbf{m}_h, \mathbf{u}_h \rangle|}{\|\mathbf{u}_h\|^2} \leq \lim_h \frac{\|\mathbf{m}_h\|}{\|\mathbf{u}_h\|} = 0 \text{ in probability.}$$

If (ii) holds, we have that $|w_h| \leq \frac{\|\mathbf{u}_h\|}{\|\mathbf{m}_h\|}$. Since $E\left[\|\mathbf{u}_h\|^2\right] = \operatorname{trace}(S_d)$, we have that $\frac{\|\mathbf{u}_h\|^2}{\|\mathbf{m}_h\|^2} \xrightarrow{P} 0$, and, also in this case $w_h \xrightarrow{P} 0$ as $h \to \infty$.

In case (iii), taking into account that equation (23) now holds, it is enough to show that

$$\frac{\langle \mathbf{m}_h, \mathbf{u}_h \rangle}{C \operatorname{trace}(S_h)} \xrightarrow{P} 0 \text{ as } h \to \infty,$$

Fix $\epsilon > 0$. We have that

$$\mathbb{P}\left[\left|\frac{\langle \mathbf{m}_h, \mathbf{u}_h\rangle}{C \text{ trace}(S_h)}\right| > \epsilon\right] \quad \leq \quad \frac{1}{C^2\epsilon^2}\sum_{i=1}^{h}\frac{m_{h,i}^2\alpha_i^h}{\left(\sum_{i=1}^{h}\alpha_i^h\right)^2} \leq \frac{1}{C^2\epsilon^2}\frac{\|\alpha^h\|_\infty}{\sum_{i=1}^{h}\alpha_i^h}\frac{\|\mathbf{m}_h\|^2}{\text{trace}(S_h)},$$

which converges to zero by assumptions (3) and (4). •

B On Assumptions (3) and (4)

The next lemma shows that if $L_S < \infty$, then assumption (3) implies assumption (4).

Lemma B.1 *Let* $\{a_d\}_{d\geq 1}$ *be a sequence of real positive numbers such that* $\lim_d \frac{1}{d}\sum_{i=1}^d a_i$ *exists, and it is finite. Then, it happens that* $\lim_d \frac{1}{d}\|a^d\|_\infty = 0$.

Proof: Fix $d \in \mathbb{N}$, and denote $A_d = \sum_{i=1}^d a_i$. We have that

$$\frac{a_d}{d} = \frac{A_d}{d} - \frac{A_{d-1}}{d-1}\frac{d-1}{d}$$

and consequently, $0 = \lim_d \frac{a_d}{d}$. Given $\epsilon > 0$, there exists $d_1 > 0$ such that if $d > d_1$, then $\frac{a_d}{d} \leq \epsilon$ and $d_2 \geq d_1$ such that

$$\sup_{1\leq i\leq d_1}\frac{a_i}{d_2} \leq \epsilon.$$

Let $d > d_2$ and take $1 \leq i \leq d$. So, we have that if $i \leq d_1$, then $\frac{a_i}{d} < \frac{a_i}{d_2} \leq \epsilon$ and if $i > d_1$, then $\frac{a_i}{d} \leq \frac{a_i}{i} \leq \epsilon$. This completes the proof. •

C Proof of Theorem 2.2

First, note that $(\mathbf{Z}_1 - \mathbf{Z}_2)_d$ is a d-dimensional normal vector, with mean $(\mu_h - \mu_k)_d$ and covariance $\Sigma_{hd} + \Sigma_{kd}$.

To prove (a) and (b) we will assume that (c) holds. Statement (c) is proved later, and its proof is independent of (a) and (b).

In case (a), we have $h = k$. So, $(\mu_k - \mu_h)_d = 0_d$ and $\Sigma_{hd} + \Sigma_{kd} = 2\Sigma_{hd}$. If we take $A_d = S_d^h$, according to Remark 2.1.2, (c) gives that assumption (4) holds for this selection of A_d. Therefore, (7) follows from Theorem 2.1 because in this case $L_\mu^h = 0$.

In case (b), we have $h \neq k$. We take $A_d = S_d^{hk}$ and $b = \mu_h - \mu_k$. Similarly as in (a), we have that assumption (4) also holds in this case and Theorem 2.1 implies

$$D_d^{\Sigma_d^{\mathbf{Z}}}(\mathbf{Z}_1, \mathbf{Z}_2) \xrightarrow{P} L^{hk} := L_\mu^{hk} + L_S^{hk} \text{ as } d \to \infty.$$

Now, (8) follows because (c) gives that $L_\mu^{hk} = 0$.

To prove (c), let us denote $\Sigma^* = \pi_1\Sigma_1 + \pi_2\Sigma_2$, $\mu = (\mu_1 - \mu_2)$ and $\pi_{12} = \pi_1\pi_2$, from (5), we have that

$$\Sigma_d = \Sigma_d^* + \pi_{12}\mu_d\mu_d^T.$$

From here, the Sherman-Morrison formula gives

$$\Sigma_d^{-1} = (\Sigma_d^*)^{-1} - \frac{\pi_{12}(\Sigma_d^*)^{-1}\mu_d\mu_d^T(\Sigma_d^*)^{-1}}{1 + \pi_{12}\mu_d^T(\Sigma_d^*)^{-1}\mu_d}.$$

Since $(\Sigma_d^*)^{-1}$ is positive definite for all $d \in \mathbb{N}$, this now implies that

$$0 \leq \mu_d^T \Sigma_d^{-1} \mu_d = \mu_d^T (\Sigma_d^*)^{-1} \mu_d - \frac{\pi_{12}(\mu_d^T (\Sigma_d^*)^{-1} \mu_d)^2}{1 + \pi_{12}(\mu_d^T (\Sigma_d^*)^{-1} \mu_d)} = \frac{\mu_d^T (\Sigma_d^*)^{-1} \mu_d}{1 + \pi_{12} \mu_d^T (\Sigma_d^*)^{-1} \mu_d} \leq \frac{1}{\pi_{12}},$$

and the proof that $L_\mu^{hk} = 0$ trivially ends from definition of L_μ^{hk}.

To handle the terms L_S^h and L_S^{hk}, recall the Woodbury matrix identity:

$$(U + V)^{-1} = U^{-1} - (U + UV^{-1}U)^{-1}.$$

Using this identity, we have

$$\Sigma_d^{-1} = 1/\pi_1 \Sigma_{1d}^{-1} - B_d,$$

where $B_d = (\pi_1 \Sigma_{1d} + \pi_1^2 \Sigma_{1d} (\pi_2 \Sigma_{2d} + \pi_{12} \mu_d \mu_d^T)^{-1} \Sigma_{1d})^{-1}$.

If U and V are positive definite (p.d.), then $U^T V U$ is p.d. In B_d, both the matrices Σ_{1d} and $(\pi_2 \Sigma_{2d} + \pi_{12} \mu_d \mu_d^T)$ are symmetric and p.d., and this implies that B_d is also p.d. Further, $\Sigma_{1d}^{1/2}$ and B_d are p.d. which now implies that $\Sigma_{1d}^{1/2} B_d \Sigma_{1d}^{1/2}$ is p.d. Recall that *trace* is a linear map. Now,

$$\begin{aligned}
L_S^1 &= \lim_d \frac{1}{d} trace(\Sigma_d^{-1/2} (2\Sigma_{1d}) \Sigma_d^{-1/2}) \\
&= \lim_d \frac{2}{d} trace(\Sigma_{1d} \Sigma_d^{-1}) \\
&= \lim_d \frac{2}{d} trace(1/\pi_1 I_d) - \lim_d \frac{2}{d} trace(\Sigma_{1d} B_d) \\
&= \lim_d \frac{2}{d} trace(1/\pi_1 I_d) - \lim_d \frac{2}{d} trace(\Sigma_{1d}^{1/2} B_d \Sigma_{1d}^{1/2}) \\
&\leq \lim_d \frac{2}{d} trace(1/\pi_1 I_d) = \frac{2}{\pi_1}.
\end{aligned}$$

Similarly, we can also prove that $L_S^2 < \dfrac{2}{\pi_2}$. Again,

$$\begin{aligned}
L_S^{12} &= \lim_d \frac{1}{d} trace(\Sigma_d^{-1/2} (\Sigma_{1d} + \Sigma_{2d}) \Sigma_d^{-1/2}) \\
&= \lim_d \frac{1}{d} trace(\Sigma_d^{-1/2} \Sigma_{1d} \Sigma_d^{-1/2}) + \lim_d \frac{1}{d} trace(\Sigma_d^{-1/2} \Sigma_{2d} \Sigma_d^{-1/2}) \\
&< \frac{1}{\pi_1} + \frac{1}{\pi_2} = \frac{1}{\pi_1 \pi_2}.
\end{aligned}$$

•

D Proof of Proposition 2.3

Under the conditions of Proposition 2.3, the number of significant (unique) eigenvalues of the matrix Γ is 2. Recall that N is fixed here.

Consider the standardized distance matrix D_d with the (i, j)-th element as $D_d^{\Sigma_d^{\mathbf{z}}}(\mathbf{z}_i, \mathbf{z}_j)$ for $1 \leq i, j \leq N$ and $d \in \mathbb{N}$. We have a sequence of matrices $D_d \xrightarrow{P} D_0$ as $d \to \infty$ (componentwise). Since the map D to Γ is clearly continuous w.r.t. this convergence, we have that $\Gamma_d \xrightarrow{P} \Gamma$ as $d \to \infty$. Let us denote the eigenvalues of Γ_d (respectively, Γ) to be $\beta_1^d, \ldots, \beta_N^d$ (respectively, $\beta_1, \ldots, \beta_N$). Since eigenvalues are continuous functions of the respective matrices, we have $\beta_j^d \xrightarrow{P} \beta_j$ as $d \to \infty$ for all $1 \leq j \leq N$.

Let us now look into the following:

$$\sum_{i=1}^{N} I(|\beta_i^d| > a_d) \xrightarrow{P} \sum_{i=1}^{N} I(|\beta_i^0| > 0) \text{ as } d \to \infty$$

with $a_d \downarrow 0$ as $d \to \infty$ at an appropriate rate. Recall that the limiting quantity on the right should give us the correct number of clusters. Consider the sequence $\{1/m\}_{m\in\mathbb{N}}$. Let us take i such that $\beta_i^d \xrightarrow{P} 0$ as $d \to \infty$. Thus, for every $\epsilon, \delta > 0$ there exists $D^i_{\delta,\epsilon}$ such that if $d \geq D^i_{\delta,\epsilon}$ then

$$\mathbb{P}[|\beta_i^d| > \delta] < \epsilon.$$

In particular, if we take $\delta = \epsilon = 1/m$, there exists D^i_m such that if $d \geq D^i_m$:

$$\mathbb{P}\left[|\beta_i^d| > \frac{1}{m}\right] < \frac{1}{m}.$$

Without loss of generality, we can assume that $D^i_1 < D^i_2 < \cdots$, and consider the sequence

$$a^i_d = \begin{cases} 2 & \text{if } 1 \leq i < D^i_1, \\ \frac{1}{m} & \text{if } D^i_m \leq i < D^i_{m+1}, \text{ for some } m \geq 1. \end{cases}$$

Then, obviously $a^i_d \to 0$, and

$$\mathbb{P}\left[I(|\beta_i^d| > a^i_d) > 0\right] = \mathbb{P}\left[|\beta_i^d| > a^i_d\right] < a^i_d.$$

If we define $a_d = \sup\{a^i_d : \beta^0_i = 0\}$, and i satisfies that $\beta^0_i = 0$, then $I(|\beta^d_i| > a_d) \xrightarrow{P} 0$ as $d \to \infty$. A similar reasoning allows us also to conclude that if $|\beta^0_i| > 0$, then $I(|\beta^d_i| > a_d) \xrightarrow{P} 1$ as $d \to \infty$. •

E Proof of Theorem 2.5

In this proof, we use the superindex d in $\mathcal{G}^d_i$ to emphasize that the groupings can change with the dimension $d \in \mathbb{N}$. Proposition 2.3 implies that $K_d = 2$ with probability converging to one.

Note that $\phi(\mathcal{G}_1, \ldots, \mathcal{G}_J)$ has an alternative mathematical expression as

$$\sum_{h=1}^{J} \frac{1}{2|\mathcal{G}_h|} \sum_{\mathbf{u},\mathbf{v}\in\mathcal{G}_h} \|\mathbf{u} - \mathbf{v}\|^2, \tag{24}$$

where $|\mathcal{G}|$ denotes the cardinality of the set $\mathcal{G}$. Let us denote the rows/columns of Γ_d as $\boldsymbol{\gamma}^d_1, \ldots, \boldsymbol{\gamma}^d_N$. The structure of Γ^d implies that $\|\boldsymbol{\gamma}^d_i - \boldsymbol{\gamma}^d_j\|^2 \xrightarrow{P} 0$ as $d \to \infty$ iff $i, j \in \mathcal{C}_h$ for $h \in \{1, 2\}$. So, if each $\mathcal{G}^d_h$ for $h = 1, 2$ contains observations from the same population, then $\phi_d(\mathcal{G}^d_1, \mathcal{G}^d_2) \xrightarrow{P} 0$ as $d \to \infty$.

Let us assume that on the contrary, there exists a subsequence of dimensions $\{d_k\}$ such that for every k there exists at least a couple of points i_k, j_k with $i_k \in \mathcal{G}^d_1$ and $j_k \in \mathcal{G}^d_2$ (say). Since the number of points is finite, there exists a further subsequence $\{d_{k^*}\}$ such that both sequences $\{i_{k^*}\}$ and $\{j_{k^*}\}$ are constant. Therefore, for those subsequences (24) implies that

$$\liminf_d \phi_d(\mathcal{G}_1, \mathcal{G}_2) \geq \lim_d \|\boldsymbol{\gamma}^{d_{k^*}}_{i_{k^*}} - \boldsymbol{\gamma}^{d_{k^*}}_{j_{k^*}}\|^2 \xrightarrow{P} \gamma_{12} > 0.$$

So, for the minimization of $\phi_d(\mathcal{G}^d_1, \mathcal{G}^d_2)$, each $\mathcal{G}^d_h$ must contain all observations from a single population with probability converging to one as the dimension increases. This proves the convergence in probability of the Rand index $\mathbb{R}_{d,N}$ to zero as $d \to \infty$. •

F Rank of the Matrix Γ

Identifying number of clusters from the matrix Γ is not equivalent to finding the rank of the matrix Γ.

Lemma F.1 *The rank of the matrix Γ is less then or equal to J. Moreever, equality is guaranteed only when $J \leq 3$.*

Proof: Trivially, $rank(\Gamma) \leq J$. Let us denote the reduced Echelon form of $N \times N$ matrix Γ as Γ°. Thus, the matrix Γ° is a $J \times J$ symmetric matric with $\gamma_{ij} > 0$ and distinct when $i \neq j$, while $\gamma_{ii} = 0$.

Moreover, for $J = 3$, we have

$$det(\Gamma^\circ) = det \begin{pmatrix} 0 & \gamma_{12} & \gamma_{13} \\ \gamma_{12} & 0 & \gamma_{23} \\ \gamma_{13} & \gamma_{23} & 0 \end{pmatrix} = 2\gamma_{12}\gamma_{13}\gamma_{23} \neq 0.$$

In the case $J = 4$, if $\gamma_{12} = \dfrac{\gamma_{13}\gamma_{24} + \gamma_{14}\gamma_{23} + 2\sqrt{\gamma_{13}\gamma_{14}\gamma_{23}\gamma_{24}}}{\gamma_{34}}$, then a simple computation gives that $det(\Gamma^\circ) = 0$. This happens, for instance, if we consider the following matrix (with all *positive and distinct* off-diagonal entries):

$$\begin{pmatrix} 0 & t & 1 & 2 \\ t & 0 & 3 & 4 \\ 1 & 3 & 0 & 5 \\ 2 & 4 & 5 & 0 \end{pmatrix},$$

where $t = 2 + 4\sqrt{6}/5 > 0$.

•

G Proof of Theorem 2.6

In order to simplify the writing, we will write d instead of d_N. We will use the notation $\|\alpha_d\|_2 := \left(\sum_{i=1}^{d}(\alpha_i^d)^2\right)^{1/2}$. The real r.v.'s $\{u_i\}$ are assumed to be i.i.d. with standard normal distribution.

The following lemma is deduced from Lemma 1 in Laurent and Massart (2000) on p. 1325, after some simple computations, taking into account that $\|\alpha_d\|_2 \geq \|\alpha_d\|_\infty$. We state it here for further reference.

Lemma G.1 *If $Z_d = \sum_{i=1}^{d} \alpha_i^d(u_i^2 - 1)$ and $x \geq 1$, then*

$$\mathbb{P}\left[|Z_d| \geq 4x\|\alpha_d\|_\infty\right] \leq 2\exp(-x).$$

We will also employ the following well known bound for the tail of the standard normal distribution:

$$\mathbb{P}[|N(0,1)| \geq t] \leq \sqrt{\frac{2}{\pi}}\exp(-t^2/2) \text{ for all } t \geq 1. \tag{25}$$

Proof of Theorem 2.6 : Let us show part b). The proof of (14) is similar to that of (16). We use the notation $\mathbf{m}_d = (\Sigma_d)^{-1/2}(\mu_1 - \mu_2)_d$ and $\mathbf{u}_d^i = (\Sigma_d)^{-1/2}(\mathbf{Z}_i - \mu_i)_d$ with $d \in \mathbb{N}$, where $\mathbf{Z}_i$ is a generic observation with distribution $\mathbb{P}_i$ for $i = 1, 2$. Moreover, with an obvious abuse of notation, we will often write $\mathbf{u}_d^i \in \mathcal{C}_i^N$ with $d \in \mathbb{N}$ for $i = 1, 2$.

Recall that $L_\mu = 0$ and $L_S < \infty$ (see part (c) in Theorem 2.2). Repeating the first steps in the proof of Theorem 2.1, we have that

$$\begin{aligned}
&\sup_{\mathbf{Z}^1 \in \mathcal{C}_1^N, \mathbf{Z}^2 \in \mathcal{C}_2^N} \left| D_d^{\Sigma}(\mathbf{Z}_1, \mathbf{Z}_2) - \frac{1}{d}\mathrm{trace}(S_d^{12}) \right| \\
&\qquad \leq \left| \frac{1}{d}\|\mathbf{m}_d\|^2 \right| + \sup_{\mathbf{u}^1 \in \mathcal{C}_1^N, \mathbf{u}^2 \in \mathcal{C}_2^N} \left| \frac{1}{d}\|\mathbf{u}_d^1 - \mathbf{u}_d^2\|^2 - \frac{1}{d}\mathrm{trace}(S_d^{12}) \right| \qquad (26)\\
&\qquad\quad + 2 \sup_{\mathbf{u}^1 \in \mathcal{C}_1^N, \mathbf{u}^2 \in \mathcal{C}_2^N} \frac{1}{d} \left| \langle \mathbf{m}_d, \mathbf{u}_d^1 - \mathbf{u}_d^2 \rangle \right|, \qquad (27)
\end{aligned}$$

and it is enough to prove that the terms in (26) and (27) converge to zero in probability.

The `first term` in (26) converges to zero by first part of (c) in Theorem 2.2. Concerning the `second term`, let N_1, N_2 be the number of elements in $\mathcal{C}_1^N$ and $\mathcal{C}_2^N$, respectively. Since $N_1 + N_2 = N$, it is clear that $N_1 \times N_2 \leq N^2/4$. Let $\varepsilon > 0$. We have that

$$\begin{aligned}
P_N &:= \mathbb{P}\left[\sup_{\mathbf{u}^1 \in \mathcal{C}_1^N, \mathbf{u}^2 \in \mathcal{C}_2^N} \left| \frac{1}{d}\|\mathbf{u}_d^1 - \mathbf{u}_d^2\|^2 - \frac{1}{d}\mathrm{trace}(S_d^{12}) \right| > \varepsilon \right] \\
&= \mathbb{P}\left[\bigcup_{\mathbf{u}^1 \in \mathcal{C}_1^N, \mathbf{u}^2 \in \mathcal{C}_2^N} \left\{ \left| \frac{1}{d}\|\mathbf{u}_d^1 - \mathbf{u}_d^2\|^2 - \frac{1}{d}\mathrm{trace}(S_d^{12}) \right| > \varepsilon \right\} \right] \\
&\leq \frac{N^2}{4}\mathbb{P}\left[\left| \frac{1}{d}\|\mathbf{u}_d^1 - \mathbf{u}_d^2\|^2 - \frac{1}{d}\mathrm{trace}(S_d^{12}) \right| > \varepsilon \right], \qquad (28)
\end{aligned}$$

where $\mathbf{u}^1$ and $\mathbf{u}^2$ are associated with some $\mathbf{Z}_1 \in \mathcal{C}_1^N$ and $\mathbf{Z}_2 \in \mathcal{C}_2^N$, respectively. However, it is clear that

$$\frac{1}{d}\|\mathbf{u}_d^1 - \mathbf{u}_d^2\|^2 - \frac{1}{d}\mathrm{trace}(S_d^{12}) \sim \frac{1}{d}\sum_{i=1}^{d} \alpha_i^d (u_i^2 - 1).$$

Take $x = \varepsilon d/(4\|\alpha_d\|_\infty)$. By assumption (15), we have $d/\|\alpha_d\|_\infty \to \infty$ and eventually $x \geq 1$. So, from Lemma G.1, we obtain

$$P_N \leq \frac{N^2}{4}\mathbb{P}\left[\left| \sum_{i \leq d} \alpha_i^d (u_i^2 - 1) \right| > \varepsilon d \right] \leq \frac{1}{2}\exp\left(-\frac{\varepsilon d}{4\|\alpha^d\|_\infty} + 2\log N \right),$$

which converges to zero by assumption (15).

For the `third term`, in equation (27) we have that

$$\begin{aligned}
P_N^* &:= \mathbb{P}\left[\sup_{\mathbf{u}^1 \in \mathcal{C}_1^N, \mathbf{u}^2 \in \mathcal{C}_2^N} \frac{1}{d} |\langle \mathbf{m}_d, \mathbf{u}_d^1 - \mathbf{u}_d^2 \rangle| > \varepsilon \right] \\
&\leq \frac{N^2}{4}\mathbb{P}\left[\frac{1}{d} |\langle \mathbf{m}_d, \mathbf{u}_d^1 - \mathbf{u}_d^2 \rangle| > \varepsilon \right] \\
&= \frac{N^2}{4}\mathbb{P}\left[\frac{1}{d} \left| \sum_{i \leq d} m_{di} (\alpha_i^d)^{1/2} u_i \right| > \varepsilon \right] \\
&= \frac{N^2}{4}\mathbb{P}\left[|N(0,1)| > \varepsilon \frac{d}{\sqrt{\sum_{i \leq d} (m_{di})^2 \alpha_i^d}} \right] \\
&\leq \frac{1}{2^{3/2}\pi^{1/2}} \exp\left(-\frac{\varepsilon^2}{2} \frac{d^2}{\sum_{i \leq d} (m_{di})^2 \alpha_i^d} + 2\log N \right) \qquad (29)\\
&\leq \frac{1}{2^{3/2}\pi^{1/2}} \exp\left(-\frac{\varepsilon^2}{2} \frac{d^2}{\|\alpha^d\|_\infty \sum_{i \leq d} (m_{di})^2} + 2\log N \right),
\end{aligned}$$

which converges to 0 because of the fact that $L_\mu = 0$ (see part (c) in Theorem 2.2) and (15). The same assumption allows us to apply inequality (25) to equation (29). •

H Result Related to Remark 2.6.1

Proposition H.1 *Under assumptions of Theorem 2.2, if we assume that* $\frac{\log N}{d_N} \to 0$*, then conditions* (13) *and* (15) *hold.*

Proof: Fix $h \in \{1, 2\}$, and recall that

$$\Sigma_d^{-1} = (\pi_h \Sigma_{hd})^{-1} - P_d,$$

where $P_d = (\pi_h \Sigma_{hd} + \pi_h \Sigma_{hd} (T_d^h)^{-1} \pi_h \Sigma_{hd})^{-1}$ is a positive definite matrix. Further,

$$I_d + \Sigma_d P_d = \frac{1}{\pi_h} \Sigma_d \Sigma_{hd}^{-1}.$$

From here, Weyl's inequality gives

$$1 \le \alpha_{min}(\frac{1}{\pi_h} \Sigma_d \Sigma_{hd}^{-1}) = \frac{1}{\pi_h} \alpha_{min}(\Sigma_d \Sigma_{hd}^{-1}). \tag{30}$$

Note the fact that the eigenvalues of the matrices AB and BA are same. So, the matrices S_d^h and $\Sigma_{hd}\Sigma_d^{-1}$ will have the same eigenvalues. Furthermore, the eigenvalues of S_d^h are the inverses of the eigenvalues of $\Sigma_d \Sigma_{hd}^{-1}$. Thus, (30) gives that

$$\alpha_{max}(S_d^h) < \frac{2}{\pi_h} (\text{free of } d). \tag{31}$$

We now have

$$\log N = o\left(\frac{d_N}{\alpha_1^{d_N}}\right) \Leftrightarrow \frac{\alpha_1^{d_N} \log N}{d_N} \to 0.$$

Equation (31) now implies that condition (13) holds if we assume $\frac{\log N}{d_N} \to 0$.

Fix $h \ne k \in \{1, 2\}$. Our second matrix of interest is

$$S_d^{hk} = (\Sigma_d)^{-1/2} (\Sigma_{hd} + \Sigma_{kd}) (\Sigma_d)^{-1/2}.$$

Since the matrices are symmetric, we have

$$\alpha_{max}(S_d^{hk}) \le \alpha_{max}(\Sigma_d^{-1/2} \Sigma_{hd} \Sigma_d^{-1/2}) + \alpha_{max}(\Sigma_d^{-1/2} \Sigma_{kd} \Sigma_d^{-1/2}).$$

Again, the eigenvalues of $\Sigma_d^{-1/2} \Sigma_{id} \Sigma_d^{-1/2}$ and of $\Sigma_{id} \Sigma_d^{-1}$ will be equal for $i = h, k$. So,

$$\begin{aligned} \alpha_{max}(S_d^{hk}) &\le \alpha_{max}(\Sigma_{hd}\Sigma_d^{-1}) + \alpha_{max}(\Sigma_{kd}\Sigma_d^{-1}) \\ &= \frac{1}{\alpha_{min}(\Sigma_d \Sigma_{hd}^{-1})} + \frac{1}{\alpha_{min}(\Sigma_d \Sigma_{kd}^{-1})} \\ &\le \frac{1}{\pi_h} + \frac{1}{\pi_k} = \frac{1}{\pi_h \pi_k} \text{ (using equation (30))}. \end{aligned}$$

From here, similarly as before, we would obtain that $\frac{\log N}{d_N} \to 0$ implies (15) holds. •

I Proof of Theorem 3.1

Recall that in this theorem, we use the subspaces generated by the estimates of the first d eigenfunctions of the covariance of the random process $\mathbf{Z}$.

We begin with some notation and preliminary results which have been taken from Delaigle and Hall (2012) and Hall and Hosseini-Nasab (2006), or follow directly from the results there. Then, we will give the proof of Theorem 3.1. For every $n \in \mathbb{N}$, let us consider

$$\begin{aligned} \hat{\Delta}^2_{\mathbf{Z}} &= \int_0^1 \int_0^1 (\hat{\Sigma}(s,t) - \Sigma(s,t))^2 ds dt, \\ \delta_j^{\mathbf{Z}} &= \min_{k \leq j} (\lambda_k - \lambda_{k+1}). \end{aligned}$$

In Delaigle and Hall (2012) and Hall and Hosseini-Nasab (2006), it is shown that if $j \geq 1$, then

$$|\hat{\lambda}_j - \lambda_j| \leq \hat{\Delta}_{\mathbf{Z}}, \tag{32}$$

and that, if $j \leq \hat{R}_N^{\mathbf{Z}}$ (recall the definition of $\hat{R}_N^{\mathbf{Z}}$ in (17)), then

$$\begin{aligned} \|\hat{\phi}_j - \phi_j\| &\leq 8^{1/2} \hat{\Delta}_{\mathbf{Z}} (\delta_j^{\mathbf{Z}})^{-1}, \qquad (33) \\ \hat{\Delta}_{\mathbf{Z}} &= O_p(N^{-1/2}), \qquad (34) \\ R_N^{\mathbf{Z}} \to \infty \text{ and } \hat{R}_N^{\mathbf{Z}} &\leq \hat{\lambda}_1^{\mathbf{Z}} \eta_N^{-1}. \qquad (35) \end{aligned}$$

Moreover, if $j \leq \hat{R}_N^{\mathbf{Z}}$, there exists a $k \leq j$ such that

$$\delta_j^{\mathbf{Z}} = \lambda_k - \lambda_{k+1} \geq \hat{\lambda}_k - \hat{\lambda}_{k+1} - 2\hat{\Delta}_{\mathbf{Z}} \geq \eta_N - 2\hat{\Delta}_{\mathbf{Z}} = \eta_N + o_P(\eta_N), \tag{36}$$

where we have applied (32) and (17) and that, from (34) and the assumption on η_N, we can conclude that $\eta_N > 2\hat{\Delta}_{\mathbf{Z}}$ from an index onward. Thus, (36) and (33) yield

$$\|\hat{\phi}_j - \phi_j\| \leq 8^{1/2} \frac{\hat{\Delta}_{\mathbf{Z}}}{\eta_N - 2\hat{\Delta}_{\mathbf{Z}}}. \tag{37}$$

From (32), (17) and (34), we obtain that

$$\lambda_j \geq \hat{\lambda}_j - \hat{\Delta}_{\mathbf{Z}} \geq \eta_N - \hat{\Delta}_{\mathbf{Z}} = \eta_N + o_P(\eta_N). \tag{38}$$

Now, we are in a position to prove Theorem 3.1.

Proof of Theorem 3.1: The proof is based on Lemma I.1. The result follows trivially from this lemma, the fact that $\hat{R}_N^{\mathbf{Z}} \xrightarrow{P} \infty$ as $n \to \infty$ and the result in Theorem 2.2.

Lemma I.1 *Under the assumptions in Theorem 3.1, it happens that*

$$\left| \hat{D}_{\hat{R}_N^{\mathbf{Z}}}(\mathbf{Z}_1, \mathbf{Z}_2) - D_{\hat{R}_N^{\mathbf{Z}}}(\mathbf{Z}_1, \mathbf{Z}_2) \right| \xrightarrow{P} 0 \text{ as } n \to \infty.$$

Proof. For fixed $\mathbf{Z}_1, \mathbf{Z}_2$, let us denote $\mathbf{u} = \mathbf{Z}_1 - \mathbf{Z}_2$. Obviously, $\|\mathbf{u}\| = O(1)$ a.s. Let us denote $(u_1, \ldots, u_{\hat{R}_n^1})^T$ and $(\hat{u}_1, \ldots, \hat{u}_{\hat{R}_n^1})^T$ to be the projections of $\mathbf{u}$ on the subspaces generated by the first $\hat{R}_N^{\mathbf{Z}}$ eigenvectors of the matrices $\Sigma_{\hat{R}_N^{\mathbf{Z}}}$ and $\hat{\Sigma}_{\hat{R}_N^{\mathbf{Z}}}$, respectively, when written in the basis generated by those eigenvectors. Let $n \in \mathbb{N}$, and take $j \leq \hat{R}_N^{\mathbf{Z}}$. We now have

$$\begin{aligned} \left| \frac{(u_j)^2}{\lambda_j^1} - \frac{(\hat{u}_j)^2}{\hat{\lambda}_j^1} \right| &= \left| \frac{u_j}{(\lambda_j^1)^{1/2}} - \frac{\hat{u}_j}{(\hat{\lambda}_j^1)^{1/2}} \right| \left| \frac{u_j}{(\lambda_j^1)^{1/2}} + \frac{\hat{u}_j}{(\hat{\lambda}_j^1)^{1/2}} \right| \\ &\leq \left(\left| \frac{u_j - \hat{u}_j}{(\lambda_j^1)^{1/2}} \right| + \left| \hat{u}_j \frac{(\lambda_j^1)^{1/2} - (\hat{\lambda}_j^1)^{1/2}}{(\lambda_j^1 \hat{\lambda}_j^1)^{1/2}} \right| \right) \left| \frac{u_j}{(\lambda_j^1)^{1/2}} + \frac{\hat{u}_j}{(\hat{\lambda}_j^1)^{1/2}} \right|. \end{aligned}$$

We analyze each term in this expression separately as follows:

$$\begin{aligned}\left|\frac{u_j-\hat u_j}{(\lambda_j^1)^{1/2}}\right| &\leq \frac{1}{(\lambda_j^1)^{1/2}}\int_0^1 |\mathbf{u}(t)||\phi_j^1(t)-\hat\phi_j^1(t)|dt\\ &\leq \frac{\|\mathbf{u}\|\ \|\phi_j^1-\hat\phi_j^1\|}{(\lambda_j^1)^{1/2}}\\ &\leq 8^{1/2}\|\mathbf{u}\|\frac{\hat\Delta_{\mathbf{X}}}{(\lambda_j^1)^{1/2}(\eta_n-2\hat\Delta_{\mathbf{X}})}\\ &\leq 8^{1/2}\|\mathbf{u}\|\hat\Delta_{\mathbf{X}}(\eta_n^{-3/2}+o_P(\eta_n^{-3/2})),\end{aligned}\tag{39}$$

where we have applied the Cauchy-Schwartz inequality, (37), (34) and (38). On the other hand, we have

$$\begin{aligned}\left|\hat u_j\frac{(\lambda_j^1)^{1/2}-(\hat\lambda_j^1)^{1/2}}{(\lambda_j^1\hat\lambda_j^1)^{1/2}}\right| &\leq \int_0^1|\mathbf{u}(t)||\hat\phi_j^1(t)|dt\frac{|\lambda_j^1-\hat\lambda_j^1|}{\left((\lambda_j^1)^{1/2}+(\hat\lambda_j^1)^{1/2}\right)(\lambda_j^1\hat\lambda_j^1)^{1/2}}\\ &\leq \|\mathbf{u}\|\frac{\hat\Delta_{\mathbf{X}}}{\left((\lambda_j^1)^{1/2}+(\hat\lambda_j^1)^{1/2}\right)(\lambda_j^1\hat\lambda_j^1)^{1/2}}\\ &\leq \frac{1}{2}\|\mathbf{u}\|\hat\Delta_{\mathbf{X}}(\eta_n^{-3/2}+o_P(\eta_n^{-3/2})),\end{aligned}\tag{40}$$

where we have applied (17) and (38). Concerning the final term, using (38) and (17) again, we obtain that

$$\left|\frac{u_j}{(\lambda_j^1)^{1/2}}+\frac{\hat u_j}{(\hat\lambda_j^1)^{1/2}}\right| \leq \|\mathbf{u}\|\left(\frac{1}{(\lambda_j^1)^{1/2}}+\frac{1}{(\hat\lambda_j^1)^{1/2}}\right)\leq\|\mathbf{u}\|(\eta_n^{-1/2}+o_P(\eta_n^{-1/2})).\tag{41}$$

Now, if we define $C=8^{1/2}+1$, combining (39), (40), (41), (35) and (34), we get the following:

$$\begin{aligned}\left|\hat D_{\hat R_N^{\mathbf{Z}}}(\mathbf{Z},\mathbf{Z}_2)-D_{\hat R_N^{\mathbf{Z}}}(\mathbf{Z},\mathbf{Z}_2)\right| &\leq \frac{1}{\hat R_N^{\mathbf{Z}}}\sum_{j=1}^{\hat R_N^{\mathbf{Z}}}\left|\frac{(u_j)^2}{\lambda_j^1}-\frac{(\hat u_j)^2}{\hat\lambda_j^1}\right|\\ &\leq C\|\mathbf{u}\|^2\hat\Delta_{\mathbf{X}}(\eta_n^{-2}+o_P(\eta_n^{-2}))=O_P(n^{-1/2}\eta_n^{-2}).\end{aligned}$$

By construction, η_n is such that $n\eta_n^5\to\infty$. So, we have $|\hat D_{\hat R_N^{\mathbf{Z}}}(\mathbf{Z}_1,\mathbf{Z}_2)-D_{\hat R_N^{\mathbf{Z}}}(\mathbf{Z}_1,\mathbf{Z}_2)|\xrightarrow{P}0$ as $n\to\infty$, and the lemma is proved. •

J Proof of Theorem 3.2

We will need the following lemma:

Lemma J.1 *Under the assumptions in Theorem 3.2, we have that* $\mathbb{P}[\hat R_N\geq R_N]\to 1$.

Proof : Let $N\in\mathbb{N}$. From (32), we have that

$$\inf_{j\leq R_N}(\hat\lambda_j-\hat\lambda_{j+1})\geq\inf_{j\leq R_N}(\lambda_j-\lambda_{j+1})-2\hat\Delta_{\mathbf{Z}}\geq(1+\delta)\eta_N-2\hat\Delta_{\mathbf{Z}},$$

and the proof ends because (34) and the fact that $\eta_N\geq N^{-1/5}$ imply that $\mathbb{P}[\delta\eta_N-2\hat\Delta_{\mathbf{Z}}\geq 0]\to 1$. •

In this setting, recall that $L_\mu=0$ and $L_S<\infty$ (see (c) in Theorem 2.2). We will only prove part b); part a) being similar. W.l.o.g. we will assume that $h=1$ and $k=2$. Remember that for every $\mathbf{Z}_1,\mathbf{Z}_2$, we have

$$D_{\hat R_N}(\mathbf{Z}_1,\mathbf{Z}_2)=\frac{1}{\hat R_N}\sum_{j=1}^{\hat R_N}\frac{\langle\mathbf{Z}_1-\mathbf{Z}_2,\phi_j\rangle^2}{\lambda_j}\text{ and }\hat D_{\hat R_N}(\mathbf{Z}_1,\mathbf{Z}_2)=\frac{1}{\hat R_N}\sum_{j=1}^{\hat R_N}\frac{\langle\mathbf{Z}_1-\mathbf{Z}_2,\hat\phi_j\rangle^2}{\hat\lambda_j}.$$

We are going to consider the function

$$\tilde{D}_{\hat{R}_N}(\mathbf{Z}_1,\mathbf{Z}_2)=\frac{1}{\hat{R}_N}\sum_{j=1}^{\hat{R}_N}\frac{\langle \mathbf{Z}_1-\mathbf{Z}_2,\phi_j\rangle^2}{\hat{\lambda}_j}.$$

Obviously,

$$\begin{aligned}
\sup_{\mathbf{Z}_1\in\mathcal{C}_1^N,\mathbf{Z}_2\in\mathcal{C}_2^N}\left|\hat{D}_{\hat{R}_N}(\mathbf{Z}_1,\mathbf{Z}_2)-L_S^{12}\right| \quad\leq\quad & \sup_{\mathbf{Z}_1\in\mathcal{C}_1^N,\mathbf{Z}_2\in\mathcal{C}_2^N}\left|\hat{D}_{\hat{R}_N}(\mathbf{Z}_1,\mathbf{Z}_2)-\tilde{D}_{\hat{R}_N}(\mathbf{Z}_1,\mathbf{Z}_2)\right|\\
&+\sup_{\mathbf{Z}_1\in\mathcal{C}_1^N,\mathbf{Z}_2\in\mathcal{C}_2^N}\left|\tilde{D}_{\hat{R}_N}(\mathbf{Z}_1,\mathbf{Z}_2)-D_{\hat{R}_N}(\mathbf{Z}_1,\mathbf{Z}_2)\right|\\
&+\sup_{\mathbf{Z}_1\in\mathcal{C}_1^N,\mathbf{Z}_2\in\mathcal{C}_2^N}\left|D_{\hat{R}_N}(\mathbf{Z}_1,\mathbf{Z}_2)-L_S^{12}\right|\\
=:\quad & T_1+T_2+T_3.
\end{aligned}$$

Lemma J.1, and equations (35) and (32) imply that there exists $C>0$ such that

$$\mathbb{P}[R_N\leq\hat{R}_N\leq CN^{1/5}]\to 1.$$

Consequently, with probability going to 1, it happens that

$$D_{R_N}(\mathbf{Z}_1,\mathbf{Z}_2)\leq D_{\hat{R}_N}(\mathbf{Z}_1,\mathbf{Z}_2)\leq D_{CN^{1/5}}(\mathbf{Z}_1,\mathbf{Z}_2).$$

Since, by assumption (15), $\log N=o\left(\frac{R_N}{\lambda_1}\right)$ and trivially we have $\log N=o\left(\frac{CN^{1/5}}{\lambda_1}\right)$, b) in Theorem 2.6 gives that T_3 converges in probability to zero as $N\to\infty$. Since $L_S^{12}<\infty$, this fact implies that

$$\sup_{\mathbf{Z}_1\in\mathcal{C}_1^N,\mathbf{Z}_2\in\mathcal{C}_2^N}D_{\hat{R}_N}(\mathbf{Z}_1,\mathbf{Z}_2)=O_P(1). \tag{42}$$

With respect to T_2, we have

$$\begin{aligned}
T_2 \quad&\leq\quad \sup_{\mathbf{Z}_1\in\mathcal{C}_1^N,\mathbf{Z}_2\in\mathcal{C}_2^N}\frac{1}{\hat{R}_N}\sum_{j=1}^{\hat{R}_N}\frac{\langle \mathbf{Z}_1-\mathbf{Z}_2,\phi_j\rangle^2}{\lambda_j}\frac{|\lambda_j-\hat{\lambda}_j|}{\hat{\lambda}_j}\\
&\leq\quad \sum_{j=1}^{\hat{R}_N}\frac{|\lambda_j-\hat{\lambda}_j|}{\hat{\lambda}_j}\sup_{\mathbf{Z}_1\in\mathcal{C}_1^N,\mathbf{Z}_2\in\mathcal{C}_2^N}D_{\hat{R}_N}(\mathbf{Z}_1,\mathbf{Z}_2)=O_p(N^{-1/10}),
\end{aligned}$$

where last equality follows from (42), (32), (34), (35) and (17).

Finally, given $\mathbf{Z}_1\in\mathcal{C}_1^N,\mathbf{Z}_2\in\mathcal{C}_2^N$, the Cauchy-Schwartz inequality and the fact that $\|\hat{\phi}_j\|=\|\phi_j\|=1$ imply

$$\begin{aligned}
\left|\hat{D}_{\hat{R}_n}(\mathbf{Z}_1,\mathbf{Z}_2)-\tilde{D}_{\hat{R}_n}(\mathbf{Z}_1,\mathbf{Z}_2)\right| \quad&\leq\quad \frac{1}{\hat{R}_N}\sum_{j=1}^{\hat{R}_N}\frac{\left|\langle \mathbf{Z}_1-\mathbf{Z}_2,\hat{\phi}_j\rangle^2-\langle \mathbf{Z}_1-\mathbf{Z}_2,\phi_j\rangle^2\right|}{\hat{\lambda}_j}\\
&=\quad \frac{1}{\hat{R}_N}\sum_{j=1}^{\hat{R}_N}\frac{\left|\langle \mathbf{Z}_1-\mathbf{Z}_2,\hat{\phi}_j-\phi_j\rangle\right|\left|\langle \mathbf{Z}_1-\mathbf{Z}_2,\hat{\phi}_j+\phi_j\rangle\right|}{\hat{\lambda}_j}\\
&\leq\quad \|\mathbf{Z}_1-\mathbf{Z}_2\|^2\frac{1}{\hat{R}_N}\sum_{j=1}^{\hat{R}_N}\frac{\|\hat{\phi}_j-\phi_j\|\,\|\hat{\phi}_j+\phi_j\|}{\hat{\lambda}_j}\\
&\leq\quad 2\|\mathbf{Z}_1-\mathbf{Z}_2\|^2\frac{1}{\hat{R}_N}\sum_{j=1}^{\hat{R}_N}\frac{\|\hat{\phi}_j-\phi_j\|}{\hat{\lambda}_j}\\
&=\quad 2\left\|\mathbf{Z}_1-\mathbf{Z}_2\right\|^2H_N.
\end{aligned}$$

Moreover, the application of (33), (34), (36) and (17) gives that $H_N = O_P(N^{-1/10})$, which in turn is equivalent to saying that there exists $C > 0$ such that $\mathbb{P}[H_n < CN^{-1/10}] \to 1$. This and the reasoning leading to (28) imply that to prove $T_1 \xrightarrow{P} 0$, it is enough to show that for every $C > 0$

$$N^2 \mathbb{P}\left[\|\mathbf{Z}_1 - \mathbf{Z}_2\|^2 > CN^{1/10}\right] \to 0 \text{ as } N \to \infty, \tag{43}$$

where $\mathbf{Z}_1$ and $\mathbf{Z}_2$ came from distributions $\mathbb{P}_1$ and $\mathbb{P}_2$, respectively.

To show (43), notice that $\mathbf{Z}_1 - \mathbf{Z}_2$ follows a Gaussian distribution whose mean function is $\mu_1 - \mu_2$ and its covariance is $\Sigma_{12} = \Sigma_1 + \Sigma_2$. Let γ_j (with $j \in \mathbb{N}$) denote the ordered eigenvalues of Σ_{12}. Consider a basis composed by the eigenfunctions of Σ_{12}, we denote by $(\mu_1 - \mu_2)_j$ the components of $\mu_1 - \mu_2$ in this basis and $\{u_j\}$ is a sequence of i.i.d. real standard normal variables with $j \in \mathbb{N}$. Now, we have the following

$$\begin{aligned}
\|\mathbf{Z}_1 - \mathbf{Z}_2\|^2 &\sim \sum_{j=1}^{\infty} \left(\gamma_j^{1/2} u_j + (\mu_1 - \mu_2)_j\right)^2 \\
&= \sum_{j=1}^{\infty} \left(\gamma_j (u_j^2 - 1) + \gamma_j + (\mu_1 - \mu_2)_j^2 + 2(\mu_1 - \mu_2)_j \gamma_j^{1/2} u_j\right) \\
&= \sum_{j=1}^{\infty} \left(\gamma_j (u_j^2 - 1) + 2(\mu_1 - \mu_2)_j \gamma_j^{1/2} u_j\right) + \operatorname{trace}(\Sigma_{12}) + \|\mu_1 - \mu_2\|^2.
\end{aligned}$$

Notice that $K := \operatorname{trace}(\Sigma_{12}) + \|\mu_1 - \mu_2\|^2 < \infty$. Thus,

$$\begin{aligned}
\mathbb{P}\left[\|\mathbf{Z}_1 - \mathbf{Z}_2\|^2 > CN^{1/10}\right] &= \mathbb{P}\left[\sum_{j=1}^{\infty} \left(\gamma_j (u_j^2 - 1) + 2(\mu_1 - \mu_2)_j \gamma_j^{1/2} u_j\right) > CN^{1/10} - K\right] \\
&\leq \mathbb{P}\left[\sum_{j=1}^{\infty} \gamma_j (u_j^2 - 1) > \frac{1}{2}\left(CN^{1/10} - K\right)\right] \\
&\quad + \mathbb{P}\left[\sum_{j=1}^{\infty} (\mu_1 - \mu_2)_j \gamma_j^{1/2} u_j > \frac{1}{4}\left(CN^{1/10} - K\right)\right] \\
&=: P_1 + P_2.
\end{aligned} \tag{44}$$

Obviously, $\frac{1}{4}\left(CN^{1/10} - K\right) \to \infty$. Thus, eventually $\frac{1}{4}\left(CN^{1/10} - K\right) > 1$ and from Lemma G.1, we have that

$$P_1 \leq \lim_{d \to \infty} \mathbb{P}\left[\sum_{j=1}^{d} \gamma_j (u_j^2 - 1) > \frac{1}{2}\left(CN^{1/10} - K\right)\right] \leq 2 \exp\left(-\frac{1}{8\gamma_1}\left(CN^{1/10} - K\right)\right). \tag{45}$$

Concerning to P_2, first notice that for every $d \in \mathbb{N}$, the real r.v. $\sum_{j=1}^{d} (\mu_1 - \mu_2)_j \gamma_j^{1/2} u_j$ is centered normal, with variance equal to $\displaystyle\sum_{j=1}^{d} (\mu_1 - \mu_2)_j^2 \gamma_j \leq \gamma_1 \sum_{j=1}^{d} (\mu_1 - \mu_2)_j^2 \leq \gamma_1 \|\mu_1 - \mu_2\|^2$. Therefore,

$$\begin{aligned}
P_2 &\leq \lim_{d \to \infty} \mathbb{P}\left[\left|\sum_{j=1}^{d} (\mu_1 - \mu_2)_j \gamma_j^{1/2} u_j\right| > \frac{1}{4}\left(CN^{1/10} - K\right)\right] \\
&\leq \mathbb{P}\left[|N(0,1)| > \frac{1}{4\gamma_1^{1/2} \|\mu_1 - \mu_2\|}\left(CN^{1/10} - K\right)\right] \\
&\leq \sqrt{\frac{2}{\pi}} \exp\left(-\frac{1}{2\gamma_1 (4\|\mu_1 - \mu_2\|)^2}\left(CN^{1/10} - K\right)^2\right),
\end{aligned} \tag{46}$$

where last inequality comes from (25) because, eventually $1 < \left(CN^{1/10} - K\right) / (4\gamma_1^{1/2} \|\mu_1 - \mu_2\|)$. Finally, (44), (45), and (46) give (43) and consequently, $T_1 \xrightarrow{P} 0$ as $N \to \infty$. •

Appendix II: Additional Material

K Extension to non-Gaussian Processes

Obviously, non-Gaussian processes can also be mutually singular. In fact, Theorem 4.3 in Rao and Varadarajan (1963) contains a sufficient condition for this property to be satisfied. This allows us to consider the possibility to extend previous results to cover non-Gaussian distributions. It is obvious that the developed proofs can cover non-Gaussian distributions as long as they satisfy the due properties. In this subsection, we state the properties a distribution should satisfy in order the proofs can be extended. Let $\mathbb{P}_1$ and $\mathbb{P}_2$ be two probabilities on the Hilbert space $\mathbb{H}$. Here, $\mathbf{Z}$ will denote a $L_2[0,1]$-valued random element with distribution $\pi_1\mathbb{P}_1 + \pi_s\mathbb{P}_2$ for some $\pi_1, \pi_2 > 0$ with $\pi_1 + \pi_2 = 1$.

The basic assumption is the existence of a covariance of $\mathbf{Z}$. We will also consider assumptions *A.1* and *A.2* (see Section 3 of the main paper) and $b \in L_2[0,1]$. Given a positive-definite $d \times d$ matrix A_d and a d-dimensional subspace $V_d \subset L_2[0,1]$, we need to consider the d-dimensional random vector $\mathbf{U}_d = (A_d)^{-1/2}(\mathbf{Z} - b)_d$ and the covariance matrix $S_d = A_d^{-1/2}\Sigma_d A_d^{-1/2}$, where Σ_d is the covariance matrix of $\mathbf{Z}_d$ and $(\mathbf{Z} - b)_d$ is the projection on V_d of $(\mathbf{Z} - b)$ with $d \in \mathbb{N}$.

Let us write $\mathbf{U}_d - \mathbb{E}[\mathbf{U}_d] = (u^1, \ldots, u^d)^T$ in the basis of the eigenvectors of S_d and let $\alpha_1^d, \ldots, \alpha_d^d$ denote the eigenvalues of S_d. Therefore, u_i/α_i^d for $1 \le i \le d$ are real, standardised random variables which we need to assume to be i.i.d. Similar properties must hold for the decomposition of $\mathbf{Z}$ in its eigenfunction basis (also see Dai et al (2017)). We finally need two exponential inequalities as those stated in (25) of Lemma G.1.

L Discussion on GP Clustering for the 'Location Only' Case

We have some ideas to fix the problem with the 'location only' case. Recall the notation used in Subsection 2.1 of the main paper. As stated there, the problem in this case is that

$$D_d^{\Sigma_d^{\mathbf{Z}}}(\mathbf{u},\mathbf{v}) = \frac{1}{d}\left\|\Sigma_d^{-1/2}(\mathbf{u}-\mathbf{v})_d\right\|^2 = \frac{1}{d}\sum_{i=1}^{d}\frac{(u_i - v_i)^2}{\lambda_i} \xrightarrow{P} 0 \text{ as } d \to \infty.$$

Our idea is to replace the terms in the sum with some others going to 0 slowly enough (or, if possible, not converging to zero at all). To use this idea, our proposal is as follows:

$$D_d^{\Sigma_d^{\mathbf{Z}},r}(\mathbf{u},\mathbf{v}) := \frac{1}{d}\left\|(\Sigma_d^{-1/2})^r(\mathbf{u}-\mathbf{v})_d\right\|^2 = \frac{1}{d}\sum_{i=1}^{d}\frac{(u_i - v_i)^2}{\lambda_i^r}, \text{ with } r \in \mathbb{I}. \tag{47}$$

Here, $\mathbb{I}$ is the set of integers. In this article, we have studied the case when $r = 1$, i.e., $D_d^{\Sigma_d^{\mathbf{Z}},1}$. However, this was not a strict requirement and we look into some possible scenarios below:

- If $r \in \{0, -1, -2, \ldots\}$, assumption *A.2* in the main paper trivially gives that $\frac{(u_i-v_i)^2}{\lambda_i^r} \le \frac{(u_i-v_i)^2}{\lambda_i}$ eventually for large i, and consequently, $D_d^{\Sigma_d^{\mathbf{Z}},r}(\mathbf{u},\mathbf{v}) \xrightarrow{P} 0$ as $d \to \infty$.
- When $r \in \{2, 3, \ldots\}$, the transformation $D_d^{\Sigma_d^{\mathbf{Z}},r}$ may be useful because $1/\lambda_i^r$ will start to take high values (recall assumption *A.2*) and this may lead to separation between the observations of corresponding to different clusters.

Keeping the viewpoint stated above in mind, we consider the transformation $D_d^{\Sigma_d^{\mathbf{Z}},4}$ (using $r = 4$ in (47)). Numerical results for the difference in `location only` setting stated in Section 4 are reported below. We have excluded Example II from this comparison because, as stated earlier, the two GPs have no difference in their means.

Table L.1: Adjusted Rand distances for different GPs with difference in location (with standard error in brackets), taking $r = 4$ in (47).

GP ↓	k-means	funclust	CL	DHP	CD
I	**0.0001** (0.0001)	0.0002 (0.0001)	**0.0001** (0.0001)	**0.0001** (0.0000)	0.0012 (0.0002)
III	**0.0646** (0.0015)	*0.0795* (0.0009)	0.0945 (0.0045)	0.1480 (0.0047)	0.1649 (0.0017)
IV	0.1606 (0.0007)	*0.0318* (0.0003)	0.1015 (0.0000)	**0.0134** (0.0004)	0.1257 (0.0019)

As expected, the performance of k-means is quite good in Examples I and III. Both DHP and CL also perform quite well securing a first place in some cases. The proposed statistic $D_d^{\Sigma_d^{\mathbf{Z}},4}$ shows significant improvement (recall from part (c) of Theorem 2.2 that $L_\mu = 0$ for the earlier transformation $D_d^{\Sigma_d^{\mathbf{Z}},1}$), and this is reflected in the numerical figures of Table L.1.

Clearly, there is scope of further work with the proposed transformation $D_d^{\Sigma_d^{\mathbf{Z}},r}$ for $r \in \{2, 3, \ldots\}$, both theoretically as well as numerically.

M Review of the paper Delaigle et al (2019)

As stated, Delaigle et al (2019) is related to *perfect clustering* and it is the only paper on perfect clustering we are aware of. In this section, we analyze the relation between our proposal and this paper.

The proposal by Delaigle et al (2019) is based on finding a finite-dimensional subspace in which the data are projected, and clustering is done by applying a modification of the k-means algorithm on those projections. A theoretical result related to perfect clustering is stated in Theorem 1 of this paper. In the homoscedastic case, Delaigle et al (2019) gives an explicit expression of the subspace in which the data should be projected (see Theorem 2 of this paper).

The technique proposed in this paper has some advantage over our proposal in the sense that they can `handle the homoscedastic (differences only in location) case`. However, it suffers from several limitations, the main one being that `Delaigle et al (2019) is able to deal with mixtures involving only two components. On the technical side, the theory of Delaigle et al (2019) has some limitations.` It requires to arbitrarily fix $p \in \mathbb{N}$. Then, the data are projected on a p-dimensional subspace in which the clustering is to be done. New issues appear in the way in which the subspace should be chosen, and the way in which the clusters can be constructed. According to Theorem 1 of this paper, the generators of the subspace must be chosen in a finite set with cardinality $a_n \to \infty$ as the sample size $n \to \infty$. Moreover, the partition of the data set must be chosen between those in a finite set of Voronoi tessellations of $\mathbb{R}^p$ with cardinality $b_n \to \infty$ as $n \to \infty$. Additionally, the result needs technical conditions like the existence of some $c \in (0, 1)$ such that for every $C > 0$ it happens that $a_n^p b_n \exp(-Cn^c) \to \infty$ as $n \to \infty$.

N Full Numerical Results

Full results for `two scenarios` are given below.

Full result for the `location only` case (using the transformation $D_d^{\Sigma_d,4}$ stated in Section L of Appendix II) is given next.

R codes for our clustering methods are available from this link: GP clustering.

Table N.1: Adjusted Rand distances for different GPs with difference in location and scale (with standard error in brackets).

GP ↓	CD-*k*-means	CD-Spectral	CD-mclust	CL1	CL2	DHP1	DHP2
I	0.1678	0.0082	0.0001	0.0239	0.0554	0.8386	0.0818
	(0.0010)	(0.0002)	(0.0001)	(0.0007)	(0.0005)	(0.0064)	(0.0025)
II	0.9858	0.9847	0.4240	0.5767	0.9967	0.5470	0.5149
	(0.0003)	(0.0004)	(0.0030)	(0.0045)	(0.0018)	(0.0047)	(0.0049)
III	0.4191	0.9857	0.0625	0.2891	0.9962	0.4137	0.5613
	(0.0042)	(0.0099)	(0.0006)	(0.0000)	(0.0000)	(0.0054)	(0.0060)
IV	0.0316	0.0000	0.0000	0.1833	0.6660	0.1379	0.5211
	(0.0001)	(0.0000)	(0.0000)	(0.0000)	(0.0000)	(0.0033)	(0.0061)

Table N.2: Adjusted Rand distances for different GPs with difference only in scales (with standard error in brackets).

GP ↓	CD-*k*-means	CD-Spectral	CD-mclust	CL1	CL2	DHP1	DHP2
I	0.0063	0.0001	0.0000	0.8269	1.0017	0.9989	0.9966
	(0.0002)	(0.0001)	(0.0000)	(0.0000)	(0.0000)	(0.0005)	(0.0008)
II	0.0091	0.0100	0.0084	0.9065	1.0019	1.0001	0.9999
	(0.0010)	(0.0019)	(0.0003)	(0.0007)	(0.0005)	(0.0002)	(0.0003)
III	0.5549	0.9805	0.0856	0.9994	0.9998	0.9984	0.9967
	(0.0052)	(0.0099)	(0.0006)	(0.0000)	(0.0000)	(0.0004)	(0.0007)
IV	0.0102	0.0014	0.0005	0.8464	0.9928	0.9994	0.9980
	(0.0021)	(0.0013)	(0.0004)	(0.0000)	(0.0000)	(0.0003)	(0.0006)

Table N.3: Adjusted Rand distances for different GPs with difference in locations (with standard error in brackets).

GP ↓	CD-*k*-means	CD-Spectral	CD-mclust	C1	C2	DHP1	DHP2
I	0.0012	0.0814	0.0016	0.0001	0.0001	0.9896	0.0001
	(0.0002)	(0.0272)	(0.0003)	(0.0000)	(0.0000)	(0.0001)	(0.0001)
III	0.1649	0.3660	0.3007	0.0945	0.9975	0.1480	0.1623
	(0.0017)	(0.0076)	(0.0024)	(0.0010)	(0.0043)	(0.0047)	(0.0075)
IV	0.1257	0.3777	0.1784	0.1015	0.9001	0.0134	0.1473
	(0.0019)	(0.0085)	(0.0021)	(0.0000)	(0.0000)	(0.0004)	(0.0039)