



HAL
open science

Spectral Properties of Radial Kernels and Clustering in High Dimensions

Alba Chiara de Vitis, David Cohen-Steiner

► **To cite this version:**

Alba Chiara de Vitis, David Cohen-Steiner. Spectral Properties of Radial Kernels and Clustering in High Dimensions. 2019. hal-01969956v5

HAL Id: hal-01969956

<https://inria.hal.science/hal-01969956v5>

Preprint submitted on 27 Jun 2019 (v5), last revised 6 Jan 2020 (v7)

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Spectral Properties of Radial Kernels and Clustering in High Dimensions*

David Cohen-Steiner [†] Alba Chiara De Vitis [‡]

June 27, 2019

Abstract

In this paper, we study the spectrum and the eigenvectors of radial kernels for mixtures of distributions in \mathbb{R}^n . Our approach focuses on high dimensions and relies solely on the concentration properties of the components in the mixture. We give several results describing of the structure of kernel matrices for a sample drawn from such a mixture. Based on these results, we analyze the ability of kernel PCA to cluster high dimensional mixtures. In particular, we exhibit a specific kernel leading to a simple spectral algorithm for clustering mixtures with possibly common means but different covariance matrices. We show that the minimum angular separation between the covariance matrices that is required for the algorithm to succeed tends to 0 as n goes to infinity.

1 Introduction

Given a set of data points drawn from a mixture of distributions, a basic problem in data analysis is to cluster the observations according to the component they belong to. For this to be possible, it is clearly necessary to impose separation conditions between the different components in the mixture.

Many approaches have been proposed to solve the problem of clustering mixtures of distributions. We give below a brief historical account of the algorithms that come with theoretical guarantees, focusing on the high dimensional situation. Unlike in the low dimensional case, approaches based *e.g.* on single linkage or spectral clustering cannot be employed, because such methods require dense samples which would have an unreasonably large cardinality. The first result in this field, due to

*This work was partially supported by the Advanced Grant of the European Research Council GUDHI

[†]UCA INRIA, david.cohen-steiner@inria.fr

[‡]UCA INRIA, alba.de-vitis@inria.fr

Dasgupta, used random projection onto a low dimensional subspace [5]. It was shown that a mixture of Gaussians with unit covariance in dimension n could be provably well clustered if the separation between the means of the components was $O(\sqrt{n})$. The result was later improved by Dasgupta and Schulman [6] using a variant of EM for unit covariance Gaussians, and by Arora and Kannan [2], using a distance-based algorithm, for Gaussians with at most unit covariance. These methods, to correctly classify the components, require a $O(n^{1/4})$ separation between the centers of the Gaussians. For mixtures of unit covariance Gaussians, Vempala and Wang [23] used PCA to obtain a dimension-free separation bound that depends only on the number of components. Their method is based on the fact that the space spanned by the k top singular vectors of the mixture's covariance matrix contains the centers of the components. Projecting to this space has the effect of reducing the variance of each component while maintaining the separation between the centers. Kannan et al. [13] extended this idea to mixtures of log concave distributions with at most unit covariance, also requiring a separation between the centers that depends only on the number of components. Achlioptas and McSherry [1] further improved the dependency of the separation bound on the number of components. A combination of PCA with a reweighting technique was proposed by Brubaker and Vempala [4]. This method is affine invariant and can deal with highly anisotropic inputs as a result. When applied to a sample from a mixture of two Gaussians, the algorithm correctly classifies the sample under the condition that there exists a half space containing most of the mass of one Gaussian and almost none of the other. Finally, a different family of approaches uses the moments of the mixture to learn the parameters of the components. Strong results have been obtained in this direction (see *e.g.* [9, 3]). These methods do not require any separation assumption, however their downside is that they require a priori knowledge of a small parametric family containing the component's distributions. They also become inefficient when applied to high dimensional data, since the number of moments involved grows rapidly with the dimension. For example, the currently fastest algorithm [9] for learning mixtures of Gaussians runs in time $O(n^6)$.

Another possible approach to the analysis of mixtures uses kernel matrices. On a dataset $\{x_1, \dots, x_N\}$ of N points in \mathbb{R}^n a kernel function $k : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ defines a $N \times N$ kernel matrix whose ij entry is $k(x_i, x_j)$. An important class of kernels are positive definite kernels, which are those for which the associated kernel matrix is positive definite for any dataset. The use of such kernel matrices, and in particular of their spectral decomposition as in the popular kernel PCA algorithm, has long become commonplace in data analysis. Still, surprisingly little is known regarding theoretical justifications for kernel based clustering methods. Notably, the analysis in [20] implies that a kernel PCA type algorithm will correctly cluster mixtures when the components are sufficiently separated. However, the arguments used in this paper follow the low (or constant) dimensional intuition and the required separation between the components is of the order of the width of the kernel, which typically leads to a separation that grows like the square root of the dimension.

In order to improve the above analysis of kernel PCA, it is necessary to better understand the behavior of kernel matrices and of their spectra as the dimension increases. Again, while the literature on eigenvalues of random matrices is vast and growing rapidly, the knowledge about random kernel matrices is much scarcer. A notable exception is [14], which gives an asymptotic description of radial kernel matrices of the form $k(x_i, x_j) = h(\|x_i - x_j\|^2/n)$ as the dimension n tends to infinity, for a fixed function h . In the case of distributions whose coordinates are independent after some linear change of coordinate, *e.g.* Gaussians, it is shown that the kernel matrices converge in the operator norm to a certain matrix related to the covariance of the data, suggesting that such kernels do not provide additional information compared to standard PCA. Under the weaker condition that the distribution enjoys concentration properties, the corresponding convergence result is proved to hold at the level of spectral distributions, but no result is derived for individual eigenvalues.

In this paper, we prove new results about radial kernel matrices of mixtures of high dimensional distributions. Unlike [14], we do not assume independence of coordinates. Rather, we only assume that the components in the mixtures have exponential concentration. Specifically, we show that such matrices can be very well approximated by the sum of a matrix that is row constant within each component and a matrix that is column constant within each component. For distance matrices of mixtures with a single component, the result implies a large spectral gap between the two largest singular values: The ratio between these singular values is of the order of the dimension, rather than that of the square root of the dimension, as one might naively expect from basic concentration results. When the input distributions are supported on a sphere, this “double concentration” phenomenon is enhanced and large eigenvalue gaps arise for kernel matrices more general than distance matrices. The proof technique is geometric and very different from the one used in [14].

For positive kernels, a consequence of the above result is that kernel PCA is a valid clustering method as long as the Gram matrix of the mixture’s components, when viewed as elements of the corresponding Reproducing Kernel Hilbert Space (RKHS), is sufficiently well conditioned. In particular, this allows to check that kernel PCA allows to correctly clusters mixtures of two Gaussians with a required separation between centers that does not depend on the dimension.

In the case of even distributions supported on a sphere and satisfying a Poincaré inequality, we further show that our main result can be strengthened, so that kernel matrices are well approximated by block constant matrices, provided the kernel, which may or may not be positive, is smooth enough. We also design a specific non positive kernel for which this result can be extended to non necessarily even (and non necessarily centered) distributions. This kernel is not of the form studied in [14], so the results of that paper do not apply even for Gaussian mixtures. Based on this kernel, we derive a simple spectral algorithm for clustering mixtures with possibly common means. This algorithm will succeed if the angle between any two covariance matrices in the mixture (seen as vectors in \mathbb{R}^{n^2}) is larger than $O(n^{-1/6} \log^{5/3} n)$. In particular, the required angular separation tends to 0 as the dimension tends to infinity. To the best of our knowledge, this is the first polynomial time algorithm for

clustering such mixtures beyond the Gaussian case.

2 Kernels in high dimensions

Our analysis of kernel matrices for high dimensional data hinges on the concentration of measure phenomenon. Concentration of measure is a property of metric measure spaces that roughly says that regular functions are nearly constant [18, 16, 10]. It can be observed in many spaces, typical examples being Gaussian spaces or manifolds with Ricci curvature bounded below. We give precise definitions below for a probability measure μ on \mathbb{R}^n . We say that $f : \mathbb{R}^n \rightarrow \mathbb{R}$ has exponential σ -concentration, or σ -concentration for short, for some $\sigma > 0$, if for any $\varepsilon > 0$:

$$\mu\{x : |f(x) - M(f)| \geq \varepsilon\} \leq O(e^{-\frac{\varepsilon}{\sigma}})$$

where $M(f)$ is a median of f . The measure μ is said to have σ -concentration if all 1-Lipschitz functions have σ -concentration. In particular, we have that f equals $M(f)$ plus or minus $O(\sigma)$ with high probability.

Levy's lemma [17] states that an isotropic Gaussian with covariance $\sigma^2 I$ has Gaussian concentration, which is a stronger property implying $O(\sigma)$ -concentration. This result is also true for anisotropic Gaussians if one takes σ^2 to be the maximum eigenvalue of the covariance matrix. In particular, it implies that for high dimensional Gaussian spaces, most of the points are at about the same distance from the center. More precisely, almost all the mass of an isotropic Gaussian is concentrated in a spherical shell of radius $\sigma\sqrt{n}$ and thickness $O(\sigma)$. Indeed, for an isotropic Gaussian vector x , $\mathbb{E}(\|x\|^2) = \sigma^2 n$. As distance functions are 1-Lipschitz, by Levy's lemma, they have $O(\sigma)$ -concentration. Hence the distance from a random point to the center differ by at most $O(\sigma)$ from $\sigma\sqrt{n}$, with high probability.

A stronger form of concentration that we will also consider is based on Poincaré inequality. We will say that a probability measure μ satisfies a Poincaré inequality if for any Lipschitz function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ whose mean is zero with respect to μ , we have

$$\int f^2 d\mu \leq O(1) \int \|\nabla f\|^2 d\mu$$

A probability measure that satisfies a Poincaré inequality necessarily has $O(1)$ -concentration [19]. Gaussians distributions whose covariance have $O(1)$ eigenvalues are known to satisfy a Poincaré inequality. The famous KLS conjecture [12] states that uniform distributions over isotropic convex bodies, and more generally isotropic measures with log-concave densities also do.

2.1 Main result

We consider a mixture μ of k distributions μ_i in \mathbb{R}^n , with weights w_i , which we treat as numerical constants. We assume that each component μ_i has $O(1)$ -concentration.

Drawing a sample of N points independently from the mixture gives a point set X that is, with probability 1, the disjoint union of subsets X_i , corresponding to each component. The *radius* of μ_i is the quantity $(\mathbb{E}_{\mu_i} \|x - \mathbb{E}_{\mu_i} x\|^2)^{1/2}$ for a random variable x with law μ_i , and we denote by R the smallest radius of the μ_i . We consider a function $h : \mathbb{R}_+ \rightarrow \mathbb{R}$ and the associated radial kernel. This defines a kernel matrix $\Phi_h(X)$ whose entries are $h(\|x_i - x_j\|)/N$, for x_i, x_j in X . We assume that the indices are ordered in such a way that the components form contiguous intervals ; in particular, we have a natural block structure (doubly)-indexed by the components.

Theorem 1. *If the number of samples N is drawn according to the Poisson distribution with mean N_0 , then with arbitrarily high probability, we have:*

$$\|\Phi_h(X) - A\| \leq O \left(c_h + \|h\|_\infty \sqrt{\frac{n \log N_0}{N_0}} \right)$$

where the entries of A in the ij block are given by

$$A_{xy} = \frac{1}{N} \left(\int h(\|x - z\|) d\mu_j(z) + \int h(\|y - z'\|) d\mu_i(z') - \int h(\|z - z'\|) d\mu_i(z) d\mu_j(z') \right)$$

and with

$$c_h = \sup_{r \geq R/2} \left(|h''(r)| + \frac{1}{r} |h'(r)| \right) + \|h'\|_\infty \exp(-\Theta(R))$$

Furthermore, if the components μ_i are supported on the sphere centered at 0 with radius \sqrt{n} , and have mean at distance $O(1)$ from the origin, the conclusions above hold with c_h replaced by

$$c'_h = \sup_{r \geq R/\Theta(\log(R))} \left(\frac{\log^2(R) |h''(r)| + |h'(r)|}{r} \right) + \|h'\|_\infty / R$$

The proof of Theorem 1 follows from the analysis of the map sending each point x in \mathbb{R}^n to its kernel function $h(\|x - \cdot\|)$ in $L^2(\mathbb{R}^n, \mu)$ or, more precisely, of a finite sample version of this map. That analysis crucially depends on the fact that in Euclidean spaces, the cross derivative of the distance $\frac{\partial^2}{\partial x \partial y} \|x - y\|$ is upper bounded by $O(1/\|x - y\|)$. A first consequence of Theorem 1 is the following result about the spectrum of $\Phi_h(X)$, which follows directly from the variational characterization of eigenvalues:

Corollary 1. *Under the assumptions of Theorem 1, the spectrum of $\Phi_h(X)$ has at most k eigenvalues larger than $O \left(c_h + \|h\|_\infty \sqrt{\frac{n \log N_0}{N_0}} \right)$, and at most k eigenvalues smaller than $-O \left(c_h + \|h\|_\infty \sqrt{\frac{n \log N_0}{N_0}} \right)$, with arbitrarily high probability.*

2.2 Distance matrices

To illustrate Theorem 1, setting for example $h(r) = r$ gives a description of distance matrices. Consider the case of a sample drawn from a mixture of k Gaussians with unit covariance. If x_i and x_j are drawn independently from two Gaussians in the mixture, $x_i - x_j$ is a Gaussian with covariance $2I$. Concentration of measure then implies that the entries $\|x_i - x_j\|$ of each block concentrate around their mean value, i.e. they differ by at most $O(1)$ from the mean of the block with high probability:

$$\Phi_h(X) = \left(\begin{array}{c|c|c} \Phi_{11} & \cdots & \Phi_{1k} \\ \vdots & \ddots & \vdots \\ \hline \Phi_{k1} & \cdots & \Phi_{kk} \end{array} \right) = \frac{1}{N} \left(\begin{array}{c|c|c} m_1 \pm O(1) & \cdots & m_{1k} \pm O(1) \\ \vdots & \ddots & \vdots \\ \hline m_{k1} \pm O(1) & \cdots & m_{kk} \pm O(1) \end{array} \right) \quad (1)$$

A finer description of $\Phi_h(X)$ is given by Theorem 1. For an isotropic Gaussian, the radius R is $\Theta(\sqrt{n})$, and from $|h'| = 1$, $|h''| = 0$ we get $c_h = \Theta(1/\sqrt{n})$.

The dependency on the average number of samples N_0 in Theorem 1 involves $\|h\|_\infty$, which is unbounded. However, assuming for example that the centers of the components are at distance $O(1)$, then the fraction of pairs of sample points whose distance is larger than an appropriate constant times \sqrt{n} is exponentially small by concentration. Hence we can first modify h by thresholding such that $\|h\|_\infty$ becomes $O(\sqrt{n})$, with an exponentially small change in $\Phi_h(X)$. Furthermore, by making the transition between the linear part and the constant part smooth enough, we can ensure that the second derivatives of the modified kernel g are $O(1/\sqrt{n})$, so that $c_g = O(1/\sqrt{n})$. Applying the theorem to g implies that with a polynomial number of samples ($N_0 = \Omega(n^3 \log n)$ suffices), with arbitrarily high probability, each block of $\Phi_h(X)$ has the following structure

$$\Phi_{ij} = \frac{1}{N} \left(\begin{array}{cccc} a_1 & a_2 & \cdots & a_{N_i} \\ a_1 & a_2 & \cdots & a_{N_i} \\ \vdots & \vdots & \ddots & \vdots \\ a_1 & a_2 & \cdots & a_{N_i} \end{array} \right) + \frac{1}{N} \left(\begin{array}{cccc} b_1 & b_1 & \cdots & b_1 \\ b_2 & b_2 & \cdots & b_2 \\ \vdots & \vdots & \ddots & \vdots \\ b_{N_j} & b_{N_j} & \cdots & b_{N_j} \end{array} \right) + B$$

with $\|B\| = O(1/\sqrt{n})$. Note that the error term B is now much smaller than the one in (1), which is a priori up to $O(1)$ in the operator norm.

Furthermore, for each block the vectors (a_s) and (b_t) are, up to a constant, averages of the columns of the distance matrix. As a result these vectors are 1-Lipschitz and thus have $O(1)$ -concentration. Also, we can assume they have the same mean, namely half the average distance m_{ij} within the block, that is, at least $\Omega(\sqrt{n})$. So we can write $a_s = m_{ij}(1 + \varepsilon_s)/2$ and $b_t = m_{ij}(1 + \delta_t)/2$ with ε_s and δ_t in $O(1/\sqrt{n})$ with high probability. This implies that each block is very well approximated by a rank one matrix. Indeed

$$a_s + b_t = m_{ij}(2 + \varepsilon_s + \delta_t)/2 = m_{ij}((1 + \varepsilon_s/2)(1 + \delta_t/2) + O(1/n))$$

In particular, the normalized distance matrix of points drawn according to a single Gaussian has only one singular value that is larger than $O(1/\sqrt{n})$, this top singular value being $\Theta(\sqrt{n})$. This observation, which we stated for isotropic Gaussians for concreteness, applies to any distribution with $O(1)$ -concentration and variance $\Theta(n)$ as well.

We also remark that in the case of distributions on the sphere with $O(1)$ -concentration and variance $\Theta(n)$, the contribution of h'' in the error bound in Theorem 1 is divided by $\Omega(\sqrt{n}/\log^3 n)$, which makes it possible to extend the above discussion to kernels other than distance functions. We do not elaborate further as the spherical case will be studied in more detail in the sequel of the paper.

3 Positive definite kernels and clustering

For radial kernels that are positive definite, *i.e.* that define positive definite kernel matrices, Corollary 1 implies that there are at most k significant eigenvalues for mixtures of k probability measures that concentrate. We can use this result to provide guarantees for a simple clustering algorithm. First, assuming a certain gap condition, we can relate eigenspaces of the kernel matrix to the space of piecewise constant vectors, *i.e.* vectors that are constant on each component in the mixture.

The required gap condition can be conveniently formulated in terms of *kernel distances* [21, 11]. Recall that kernel distances are Hilbertian metrics on the set of probability measures, which are obtained by embedding the ambient Euclidean space into a universal RKHS. More precisely, given two probability measures μ_1 and μ_2 on \mathbb{R}^n , the expression

$$\langle \mu_1, \mu_2 \rangle = \int h(\|x - y\|) d\mu_1(x) d\mu_2(y)$$

is a positive definite kernel and the kernel distance is the associated distance.

Proposition 1. *Assume h defines a positive definite kernel, and that the conditions of Theorem 1 are satisfied. Let*

$$G_h = (\langle \mu_i, \mu_j \rangle)_{i,j=1\dots k}$$

be the Gram matrix of the components in the kernel distance.

If the smallest eigenvalue of G_h is at least Kc_h , then the maximum angle formed by the space spanned by the top k eigenvectors of $\Phi_h(X)$ and the space of piecewise constant vectors is at most $O(1/\sqrt{K})$, with arbitrarily high probability, provided $N_0 \geq N_1$, with:

$$N_1 = O\left(\frac{\|h'\|_\infty^2}{c_h^2} + \frac{n\|h\|_\infty^2}{c_h^2} \log\left(\frac{n\|h\|_\infty^2}{c_h^2}\right)\right)$$

Under these assumptions we can provide a guarantee for the following basic kernel PCA clustering algorithm. First, we perform a spectral embedding using the k top

eigenvectors of $\Phi_h(X)$. Namely, each data point x is mapped to $(\phi_1(x), \dots, \phi_k(x))$, ϕ_1, \dots, ϕ_k being the k dominant eigenvectors of $\Phi_h(X)$. In order to have the right dependency on the total number of points, these eigenvectors are scaled to have norm \sqrt{N} . By the above proposition, this will give a point cloud that is $O(\sqrt{1/K})$ close in the transportation distance W_2 to a point cloud obtained using the embedding provided by an orthogonal basis of piecewise constant vectors, scaled to have norm \sqrt{N} . Note that in the latter point cloud, each component becomes concentrated at a single location, the distance between any two such locations being $\Omega(1)$. In such a situation, any constant factor approximation algorithm for the k -means problem will find a clustering with a fraction of at most $O(1/K)$ misclassified points. We just proved:

Corollary 2. *If the assumptions of Proposition 1 are satisfied, kernel PCA allows to correctly cluster a $1 - O(1/K)$ fraction of the mixture, with arbitrarily high probability.*

As an example, we consider the case of a mixture of two Gaussians using a Gaussian kernel $h(r) = \exp(-r^2/(2\tau^2))$. In this case, matrix G_h can be computed in closed form, so that the conditions of Proposition 1 can be checked explicitly.

Corollary 3. *Consider a mixture of two Gaussians with $O(1)$ -concentration in \mathbb{R}^n . Assuming that the variance of each Gaussian is $\Theta(n)$, for $\tau = \Theta(\sqrt{n})$, Gaussian kernel PCA allows to correctly cluster a $1 - O(1/K)$ fraction of the mixture if the distance between the centers is K .*

The choice of variance for the components in the above corollary is to fix ideas, similar conclusions would hold with other behaviors. The above guarantee matches the dimension-independent separation required by the PCA-based algorithms described in [13, 1] for example. Finally, the results in this section are in fact not strongly tied to the Hilbertian nature of positive kernels. More precisely, they may be easily extended to conditionally positive kernels, by simply restricting the involved quadratic forms to the space of zero mean functions. We omit further details.

4 Covariance based clustering

As shown in the above section, the approximation of kernel matrices provided by Theorem 1 is sufficient to conclude that their top eigenvectors are nearly constant on the clusters if the kernel is positive, which allows to correctly cluster the data. Unfortunately, while we showed that positive kernels could allow to cluster *e.g.* mixtures of Gaussians with different enough centers, the range of cases that can be successfully clustered using positive kernels remains unclear at this stage. In this section we show that by relaxing the positivity constraint, one can design kernels that can deal with more difficult situations, such as mixtures of distributions with common centers but different covariances. While Theorem 1 alone is insufficient for this purpose, we show that stronger conclusions can be obtained assuming that the components of the mixtures are supported on the sphere S with radius \sqrt{n} and

centered at the origin, and satisfy a Poincaré inequality. Namely, kernel matrices can then be approximated by block constant matrices, rather than a sum of column and row constant matrices within each block. We state below such a result for general kernels, assuming the input distributions are even. We also consider the case of non necessarily even distributions with small enough means. Similar conclusions can then be drawn for the kernel

$$h_t(r) = \cos\left(\frac{t}{\sqrt{n}}(n - r^2/2)\right)$$

where t is a parameter. The argument is more direct and avoids the use of Poincaré inequality. A more transparent way to write this kernel is to remark that for x and y on S ,

$$h_t(\|x - y\|) = \cos\left(\frac{t}{\sqrt{n}} \langle x, y \rangle\right)$$

Note that h_t has a perhaps non intuitive behavior compared to the most commonly used kernels as it oscillates $\Theta(\sqrt{n})$ times over the sphere S for $t = \Theta(1)$ for example.

Theorem 2. *Assume measures μ_i are supported on S , even, and satisfy a Poincaré inequality. Let $\tilde{h}(r) = h'(r)/r$. If the number of samples N is drawn according to the Poisson distribution with mean N_0 , then with arbitrarily high probability, we have:*

$$\|\Phi_h(X) - B\| \leq O\left(c'_h + \sqrt{n}c'_h + \|h\|_\infty \sqrt{\frac{n \log N_0}{N_0}}\right)$$

where the entries of B in the ij block are all equal to

$$G_h(i, j)/N = \frac{1}{N} \left(\int h(\|z - z'\|) d\mu_i(z) d\mu_j(z') \right)$$

For the kernel h_t , under the weaker assumption that measures μ_i are supported on S , have $O(1)$ -concentration and have means at distance $O(1)$ from the origin, we have:

$$\|\Phi_{h_t}(X) - B\| \leq O\left(\frac{t \log^3 n}{\sqrt{n}} + \sqrt{\frac{n \log N_0}{N_0}}\right)$$

with arbitrarily high probability for $t = O(1)$.

In particular, in the case of even distributions satisfying a Poincaré inequality, letting the sample size go to infinity, expliciting the upper bound in the first part of the theorem implies that for any fixed bounded function h with bounded derivatives up to the third order, the radial convolution operator from $L^2(\mathbb{R}^n, \mu_i)$ to $L^2(\mathbb{R}^n, \mu_j)$ associated with kernel $r \mapsto h(r^2/\sqrt{n})$ has at most one singular value larger than $O(\log^3 n/\sqrt{n})$. It seems likely that the logarithmic factor can in fact be removed, by replacing the Lipschitz extension argument by a Dirichlet energy estimate in the proof of Theorem 1.

We now show that the second part of the above theorem can be used to cluster high dimensional mixtures based on the components covariance matrices. We assume that the components μ_i have $O(1)$ -concentration and variance $\Theta(n)$. As the PCA algorithm of [13] allows to separate components whose means are at distance at least $\Omega(1)$ from the other means, it is sufficient to consider the case where all means are at distance $O(1)$ from the origin. We denote by Σ_i the non centered covariance matrix of μ_i . Given $s > 0$ and a symmetric matrix M , we define $f_s(M)$ to be the matrix having the same eigenvectors as M , eigenvalues being transformed by function $\lambda \mapsto f_s(\lambda)$, with $f_s(\lambda) = \max(0, |\lambda| - s)$. Let

$$\Delta = \sqrt{n} \min_{u \neq v} \left\| \frac{\Sigma_u}{\text{trace}\Sigma_u} - \frac{\Sigma_v}{\text{trace}\Sigma_v} \right\|_2$$

As covariance matrices have trace $\Theta(n)$, they have Frobenius norm $\Theta(\sqrt{n})$, so that $\Delta = \Omega(\alpha_{min})$, α_{min} being the minimum angle between any two covariance matrices. Let further C_1, C_2 be two appropriate universal constants. The algorithm we propose is the following:

Algorithm 1 CovarianceClustering(X)

\tilde{X} = data points projected on S

$\Phi = \Phi_{h_t}(\tilde{X})$, with $t = C_1\Delta$

Approximately solve the k-means problem for the columns of $f_{C_2\Delta^4}(\Phi)$

To prove that this algorithm succeeds, we apply Theorem 2 to the data projected on S , which tells us that $\Phi_{h_t}(\tilde{X})$ is well approximated by block constant matrix B . We then show that under our separation assumptions, matrices G_{h_t} are well-conditioned in the case of mixtures of two components. Using this fact, we show that the columns $f_{C_2\Delta^4}(B)$ corresponding to different components are sufficiently far apart. Applying a perturbation bound then allows to conclude, and obtain the following guarantee:

Theorem 3. *If $\Delta \geq Kn^{-1/6} \log^{5/3} n$, the above algorithm allows to correctly cluster a $O(1/K^6)$ fraction of the mixture with arbitrarily high probability, provided $N_0 \geq N_1$, with:*

$$N_1 = O(\log(n/\Delta)n^2/\Delta^2)$$

Hence clustering will succeed if the minimum angle α_{min} between the components covariances is larger than $O(n^{-1/6} \log^{5/3} n)$. First note that one case is not covered by this algorithm, namely the case where different components have covariance matrices differing only by a scaling. This situation can be dealt with easily by clustering the data according to the distance to the origin. A second remark can be made about the sample size. The guarantee given above aims for the smallest angular separation, and as a result requires a number of points that is more than quadratic in the dimension. While it is possible that a better analysis would give

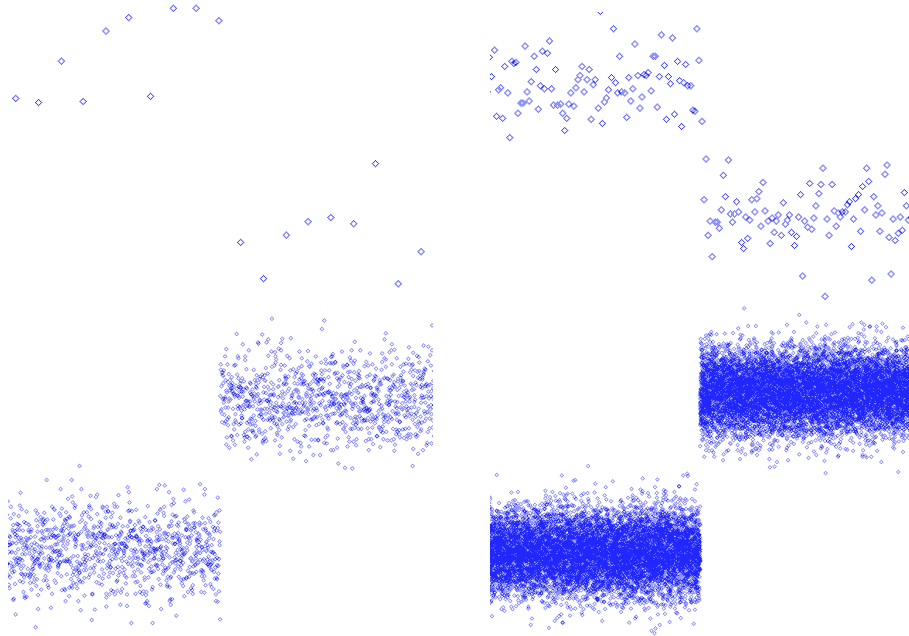


Figure 1: Second singular vector of Φ for isotropic mixtures of centered Gaussians.

smaller sample sizes in this regime, we remark that if $\alpha_{min} = \Omega(1)$, the proof can be modified to show that correct clustering will require only $O(n \log n)$ points. Indeed, in this situation, the error bound in Theorem 2 is dominated by the contribution of the sample size, and having $O(n \log n)$ points will make it small enough so that the rest of the analysis can be applied.

To conclude, we give some numerical results on specific examples of equal weight mixtures of two Gaussian distributions μ_1 and μ_2 with mean zero on \mathbb{R}^n , with n even. The covariances Σ_1 and Σ_2 are both diagonal in the standard basis. For a parameter $s > 0$, the eigenvalues of Σ_1 are $1 + s$ on the first $n/2$ coordinates, and $1 - s$ on the last $n/2$ coordinates. Eigenvalues of Σ_2 are reversed, so that $\Sigma_1 + \Sigma_2 = 2I$, meaning that the whole distribution is isotropic. Under the assumptions of Theorem 3, as shown in the proof, the spectral soft thresholding operation used in the algorithm will leave at most 2 non zero eigenvalues. Rather than implementing the full algorithm, we just plot the second dominant singular vector of Φ , as the first one turns out not to separate the components. Figure 1 shows it for $s = 0.9$, $n = 10$, $s = 0.6$, $n = 100$, $s = 0.33$, $n = 1000$ and $s = 0.2$, $n = 10000$, with $t = 0.1$. In all cases each Gaussian has n sample points. We see that the clusters are easily detected. Note that in the latter case, the Gaussians are nearly spherical, the relative error being of roughly 10% in terms of standard deviation.

5 Proofs

We give the proof of Theorem 1 in section 5.1, of Proposition 1 in Section 5.2, and of Corollaries 1 and 3 in Sections 5.3 and 5.4. Theorems 2 and 3 are proved in Sections 5.5 and 5.6.

5.1 Proof of Theorem 1

For technical reasons we will not work directly with the input measure μ , but rather with its empirical measure $\bar{\mu} = \sum_i w_i \bar{\mu}_i$, the number of samples being drawn according to a Poisson distribution with appropriately large mean M_0 . Since the μ_i have $O(1)$ -concentration, a vector X with law μ_i satisfies $\mathbb{E}(\|X - \mathbb{E}X\|^q)^{1/q} = O(\sqrt{n})$ for constant $q \geq 1$, which implies (see *e.g.* [8]) that

$$\mathbb{E}(W_l(\mu_i, \bar{\mu}_i)) = O(nM_0^{-1/n})$$

where W_l are the transportation distances for $l = 1$ or 2 . By Markov inequality, for any $\delta > 0$, these distances are at most δ with probability at least $1 - p$, with

$$p = O\left(\frac{nM_0^{-1/n}}{\delta}\right)$$

Consider the map

$$\begin{aligned} \phi_{\bar{\mu}} : \mathbb{R}^n &\rightarrow L^2(\mathbb{R}^n, \bar{\mu}) \\ x &\mapsto \phi_{\bar{\mu}}(x) = h(\|x - \cdot\|) \end{aligned}$$

The gist of our proof of Theorem 1 is as follows. We first observe that the directional derivatives of $\phi_{\bar{\mu}}$ at each point satisfy a Lipschitz condition with a small constant. More precisely, this is true after modifying them in a small region, which is enough for our purposes. Using concentration of measure, this implies that these derivatives, modulo piecewise constant functions on the components, are small. This can be further reinterpreted as saying that $\phi_{\bar{\mu}}$, after centering on each component, has a small Lipschitz constant. Because each component has constant concentration by assumption, this implies that the image of each component by $\phi_{\bar{\mu}}$, after centering on each component, has small concentration. The desired claim on the block structure of $\Phi_h(X)$ can then be deduced.

5.1.1 A property of $\phi_{\bar{\mu}}$

Let $E \in L^2(\mathbb{R}^n, \bar{\mu})$ be the space of functions that are constant on the support of each $\bar{\mu}_i$, and P_E and P_{E^\perp} denote the orthogonal projectors onto E and E^\perp . Further denote by S the sphere with radius \sqrt{n} centered at 0.

Proposition 2. *With probability at least $1 - p$, for any x_1 and $x_2 \in \mathbb{R}^n$,*

$$\|P_{E^\perp} \phi_{\bar{\mu}}(x_1) - P_{E^\perp} \phi_{\bar{\mu}}(x_2)\| \leq O(c_h(\delta)) \|x_1 - x_2\|$$

Furthermore if measures μ_i are supported on S and their mean is $O(1)$, then with probability at least $1 - p$, for any x_1 and x_2 in S :

$$\|P_{E^\perp} \phi_{\bar{\mu}}(x_1) - P_{E^\perp} \phi_{\bar{\mu}}(x_2)\| \leq O(c'_h(\delta)) \|x_1 - x_2\|$$

with

$$\begin{aligned} c_h(\delta) &= (1 + \delta)c_h + \sqrt{\delta} \|h'\|_\infty \\ c'_h(\delta) &= (1 + \delta)c'_h + \sqrt{\delta} \|h'\|_\infty \end{aligned}$$

To prove the first part of Proposition 2 we argue that

$$\begin{aligned} \|P_{E^\perp} \phi_{\bar{\mu}}(x_1) - P_{E^\perp} \phi_{\bar{\mu}}(x_2)\|_2 &\leq \sup_{x_0, v, \|v\|=1} \left\| \frac{d}{dx} \Big|_{v, x=x_0} P_{E^\perp} \phi_{\bar{\mu}} \right\|_2 \|x_1 - x_2\| \\ &\leq \sup_{x_0, v, \|v\|=1} \left\| P_{E^\perp} \frac{d}{dx} \Big|_{v, x=x_0} \phi_{\bar{\mu}} \right\|_2 \|x_1 - x_2\| \\ &\leq \sup_{x_0, v, \|v\|=1} \left(\sum_i w_i \left\| f_i - \int f_i d\bar{\mu}_i \right\|_2^2 \right)^{1/2} \|x_1 - x_2\| \end{aligned}$$

where in the last line f_i denotes the directional derivative of $\phi_{\bar{\mu}_i}$ at x_0 in direction v . To conclude, it is sufficient to prove that

$$\sup_{x_0, v, \|v\|=1} \left\| f_i - \int f_i d\bar{\mu}_i \right\|_2 \leq O(c_h(\delta)) \quad (2)$$

For the second part, we use a similar argument except that we interpolate between x_1 and x_2 using a great circle on S instead of a straight line. This shows that establishing

$$\sup_{x_0, v, \|v\|=1, \langle v, x_0 \rangle = 0} \left\| f_i - \int f_i d\bar{\mu}_i \right\|_2 \leq O(c'_h(\delta)) \quad (3)$$

suffices to conclude. Proving these two inequalities is the point of the rest of this section. For some $\rho > 0$, let

$$L_{v, \rho} = \{y \mid |\langle y, v \rangle| \leq 1/\rho\}$$

Further define:

$$\begin{aligned} d_h &= \sup_{r \geq \rho R} \left(|h''(r)| + \frac{1}{r} |h'(r)| \right) \\ d'_h &= \sup_{r \geq \rho R} \left(\frac{|h''(r)|}{\rho^2 r} + \frac{1}{r} |h'(r)| \right) \end{aligned}$$

Lemma 1. *Function f_i is d_h -Lipschitz outside $B(x_0, \rho R)$ and $|f_i|$ is bounded everywhere by $\sup |h'|$. Furthermore, if v is a unit tangent vector at $x_0 \in S$, then f_i is d'_h -Lipschitz on $L_{v,\rho} \setminus B(x_0, \rho R)$.*

Proof. We consider the radial coordinate system (r, θ) centered at x_0 , where θ denotes the angle formed by $y - x_0$ and v . A direct calculation shows that

$$f_i(y) = \frac{d}{dx} \Big|_{v, x=x_0} \phi_{\bar{\mu}_i}(x)(y) = h'(r) \cos \theta$$

Hence

$$\begin{aligned} \frac{d}{dr} f_i(r(y), \theta(y)) &= h''(r) \cos \theta \\ \frac{d}{d\theta} f_i(r(y), \theta(y)) &= -h'(r) \sin \theta \end{aligned}$$

Noticing that r is a 1-Lipschitz function of y , and that $|d\theta/dy| \leq 1/r$ allows to bound the derivatives of f_i in the radial and tangent directions using the chain rule, implying:

$$\begin{aligned} \|\nabla f_i(y)\| &= \left((h''(r(y)) \cos \theta(y))^2 + \left(\frac{h'(r(y))}{r(y)} \sin \theta(y) \right)^2 \right)^{1/2} \\ &\leq \max \left(h''(r(y)) |\cos \theta(y)|, \frac{h'(r(y))}{r(y)} \right) \end{aligned}$$

Using that $|\cos \theta(y)| \leq 1/(\rho^2 r)$ on $L_{v,\rho} \setminus B(x_0, \rho R)$, the conclusion follows. \square

Lemma 2. *We can write $f_i = \tilde{f}_i + g_i$, where \tilde{f}_i is d_h -Lipschitz, and g_i is supported on $B(x_0, \rho R)$ with $\|g_i\|_\infty \leq 2 \sup_r |h'(r)|$. If v is a unit tangent vector at $x_0 \in S$, then we can find a similar decomposition with \tilde{f}_i d'_h -Lipschitz and g_i supported on $B(x_0, \rho R) \cup \mathbb{R}^n \setminus L_{v,\rho}$ with $\|g_i\|_\infty \leq 2 \sup_r |h'(r)|$.*

Proof. Define \tilde{f}_i to be a d_h -Lipschitz extension of $f_i|_{\mathbb{R}^n \setminus B(x_0, \rho R)}$ to \mathbb{R}^n , which exists by Kirszbraun's extension theorem [15]. We choose \tilde{f}_i such that $\sup_{B(x_0, \rho R)} |\tilde{f}_i| = \sup_{\partial B(x_0, \rho R)} |\tilde{f}_i|$, which can be done by thresholding if necessary. The result follows by letting $g_i = f_i - \tilde{f}_i$. The spherical case is proved similarly. \square

Lemma 3. *With probability at least $1 - p$, we have $\text{Var}_{\bar{\mu}_i}(f_i) = O(c_h(\delta)^2)$. If measures μ_i are supported on S with mean $O(1)$, then with probability at least $1 - p$, for v a unit tangent vector at $x_0 \in S$, $\text{Var}_{\bar{\mu}_i}(f_i) = O(c'_h(\delta)^2)$.*

Proof. For the first claim, we write

$$\begin{aligned} \sqrt{\text{Var}_{\bar{\mu}_i}(f_i)} &\leq \sqrt{\text{Var}_{\bar{\mu}_i}(\tilde{f}_i)} + \sqrt{\text{Var}_{\bar{\mu}_i}(g_i)} \\ &\leq \sqrt{\text{Var}_{\bar{\mu}_i}(\tilde{f}_i)} + \|g_i\|_2 \\ &\leq \sqrt{\text{Var}_{\bar{\mu}_i}(\tilde{f}_i)} + \sup |g_i| \bar{\mu}_i(B(x_0, \rho R))^{1/2} \end{aligned}$$

Because \tilde{f}_i is d_h -Lipschitz, the pushforwards of μ_i and $\bar{\mu}_i$ satisfy

$$W_2(\tilde{f}_{i\#}\bar{\mu}_i, \tilde{f}_{i\#}\mu_i) \leq d_h W_2(\bar{\mu}_i, \mu_i) \leq d_h \delta$$

And since μ_i has $O(1)$ -concentration, $\tilde{f}_{i\#}\mu_i$ has at most $O(d_h^2)$ variance. As a result

$$\text{Var}_{\bar{\mu}_i}(\tilde{f}_i) = \text{Var}_{\tilde{f}_{i\#}\bar{\mu}_i} \leq O((1 + \delta^2)d_h^2)$$

Also, letting d_{x_0} be the distance function to x_0 , we have that

$$W_1(d_{x_0\#}(\bar{\mu}_i), d_{x_0\#}(\mu_i)) \leq \delta$$

since distance functions are 1-Lipschitz. Consider an optimal coupling (X, Y) between $d_{x_0\#}(\bar{\mu}_i)$ and $d_{x_0\#}(\mu_i)$. By Markov inequality, the probability that $X \leq \rho R$ and $Y \geq \rho R + 1$ is at most δ . This implies that

$$\bar{\mu}_i(B(x_0, \rho R)) \leq \delta + \mu_i(B(x_0, \rho R + 1))$$

Since d_{x_0} $O(1)$ -concentrates on μ_i , its median is $O(1)$ close to $(\int d_{x_0}^2 d\mu_i)^{1/2}$. As the latter quantity is at least R , we have by concentration

$$\mu_i(B(x_0, \rho R + 1)) \leq \exp(-\Omega(1 - \rho)R + O(1))$$

As a consequence

$$\sqrt{\text{Var}_{\bar{\mu}_i}(f_i)} \leq O\left((1 + \delta^2)^{1/2}d_h + \sup_r |h'(r)| (\delta + \exp(-\Omega(1 - \rho)R))^{1/2}\right)$$

The first claim follows by setting $\rho = 1/2$. The spherical case is proved similarly, except that we use the inequalities

$$\bar{\mu}_i(B(x_0, \rho R) \cup \mathbb{R}^n \setminus L_{v,\rho}) \leq \bar{\mu}_i(B(x_0, \rho R)) + \bar{\mu}_i(\mathbb{R}^n \setminus L_{v,\rho})$$

and

$$\begin{aligned} \bar{\mu}_i(\mathbb{R}^n \setminus L_{v,\rho}) &\leq \delta + \mu_i(\{y \mid |\langle y, v \rangle| \geq 1/\rho - 1\}) \\ &\leq \delta + 2 \exp(-\Omega(1/\rho) + O(1)) \\ &\leq \delta + O(\exp(-\Omega(1/\rho))) \end{aligned}$$

which follows as above from the fact that linear functions $O(1)$ -concentrate on μ_i and have mean $O(1)$. Choosing appropriate $\rho = \Theta(\log(R)^{-1})$, the bound above becomes $\delta + 1/R^2$, hence

$$\begin{aligned} \sqrt{\text{Var}_{\bar{\mu}_i}(f_i)} &\leq O\left((1 + \delta^2)^{1/2}d'_h + \sup_r |h'(r)| (\delta + 1/R^2)^{1/2}\right) \\ &\leq O(c'_h(\delta)) \end{aligned}$$

□

This proves (2) and (3) and concludes the proof of Proposition 2.

5.1.2 Decomposition of $\Phi_h(X)$

We first show the following variant of Theorem 1:

Proposition 3. *If the number of samples M is drawn according to the Poisson distribution with mean M_0 , then with probability at least $1-p$, we have $\|\Phi_h(X) - A\| = O(e_h(\delta))$ with $e_h(\delta) = c_h(\delta)(1 + \delta) + \delta\|h'\|_\infty$, and $\|\Phi_h(X) - A\| = e'_h(\delta)$ with $e'_h(\delta) = c'_h(\delta)(1 + \delta) + \delta\|h'\|_\infty$ in the spherical case.*

The argument is the same for the spherical and for the non-spherical case, so we only consider the non spherical case. Let M be the number of samples of $\bar{\mu}$. First decompose the unnormalized kernel matrix $D_h(X) = M\Phi_h(X)$ as follows:

$$D_h(X) = P_E D_h(X) + P_{E^\perp} D_h(X)$$

The first term $P_E D_h(X)$ is column constant within each block. We now focus on the second one.

Lemma 4. *With probability at least $1-p$, the centered covariance matrix of the columns of $P_{E^\perp} D_h(X)$ corresponding to any component has eigenvalues at most $O(Mc_h(\delta)^2(1 + \delta^2))$.*

Proof. The columns of $P_{E^\perp} D_h(X)$ are the images of the sample points by $P_{E^\perp} \phi_{\bar{\mu}}$, expressed in the standard basis. Hence by Proposition 2, the map $\bar{\phi}$ associating each sample point with its column in $P_{E^\perp} D_h(X)$ is $O(\sqrt{M}c_h(\delta))$ -Lipschitz with probability at least $1-p$. Let $\tilde{\phi}$ be a $O(\sqrt{M}c_h(\delta))$ -Lipschitz extension of $\bar{\phi}$ to \mathbb{R}^n . Consider a unit vector $v \in \mathbb{R}^M$ and let U be a random column of $P_{E^\perp} D_h(X)$. Variable $\langle U, v \rangle$ is equal to $\langle \bar{\phi}(V), v \rangle = \langle \tilde{\phi}(V), v \rangle$, where V is drawn according to $\bar{\mu}_i$. Let now W be drawn according to μ_i . Since μ_i has $O(1)$ -concentration, $\langle \tilde{\phi}(W), v \rangle$ has variance $O(Mc_h(\delta)^2)$. Because with probability at least $1-p$, $W_2(\bar{\mu}_i, \mu_i) < \delta$, the distributions of $\langle \tilde{\phi}(W), v \rangle$ and $\langle \tilde{\phi}(V), v \rangle$ are $O(\sqrt{M}c_h(\delta)\delta)$ away in the W_2 distance. As a consequence

$$\text{Var}(\langle \tilde{\phi}(V), v \rangle) = O(\text{Var}(\langle \tilde{\phi}(V), v \rangle) + Mc_h(\delta)^2\delta^2) = O(Mc_h(\delta)^2(1 + \delta^2))$$

□

Let us further decompose

$$P_{E^\perp} D_h(X) = P_{E^\perp} D_h(X) P_E + P_{E^\perp} D_h(X) P_{E^\perp}$$

as a sum of matrix $P_{E^\perp} D_h(X) P_E$ which is row constant within each block, and a remainder $M.B = P_{E^\perp} D_h(X) P_{E^\perp}$ whose columns are the columns of $P_{E^\perp} D_h(X)$ centered in each block. By Lemma 4, the non centered covariance matrix of all the columns of $M.B$ has eigenvalues at most $O(Mc_h(\delta)^2(1 + \delta^2))$. As this covariance matrix is $M.BB^t$, this shows that $\|B\| = O(c_h(\delta)(1 + \delta))$. Thus we get:

$$\Phi_h(X) = P_E \Phi_h(X) + P_{E^\perp} \Phi_h(X) P_E + B$$

Letting $\bar{A} = P_E \Phi_h(X) + P_{E^\perp} \Phi_h(X) P_E$, we see that for $x \in \text{support}(\bar{\mu}_i)$ and $y \in \text{support}(\bar{\mu}_j)$, the xy entry of \bar{A} is given by

$$M \cdot \bar{A}_{xy} = \int h(\|x - z\|) d\bar{\mu}_j(z) + \int h(\|y - z'\|) d\bar{\mu}_i(z') - \int h(\|z - z'\|) d\bar{\mu}_i(z) d\bar{\mu}_j(z')$$

By Kantorovich-Rubinstein theorem,

$$\|A - \bar{A}\| \leq \sup_{xy} |M \cdot \bar{A}_{xy} - M \cdot A_{xy}| \leq O(\delta \|h'\|_\infty)$$

which concludes the proof.

5.1.3 Sample size

In order to prove that Theorem 1 also holds for small sample size, we use the following result in [22]. For a random variable W , let $E_k W$ denotes the L_k norm of W . For a matrix U , $\|U\|_\infty$ is the maximum entry of U , and $\|U\|_{1,2}$ is the maximum norm of the columns of U .

Theorem. *Let Z be a $M \times M$ Hermitian matrix, decomposed into diagonal and off-diagonal parts: $Z = D + H$. Fix k in $[2, \infty)$, and set $q = \max\{k, 2 \log M\}$. Then*

$$E_k \|RZR\| \leq O(q E_k \|RHR\|_\infty + \sqrt{\eta q} E_k \|HR\|_{1,2} + \eta \|H\|) + E_k \|RDR\|$$

where R is a diagonal matrix with independent 0 – 1 entries with mean η .

Let us apply this theorem to $Z = M(\Phi_h(X) - A_M)$, where X is an iid sample of μ with cardinality M distributed according to a Poisson distribution with mean M_0 , and A_M is the matrix specified in Theorem 1. In any case $\|RZR\| \leq O(\text{trace}(R) \|h\|_\infty)$, and by Proposition 3, with probability at least $1 - p$, we have $\|Z\| \leq O(M e_h(\delta))$ (and similarly for the spherical case). Clearly $E_k \|RDR\|$ and $E_k \|RHR\|_\infty$ are both bounded by $O(\|h\|_\infty)$, and $E_k \|HR\|_{1,2}$ is at most $O(\|h\|_\infty E_k \sqrt{M})$. Also $\|H\| \leq \|Z\| + \|D\| \leq O(M e_h(\delta) + \|h\|_\infty)$ with probability at least $1 - p$. Hence the theorem above gives:

$$E_k \|RZR\| \leq \|h\|_\infty O(p E_k \text{trace}(R) + q + \sqrt{\eta q} E_k \sqrt{M} + \eta) + O(\eta e_h(\delta) E_k M)$$

Taking $k = 2$ and $\eta = N_0/M_0$, we have $E_k \text{trace}(R) = O(N_0)$, $E_k \sqrt{M} = O(\sqrt{M_0})$ and $E_k M = O(M_0)$. With $q = 2 \log M_0$, we get

$$\begin{aligned} E_2 \left(\frac{\|RZR\|}{\text{trace}(R)} \right) &\leq O \left(E_2 \left(\frac{\|RZR\|}{N_0} \right) \right) \\ &\leq \|h\|_\infty O \left(p + \frac{\log M_0}{N_0} + \sqrt{\frac{\log M_0}{N_0}} + \frac{1}{M_0} \right) + O(e_h(\delta)) \\ &\leq \|h\|_\infty O \left(\frac{n}{\delta M_0^{1/n}} + \sqrt{\frac{\log M_0}{N_0}} \right) + O(e_h(\delta)) \\ &\leq \|h\|_\infty O \left(\frac{n}{\delta M_0^{1/n}} + \sqrt{\frac{\log M_0}{N_0}} + \delta + (1 + \delta) \sqrt{\delta} \right) + (1 + \delta)^2 O(c_h) \end{aligned}$$

assuming $N_0 \geq \log M_0$. Matrix $RZR/\text{trace}(R)$ is simply $\Phi_h(Y) - A_N$, where Y is an iid sample of μ with cardinality N distributed according to a Poisson distribution with mean N_0 . Continuing the last equation, taking $M_0 = N_0^{3n/2}$ and $\delta = (n/M_0^{1/n})^{2/3}$ so that $p = \Theta(\sqrt{\delta})$, we have

$$\begin{aligned} E_2(\|\Phi_h(Y) - A_N\|) &\leq \|h\|_\infty O\left(\frac{n}{\delta M_0^{1/n}} + \sqrt{\frac{\log M_0}{N_0}}\right) + O(c_h) \\ &\leq O\left(c_h + \|h\|_\infty \sqrt{\frac{n \log N_0}{N_0}}\right) \end{aligned}$$

The conclusion follows by applying Markov inequality.

5.2 Proof of Proposition 1

We want to show that for a positive kernel, the space spanned by the k top eigenvectors of $\Phi_h(X)$ is close to the space of piecewise constant functions E . We first observe that for a large enough number of samples, matrix G_h is close to its finite sample version \widehat{G}_h , whose ij entry is the average of the kernel over $X_i \times X_j$:

Lemma 5. *For any $c > 0$, we have:*

$$P\left(\|G_h - \widehat{G}_h\| \geq c\right) \leq 1 - O\left(N_0 \exp\left(-N_0 \Omega\left(\min\left(\frac{c}{\|h'\|_\infty}, \frac{c^2}{\|h'\|_\infty^2}\right)\right)\right)\right)$$

Proof. The desired operator norm can be bounded using entries magnitude as follows:

$$\begin{aligned} P\left(\|G_h - \widehat{G}_h\| \geq c\right) &\leq P\left(\|G_h - \widehat{G}_h\|_2^2 \geq c^2\right) \\ &\leq \max_{ij} P\left(|G_h(i, j) - \widehat{G}_h(i, j)| \geq c/k\right) \end{aligned} \quad (4)$$

In order to control the error on entry ij , we write:

$$\begin{aligned} G_h(i, j) - \widehat{G}_h(i, j) &= \frac{1}{N_i N_j} \sum_{x \in X_i, y \in X_j} h(\|x - y\|) - \int h(\|x - y\|) d\mu_i(x) d\mu_j(y) \\ &= \frac{1}{N_i} \sum_{x \in X_i} \frac{1}{N_j} \sum_{y \in X_j} \left(h(\|x - y\|) - \int h(\|x - y\|) d\mu_j(y) \right) \\ &\quad + \frac{1}{N_i} \sum_{x \in X_i} \left(\int h(\|x - y\|) d\mu_j(y) - \int h(\|x - y\|) d\mu_i(x) d\mu_j(y) \right) \end{aligned}$$

Since $\|h'\|_\infty$ is the Lipschitz constant of $\|h(x - \cdot)\|$, we see by concentration that for fixed x and for y distributed according to μ_j :

$$\|h(\|x - y\|) - \int h(\|x - y\|) d\mu_j(y)\|_{\psi_1} = O(\|h'\|_\infty)$$

where for a random variable U , $\|U\|_{\psi_1} = \sup_{p \geq 1} p^{-1} (E\|U\|^p)^{1/p}$ is its Orlicz ψ_1 norm. As a consequence, conditionally to N_j , this implies (Corollary 5.17 in [24]) that for any $\varepsilon > 0$:

$$P(|S_x| \geq \varepsilon) \leq 2 \exp \left(-N_j \Omega \left(\min \left(\frac{\varepsilon}{\|h'\|_\infty}, \frac{\varepsilon^2}{\|h'\|_\infty^2} \right) \right) \right)$$

with

$$S_x = \frac{1}{N_j} \sum_{y \in X_j} \left(h(\|x - y\|) - \int h(\|x - y\|) \right)$$

Hence by the union bound:

$$\begin{aligned} P \left(\left| \frac{1}{N_i} \sum_{x \in X_i} S_x \right| \geq \varepsilon \right) &\leq 2N_i \exp \left(-N_j \Omega \left(\min \left(\frac{\varepsilon}{\|h'\|_\infty}, \frac{\varepsilon^2}{\|h'\|_\infty^2} \right) \right) \right) \\ &\leq O \left(N_0 \exp \left(-N_0 \Omega \left(\min \left(\frac{\varepsilon}{\|h'\|_\infty}, \frac{\varepsilon^2}{\|h'\|_\infty^2} \right) \right) \right) \right) \end{aligned}$$

Similarly, as the Lipschitz constant of $\int h(\|\cdot - y\|) d\mu_j(y)$ is at most $\|h'\|_\infty$ as well, we get:

$$P(|U| \geq \varepsilon) \leq 2 \exp \left(-N_0 \Omega \left(\min \left(\frac{\varepsilon}{\|h'\|_\infty}, \frac{\varepsilon^2}{\|h'\|_\infty^2} \right) \right) \right)$$

with

$$U = \frac{1}{N_i} \sum_{x \in X_i} \left(\int h(\|x - y\|) d\mu_j(y) - \int h(\|x - y\|) d\mu_i(x) d\mu_j(y) \right)$$

The last two inequalities together with (4) imply the desired claim. \square

Let now \widehat{M}_h be the matrix obtained from \widehat{G}_h by multiplying the ij entry by $\sqrt{w_i w_j}$. Applying the above lemma with $c = c_h$, its smallest eigenvalue can be lower bounded as follows:

$$\lambda_1(\widehat{M}_h) = \Omega(\lambda_1(\widehat{G}_h)) = \Omega(\lambda_1(G_h) - c_h) = \Omega(Kc_h)$$

with arbitrarily high probability, assuming $N_0 \gg \|h'\|_\infty^2 / c_h^2$ and $K \geq 2$.

Now, note that \widehat{M}_h is the matrix of the quadratic form $\Phi_h(X)$ restricted to E . More precisely, the indicator functions of the clusters, normalized to have unit L_2 -norm, form an orthonormal basis of E , and writing that quadratic form in this basis gives \widehat{M}_h . Let λ be the smallest eigenvalue of \widehat{M}_h . By the variational characterization of eigenvalues, there exist at least k eigenvalues of $\Phi_h(X)$ that are at least λ . Let H denote the space spanned by the k -top eigenvectors of $\Phi_h(X)$, and let L denote the space spanned by the remaining $N - k$. We show using a perturbation argument that the maximum of the principal angles between space E and space H is small.

Let $x \in E^\perp$ be a unit vector. We may write $x = \alpha x_L + \beta x_H$ with $\alpha^2 + \beta^2 = 1$, and x_L and x_H are unit vectors belonging respectively to L and H . Then:

$$x^t \Phi_h(X) x = \alpha^2 x_L^t \Phi_h(X) x_L + \beta^2 x_H^t \Phi_h(X) x_H$$

Since $x \in E^\perp$, we have $x^t A x = 0$, where A is the matrix defined in Theorem 1. Hence by Theorem 1, with arbitrarily high probability:

$$x^t \Phi_h(X) x \leq O(c_h)$$

provided

$$N_0 \geq N_1 = O\left(\frac{n \|h\|_\infty^2}{c_h^2} \log\left(\frac{n \|h\|_\infty^2}{c_h^2}\right)\right)$$

Also, by assumption:

$$x_H^t \Phi_h(X) x_H \geq \lambda \geq K \Omega(c_h)$$

As a consequence:

$$d(x, L) = \beta \leq O(1/\sqrt{K})$$

That is, the maximum angle between the $(N - k)$ -flats E^\perp and L is $O(1/\sqrt{K})$. Hence, so is the maximum angle between their orthogonals E and H , which is the desired claim.

5.3 Proof of Corollary 2

Let $E^\perp \in \mathbb{R}^N$ be the space of vectors whose mean is zero on each block. This space has codimension k . Now, for any vector $x \in E^\perp$, we see that $x^t A x = 0$, where A is the matrix from Theorem 1. As a result, the quadratic form $\Phi_h(X)$ is at most $O\left(c_h + \|h\|_\infty \sqrt{\frac{n \log N_0}{N_0}}\right) I$ on E^\perp with arbitrarily high probability, implying that $\Phi_h(X)$ has at least $(N - k)$ eigenvalues that are at most $O\left(c_h + \|h\|_\infty \sqrt{\frac{n \log N_0}{N_0}}\right)$. Applying the same argument to $-\Phi_h(X)$, the result follows.

5.4 Proof of Corollary 3

Matrix G_h has entries

$$G_h(i, j) = \mathbb{E}h(\|x_i - x_j\|)$$

where x_i are independent random variables with law $\mathcal{N}(\mu_i, \Sigma_i)$, where μ_i and Σ_i are the means and covariances of the two Gaussians in the mixture.

Lemma 6. *If u is a centered Gaussian random variable with covariance Σ , then:*

$$\mathbb{E}(h(\|u\|)) = \det\left(I + \frac{1}{\tau^2} \Sigma\right)^{-\frac{1}{2}}$$

Proof.

$$\begin{aligned}
\mathbb{E}(h(\|u\|)) &= \int \frac{1}{\sqrt{(2\pi)^n \det(\Sigma)}} \exp\left(-\frac{1}{2}x^t \left(\Sigma^{-1} + \frac{1}{\tau^2}I\right)x\right) dx \\
&= \frac{\det\left(\left(\Sigma^{-1} + \frac{1}{\tau^2}I\right)^{-1}\right)^{1/2}}{\det(\Sigma)^{1/2}} \\
&= \det\left(I + \frac{1}{\tau^2}\Sigma\right)^{-\frac{1}{2}}
\end{aligned}$$

□

By standard algebraic manipulations, shifting the center amounts to scaling the expectation by a certain factor:

Lemma 7. *If u is a Gaussian random variable with covariance Σ and mean μ , then:*

$$\mathbb{E}(h(\|u\|)) = \exp\left(-\frac{1}{\tau^2}\mu^t(I - (I + \tau^2\Sigma^{-1})^{-1})\mu\right) \det\left(I + \frac{1}{\tau^2}\Sigma\right)^{-\frac{1}{2}}$$

In particular, letting B_h be the 2×2 matrix with entries

$$B_h(i, j) = \mathbb{E}h(\|y_i - y_j\|)$$

where y_i are independent random variables with law $\mathcal{N}(0, \Sigma_i)$, we see that G_h is obtained from B_h by scaling the off diagonal entries by a factor λ that satisfies

$$\begin{aligned}
\lambda &\leq \exp\left(-\frac{1 - (1 + \Omega(\tau^2))^{-1}}{\tau^2} \|\mu_1 - \mu_2\|^2\right) \\
&\geq 1 - \Theta\left(\frac{\|\mu_1 - \mu_2\|^2}{n}\right)
\end{aligned}$$

Because $\det B_h$ is non negative and the entries of B_h are $\Theta(1)$, we deduce that

$$\begin{aligned}
\det G_h &= \det B_h + (B_h)_{12}^2 - \lambda^2 (B_h)_{12}^2 \\
&\geq (1 - \lambda^2)(B_h)_{12}^2 \\
&\geq \Theta\left(\frac{\|\mu_1 - \mu_2\|^2}{n}\right)
\end{aligned}$$

Now, the largest entries of G_h are the same as for B_h , that is, $\Theta(1)$, which implies that the maximal eigenvalue of G_h is $\Theta(1)$ as well. From this we see that:

$$\lambda_1(G_h) = \Theta\left(\frac{\|\mu_1 - \mu_2\|^2}{n}\right)$$

To conclude, it suffices to check that for our choice of kernel and assumptions on the variance of the Gaussians, $c_h = \Theta(1/n)$.

5.5 Proof of Theorem 2

We first show that constant functions are sent to nearly constant functions by the convolution operator with kernel h from $L^2(\mathbb{R}^n, \mu_i)$ to $L^2(\mathbb{R}^n, \mu_j)$.

Lemma 8. *Let $f_i(x) = \int h(\|y - x\|)d\mu_i(y)$. If μ_i and μ_j are supported on the sphere S , even, and satisfy a Poincaré inequality, then:*

$$\text{Var}_{\mu_j} f_i = O\left(nc\frac{t^2}{h}\right)$$

Proof. The gradient of f_i is as follows:

$$\nabla f_i(x) = \int (x - y)\tilde{h}(\|x - y\|)d\mu_i(y)$$

For $x \in S$, the gradient of the restriction of f_i to S is

$$\nabla f_{i|S}(x) = P_{T_x S} \nabla f_i(x) = -P_{T_x S} \left(\int y\tilde{h}(\|x - y\|)d\mu_i(y) \right) \quad (5)$$

Denote by $M : L^2(\mathbb{R}^n, \mu_i) \rightarrow L^2(\mathbb{R}^n, \mu_j)$ the operator defined by

$$Mg(x) = \int g(y)\tilde{h}(\|x - y\|)d\mu_i(y)$$

From the structure of blocks described in Theorem 1, and letting the sample size go to infinity, we get that $\|M - M'\| = O(c'_h)$, where

$$M'g(x) = \int g(y)M'_{xy}d\mu_i(y)$$

and

$$M'_{xy} = \int \tilde{h}(\|y - z'\|)d\mu_i(z') + \int \tilde{h}(\|x - z\|)d\mu_j(z) - \int \tilde{h}(\|z - z'\|)d\mu_i(z)d\mu_j(z')$$

Calling y the coordinate vector of S , that is, the identity map of S , the above equation expresses $M'y$ as the sum of two terms T_1 and T_2 . The first one is

$$T_1 = \int y \left(\int \tilde{h}(\|y - z'\|)d\mu_i(z') \right) d\mu_i(y)$$

we see that as μ_i is even, $\int \tilde{h}(\|y - z'\|)d\mu_i(z')$ is an even function of y . Hence multiplying it by y gives an odd function whose integral against μ_j must be zero as μ_j is even as well. Hence T_1 vanishes. The second term T_2 is

$$T_2 = \left(\int y d\mu_i(y) \right) \left(\int \tilde{h}(\|x - z\|)d\mu_j(z) - \int \tilde{h}(\|z - z'\|)d\mu_i(z)d\mu_j(z') \right)$$

As μ_i is even, it has zero mean so T_2 cancels. From (5), the above discussion gives:

$$\begin{aligned}\|\nabla f_{i|S}\|^2 &\leq \|My\|^2 \\ &\leq \|(M - M')y\|^2 \\ &\leq O\left(c_h'^2 \|y\|^2\right) \\ &\leq O\left(nc_h'^2\right)\end{aligned}$$

The desired claim follows using Poincaré inequality. \square

Lemma 9. *Taking $h = h_t$, we have:*

$$\text{Var}_{\mu_j} f_i \leq O(t^2/n)$$

assuming μ_i and μ_j are supported on S , have $O(1)$ means and $O(1)$ -concentration.

Proof. For any x, y in S we can write:

$$h_t(\|x - y\|) = \text{Re} \exp\left(\frac{it}{\sqrt{n}} \langle x, y \rangle\right)$$

Hence we can express f_i using a Fourier transform:

$$f_i(x) = \text{Re} \left(\exp(2nit) \widehat{\mu}_i(-tx/\sqrt{n}) \right)$$

As a consequence, for any unit vector u :

$$\begin{aligned}|\langle \nabla f_i(x), u \rangle| &\leq \frac{t}{\sqrt{n}} |\langle \nabla \widehat{\mu}_i(-tx/\sqrt{n}), u \rangle| \\ &\leq \frac{t}{\sqrt{n}} |\widehat{\mu}_i^u(-tx/\sqrt{n})| \\ &\leq \frac{t}{\sqrt{n}} O(\|\mu_i^u\|_1) \\ &\leq O(t/\sqrt{n})\end{aligned}$$

where μ_i^u is μ_i multiplied by function $x \mapsto \langle x, u \rangle$, the last line using the fact that μ_i has $O(1)$ -concentration and $O(1)$ mean. Hence f_i is $O(t/\sqrt{n})$ -Lipschitz. The lemma follows since μ_j has $O(1)$ -concentration. \square

To prove the first part of Theorem 2, using Theorem 1, it is sufficient to show that with arbitrarily high probability $\|A - B\| = O(\sqrt{nc_h'})$, A being the matrix given by Theorem 1. By definition of A , we see that the entries of $A - B$ in the ij block are given by

$$\begin{aligned}(A - B)_{xy} &= \frac{1}{N} \left(\int h(\|x - z\|) d\mu_j(z) - \int h(\|x - z\|) d\mu_j(z) d\mu_i(x) \right) \\ &\quad + \frac{1}{N} \left(\int h(\|y - z'\|) d\mu_i(z') - \int h(\|y - z'\|) d\mu_i(z') d\mu_j(y) \right) \\ &= \frac{1}{N} \left(\left(f_j(x) - \int f_j(x) d\mu_i(x) \right) + \left(f_i(y) - \int f_i(y) d\mu_j(y) \right) \right)\end{aligned}$$

Hence by Lemma 8, the entries of $A-B$ have, conditionally to N , variance $O(nc_h^{\prime 2}/N^2)$. In particular, $A-B$ has expected squared Frobenius norm at most $O(nc_h^{\prime 2})$. Bounding the operator norm by the Frobenius norm and applying Markov inequality proves the desired bound on $\|A-B\|$ and concludes the proof of the first part of the theorem. For the second part of Theorem 2, the argument is the same except one uses the bound given in Lemma 9 instead of Lemma 8. Expliciting the constant $c'_{h_t} = O(t \log^3 n / \sqrt{n})$ then gives the desired bound.

5.6 Proof of Theorem 3

Since the desired conclusions are unchanged by scaling the components by a constant factor, and as we assume their variance is $\Theta(n)$, we can assume that their variance is n . Let $\tilde{\mu}_i$ be the pushforwards of μ_i by the closest point projection on S . The following lemma is easily proved:

Lemma 10. *Measure $\tilde{\mu}_i$ has $O(1)$ -concentration and mean $O(1)$.*

Proof. Let $f : S \rightarrow \mathbb{R}$ be a 1-Lipschitz function. To prove that $\tilde{\mu}_i$ has $O(1)$ -concentration, we prove that for X distributed according to $\tilde{\mu}_i$, there exists a number c such that $\|f(X) - c\|_{\psi_1} = O(1)$. The range of f on S is contained in an interval of length $2\sqrt{n}$. By shifting f if necessary, we can assume that $\|f\|_\infty = O(\sqrt{n})$. We also assume f is smooth, which is sufficient. Define

$$\begin{aligned} g : \mathbb{R}^n &\rightarrow \mathbb{R} \\ x &\mapsto f\left(\frac{x}{\|x\|}\right) \text{ if } \|x\| \geq \sqrt{n}/2 \\ x &\mapsto \frac{2\|x\|}{\sqrt{n}} f\left(\frac{x}{\|x\|}\right) \text{ else} \end{aligned}$$

We have:

$$\begin{aligned} \nabla g(x) &= \frac{\sqrt{n}}{\|x\|} \nabla f\left(\frac{x}{\|x\|}\right) \text{ if } \|x\| \geq \sqrt{n}/2 \\ &= \frac{2}{\sqrt{n}} \left(\frac{x}{\|x\|} f\left(\frac{x}{\|x\|}\right) + \sqrt{n} \nabla f\left(\frac{x}{\|x\|}\right) \right) \text{ else} \end{aligned}$$

As a consequence function g is $O(1)$ -Lipschitz, hence by concentration, for Y distributed according to μ_i , there exists a number c such that by $\|g(Y) - c\|_{\psi_1} = O(1)$. Letting now $\bar{f} : x \mapsto f(x/\|x\|)$, we have that $P(g(Y) \neq \bar{f}(Y)) \leq \exp(-\Theta(1)\sqrt{n})$ since g and \bar{f} only differ on $B(0, \sqrt{n}/2)$, which has exponentially small measure by concentration. Also clearly $\|g(Y) - \bar{f}(Y)\|_\infty \leq O(\sqrt{n})$. As a consequence, the ψ_1 norm of $g(Y) - \bar{f}(Y)$ is at most $O(\sqrt{n})$ times the ψ_1 norm of a Bernoulli variable with expectation $\exp(-\Theta(1)\sqrt{n})$. Since the ψ_1 norm of such variables is $O(1/\sqrt{n})$, $\|g(Y) - \bar{f}(Y)\|_{\psi_1} = O(1)$, from which we get $\|\bar{f}(Y) - c\|_{\psi_1} = O(1)$. This is what we wanted to prove, as $\bar{f}(Y)$ and $f(X)$ have the same distribution.

To relate the means of μ_i and $\tilde{\mu}_i$, we notice that by concentration of the distance to the origin, the 1-transportation distance between both measures is $O(1)$. In particular the means of μ_i and $\tilde{\mu}_i$ differ by $O(1)$, hence the mean of $\tilde{\mu}_i$ is $O(1)$. \square

The above lemma shows that we can apply Theorem 2 to the projected point cloud \tilde{X} : With arbitrarily high probability, matrix $\Phi_{h_t}(\tilde{X})$ is $\delta = O(t \log^3 n / \sqrt{n})$ close to B in the operator norm, assuming N_0 is $\Omega(\log(n/t)n^2/t^2)$.

We would now like to argue that B retains enough information about the components so that we can separate them. To do so, we restrict B to the subspace $E_{u,v}$ of piecewise constant vectors supported on the two components \tilde{X}_u and \tilde{X}_v , for some indices u and v . In the orthonormal basis formed by the normalized indicator vectors of the two components, the ij entry ($i, j \in \{u, v\}$) matrix of this restriction is $(\bar{w}_i \bar{w}_j)^{-1/2} \tilde{G}_{h_t}(i, j)$, \tilde{G}_{h_t} being the 2×2 matrix associated with $\tilde{\mu}_u$ and $\tilde{\mu}_v$, and \bar{w}_i being the fraction of data points in the i^{th} component. As the \bar{w}_i 's are $\Theta(1)$, the singular values of B restricted to $V_{u,v}$ are within a constant factor of those of \tilde{G}_{h_t} .

Now, using the power series expansion of h_t , one can show the following lower bound on the smallest singular value of the 2×2 matrix G_{h_t} associated with μ_u and μ_v , based on the difference between their covariance matrices:

Lemma 11. *There exists $C_1 = \Theta(1)$ such that if $t \leq C_1 \|\Sigma_u - \Sigma_v\|_2 / \sqrt{n}$, the smallest singular value of G_{h_t} is at least $\Omega(t^2 \|\Sigma_u - \Sigma_v\|_2^2 / n)$. Furthermore:*

$$\|\tilde{G}_{h_t} - G_{h_t}\| = O(t/\sqrt{n})$$

Proof. By Taylor's theorem, for $i, j \in \{u, v\}$, we have:

$$\begin{aligned} G_{h_t}(i, j) &= \int \cos\left(\frac{t}{\sqrt{n}} \langle x, y \rangle\right) d\mu_i(x) d\mu_j(y) \\ &= \sum_{l=0}^{\infty} \int (-1)^l \frac{(t/\sqrt{n})^{2l}}{(2l)!} \langle x, y \rangle^{2l} d\mu_i(x) d\mu_j(y) \end{aligned}$$

Let x and y be two independent random vectors distributed respectively according to μ_i and μ_j . Conditioned to $x = x_0 \in \mathbb{R}^n$, $\langle x, y \rangle$ has $O(\|x_0\|)$ -concentration and mean $O(\|x_0\|)$, so its ψ_1 norm is $O(\|x_0\|)$. Hence

$$\|\langle x, y \rangle\|_{\psi_1} \leq O(\mathbb{E}\|x\|) \leq O(\sqrt{n})$$

As a consequence the distribution of $|\langle x, y \rangle|/\sqrt{n}$ decays exponentially. Hence its l^{th} moment is controlled by the l^{th} moment of an exponential distribution with mean $\Theta(1)$, that is, $\Theta(1)^{l!}$. This implies

$$\begin{aligned} |G_{h_t}(i, j) - 1 + \int \frac{t^2}{2n} \langle x, y \rangle^2 d\mu_i(x) d\mu_j(y)| &\leq \sum_{l=2}^{\infty} \frac{t^{2l}}{(2l)!} \Theta(1)^{2l} (2l)! \\ &\leq O(t^4) \end{aligned}$$

for t less than some numerical constant. Now

$$\begin{aligned} \int \langle x, y \rangle^2 d\mu_i(x)d\mu_j(y) &= \int y^t \Sigma_i y d\mu_j(y) \\ &= \int \text{trace } \Sigma_i y y^t d\mu_j(y) \\ &= \text{trace } \Sigma_i \Sigma_j \end{aligned}$$

We may thus expand the determinant of G_{h_t} as follows:

$$\begin{aligned} \det G_{h_t} &= G_{h_t}(u, u)G_{h_t}(v, v) - G_{h_t}(u, v)^2 \\ &= \left(1 - \frac{t^2}{2n} \langle \Sigma_u, \Sigma_u \rangle + O(t^4)\right) \left(1 - \frac{t^2}{2n} \langle \Sigma_v, \Sigma_v \rangle + O(t^4)\right) \\ &\quad - \left(1 - \frac{t^2}{2n} \langle \Sigma_u, \Sigma_v \rangle + O(t^4)\right)^2 \\ &= -\frac{t^2}{2n} \|\Sigma_u - \Sigma_v\|_2^2 + O(t^4) \end{aligned}$$

Hence by assumption, for well chosen C_1 , the first term in the expansion above dominates, so $|\det G_{h_t}|$ satisfies the desired lower bound. Since the entries of G_{h_t} have absolute value less than 1, the lower bound also holds for the smallest singular value of G_{h_t} .

To relate matrices G_{h_t} and \tilde{G}_{h_t} , we let δx (resp. δy) be the difference between x (resp. y) and its projection on S , so that $x - \delta x$ (resp. $y - \delta y$) is distributed according to $\tilde{\mu}_i$ (resp. $\tilde{\mu}_j$). We can write

$$\tilde{G}_{h_t}(i, j) = \int \cos\left(\frac{t}{\sqrt{n}} \langle x - \delta x, y - \delta y \rangle\right) d\mu_i(x)d\mu_j(y)$$

Also

$$\langle x - \delta x, y - \delta y \rangle = \langle x, y \rangle - \langle \delta x, y \rangle - \langle \delta y, x \rangle + \langle \delta x, \delta y \rangle$$

By concentration and since μ_j has $O(1)$ mean, $|\langle \delta x, y \rangle|$ has expectation $O(\|\delta x\|)$ conditioned to δx . Since $\mathbb{E}\|\delta x\| = O(1)$ by concentration of the distance to the origin, we have $\mathbb{E}|\langle \delta x, y \rangle| = O(1)$. The last two terms above can be dealt with similarly, yielding that the distributions of $\langle x - \delta x, y - \delta y \rangle$ and of $\langle x, y \rangle$ are at 1-transportation distance $O(1)$. Since $\cos(t/\sqrt{n})$ is $O(t/\sqrt{n})$ -Lipschitz, we see that

$$|\tilde{G}_{h_t}(i, j) - G_{h_t}(i, j)| = O(t/\sqrt{n})$$

which concludes the proof. \square

In particular, choosing $t = C_1 \min_{u \neq v} \|\Sigma_u - \Sigma_v\|_2 / \sqrt{n} = C_1 \Delta$, we see that for any $u \neq v$, the smallest singular value of B restricted to $E_{u,v}$ is at least $\Omega(\Delta^4 - O(\Delta/\sqrt{n}))$, which by assumption on Δ is also $\Omega(\Delta^4)$.

Lemma 12. *For sufficiently small $C_2 = \Theta(1)$, the columns of $f_{C_2\Delta^4}(B)$ with indices i and j are equal if i and j belong to the same component. If i and j belong to different components, their distance is $\Omega(\Delta^4/\sqrt{N})$.*

Proof. Eigenvectors of B with non zero eigenvalue are piecewise constant, so the first part is clear. Assume indices i and j respectively belong to distinct components u and v . The distance between their columns is $\|f_{C_2\Delta^4}(B)e_{uv}\|$, where e_{uv} has entries $1/\#X_u$ (resp. $-1/\#X_v$) at indices corresponding to component u (resp. v), and 0 else.

Vector e_{uv} is in E_{uv} and has norm $\Theta(1/\sqrt{N})$. From the singular value lower bound, there must exist a unit vector x such that $|\langle e_{uv}, Bx \rangle| = \Omega(\Delta^4/\sqrt{N})$. Denote by $E_{2C_2\Delta^4}$ the vector space generated by the singular vectors of B with singular values at least $2C_2\Delta^4$, and write $x = \alpha y + \beta z$, where y and z are unit vectors respectively lying in $E_{2C_2\Delta^4}$ and in $E_{2C_2\Delta^4}^\perp$, and $\alpha^2 + \beta^2 = 1$. We have

$$\begin{aligned} |\langle e_{uv}, Bx \rangle| &= |\alpha \langle e_{uv}, By \rangle + \beta \langle e_{uv}, Bz \rangle| \\ &= O(|\langle e_{uv}, By \rangle|) + O(C_2\Delta^4/\sqrt{N}) \\ &\leq \max(C_3|\langle e_{uv}, By \rangle|, C_4C_2\Delta^4/\sqrt{N}) \end{aligned}$$

for some constant C_3 and C_4 . For small enough $C_2 = \Theta(1)$, we will have $C_4C_2\Delta^4/\sqrt{N} < |\langle e_{uv}, Bx \rangle|$, implying

$$|\langle e_{uv}, By \rangle| \geq |\langle e_{uv}, Bx \rangle|/C_3 = \Omega(\Delta^4/\sqrt{N})$$

Now because $y \in E_{2C_2\Delta^4}$, as $f_{C_2\Delta^4}$ modifies eigenvalues by a factor at most 2 in that range, there exists a matrix F with the same eigenvectors as B , and with singular values between $1/2$ and 2 , such that $FBy = f_{C_2\Delta^4}(B)y$. Hence

$$\begin{aligned} |\langle f_{C_2\Delta^4}(B)F^{-1}e_{uv}, y \rangle| &= |\langle F^{-1}e_{uv}, f_{C_2\Delta^4}(B)y \rangle| = |\langle F^{-1}e_{uv}, FBy \rangle| \\ &= |\langle e_{uv}, By \rangle| = \Omega(\Delta^4/\sqrt{N}) \end{aligned}$$

In particular $f_{C_2\Delta^4}(B)F^{-1}e_{uv}$ has norm at least $\Omega(\Delta^4/\sqrt{N})$. But that vector equals $F^{-1}f_{C_2\Delta^4}(B)e_{uv}$, and as F^{-1} doesn't change distances by more than a factor of 2, we see that $\|f_{C_2\Delta^4}(B)e_{uv}\| = \Omega(\Delta^4/\sqrt{N})$, as claimed. \square

Now, as $f_{C_2\Delta^4}$ is 1-Lipschitz, the perturbation inequality proved in [7] states that

$$\begin{aligned} \|f_{C_2\Delta^4}(B) - f_{C_2\Delta^4}(\Phi_{h_t}(\tilde{X}))\| &\leq O\left(\log \frac{\|B\| + \|\Phi_{h_t}(\tilde{X})\|}{\|\Phi_{h_t}(\tilde{X}) - B\|} + 2\right)^2 \|\Phi_{h_t}(\tilde{X}) - B\| \\ &\leq O(\delta \log^2 \delta) \end{aligned}$$

Our assumption on Δ is chosen so that $\Delta^4/(\delta \log^2 \delta) = \Omega(K^3)$. Hence we may assume that $\|\Phi_{h_t}(\tilde{X}) - B\| < C_2\Delta^4$. By Weyl's theorem on eigenvalue perturbations, $f_{C_2\Delta^4}(\Phi_{h_t}(\tilde{X}))$ thus has at most $k = \Theta(1)$ non zero eigenvalues. As a result

$$\|f_{C_2\Delta^4}(B) - f_{C_2\Delta^4}(\Phi_{h_t}(\tilde{X}))\|_2^2 \leq O(\delta^2 \log^4 \delta) = O(\Delta^8/K^6)$$

This means that within each component, the expected square distance between a random column of $f_{C_2\Delta^4}(\Phi_{h_t}(\tilde{X}))$ and the column of $f_{C_2\Delta^4}(B)$ associated with that component is at most $O(\Delta^8/(NK^6))$. By Lemma 12, this implies that after mapping data points to columns of $f_{C_2\Delta^4}(\Phi_{h_t}(\tilde{X}))$, the ratio between the maximum variance of the components and the minimum squared distance between their centers in an optimal solution to the k -means problem is $O(K^{-6})$. Applying any constant factor approximation algorithm for the k -means problem will thus cluster the data with the claimed error rate.

Acknowledgements

The authors would like to thank Jean-Daniel Boissonnat for his help throughout the elaboration of this paper. This work is partially supported by the Advanced Grant of the European Research Council GUDHI (Geometric Understanding in Higher Dimensions).

References

- [1] Dimitris Achlioptas and Frank McSherry. On spectral learning of mixtures of distributions. In *Learning Theory: 18th Annual Conference on Learning Theory, COLT 2005, Bertinoro, Italy, June 27-30, 2005. Proceedings*, pages 458–469. Springer, 2005.
- [2] S. Arora and R. Kannan. Learning mixtures of separated non-spherical Gaussians. *The Annals of Applied Probability*, 162(3-4):707–738, 2015.
- [3] M. Belkin and K. Sinha. Polynomial learning of distribution families. *SIAM J. Comput.*, 44(4):889–911, 2015.
- [4] S. Charles Brubaker and Santosh S. Vempala. *Isotropic PCA and Affine-Invariant Clustering*, pages 241–281. Springer Berlin Heidelberg, 2008.
- [5] S. Dasgupta. Learning mixtures of Gaussians. In *Proceedings of the 40th Annual IEEE Symposium on Foundations of Computer Science, FOCS 99*, pages 634–644, 1999.
- [6] S. Dasgupta and L. Schulman. A Probabilistic Analysis of EM for Mixtures of Separated Spherical Gaussians. *JMLR*, 8:203–26, 2007.
- [7] Yu. B. Farfarovskaia. An estimate of the norm $\|f(A) - f(B)\|$ for selfadjoint operators A and B (in Russian). *Zap. Nauchn. Sem. LOMI*, (56):143–162, 1976.
- [8] N. Fournier and A. Guillin. On the rate of convergence in Wasserstein distance of the empirical measure. *Probability Theory and Related Fields*, 15(1A):69–92, 2005.
- [9] Rong Ge, Qingqing Huang, and Sham M. Kakade. Learning mixtures of gaussians in high dimensions. In *Proceedings of the Forty-seventh Annual ACM*

Symposium on Theory of Computing, STOC '15, pages 761–770, New York, NY, USA, 2015. ACM.

- [10] M. Gromov. *Metric structures for Riemannian and non-Riemannian spaces*. Birkhäuser Verlag Basel, 1999.
- [11] M. Hein and O. Bousquet. Hilbertian metrics and positive definite kernels on probability measures. In *Proceedings of AISTATS 2005*, pages 136–143, 2005.
- [12] R. Kannan, L. Lovász, and M. Simonovits. Isoperimetric problems for convex bodies and a localization lemma. *Discrete Comput. Geom.*, 3-4(13):541–559, 1995.
- [13] R. Kannan, S. Vempala, and H. Salmasian. The spectral method for general mixture models. *SIAM J. Computing*, 38(3):1141–1156, 2008.
- [14] N. El Karoui. The spectrum of random kernel matrices. *The Annals of Statistics*, 38(1):1–50, 2010.
- [15] M.D. Kirzbraun. Über die zusammenziehende und Lipschitzsche transformationen. *Fundamenta Math.*, 22:77–108, 1934.
- [16] M. Ledoux. *The Concentration of Measure Phenomenon*. AMS Mathematical Surveys & Monographs, Providence, 2001.
- [17] P. Lévy and F. Pellegrino. *Problèmes concrets d'analyse fonctionnelle*. Collection de monographies sur la théorie des fonctions. Gauthier-Villars Paris, 1951.
- [18] V. Milman. A certain property of functions defined on infinite-dimensional manifolds. *Dokl. Akad. Nauk SSSR 200*, pages 781–784, 1971.
- [19] M. Ledoux S. Bobkov. Poincaré's inequality and Talagrand's concentration phenomenon for the exponential distribution. *Probab. Theory Relat. Fields*, (107):383–400, 1997.
- [20] Tao Shi, Mikhail Belkin, and Bin Yu. Data spectroscopy: Eigenspaces of convolution operators and clustering. *The Annals of Statistics*, 37, 6B:3960–3984, 2009.
- [21] C. Suquet. Distances euclidiennes sur les mesures signées et application à des théorèmes de Berry-Esseen. *Bull. Belg. Math. Soc. Simon Stevin*, 2(2):161–181, 1995.
- [22] Joel A. Tropp. Norms of random submatrices and sparse approximation. *Comptes Rendus Mathematiques*, 346(23):1271 – 1274, 2008.
- [23] S. Vempala and G. Wang. A spectral algorithm for learning mixture models. *Journal of Computer and System Sciences Special issue on FOCS 2002 archive*, 68(4):841–860, June 2004.
- [24] R. Vershynin. Introduction to the non-asymptotic analysis of random matrices. In Yonina C. Eldar and Gitta Kutyniok, editors, *Compressed Sensing: Theory and Applications*, pages 210–268. Cambridge University Press, 2012.