A Fourier analytic approach to Gaussian mixture learning

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Abstract Suppose that we are given independent, identically distributed random samples x_1, \dots, x_n from a mixture at most k many d-dimensional spherical Gaussian distributions μ_1, \cdots, μ_{k_0} of identical and known variance σ^2 in each coordinate, such that the minimum ℓ^2 distance between two distinct centers y_l and y_j is greater than $2\Delta\sigma \min\{\sqrt{d}, \sqrt{k}\}\$, where $\Delta > C_0$, and C_0 is a sufficiently large universal constant. We develop a randomized algorithm that learns the centers y_l 's of the Gaussian components to within an ℓ^2 distance of $k^{-\tilde{C}_0}$ — in presence of arbitrarily large number of components and in arbitrary dimension, when the weights are known to be uniform. Furthermore, if the number of components is $k = \Omega(2^d)$, then for arbitrary universal constant c > 0, even for unknown weights, the algorithm learns the centers to within an ℓ^2 distance of $d^{-\tilde{C}_0}$ and the weights up to an accuracy of cw_{min} , with probability greater than $1 - \exp(-k/c)$, provided that the weights lie in [c/k, 1/ck], and the minimum separation is just $2c\sqrt{d}$. The number of samples and the computational time is bounded above by poly(k, d) in either case. Such a bound on the sample and computational complexity was previously unknown in the regime of non-constant dimension, and in particular, when d is not O(1), When d = O(1), this complexity bound follows from [15], where it has also been shown that the sample complexity of learning a random mixture of Gaussians in a ball of radius $o(\sqrt{d})$ in d dimensions, when d is $\Theta(\log k)$, is at least super-polynomial in k, d, showing that our result is tight in this case.

Key words: mixtures of Gaussians, Lipschitz function, Hausdorff distance, sample complexity bound, approximate log-concave functions, PCA, Fourier transform, Johnson-Lindenstrauss lemma, (de)convolution, Hoeffding's inequality

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1 Introduction

Designing efficient algorithms that estimate the parameters of an underlying probability distribution is a central theme in statistical learning theory. An important special instance of this learning problem is the case when the underlying distribution is known to be a finite mixture of Gaussian distributions in d-dimensional Euclidean space. Such mixtures are popular models for high-dimensional data clustering, and learning mixture of Gaussians in an unsupervised setting has been a topic of intensive research for the last few decades.

In its most general form, the underlying problem is as follows: we have access to random samples drawn independently from some Gaussian mixture $\mu := \omega_1 \mu_1 + \cdots + \omega_{k_0} \mu_{k_0}$, where $(\omega_1, \cdots, \omega_{k_0})$ is a probability vector with strictly positive components, and each μ_l is a Gaussian density in \mathbb{R}^d , with mean $y_l \in \mathbb{R}^d$ and covariance Σ_l . The algorithmic task is to estimate each component of the parameter set $\{(\omega_1, y_1, \Sigma_1), \cdots, (\omega_{k_0}, y_{k_0}, \Sigma_{k_0})\}$ of the density function μ , within a pre-specified accuracy $\epsilon > 0$, with success probability at least $1-\delta$ for a pre-specified $\delta > 0$. For the purposes of this paper, we will restrict ourselves to the case where all the Gaussian components are spherical, with identical variance in each coordinates.

Recently, [7] and [8] devised polynomial time learning algorithms that work with minimum separation of k^{ϵ} (for any $\epsilon > 0$), although, the sucess of these algorithms appear to be guaranteed only in some restricted region in the (d,k)-space (see table 1.1). In [15], Regev-Vijayaraghavan considered the question of obtaining a lower bound on the separation of centers necessary for the polynomial learnability of Gaussian mixtures. They devised an *iterative algorithm for amplifying the accuracy of parameter estimation* that, given initializer $y_1^0, \cdots, y_{k_0}^0$ and a desired accuracy parameter $\epsilon > 0$, uses polynomially many samples from the underlying mixture and computation steps to return y_1', \cdots, y_{k_0}' , that lie within Hausdorff distance (see definition 1) at most ϵ from the true centers; for more details, see Theorem 4.1 of [15]. One of their results establishes that, in constant dimension d = O(1), with minimum separation at least $\Omega(1)$, any uniform mixture of spherical Gaussians can be learned to desired accuracy δ (with high probability) in number of samples and computation time depending polynomially on the number of components and ϵ^{-1} .

In the present paper we answer the question of learning the centers of uniform mixture of spherical Gaussians, up to accuracy $k^{-\tilde{C}_0}$ for arbitrary large constant $\tilde{C}_0 > 0$ — where the minimum separation of the centers is $2\Delta\sigma\min\{\sqrt{d},\sqrt{k}\}$ — in number of samples and computational time that depends polynomially on the ambient dimension d, and the number of components k, provided that Δ is larger than a certain absolute constant C_0 . Moreover, when $d = O(\log k)$, our algorithm can recover the centers within accuracy $d^{-\tilde{C}_0}$, even if the minimum separation of the centers is $2c\sigma\sqrt{d}$ for any absolute constant $c \in (0,1)$. We note that our minimum separation requirement is independent of k, the number of components, and for $d = O(\log k)$, this is the weakest minimum separation required for polynomial learnability of the mixture: see theorem 3.1 of [15]. We employ deconvolution in the Fourier domain — a heavily-studied technique in the realm of statistical data analysis;

see, for example, [12], or the references therein. However, a carefully chosen cutoff has to be used in course of performing this deconvolution, because deconvolution by a Gaussian is an unstable operation which — when applied to functions that are not in the trajectory of a heat flow — does not give rise to functions. Here is the main theorem of this paper:

Main Theorem: Let \tilde{C}_0 , c > 0 be arbitrary absolute constants — with $c \in (0, 1)$, and let $\Delta > C_0$ for a sufficiently large absolute constant $C_0 > 0$. Given a mixture of at most k standard spherical Gaussians in \mathbb{R}^d — having identical known variance σ^2 in each direction — for which a) all the mixing weights are in $[ck^{-1}, (ck)^{-1}]$, and b) the minimum separation of the centers of the components satisfies

$$\min_{1 \le l \ne j \le k_0} ||y_l - y_j||_2 \ge 2\Delta\sigma \min\{\sqrt{d}, \sqrt{k}\}$$

There is an efficient randomized algorithm that accomplishes the following task:

- 1. if the weights are known to be uniform, then in arbitrary dimension d, the algorithm recovers (with high probability) the centers of the mixture, up to accuracy $k^{-\tilde{C}_0}$ in time (and samples) poly (k, d);
- 2. if the weights are unknown, but the number of components satisfies $k \geq 2^d$, then the algorithm recovers (with high probability) the centers and the weights up to accuracy $d^{-\tilde{C}_0}$ and cw_{min} , respectively, in time (and samples) poly (k, d), even if the minimum separation is $2c\sigma\sqrt{d}$.

Note that, by scale invariance nature of the problem, we may assume $\sigma = 1$ without loss of generality. We will denote the actual number of Gaussian components in the mixture by k_0 , so that $k_0 \le k$. It is evident that the results in this paper generalize the main upper bound in theorem 5.1 of [15] to the regime of dimension $k = \Omega(2^d)$ and arbitrary dimension (d), when the (identical) variance and uniform weights of the underlying mixture is known, as was also the underlying assumption in [15].

1.1 Earlier works on Gaussian mixture learning

Many of the earlier approaches to the problem of Gaussian mixture learning were based on local search heuristics, e.g. the EM algorithm and k-means heuristics, that resulted in weak performance guarantees. There is a very extensive body of work on this question, and it would take a large survey to cover all of it. We make a modest attempt at surveying some of the results in this area that are most in line with our results; for more elaborate history on some interesting lines of works, see (for example) [1], [9], and the references therein.

In [5], Dasgupta presented the first provably correct algorithm for learning a mixture of Gaussians, with a common unknown covariance matrix, using only polynomially many (in dimension as well as number of components) samples and

computation time, under the assumption that the minimum separation between the centers of component Gaussians is at least $\Omega(\text{poly}\log(kd)\sqrt{d})$. In a consequent work, [6] showed a variation of EM to work with minimum separation only poly $\log(kd)d^{\frac{1}{4}}$, when the components are all spherical. Subsequently, many more algorithms (see [14] and the references therein) with improved sample complexity and/or computational complexity have since been devised, that work on somewhat weaker separation assumption; in particular, the SVD-based algorithm of [16] learns a mixture of spherical Gaussians with poly-sized samples and polynomially many steps, under the separation assumption

$$\min_{1 \leq l \neq j \leq k} ||y_l - y_j||_2 \geq C \max\{\sigma_l, \sigma_j\} \left(\min(k, d)^{\frac{1}{4}} \log^{\frac{1}{4}} (dk/\epsilon) + \log^{\frac{1}{2}} (dk/\epsilon) \right)$$

Here $\epsilon > 0$ denotes the desired ℓ^2 -accuracy to which the centers are learned. We note that when $k = \Theta(2^{2^d})$ and $\epsilon = k^{-C_{200}}$ for some constant $C_{200} > 0$, the above separation requirement translates to minimum separation much larger than $d^{\frac{1}{2}}$ —this is due to the presence of $\log^{\frac{1}{2}}(dk/\epsilon)$, which dominates the rest in the regime $k = \Omega(2^{2^d})$; whereas, when $k = \Theta(2^d)$, the separation requirement is of order \sqrt{d} . On the other hand, consideration of Gaussian concentration phenomenon in higher dimension intuitively suggests that minimum separation of order \sqrt{d} should help in clustering the samples into respective components and therefore, should help in tackling the problem in arbitrary dimension.

In another line of work (see [10] and [14], for example) the question of polynomial learnability of arbitrarily separated mixture of Gaussians (and more general families of distributions have been investigated by [2]), it has been established that, for Gaussian mixture with a fixed number of components and the components having a known minimum statistical separation (*i.e.*, a minimum total variation distance of some constant $\eta > 0$), there is an algorithm that runs in polynomial time and uses polynomially many samples to learn the parameters of the mixture to any desired accuracy, with arbitrarily high probability.

The table below contains an explicit comparison of the guarantees derived (when the covariance matrices are all diagonal and identical) — and the assumptions under which they are proved to be true — in this paper to the ones in some of the most recent works that we are aware of.

Table 1.1 table

Comparisons	with	previous	works

References	separation, regime	complexity gurantees
[15]	$C\sqrt{d}, d = O(1)$	poly (k, d)
[16]	$C\log^{\frac{1}{2}}\left(dk/\epsilon ight)$, all d,k	poly (k, d, ϵ^{-1})
[7]	$C\sqrt{\log(k/\epsilon)}$, all d, k	$\operatorname{poly}\left(d,k,\frac{1}{\epsilon}\right)$
[8]		$\max\{(dk)^{\frac{1}{\epsilon^2}}, k^{O(1)}d^{O(\frac{1}{\epsilon})}\}$
This paper	$C_0 \min{\{\sqrt{d}, \sqrt{k}\}}$, all d, k	poly(k, d)
This paper	$c\sqrt{d}$, $c > 0$ arbitrary, $k = \Omega(2^d)$	poly(k, d)

1.2 Our contributions

Our main contributions can be summarized as follows:

- 1. We establish that, when the component Gaussians are spherical with identical known covariance the minimum separation needed to learn the centers in polynomial time, is of order min $\{\sqrt{d}, \sqrt{k}\}$.
 - a. In particular, when the number of component Gaussians in the mixture overwhelms the ambient dimension $(k = \Omega(2^d))$, the minimum separation needed to learn the centers, within inverse polynomial (in k) accuracy, is $O(\sqrt{d})$, which improves upon all the previously known separation requirements with respect to the constant overhead, as indicated in table 1.1.
 - b. Moreover, in the setting of $d = O(\log k)$, this is the best possible, as established by (theorem III.2 of) [15].
- 2. We have made a novel application of Fourier analysis to the problem of learning mixture of Gaussians; to the best of our knowledge, this has not been rigorously considered before. An earlier attempt on deconvolution via Fourier analysis appeared in [12], which addressed a related but different problem, based on different techniques. The success of our techniques relies on the truncation in Fourier domain (see section 4.1, especially eq. (1.3) and lemma 4), which is the crux of the methodological contributions in this paper.

1.3 Organization of the paper

In section 2, we give a brief overview of the key technical ideas in the paper. Next, section 3 contains preprocessing and reduction steps, whereby we reduce the problem to one where the centers of the mixtures are all contained in a ball of radius $\Omega(k\sqrt{d\ln(C_1dn)})$, in a $d=O(\log k)$ dimensional space, for some $n=\operatorname{poly}(d,k)$. Then, section 4 contains bulk of the technical results needed to carry out the Fourier deconvolution, which results in obtaining black-box oracle access to good additive approximation of the underlying atomic mixture. Next, section 5 contains weight estimation. The final section 7 briefly mentions a problem that still remains open (to the best of our knowledge).

2 Outline of techniques used

We observe that if two clusters of centers are very far (*i.e.*, the minimum distance of a center in one cluster is at least \sqrt{d} away from every center of the other cluster), then the samples are unambiguously of one cluster only. This is shown in lemma 1,

allowing us to reduce the question to the case when a certain proximity graph — defined on the centers — is connected. This lemma, along with theorem C.1 of [15], also allows us to reduce the problem to dimension $d \le k$.

In algorithm 2, we use the standard Johnson-Lindenstrauss lemma and project the data in the ambient space to at most $d = O(\log k)$ many carefully chosen subspaces of dimension at most $O(1 + \min(\log k, d))$, and show that if we can separate the Gaussians in these subspaces, the resulting centers can be used to obtain a good estimate of the centers in the original question. Thus the question is further reduced to one where the dimension $d = O(\log k)$.

Next, in lemma 2, we show that if the number of samples is chosen to be an appropriately large polynomial in k, then all the k_0 centers are with high probability contained in a union of balls B_i of radius $2\sqrt{d}$ centered around the n data points. This allows us to focus our attention to n balls of radius $2\sqrt{d}$.

The main idea is that in low dimensions, it is possible to efficiently implement a deconvolution on a mixture of identical standard Gaussians having variance 1 in each direction, and recover a good approximation to a mixture of Gaussians with the same centers and weights, but in which each component now has standard deviation $\bar{\Delta} < c\Delta$, where $2\Delta\sqrt{d}$ is the minimum separation between two centers. Once this density is available within small L^{∞} error, the local maxima can be approximately obtained using a robust randomized zeroth order concave optimization method developed in [3] started from all elements of a sufficiently rich ℓ^{∞} net on $\bigcup_j B_j$ (which has polynomial size by lemma 9), and the resulting centers are good approximations (i.e. within $k^{-\tilde{C}_0/2}$ of the true centers in Hausdorff distance) of the projections of true centers with high probability. We then feed these $d^{-\frac{5}{2}}$ approximate projected centers into the iterative procedure developed in [15] and by Theorem 4.1 in there, a seed of this quality, suffices to produce in poly (k,d,δ^{-1}) time, a set of centers whose projections are within $k^{-\tilde{C}_0}$ of the true projections, in Hausdorff distance.

The deconvolution is achieved by convolving the empirical measure μ_e obtained from independent random samples from the mixture, with the Fourier transform of a certain carefully chosen $\hat{\zeta}$. The function $\hat{\zeta}$ is, upto scalar multiplication, the reciprocal of a Gaussian with standard deviation $\sqrt{1-\bar{\Delta}^2}$ multiplied by the indicator of a ball of radius $(\sqrt{\log k}+\sqrt{d})\bar{\Delta}^{-1}$. It follows from lemma 4, that the effect of this truncation (*i.e.*, multiplication by the indicator) on the deconvolution process can be controlled. The pointwise evaluation of the convolution is done using the Monte Carlo method. The truncation plays an important role; without it, the reciprocal of a Gaussian would not have well-defined Fourier transform.

3 Preprocessing & Reduction

Suppose we are given independent, identically distributed samples x_1, \ldots, x_n from a mixture μ of no more than k of d-dimensional spherical Gaussian distributions μ_j with variance 1, such that the minimum ℓ^2 distance between two distinct centers y_l and y_j is greater than $\Delta \min\{\sqrt{d}, \sqrt{k}\}$ for some $\Delta \geq C_0$, where $C_0 > 0$ is a sufficiently large universal constant. We write

$$\mu(x) := (2\pi)^{-\frac{d}{2}} \sum_{l=1}^{k_0} w_l \exp\left(-\frac{1}{2}||x - y_l||^2\right),$$

where $k_0 \le k$, and (w_1, \dots, w_{k_0}) is an unknown probability vector such that $w_{min} := \min_{l \in [k_0]} w_l$ satisfies $w_{min} \ge \frac{c}{k}$, and also $Y := \{y_1, \dots, y_{k_0}\}$ is the set of centers of the component Gaussians in the mixture μ . Let us fix $1 - \eta := \frac{9}{10}$, to be the success probability we will require. This can be made $1 - \eta_0$ that is arbitrarily close to 1 by the following simple clustering technique in the metric space associated with Hausdorff distance, applied to the outputs of $100(\log \eta_0^{-1})$ runs of the algorithm.

Algorithm 1 Boost

find the median of all the number of centers output by the different runs of algorithm 2, and set that to be k_0

pick a set of centers Y (that is the output of one of the runs) having the property that $|Y|=k_0$ and at least half of the runs output a set of centers that is within a Hausdorff distance of less than $\frac{\Delta\sqrt{d}}{k^C}$ to Y. It is readily seen that — provided each run succeeds with probability $(1-\eta)$ — this clustering technique succeeds in producing an acceptable set of centers $\{\hat{y}_1, \cdots, \hat{y}_{k_0}\}$ with probability at least $1-\eta_0$

once the centers are fixed, to determine the weights, we take the median of the weights assigned to the nearest center over all $100(\log \eta_0^{-1})$ runs of the algorithm, where — in determining the nearest center — ties are broken arbitrarily

return $\{\hat{y}_1, \cdots, \hat{y}_k\}$.

We record the observation that, if d > k, then by Principal Component Analysis (PCA), it is possible to find a linear subspace $S_k \subseteq \mathbb{R}^d$ of dimension k, such that all the centers y_l are within $\frac{\sqrt{d}\Delta}{k^C}$ of S_k in ℓ^2 -norm, with probability at least $1 - \frac{\eta}{100}$, using poly(d, k) samples and computational time (see Appendix C of [15]); moreover, this does not impose any constraint on the minimum separation requirement. PCA has been used previously in this context (see [16]).

Now, let $\{(x_1(y_{l_1}), y_{l_1}), \dots, (x_n(y_{l_n}), y_{l_n})\}$ be a set of n independent identically distributed random samples from the mixture μ , generated by first sampling — with probability w_l — the mixture component having mean y_l , and then picking $x_l(y_l)$ from the corresponding Gaussian. With probability 1, all the x_l 's are distinct, and this is part of the hypothesis in the lemma below, a proof of which appears in appendix 2.1.

Lemma 1 Let \mathcal{G} be a graph whose vertex set is $X = \{x_1, \ldots, x_n\}$, in which two vertices x_l and x_j are connected by an edge if the ℓ^2 distance between x_l and x_j is less than $2\sqrt{3d \ln(C_1 dn)}$. Decompose \mathcal{G} into the connected components $\mathcal{G}_1, \ldots, \mathcal{G}_r$ of \mathcal{G} . Then, the probability that there exist $l \neq j$ and $x \in \mathcal{G}_l$, $x' \in \mathcal{G}_j$ such that x, x' are both from the same Gaussian components is less than $\eta/100$.

Thanks to this lemma, we can now concentrate on any one particular connected component of the graph \mathcal{G} ; in other words, we may assume that our mixture is well-separated, and at the same time, none of the centers is a so-called outlier which translates to the case where all the centers are (after application of a deterministic linear shift, if required) within an origin-centric ball of radius $2k\sqrt{3d \ln(C_1 dn)}$.

The algorithm below helps us monitor the effect of dimension reduction, and the patching-up of the learnt projected centers. In what follows, we set ϵ to be $k^{-2\tilde{C}_0}$. We note that this algorithm is called-in only when $\omega(\log k) \leq d$; thus, we are tacitly assuming here that the weights are uniform.

Algorithm 2 LearnMixture

Input: IID samples x_1, \dots, x_N from the mixture of Gaussians. **Output:** Candidate centers $\hat{y}_1, \dots, \hat{y}_k$

- let e_1, \ldots, e_d be a uniformly random orthonormal set of vectors
- define $\bar{d} = \min(d, O(\log k))$ dimensional subspace $A_{\bar{d}}$ to be the span of $e_1, \ldots, e_{\bar{d}}$; by lemma 7, with probability greater than $1 \frac{\eta}{100}$, the distance between the projections of any two centers is at least $\left(\frac{\Delta}{2}\right)\sqrt{\bar{d}}$
- use the low dimensional Gaussian learning primitive algorithm 3 from section 4.4 on the samples $\{\Pi_{\bar{d}}x_j\}$ to solv the $\bar{d}+O(1)$ dimensional problem with high probability, if the distance between any two centers is at least $\left(\frac{\Delta}{2}\right)\sqrt{\bar{d}}$; let $(y_1^{(\bar{d})},\ldots,y_{\bar{d}}^{(\bar{d})})$ be the output of algorithm 3
 - if this fails to produce such a set of centers, go back to 1
 - **else** pass the output of algorithm 1 obtained by processing $count_{max}$ copies of M, to the iterative algorithm of [15], which will correctly output the centers to accuracy ϵ/k with the required probability $1 \exp(-k/c)$
- for any fixed $l \ge \bar{d} + 1$, let A(l) denote the span of $e_1, \ldots, e_{\bar{d}}$ augmented with the vector e_l ; suppose that we have succeeded in identifying the projections of the centers on to A(l) for $\bar{d} + 1 \le l \le d$ to within k^{-C_3} in ℓ^2 distance with high probability
- together with the knowledge of $y_1^{(\bar{d})}, \ldots, y_{\bar{d}}^{(\bar{d})}$, and the initial guarantee that (the projected) centers have large mutual distance, this allows us to patch up these projections and give us the centers $\hat{y}_1, \cdots, \hat{y}_k$ to within a Hausdorff distance of δ with high probability.

By the preceding algorithm, it is clear that it suffices to consider the case when $d \le C_{1.5}$ (log k) for an appropriate constant $C_{1.5} > 0$ (inherited from application of lemma 7 in algorithm 2).

4 Analysis in the regime $d \leq C_{1.5} (\log k)$

The following lemma help us restrict our search for the centers inside a union of "not-too-many" balls of radius \sqrt{d} . Proof appears in appendix 2.2

Lemma 2 The following statement holds with probability at least $1 - \frac{\eta}{100}$: if

$$n \ge 1 + \frac{k}{c} \log \left\lceil \frac{300k}{\eta} \right\rceil \left\lceil \log \left\lceil \frac{300k \log \left\lceil \frac{300k}{\eta} \right\rceil}{\eta} \right\rceil \right\rceil,$$

and x_1, \dots, x_n are independent random μ -samples, then

$$\{y_1,\ldots,y_k\}\subseteq\bigcup_{l\in[n]}B_2(x_l,2\sqrt{d}).$$

We recall the following definition:

Definition 1 Given two nonempty subsets $S,T \subset \mathbb{R}^d$, their Hausdorff distance $d_{\mathcal{H}}(S,T)$ is

$$\max \{ \max_{s \in S} \min_{t \in T} ||s - t||_2, \max_{t \in T} \min_{s \in S} ||s - t||_2 \}$$

Let $\mathcal{B}(S,T)$ be the set of bijections between S and T. It is evident from the definition above that the following holds when |S| = |T|:

$$d_{\mathcal{H}}(S,T) = \inf_{\pi \in \mathcal{B}(S,T)} ||\pi(s) - s||_2$$

Let \mathcal{F} denote the Fourier transform. For any function $f \in L^1(\mathbb{R}^d)$, we write $\hat{f} = \mathcal{F}(f)$, where

$$\hat{f}(\xi) = \left(\frac{1}{\sqrt{2\pi}}\right)^d \int_{\mathbb{R}^d} f(x)e^{-i\xi \cdot x} dx \tag{1.1}$$

By the Fourier inversion formula,

$$f(x) = \left(\frac{1}{\sqrt{2\pi}}\right)^d \int_{\mathbb{R}^d} \hat{f}(\xi) e^{i\xi \cdot x} d\xi,\tag{1.2}$$

The following properties of Fourier transform operator are standard and easily verified, and hence, we ommit their proofs altogether.

Lemma 3 (a) Let $\gamma(z) := (2\pi)^{-\frac{d}{2}} e^{-\frac{||z||^2}{2}}$ be the standard Gaussian density in \mathbb{R}^d ; then, $\hat{\gamma} := \mathcal{F}(\gamma) = \gamma$.

(b) If $g, h \in L^2(\mathbb{R}^d)$ are such that $f \star g \in L^2(\mathbb{R}^d)$, then $\mathcal{F}(f \star g) = (2\pi)^{\frac{d}{2}} \hat{f} \hat{g}$. Here \star denotes the convolution.

4.1 Deconvolution

We make the following conventions for the rest of this paper.

Convention: Symbol x.y represents decimal number. All constants $C_{x.y}$ are absolute constants in $[1, \infty)$, and all constants $c_{x,y}$ satisfy $c_{x.y} = C_{x.y}^{-1}$. We allow $C_{x.y}$ to depend on $C_{x'.y'}$ if x.y > x'.y'.

Let $\bar{\Delta}$ equal $\Delta/C_{3.2}$. Let $\gamma_{\sigma}(z) := \sigma^{-d}\gamma(\sigma^{-1}z)$ denote the spherical Gaussian whose one dimensional marginals have variance σ^2 , and note that $\hat{\gamma}_{\bar{\Delta}}(z) = \gamma(z\bar{\Delta})$. Define

$$\mathcal{B} := \left(\sqrt{C_{3.5} \ln k} + \sqrt{d}\right) B_2(0, \bar{\Delta}^{-1}),\tag{1.3}$$

where $B_2(0, \bar{\Delta}^{-1})$ is the Euclidean ball of radius $\bar{\Delta}^{-1}$; set $\hat{s}(z) := \gamma(z\bar{\Delta}) \mathbb{I}_{\mathcal{B}}(z)$, where \mathbb{I}_S the indicator function of S. In the lemma that follows, we write $s = \mathcal{F}^{-1}(\hat{s})$; proof of the lemma appears in appendix 2.3.

Lemma 4 For all $z \in \mathbb{R}^d$, we have $|s(z) - \gamma_{\bar{\Delta}}(z)| \le (2\pi\bar{\Delta}^2)^{-\frac{d}{2}}k^{-\frac{C_{3,5}}{2}}$.

4.2 An observation

Let x_1, \ldots, x_n be iid samples from the Gaussian mixture μ . Let μ_e denote the uniform probability measure supported on $\{x_1, \ldots, x_n\}$. Let \star denote convolution in \mathbb{R}^d . Note that the Fourier convolution identity is $(2\pi)^{-\frac{d}{2}}\mathcal{F}(f \star g) = \hat{f}\hat{g}$. Let $\hat{\zeta} := \hat{\gamma}^{-1} \cdot \hat{s}$, and $\zeta = \mathcal{F}^{-1}(\hat{\zeta})$. We will recover the centers and weights of the Gaussians from $\zeta \star \mu_e = (2\pi)^{\frac{d}{2}}\mathcal{F}^{-1}(\hat{\zeta} \cdot \hat{\mu}_e)$. The heuristics are as follows.

Let ν denote the unique probability measure satisfying $\gamma \star \nu = \mu$. Thus, $\nu = \sum_{j=1}^{k_0} w_j \delta_{y_j}$, where δ_{y_j} is a dirac delta supported on y_j . It follows, roughly speaking, that inside supp(\hat{s}), we get

$$\begin{split} \hat{v}(w) &= (2\pi)^{-d} \hat{\gamma}(w)^{-1} \mathbb{E}_{X \approx \mu} \left[e^{-iX \cdot w} \right] \approx (2\pi)^{-\frac{d}{2}} \hat{\gamma}(w)^{-1} \hat{\mu}_e(w) \\ \Rightarrow \qquad \hat{s}(w) \hat{v}(w) \approx (2\pi)^{-\frac{d}{2}} \hat{\zeta}(w) \hat{\mu}_e(w) \end{split}$$

pointwise, and this should (roughly) yield $s \star \nu \approx (2\pi)^{-\frac{d}{2}} \zeta \star \mu_e$. On the other hand, notice that lemma 4 shows that $s \star \nu \approx \gamma_{\bar{\Delta}} \star \nu$, and because the spikes of ν are approximately (up to scaling) the spikes of $\gamma_{\bar{\Delta}} \star \nu$, we restrict to learning the spikes of $\gamma_{\bar{\Delta}} \star \nu$ by accessing an approximation via $(2\pi)^{-\frac{d}{2}} \zeta \star \mu_e$. For notational convenience, we write $\xi_e := (2\pi)^{-\frac{d}{2}} \zeta \star \mu_e$.

4.3 Monte-Carlo and access to deconvolved mixture

In order to formalize the heuristics above, we proceed as follows. Recall that $\mathcal{B} = \text{supp}(\hat{s})$, so that $z \in \mathcal{B}$ if and only if $z \in \mathbb{R}^d$ satisfies $||\bar{\Delta}z|| \le \sqrt{C_{3.5} \ln k} + \sqrt{d}$.

The following proposition allows us to construct a (random) **black box** oracle that outputs a good additive approximation of $\gamma_{\bar{\Delta}} \star \nu$ at any given point x. See appendix 2.4 for a proof of the proposition.

Proposition 1 Let z_1, \dots, z_m be independent, random variables drawn from the uniform (normalized Lebesgue) probability measure on \mathcal{B} . Let x_1, \dots, x_n be independent μ -distributed random samples. If $m = C_{3.6}k^{C_{3.6}} \ln k$, and

$$n \ge C_{3.6} k^{C_{3.6} + C_{3.5}} \ln \left(C_{3.6} k^{C_{3.6} + C_{3.5}} \ln k \right),$$
 (1.4)

where $C_{3.6} \ge C_{0.1}C_{3.5} + C_{1.5} \left(\ln(2\pi) + 2 \ln\left(\frac{2C_{3.2}}{c}\right) \right) + C_{3.5} \left(8 + \frac{2C_{3.2}^2}{c^2} \right)$, then for any $x \in \mathbb{R}^d$, the random variable

$$f_x := \frac{vol(\mathcal{B})}{m} \sum_{l \in [m]} e^{ix \cdot z_l} \gamma(z_l \bar{\Delta}) e^{\frac{||z_l||^2}{2}} \hat{\mu}_e(z_l)$$
 (1.5)

satisfies the inequality $|(\gamma_{\bar{\Delta}} \star v)(x) - \Re f_x| \le 3k^{-C_{3.5}}$ with probability at least $1 - 8k^{-C_{3.5}}$: here $\Re f_x$ denotes the real part of f_x .

4.4 Low-dimensional learning algorithm

In algorithm 3 below — whose analysis will be deferred to appendix 3, at any point $z \in \bigcup_i B_2(x_i, 2\sqrt{d})$, we will assume access to the random variable f_z in \mathbb{C} , such that

$$\mathbb{P}\left[\left|f_z - (\gamma_{\bar{\Delta}} \star \nu)(z)\right| < k^{-C_4}\right] > 1 - k^{-C_4}$$

As established by proposition 1, these f_z can be constructed using polynomially many samples and computation steps, in such a way that for any subset $\{z_1, \ldots, z_m\} \subseteq \mathbb{R}^d$, the set $\{f_{z_1}, \ldots, f_{z_m}\}$ consists of independent random variables. Let $diam(Q_\ell)$ denote the ℓ^2 diameter of Q_ℓ .

In our implementation, we will employ the efficient zeroth order stochastic concave maximization algorithm, devised in [3]. We denote this algorithm of [3] as \mathfrak{A}_0 . In d-dimensional Euclidean space, the algorithm returns an ϵ -maxima of certain $d^{-1}\epsilon$ -approximate t-Lipschitz concave function, and the number of function evaluations used depends polynomially on d, ϵ , and $\log t$. The performance guarantee of algorithm \mathfrak{A}_0 is summarized in lemma 5 stated below.

Definition 2 Let $\mathcal{B} \subseteq \mathbb{R}^{\bar{d}}$ be a convex set, and $\xi > 0$. A continuous function $\phi : \mathcal{B} \to \mathbb{R}_+$ is said to be ξ -approximately log-concave if there exists a continuous

function $\psi : \mathcal{B} \to \mathbb{R}_+$ such that $\log \psi$ is concave, and $||\log \phi - \log \psi||_{L^{\infty}(\mathcal{B})} \leq \xi$. We say ϕ is approximately log-concave if it is ξ -approximately log-concave for some $\xi > 0$.

Lemma 5 (Belloni et al) Suppose that $\mathcal{B} \subseteq \mathbb{R}^{\bar{d}}$ is a convex subset, and χ, ψ : $\mathcal{B} \to \mathbb{R}$ are functions satisfying $\sup_{z \in \mathcal{B}} |\chi(z) - \psi(z)| \leq \frac{\epsilon}{\bar{d}}$. Suppose that ψ is concave and t-Lipschitz; then algorithm \mathfrak{A}_0 returns a point $q \in \mathcal{B}$ satisfying $\chi(q) \geq \max_{z \in \mathcal{B}} \chi(z) - \epsilon$, and uses $O(\bar{d}^8 \epsilon^{-2} \log t)$ computation steps.

We now present the algorithm for learning in low-dimension. In what follows, we use \bar{d} instead of d in order to keep the notation consistent with algorithm 2.

Algorithm 3 FindSpikes

Input: IID samples from well-separated mixture of Gaussians in $d = O(\log k)$ dimensions; **Output:** The centers of the components Gaussians;

let $count_{max} = C_{4.5}k$ while $count \le count_{max}$,

· for each point

$$\ell \in \left(\frac{\bar{\Delta}}{1000} \sqrt{\frac{\bar{d}}{C_{1.5} \log k}}\right) \mathbb{Z}^{\bar{d}} \bigcap \bigcup_{i} B_{2}(x_{i}, 2\sqrt{\bar{d}}),$$

let Q_{ℓ} be the ball of radius $\left(\frac{\bar{\Delta}}{400} \frac{\bar{d}}{\sqrt{C_{1.5} \log k}}\right)$, centered at ℓ use an efficient zeroth order stochastic concave maximization subroutine (see lemma 5) that

- use an efficient zeroth order stochastic concave maximization subroutine (see lemma 5) that produces a point q_ℓ in Q_ℓ at which $(2\pi)^{-\frac{\bar{d}}{2}}(\zeta\star\mu_e)(z)$ is within $k^{-C_{4.6}}$ of the maximum of $(2\pi)^{-\frac{\bar{d}}{2}}(\zeta\star\mu_e)$ restricted to Q_ℓ
- create a sequence $L=(q_{\ell_1},\ldots,q_{\ell_{k_1}})$ that consists of all those q_ℓ , such that $(2\pi)^{-\frac{\bar{d}}{2}}(\zeta\star\mu_e)(q_\ell)>(\frac{w_{min}}{2})\gamma_{\bar{\Delta}}(0)$, and $\|\ell-q_\ell\|_2< diam(Q_\ell)/4$
- reorder L, if necessary, so that $(\zeta \star \mu_e)(q_{\ell_1}) \geq \cdots \geq (\zeta \star \mu_e)(q_{\ell_{k_1}})$
 - if $k_1 < 1$, return error
 - **else**, form a subsequence $M=(\ell_{m_1},\ldots,\ell_{m_{k_2}})$ of $(\ell_1,\ldots,\ell_{k_1})$ using the following iterative procedure
 - · let $m_1 \leftarrow 1, j \leftarrow 1$ and $M := \{\ell_1\}$ while $j \leq k_1$, if ℓ_{j+1} is not contained in $B(\ell_{j'}, \sqrt{\bar{d}}\sqrt{\Delta\bar{\Delta}}/2)$ for any $j' \leq j$, append ℓ_{j+1} to M increment j
- pass

$$\{(q_{\ell_{m_i}})\}_{j\in[k_2]}$$

to algorithm 2

• increment count.

5 Estimating Weights

We find estimates for the weights of the Gaussian components, within accuracy cw_{min} , when the dimension satisfies $\bar{d} \leq O(\log k)$. The idea is that the weight of a Gaussian component in a well-separated mixture is concentrated near the center of the component, hence, can be estimated by considering the integral of the mixture in an appropriately sized ball around the (approximate) center of the component. We formulate this in the following. A proof appears in appendix 2.5.

Proposition 2 (Estimating the weights) Let q_{ℓ} be an output of algorithm 1, and let $\hat{Q}_{\ell} \subseteq \mathbb{R}^{\bar{d}}$ be the ball of radius $C_{3.3}\bar{\Delta}\sqrt{\bar{d}}$, centered at ℓ , with volume v. Let z_1, \dots, z_p be independent uniformly random points from \hat{Q}_{ℓ} ; if

$$p \ge \frac{C_{3.5}}{c_{0.1}\delta^2} k^{\frac{C_{1.5}}{2} \ln(eC_{3.3}^2)} \ln k \tag{1.6}$$

then

$$\mathbb{P}\left[\left|\frac{1}{p}\sum_{j=1}^{p}\Re(f_{z_{j}})-\int_{\hat{Q}_{\ell}}\gamma_{\bar{\Delta}}\star\nu\ dx\right|>\delta+3k^{-C_{3.5}}v\right]\leq20k^{-C_{3.5}}\tag{1.7}$$

In particular, if $y_{j_0} \in Q_{\ell}$, then

$$\mathbb{P}\left[\left|\frac{1}{p}\sum_{j=1}^{p}\Re(f_{z_{j}})-w_{j_{0}}\right|>cw_{min}\right]\leq20k^{-C_{3.5}}$$
(1.8)

6 Discussions

6.1 Why brute-force-search may not work even when $poly(2^d)$ many samples are available?

As stated in the introduction, our results are most interesting when $d = O(\log k)$. Perhaps an intelligent approach in this regime would be to get $\operatorname{poly}(k)$ independent samples $X_1, \dots, X_k c$ from the Gaussian mixture μ , and consider an ϵ -net on the union $\bigcup_j B(X_j, C'\sqrt{d})$, and perform an exhaustive brute-force search for the centers, using this net. Criterion to decide if a point is close to a center of such a mixture of Gaussians is that, in a small neighbourhood, the point is close to a maxima of the mixture density. How we ascertain whether a point is close to a local maxima is another story (and we discuss this in this paper), but for now, we consider ourselves just powerful enough to be able to do this. Note, however, that when $d = \Omega(\log k)$, such an ϵ -net has cardinality of potential order

 $\Omega(k^C(C'/\epsilon)^d d^{\frac{d}{2}}) = \Omega(k^{C+\log(C'/\epsilon)} k^{\frac{1}{2}\log\log k}) = \Omega(k^{\log\log k})$. Thus, to learn the centers, we need to be ready for $\Omega(k^{C+\log(C'/\epsilon)} k^{\frac{1}{2}\log\log k})$ many searches, which fails to be executed in $\operatorname{poly}(k)$ time. Moreover, even if one ignores $\log\log k$ in the exponent above, there is the so-called *mixture-density dilemma* that needs to be dealt with. To discuss this, let us consider a unit sphere $\mathbb{S}^{d-1} \subseteq \mathbb{R}^d$, and let $y_1, \dots, y_k \in \mathbb{S}^{d-1}$ be such that the atomic-mixture $v := k^{-1}(\delta_{y_1} + \dots + \delta_{y_k})$ is an approximation of the uniform surface measure of the sphere; equivalently, the points y_1, \dots, y_k are equidistributed. Let γ be the standard d-dimensional spherical Gaussian density of unit variance in each coordinate. In this case, the origin is a global maxima of the mixture $v \star \gamma$. This can be easily seen when the centers of the Gaussians are the roots of unity $y_r := e^{\frac{2\pi i r}{k}}$ for $r \in [k]$ with k = 2n and n odd. Let γ_t be the 2-dimensional Gaussian with mean 0 and variance t^2 , and let $\mu = v \star \gamma_t$. One has $\mu(0) = (2\pi t^2)^{-1} e^{-\frac{1}{2t^2}}$, and for any $r \in [k]$,

$$\mu\left(e^{\frac{2\pi i r}{k}}\right) = \frac{1}{4n\pi t^2} + \frac{1}{4n\pi t^2} \sum_{r=1}^{2n-1} e^{-\frac{\left|1-e^{\frac{\pi i r}{R}}\right|^2}{2t^2}}$$

$$= \frac{1+e^{-\frac{2}{t^2}}}{4n\pi t^2} + \frac{e^{-\frac{1}{t^2}}}{2n\pi t^2} \sum_{r=1}^{n-1} e^{\frac{\cos\left(\frac{\pi r}{R}\right)}{2t^2}}$$

$$\leq \frac{1+e^{-\frac{2}{t^2}}}{4n\pi t^2} + \frac{(n-1)e^{-\frac{1}{t^2}}}{4n\pi t^2} \left(e^{\frac{\cos\left(\frac{\pi}{R}\right)}{2t^2}} + e^{-\frac{\cos\left(\frac{\pi}{R}\right)}{2t^2}}\right)$$

A simple observation is that $1 + e^{-\frac{2}{t^2}} < 2e^{-\frac{1}{2t^2}}$ when $t \ge 1$; hence,

$$\begin{split} \left(e^{\frac{\cos(\frac{\pi}{n})}{2t^2}} + e^{-\frac{\cos(\frac{\pi}{n})}{2t^2}}\right) &< 2e^{\frac{\cos(\frac{\pi}{n})}{2t^2}} \\ \Rightarrow & \mu\left(e^{\frac{2\pi i r}{k}}\right) & < \frac{2e^{-\frac{1}{2t^2}}}{4n\pi t^2} + \frac{2(n-1)e^{\frac{\cos(\frac{\pi}{n})}{2t^2}}e^{-\frac{1}{t^2}}}{4n\pi t^2} \\ &< (2\pi t^2)^{-1}e^{-\frac{1}{2t^2}} \end{split}$$

In particular, the center appears to be a global maxima. This example illustrates the short-comings of naive brute-force-search.

We deal with this, by deconvolving the Gaussian mixture followed by local search. It appears from the simple computation that — as $t \to 0^+$, the situation should turn around dramatically, and this is precisely what is expected, since Gaussian kernel is an efficient approximate identity. Thus, suitable application of deconvolution technique results in a mixture that approximately resembles the underlying atomic mixture after smoothning with a thin Gaussian. Such a smooth mixture inherits the property of the underlying atomic mixture, which prohibits points away from all the centers to manifest as maxima (local or global) of the mixing density. We note that the deconvolution itself involves technicalities, since this amounts to multiplying with exponentially increasing function in Fourier domain, and in presence of noise

in computing the characteristic function using samples from the mixture, one needs to be sufficiently careful.

6.2 About assumptions on uniform variance, and almost 'uniform' mixing weights

Our motivation for considering this somewhat stylized setting — of almost 'uniform' mixing weight, and Gaussian components having uniform variance — stems from questions in manifold learning. Here, data originate from an underlying compact smooth manifold — having known positive lower-bound on the reach and known upper-bound on Hausdorff volume — isometrically embedded into a possibly exponentially large dimensional ambient space, and then get noisy by addition of independent Gaussian noise from the ambient space. The original distribution supported on the manifold usually posses almost uniform Radon-Nikodym derivative with respect to the Hausdorff measure on the manifold. Considering the set of centers of the individual Gaussian components as compact (nonsmooth) 0-dimensional manifold, the above facts account for uniform variance, and almost 'uniform' weight, respectively. We note that the usual manifold learning results currently available do not carry forward to our 0-dimensional settings, mainly because (1) the 0-dimensionality does not allow smooth analysis available for positive dimensional manifolds, and (2) the 0-dimensional case affords noise with comparatively large variance than in positive dimension.

6.3 Why is the focussed dimensionality interesting?

One of our practical technical motivation for considering the regime $d \leq \log k$ is that essentially the entire analysis on higher dimension reduces to this regime by an application of Johnson-Lindenstrauss. This is prevalent even in the more general setting of manifold learning, where the noiseless data comes from and underlying space — which is a manifold of dimension d — and gets corrupted by Gaussian noise: for example, in case of Gaussian mixture learning, the underlying space consists of the means of the Gaussians, a zero dimensional manifold. We note that this also partially explains the reason for considering mixture of spherical Gaussian with identical variance. In the general case, a standard (and reasonably well-motivated — by an urge to avoid "curse of dimensionality") trick is dimension reduction. If the manifold has standard d-dimensional volume μ_I and curvature based volume μ_I' , and if an Euclidean tubular neighbourhood of radius $\tau > 0$ of the manifold remains reasonably smooth, then Johnson-Lindenstrauss type theorem (see, for example, theorem 1.5 of [4]), asserts that a random projection onto a subspace of dimension of order

$$\epsilon^{-2} \left(d \log(1/\epsilon) + \log(1/\delta) \right) + \epsilon^{-2} \left(\log(\mu_I/\tau^d + \mu_I') \right)$$

is an ϵ -approximate isometry with probability at least $1 - \delta$. Thus, one essentially projects data onto a randomly choosen subspace of dimension specified above. In this paper too, we follow this broad strategy, whereby data from high dimensional space are first projected onto a sequence of subspaces and the resulting mean coordinates are carefully patched-up.

Many of the popular algorithms for learning mixture of Gaussians, with separation assumption — that appears to be at par or even weaker than the separation assumption in this paper — are based on EM methodology and/or moment-based methods. While these algorithms are highly efficient in learning mixture of Gaussians, it is not immediately obvious whether they generalize to the more involved case of data analysis, where the underlying space is a manifold of positive dimension. On the other hand, our approach is generic in some sense, and we expect this can be extended to the more general case of manifold learning.

7 Conclusion and open problems

We developed a randomized algorithm that learns the centers y_i of standard Gaussians in a mixture, to within an ℓ^2 distance of $\delta < \frac{\Delta \sqrt{d}}{2}$ with high probability when the minimum separation between two centers is at least $\sqrt{d}\Delta$, where Δ is larger than an universal constant in (0,1). The number of samples and the computational time is bounded above by poly $\left(k,d,\log\left(\frac{1}{\delta}\right)\right)$. Such a polynomial bound on the sample and computational complexity was previously unknown when $d \geq \omega(1)$. There is a matching lower bound due to [15] on the sample complexity of learning a random mixture of Gaussians in a ball of radius $\Theta(\sqrt{d})$ in d dimensions, when d is $\Theta(\log k)$. It remains open whether (as raised in [15]) poly $(k,d,1/\delta)$ upper bounds on computational complexity of this task can be obtained when the minimum separation between two centers in $\Omega(\sqrt{\log k})$ in general, although when $d \leq O(\log k)$, this follows from our results. It would also be interesting to extend the results of this paper to mixtures of spherical Gaussians whose variances are not necessarily equal, or even more, to the case of non-spherical Gaussian mixture.

References

- Arora, S., Kannan, R.: Learning mixtures of separated nonspherical Gaussians. Ann. Appl. Probab. 15(1A), 69–92 (2005)
- Belkin, M., Sinha, K.: Polynomial learning of distribution families. SIAM J. Comput. 44(4), 889–911 (2015)
- 3. Belloni, A., Liang, T., Narayanan, H., Rakhlin, A.: Escaping the local minima via simulated annealing: Optimization of approximately convex functions. Proceedings of Machine Learning Research (2015). URL http://arxiv.org/abs/1501.07242
- Clarkson, K.: Tighter bounds for random projections of manifolds. In: Proceedings of the 24th Annual Symposium held at the University of Maryland, College Park, MD, June 9–11, 2008, pp. 39–48. Association for Computing Machinery (ACM), New York (2008)
- Dasgupta, S.: Learning mixtures of Gaussians. In: 40th Annual Symposium on Foundations of Computer Science (New York, 1999), pp. 634–644. IEEE Computer Soc., Los Alamitos, CA (1999)
- Dasgupta, S., Schulman, L.: A probabilistic analysis of EM for mixtures of separated, spherical Gaussians. J. Mach. Learn. Res. 8, 203–226 (2007)
- Diakonikolas, I., Kempe, D., Henzinger, M.: List-decodable robust mean estimation and learning mixtures of spherical gaussians. In: STOC'18—Proceedings of the 50th Annual ACM SIGACT Symposium on Theory of Computing, pp. 1047–1060. Association for Computing Machinery (ACM), New York (2018)
- Hopkins, S.B., Li, J.: Mixture models, robustness, and sum of squares proofs. In: STOC'18—Proceedings of the 50th Annual ACM SIGACT Symposium on Theory of Computing, pp. 1021–1034. ACM, New York (2018)
- Hsu, D., Kakade, S.M.: Learning mixtures of spherical Gaussians: moment methods and spectral decompositions. In: ITCS'13—Proceedings of the 2013 ACM Conference on Innovations in Theoretical Computer Science, pp. 11–19. ACM, New York (2013)
- Kalai, A.T., Moitra, A., Valiant, G.: Efficiently learning mixtures of two Gaussians. In: STOC'10—Proceedings of the 2010 ACM International Symposium on Theory of Computing, pp. 553–562. ACM, New York (2010)
- Karatsuba, E.A.: On the asymptotic representation of the Euler gamma function by Ramanujan.
 J. Comput. Appl. Math. 135(2), 225–240 (2001)
- Koltchinskii, V.I.: Empirical geometry of multivariate data: a deconvolution approach. Ann. Statist. 28(2), 591–629 (2000)
- Laurent, B., Massart, P.: Adaptive estimation of a quadratic functional by model selection. Ann. Statist. 28(5), 1302–1338 (2000)
- Moitra, A., Valiant, G.: Settling the polynomial learnability of mixtures of Gaussians. In: 2010 IEEE 51st Annual Symposium on Foundations of Computer Science—FOCS 2010, pp. 93–102. IEEE Computer Soc., Los Alamitos, CA (2010)

- Regev, O., Vijayaraghavan, A.: On learning mixtures of well-separated Gaussians. In: 58th Annual IEEE Symposium on Foundations of Computer Science—FOCS 2017, pp. 85–96.
 IEEE Computer Soc., Los Alamitos, CA (2017)
- Vempala, S., Wang, G.: A spectral algorithm for learning mixture models. J. Comput. System Sci. 68(4), 841–860 (2004)
- 17. Vershynin, R.: High-dimensional probability, Cambridge Series in Statistical and Probabilistic Mathematics, vol. 47. Cambridge University Press, Cambridge (2018). An introduction with applications in data science, With a foreword by Sara van de Geer

1 Technical Discussions

1.1 Gaussian concentration

In all the discussions, we will employ the following tail-bound on χ^2 -statistic; this has appeared as inequality (4.3) of [13] which contains a proof of the statement.

Lemma 6 Suppose that u is χ^2 -statistic with d degrees of freedom; then, for any x > 0, the following inequality holds:

$$\mathbb{P}\left[u - d \ge 2\sqrt{dx} + 2x\right] \le e^{-x}$$

Remark 1 The reason that we are able to learn the centers (and the weights too, in suitable cases) even with Gaussian smoothing at just a constant scale (recall that we are basically scaling Δ by $C_{3,2}$) is hidden in the Gaussian concentration; the probability the scaled Gaussian exceeds $CC_{3,2}^{-1}d$ far from its center is at most $e^{-C^2C_{3,2}d}$.

Remark 2 We note that lemma 1 allows us to restrict onto any one particular cluster of centers, and we know this cluster of centers has (with high probability) diameter at most

$$\rho := 2k\sqrt{3d\ln(C_1dn)}$$

Equivalently, we are, from here on, focusing on a ρ -bounded mixture in dimension $d \le k$, a la Regev-Vijayaraghavan in [15]. For this, it is enough for us to estimate the centroid of the mixture by averaging $\operatorname{poly}(k,d)$ many samples, and apply an affine-transform so that origin is placed at this estimated centroid. Next, we take the push forward of μ via an orthoprojection of \mathbb{R}^d on to S_k , and work with that instead. This allows us to reduce the dimension d to k (if d started out being greater than k), while retaining the same Δ to within a multiplicative factor of 2.

1.2 Random projection

We now recall the Johnson-Lindenstrauss lemma for dimension reduction; this will be indispensable for dealing with high-dimensional mixture. A proof of the lemma can be found in [17] (see theorem 5.3.1).

Lemma 7 (Johnson-Lindenstrauss) *Let* \mathcal{Y} *be a set of at most k points in* \mathbb{R}^d *, and* $\epsilon > 0$ *. Assume that*

$$m \ge \left(\frac{\tilde{C}}{\epsilon^2}\right) \log k.$$

Let $E \subseteq \mathbb{R}^d$ be a random subspace drawn from the uniform distribution on Grassmannian $G_{d,m}$ — the space of d-dimensional vector subspaces of \mathbb{R}^m ; if Π_E is the orthogonal projection onto E, then with probability at least $1 - \exp(-\tilde{c}\epsilon^2 m)$, the scaled projection

$$\Pi := \sqrt{\frac{d}{m}} \Pi_E$$

is an approximate identity on \mathcal{Y} :

$$(1 - \epsilon)||y_j - y_l||_2 \le ||\Pi(y_j - y_l)||_2 \le (1 + \epsilon)||y_j - y_l||_2 \quad \forall y_j, y_l \in \mathcal{Y}$$

1.3 Remarks on proposition 1

We needed to employ Hoeffding's inequality for C-valued random variables:

Lemma 8 (Hoeffding) Let b > 0. Let Y_1, \dots, Y_r be independent identically distributed \mathbb{C} -valued random variables such that $|Y_i| \le b^{-1}$ for all $j \in [r]$. Then

$$\mathbb{P}\left[\left|\frac{1}{r}\sum_{j=1}^{r}(\mathbb{E}[Y_j] - Y_j)\right| \ge t\right] \le 2e^{-c_{0.1}rt^2b^2} \tag{.1}$$

where $c_{0.1}$ is a universal constant.

Remark 3 The main point to be noted — vis-a-vis proposition 1 — is that, for each $x \in \mathbb{R}^d$, we need polynomially many mixture samples to determine f_x ; since we need to determine f_x at polynomially many $x \in \mathbb{R}^d$, this is enough (albeit, slightly wasteful) for the desired sample complexity and time complexity.

Remark 4 We note that, for any $x \in \mathbb{R}^d$, one has

$$\xi_e(x) = \text{vol}(\mathcal{B}) \mathbb{E}_z \left[\hat{s}(z) \exp\left(||z||^2/2\right) \hat{\mu}_e(z) e^{ix \cdot z} \right]$$

Writing $\xi(z) := \hat{s}(z)e^{\frac{||z||^2}{2}}\hat{\mu}_e(z)e^{ix\cdot z}$, one has

$$\mathbb{P}\left[\left|f_{x} - \xi_{e}(x)\right| > k^{-C_{3.5}}\right] = \mathbb{P}\left[\frac{\operatorname{vol}(\mathcal{B})}{m} \left| \sum_{l \in [m]} \xi(z_{l}) - \mathbb{E}\left[\xi(z_{l})\right]\right| > k^{-C_{3.5}}\right]$$

Using Hoeffding's inequality from lemma 8 and the fact that $m = C_{3.6}k^{C_{3.6}} \ln k$, we get

$$\mathbb{P}\left[|f_x - \xi_e(x)| > k^{-C_{3.5}}\right] \le k^{-C_{3.5}} \tag{.2}$$

2 Proofs

2.1 Proof of lemma lemma 1

Proof By bounds on the tail of a χ^2 -random variable with parameter d (see lemma 6), the probability that $||x_l - y(x_l)|| \ge \sqrt{3d \ln(C_1 dn)}$ can be bounded from above as follows.

$$\mathbb{P}\left[||x - y(x)|| \ge \sqrt{3d\ln(C_1dn)}\right] \le \left(3e\ln(C_1dn)\right)^{\frac{d}{2}} (C_1dn)^{-\frac{3d}{2}} \tag{.3}$$

The union bound yields

$$\mathbb{P}\left[\exists x_{l} \text{ s.t } ||x_{l} - y(x_{l})|| \ge \sqrt{3d \ln(C_{1}dn)}\right] \le n \left(3e \ln(C_{1}dn)\right)^{\frac{d}{2}} (C_{1}dn)^{-\frac{3d}{2}} \le \frac{\eta}{100}$$

2.2 Proof of lemma 2

Proof This is essentially an application of coupon collector's problem.

Recall that $w_{min} \ge ck^{-1}$. Suppose that m > k random independent μ -samples, denoted as x_1, \dots, x_m , have been picked up. Let C := C(k) be a positive integer valued function. For any $l \in [k_0]$, the probability – that x_1, \dots, x_m contain no μ_l -sample – is at most $(1 - ck^{-1})^m \le e^{-mck^{-1}}$. Thus, the probability – that x_1, \dots, x_m contain no sample from at least one Gaussian component in μ – is at most $e^{\ln k - mck^{-1}}$. We ensure this probability is at most $\frac{\eta}{300C}$ by having

$$m \ge \frac{k}{c} \left[\log \left(\frac{300Ck}{\eta} \right) \right]$$

It follows that, if at least

$$n_0 := \frac{Ck}{c} \left[\log \left(\frac{300Ck}{\eta} \right) \right] \tag{.4}$$

random independent μ -samples were picked up, then with probability at least $1 - \frac{\eta}{300}$ all the components were needed to be sampled at least C times.

Let E denote the event that n_0 random independent μ -samples contain at least C points from each Gaussian component. For $l \in [k_0]$, let A_l be the event that none of the n_0 random samples satisfy $||x_j - y_l|| < 2\sqrt{d}$. Applying Gaussian isoperimetric inequality (see lemma 6) and union bound, we obtain

$$\mathbb{P}\left[\bigcup_{l\in[k_0]}A_l \mid E\right] \le 2^{\log k - Cd}$$

Thus, letting $C \ge \log\left(\frac{300k}{\eta}\right)$, it follows that

$$\mathbb{P}\left[\bigcap_{l\in[k]}A_{l}^{c}\right] \geq \mathbb{P}\left[\bigcap_{l\in[k_{0}]}A_{l}^{c}\mid E\right]\mathbb{P}\left[E\right]$$
$$\geq \left(1-\frac{\eta}{300}\right)^{2}$$

provided

$$n \ge \frac{k}{c} \log \left\lceil \frac{300k}{\eta} \right\rceil \left\lceil \log \left\lceil \frac{300k \log \left\lceil \frac{300k}{\eta} \right\rceil}{\eta} \right\rceil \right\rceil$$

2.3 Proof of lemma 4

Proof Let $d\hat{\kappa}^2$ be a χ^2 random variable with d degrees of freedom, *i.e.*, the sum of squares of d independent standard Gaussians. By the inequality in lemma 6, we know that

$$\mathbb{P}\left[\hat{\kappa} \ge \sqrt{\frac{C_{3.5} \ln k}{d}} + 1\right] = \mathbb{P}\left[d\hat{\kappa}^2 - d \ge C_{3.5} \ln k + 2\sqrt{C_{3.5} d \ln k}\right]$$

$$\le \exp\left(-\frac{C_{3.5} \ln k}{2}\right)$$

$$= k^{-\frac{C_{3.5}}{2}} \tag{.5}$$

For $z \in \text{supp}(\hat{s})$, one has $\hat{s}(z) = \bar{\Delta}^{-d} \gamma_{(1/\bar{\Delta})}(z)$. Therefore,

$$\begin{split} \|\hat{s} - \bar{\Delta}^{-d} \gamma_{(1/\bar{\Delta})}\|_{L^{1}} &= \int_{||\bar{\Delta}z|| \ge \sqrt{C_{3.5} \ln k} + \sqrt{d}} \gamma(\bar{\Delta}z) \ dz \\ &= \bar{\Delta}^{-d} \mathbb{P} \left[\hat{\kappa} \ge \sqrt{\frac{C_{3.5} \ln k}{d}} + 1 \right] \\ &\le \bar{\Delta}^{-d} k^{-\frac{C_{3.5}}{2}} \end{split}$$

The lemma now follows from the fact that \mathcal{F}^{-1} is a bounded linear operator from L^1 to L^{∞} with operator norm $(2\pi)^{-\frac{d}{2}}$.

2.4 Proof of proposition 1

Proof For any $x \in \mathbb{R}^d$, one has

$$\left| (\gamma_{\bar{\Delta}} \star \nu)(x) - (2\pi)^{-d} \sum_{j=1}^{k_0} w_j \int_{\mathcal{B}} e^{-\frac{\bar{\Delta}^2 ||z||^2}{2}} e^{i(x-y_j) \cdot z} dz \right|$$

$$\leq (2\pi)^{-d} \int_{\mathbb{R}^{\bar{d}} \setminus \mathcal{B}} e^{-\frac{\bar{\Delta}^2 ||z||^2}{2}} dz$$

$$\leq k^{-\frac{C_{3,5}}{4}} \tag{.6}$$

Hence, it suffices to estimate

$$I_x := (2\pi)^{-d} \sum_{i=1}^{k_0} w_i \int_{\mathcal{B}} e^{-\frac{\bar{\Lambda}^2 ||z||^2}{2}} e^{i(x-y_i)\cdot z} dz$$

Next, one has

$$\begin{split} I_{x} &= (2\pi)^{-\frac{d}{2}} \int_{\mathcal{B}} e^{ix \cdot z} \left(\hat{s}(z) \sum_{j=1}^{k_{0}} w_{j} e^{-iy_{j} \cdot z} \right) dz \\ &= (2\pi)^{-\frac{d}{2}} \text{vol}(B) \, \mathbb{E}_{z} \left[e^{ix \cdot z} \left(\hat{s}(z) \sum_{j=1}^{k_{0}} w_{j} e^{-iy_{j} \cdot z} \right) \right] \end{split}$$

where z is a sample from the uniform probability distribution on \mathcal{B} . For brevity of notation, write

$$\phi(z) = (2\pi)^{-\frac{d}{2}} \operatorname{vol}(\mathcal{B}) \left(\hat{s}(z) \sum_{j=1}^{k_0} w_j e^{-iy_j \cdot z} \right)$$
$$= \operatorname{vol}(\mathcal{B}) \hat{s}(z) \hat{v}(z)$$

so that $I_x = \mathbb{E}_z[e^{ix\cdot z}\phi(z)]$. By Ramanujan's approximation of Γ (see *theorem 1* of [11]) we get

$$\operatorname{vol}(\mathcal{B}) = \bar{\Delta}^{-d} \left(1 + \sqrt{\frac{C_{3.5} \ln k}{d}} \right)^{d} \frac{(d\pi)^{\frac{d}{2}}}{\Gamma(\frac{d}{2} + 1)}$$

$$\leq (2\pi)^{\frac{d}{2}} k^{C_{1.5} \ln\left(\frac{2C_{3.2}}{c}\right) + C_{3.5}}$$
(.7)

so that

$$|\phi(z)| \le (2\pi)^{-\frac{d}{2}} \operatorname{vol}(\mathcal{B}) |\hat{s}(z)|$$

$$< k^{C_{1.5} \ln\left(\frac{2C_{3.2}}{c}\right) + C_{3.5}}$$

$$< k^{2C_{3.5}}$$

If z_1, \dots, z_m are independent (Lebesgue) uniformly distributed points in \mathcal{B} , then by Hoeffding's inequality from lemma 8, one has

$$\mathbb{P}\left[\left|I_{X} - \frac{1}{m} \sum_{l=1}^{m} e^{ix \cdot z_{l}} \phi(z_{l})\right| \ge k^{-2C_{3.5}}\right] \le k^{-2C_{3.5}}$$
(.8)

if we set

$$m = C_{0.1}C_{3.5}k^{8C_{3.5} + \frac{2C_{3.5}C_{3.2}^2}{c^2} + 2C_{1.5}\ln\left(\frac{2C_{3.2}}{c}\right) + C_{1.5}\ln(2\pi)}\ln k. \tag{.9}$$

Recalling that $||\hat{v}||_{L^{\infty}}$, $||\hat{\mu}_e||_{L^{\infty}} \leq (2\pi)^{-\frac{d}{2}}$, and

$$\hat{v}(z) = \mathbb{E}_{X \approx \mu} \left[(2\pi)^{-\frac{d}{2}} e^{-iX \cdot z + \frac{\|z\|^2}{2}} \right] = \mathbb{E} \left[e^{\frac{\|z\|^2}{2}} \hat{\mu}_e(z) \right],$$

for any fixed $z \in \mathcal{B}$, applying Hoeffding's inequality from lemma 8 once again, we obtain

$$\mathbb{P}\left[\left|\hat{v}(z) - e^{\frac{||z||^2}{2}}\hat{\mu}_e(z)\right| > \frac{k^{-C_{3.5}}}{\text{vol}(\mathcal{B})}\right] < \exp\left(-\frac{c_{0.1}n}{(2\pi)^{-\frac{d}{2}}k^{2C_{3.5}} + \frac{2C_{3.2}^2C_{3.5}}{c^2}}\text{vol}^2(\mathcal{B})\right)$$

In particular, letting

$$C_{3.6} \ge C_{0.1}C_{3.5} + C_{1.5} \left(\ln(2\pi) + 2\ln\left(\frac{2C_{3.2}}{c}\right) \right) + C_{3.5} \left(8 + \frac{2C_{3.2}^2}{c^2} \right)$$

and

$$n \ge C_{3.6}k^{C_{3.6}+C_{3.5}} \ln \left(C_{3.6}k^{C_{3.6}+C_{3.5}} \ln k \right)$$

$$m = C_{3.6}k^{C_{3.6}} \ln k$$
(.10)

one has

$$\mathbb{P}\left[\left|\hat{v}(z) - e^{\frac{||z||^2}{2}}\hat{\mu}_e(z)\right| > \frac{k^{-C_{3.5}}}{\text{vol}(\mathcal{B})}\right] < m^{-1}k^{-C_{3.5}}$$
(.11)

By an application of the union bound, inequalities $\ref{eq:2}$ 4, $\ref{eq:3}$ 4, and $\ref{eq:4}$ 9 give us this proposition.

2.5 Proof of proposition 2

Proof Each output q_l of algorithm 1 (as mentioned in algorithm 3 above) satisfies the inequality $||q_l - l||_2 < \frac{1}{4} diam(Q_\ell)$. Let \hat{Q}_ℓ be a ball of radius $C_{3.3} \bar{\Delta} \sqrt{\bar{d}}$, centered at ℓ . We will choose $C_{3.3} = 10^{-3} C_{3.2}$ appropriately. Suppose that y_{j_0} be the center such that $||y_{j_0} - q_\ell||_2 < \frac{1}{2} diam(Q_\ell)$; such a center may or may not exist, but we are only interested when it does exist. Without loss of generality (by translating the mixture appropriately), we may assume that $y_{j_0} = 0$.

Let λ be the Lebesgue measure on $\mathbb{R}^{\bar{d}}$. We would like to have affirmative answers to each of the following three questions: a) if we can well-approximate

$$w_{j_0} = \int_{\mathbb{R}^{\bar{d}}} \gamma_{\bar{\Delta}} \star \nu_{j_0} \ d\lambda$$

using the restricted integral

$${}^{1}\hat{w} = \int_{\hat{O}_{\ell}} \gamma_{\bar{\Delta}} \star \nu_{j_0} \ d\lambda;$$

b) if we can approximate \hat{w} using the mixture integral

$${}^{2}\hat{w} = \int_{\hat{Q}_{\ell}} \gamma_{\bar{\Delta}} \star \nu \ d\lambda;$$

and c) if we can approximate $^2\hat{w}$ using Monte-Carlo.

The first approximation amounts to bounding the following:

$$\left| w_{j_0} - \int_{\hat{Q}_{\ell}} \gamma_{\bar{\Delta}} \star \nu_{j_0} \, d\lambda \right| = \int_{\mathbb{R}^{\bar{d}} \setminus \hat{Q}_{\ell}} \gamma_{\bar{\Delta}} \star \nu_{j_0} \, d\lambda$$
$$= w_{j_0} \int_{||x|| \ge C_{3,3} \sqrt{\bar{d}}} \gamma_1 \, d\lambda$$

By Gaussian concentration results, we have

$$\left| w_{j_0} - \int_{\hat{Q}_{\ell}} \gamma_{\bar{\Delta}} \star \nu_{j_0} \, d\lambda \right| \le w_{j_0} C_{3,3}^{\bar{d}} e^{-\frac{\bar{d}(C_{3,3}^2 - 1)}{2}}$$

$$\le \frac{c w_{\min}}{10}$$
(.12)

as soon as

$$C_{3.3} \ge 3 \ln \left(\frac{1}{10c} \right) \tag{.13}$$

For the second approximation, we follow the general strategy as in lemma 10. Letting $\omega_{\bar{d}}$ be the volume of unit ball in $\mathbb{R}^{\bar{d}}$, and writing $p_m := |S_m|$ where

$$S_m := \left(r \in \left[k_0\right]: \ \tfrac{m}{2} \Delta \sqrt{\bar{d}} \leq ||y_r|| < \tfrac{m+1}{2} \Delta \sqrt{\bar{d}}\right),$$

one has

$$\omega_{\bar{d}} \left(\frac{\Delta \sqrt{\bar{d}}}{2} \right)^{\bar{d}} p_m \le \omega_{\bar{d}} \left(\frac{\Delta \sqrt{\bar{d}}}{2} \right)^{\bar{d}} \left((m+2)^{\bar{d}} - (m-1)^{\bar{d}} \right)$$

$$\Rightarrow p_m \le \left((m+2)^{\bar{d}} - (m-1)^{\bar{d}} \right)$$

$$< (m+2)^{\bar{d}}$$

which gives

$$\left| \int_{\hat{Q}_{\ell}} \gamma_{\bar{\Delta}} \star \nu \, d\lambda - \int_{\hat{Q}_{\ell}} \gamma_{\bar{\Delta}} \star \nu_{j_{0}} \, d\lambda \right|$$

$$= (2\pi\bar{\Delta}^{2})^{-\frac{\bar{d}}{2}} \sum_{m=2}^{\infty} \sum_{r \in [k_{0}] \setminus \{j_{0}\}, \frac{m}{2} \leq ||\frac{y_{r}}{\Delta\sqrt{\bar{d}}}|| < \frac{m+1}{2}} w_{r} \int_{\hat{Q}_{\ell}} e^{-\frac{C_{3,2}^{2}||x-y_{r}||^{2}}{2\Delta^{2}}} \, dx$$

$$< (ck)^{-1} \sum_{m=1}^{\infty} e^{-\frac{\bar{d}C_{3,2}^{2}(248m)^{2}}{2}}$$

$$< (ck)^{-1} \sum_{m=1}^{\infty} e^{-30000\bar{d}C_{3,2}^{2}m^{2}}$$

$$< \frac{cw_{min}}{10} \frac{10}{c^{2}e^{30000\bar{d}C_{3,2}^{2}}} \qquad (.14)$$

We proceed with the third approximation as follows. Let $v := \operatorname{vol}(\hat{Q}_{\ell})$; by Ramanujan's approximation of Γ (see *theorem 1* of [11]) we get

$$v \leq \left(\frac{2\pi e C_{3.3}^2}{\bar{d}}\right)^{\frac{\bar{d}}{2}} \bar{d}^{\frac{\bar{d}}{2}} \bar{\Delta}^{\bar{d}} \leq \bar{\Delta}^{\bar{d}} k^{\frac{1}{2}C_{1.5} \log(2\pi e C_{3.3}^2)}$$

Consider the identity

$$\int_{\hat{O}_{\ell}} \gamma_{\bar{\Delta}} \star \nu \ dx = \mathbb{E}_{U_{\hat{Q}_{\ell}}} \left[v \gamma_{\bar{\Delta}} \star \nu \right]$$

where $U_{\hat{Q}_{\ell}}$ is the uniform distribution on \hat{Q}_{ℓ} . Let $z_1, \dots, z_p \in \hat{Q}_{\ell}$ be uniformly random points; since $||\gamma \star \nu||_{L^{\infty}} \leq (2\pi\bar{\Delta}^2)^{-\frac{d}{2}}$, an application of Hoeffding's lemma 8 implies

$$\mathbb{P}\left[\left|\frac{1}{p}\sum_{j=1}^{p}\gamma_{\bar{\Delta}}\star\nu(z_{j})-\mathbb{E}_{U_{\hat{Q}_{\ell}}}\left[\gamma_{\bar{\Delta}}*\nu\right]\right|>\frac{\delta}{v}\right]\leq e^{-\frac{c_{0,1}(2\pi\bar{\Delta}^{2})\frac{d}{2}p\delta^{2}}{v^{2}}}$$

Thus, for

$$p \ge \frac{C_{3.5}}{c_{0.1}\delta^2} k^{\frac{C_{1.5}}{2} \ln(eC_{3.3}^2)} \ln k,$$

an application of proposition 1 and a union bound implies

$$\mathbb{P}\left[\left|\frac{1}{p}\sum_{j=1}^{p}\Re(f_{z_{j}}) - \mathbb{E}_{U_{\bar{Q}_{\ell}}}\left[\gamma_{\bar{\Delta}} \star \nu_{j}\right]\right| > \frac{\delta}{v} + 3k^{-C_{3.7}}\right] \\
\leq \mathbb{P}\left[\exists j \in [p] \text{ s.t } \left|\Re(f_{z_{j}}) - \gamma_{\bar{\Delta}} \star \nu(z_{j})\right| > 3k^{-C_{3.7}}\right] \\
+ \mathbb{P}\left[\left|\frac{1}{p}\sum_{j=1}^{p}\gamma_{\bar{\Delta}} \star \nu(z_{j}) - \mathbb{E}_{U_{\bar{Q}_{\ell}}}\left[\gamma_{\bar{\Delta}} \star \nu_{j}\right]\right| > \frac{\delta}{v}\right] \\
\leq 20k^{-C_{3.5}}$$

We write $\tilde{v}_{j_0} = v - v_{j_0}$, and

$$\hat{w}_{\ell} := \frac{v}{p} \sum_{i=1}^{p} \Re(f_{z_j})$$

where z_1, \dots, z_p are independent uniformly random points in \hat{Q}_{ℓ} . Then

$$\begin{aligned} \left| w_{j_0} - \hat{w}_{\ell} \right| &\leq \int_{\mathbb{R}^{\bar{d}} \setminus \hat{Q}_{\ell}} \gamma_{\bar{\Delta}} \star \nu_{j_0} \, d\lambda + \left| \int_{\hat{Q}_{\ell}} \gamma_{\bar{\Delta}} \star \nu \, d\lambda - \hat{w}_{\ell} \right| + \left| \int_{\hat{Q}_{\ell}} \gamma_{\bar{\Delta}} \star \tilde{\nu}_{j_0} \, d\lambda \right| \\ &\leq \frac{cw_{min}}{5} + \left(\delta + 3vk^{-C_{3.7}} \right) \end{aligned}$$

3 Analysis of algorithm 3

The following lemma shows that the number of cubes in algorithm 3 that need to be considered is polynomial in k.

Lemma 9 For any $x \in \mathbb{R}^d$,

$$\left| \left(\frac{\bar{\Delta}}{1000} \sqrt{\frac{d}{C_{1.5} \log k}} \right) \mathbb{Z}^d \bigcap B_2(x, 2\sqrt{d}) \right| \le k^{C_7}$$

Proof Set r to \sqrt{d} . We observe that the number of lattice cubes of side length $cr/\sqrt{\log k}$ centered at a point x belonging to $\left(cr/\sqrt{\log k}\right)\mathbb{Z}^d$ that intersect a ball B of radius r in d dimensions is less or equal to to the number of lattice points inside a concentric ball B' of dimension d of radius $r + \frac{c\sqrt{d}r}{\sqrt{\log k}}$. Every lattice cube of side length $cr/\sqrt{\log k}$ centered at a lattice point belonging to $\left(cr/\sqrt{\log k}\right)\mathbb{Z}^d\cap B'$ is contained in the ball B'' with center x and radius $r + \frac{2c\sqrt{d}r}{\sqrt{\log k}}$. By volumetric considerations, $|\left(cr/\sqrt{\log k}\right)\mathbb{Z}^d\cap B'|$ is therefore bounded above by $\frac{vol(B'')}{\left(cr/\sqrt{\log k}\right)^d}$.

We write $v_d := \operatorname{vol}\left(B_2(0, \sqrt{d})\right)$. By Ramanujan's approximation of Γ (see *theorem 1* of [11]) we get

$$v_d \le \frac{1}{\sqrt{\pi}} \left(\frac{2\pi e}{d}\right)^{\frac{d}{2}} d^{\frac{d}{2}}$$

This tells us that

$$\begin{split} \frac{vol(B'')}{\left(cr/\sqrt{\log k}\right)^d} & \leq \left(\frac{C\sqrt{\log k}}{\sqrt{d}}\right)^d \\ & \leq \left(\frac{C\sqrt{\log k}}{\sqrt{d}}\right)^{\left(\frac{\sqrt{d}}{C\sqrt{\log k}}\right)} \left(C\sqrt{d\log k}\right) \\ & \leq \left(e^{1/e}\right)^{\left(C\sqrt{d\log k}\right)} \\ & \leq k^{C_7} \end{split}$$

We have used the fact that for $\alpha > 0$, $\alpha^{\alpha^{-1}}$ is maximized when $\alpha = e$, a fact easily verified using calculus.

We will need some results on the structure of $\gamma_{\bar{\Lambda}} \star \nu$.

Lemma 10 If $q_{\ell} \in B(y_j, diam(Q_{\ell}))$ for some $j \in [k_0]$, then the restriction of $\gamma_{\bar{\Delta}} \star \nu$ to Q_{ℓ} is approximately log-concave in the following sense. For $\nu_j := w_j \delta_{y_j}$, and $x \in Q_{\ell}$, we have

$$0 \leq \log(\gamma_{\bar{\Delta}} \star \nu)(x) - \log(\gamma_{\bar{\Delta}} \star \nu_j)(x) \leq \frac{C_{103}}{c^2 \bar{d}^{C_{100}}}$$

Proof Fix $x \in Q_{\ell}$, and write $a_r := x - y_r$ for $r \in [k_0]$. One has

$$||a_j|| \le \frac{1.1\Delta\sqrt{\bar{d}}}{100C_{3.2}}\sqrt{\frac{\bar{d}}{C_{1.5}\log k}} + \frac{\Delta\sqrt{\bar{d}}}{200C_{3.2}}\sqrt{\frac{\bar{d}}{C_{1.5}\log k}} \le \frac{3.2\Delta\sqrt{\bar{d}}}{200C_{3.2}}$$

and

$$||a_r - a_s|| \ge \Delta \sqrt{\bar{d}}$$

if $r \neq s$. Rewriting $\Delta = C_{3.2}\bar{\Delta}$, one has

$$(2\pi\bar{\Delta}^{2})^{\frac{\bar{d}}{2}} \left| (\gamma_{\bar{\Delta}} \star \nu)(x) - (\gamma_{\bar{\Delta}} \star \nu_{j})(x) \right| = \sum_{r \in [k_{0}] \setminus \{j\}} w_{r} e^{-\frac{||a_{r}||^{2}}{2\bar{\Delta}^{2}}}$$

$$= \sum_{m=1}^{\infty} \sum_{r \in [k_{0}] \setminus \{j\}, \ \frac{m}{2} \le ||\frac{a_{r}}{\bar{\Delta}\sqrt{\beta}}|| < \frac{m+1}{2}} w_{r} e^{-\frac{C_{3,2}^{2}||a_{r}||^{2}}{2\bar{\Delta}^{2}}}$$

We write $p_m := |S_m|$ where

$$S_m := \left(r \in [k_0] : \frac{m}{2} \Delta \sqrt{\bar{d}} \le ||a_r|| < \frac{m+1}{2} \Delta \sqrt{\bar{d}} \right)$$

Since $||a_r - a_s|| \ge \Delta \bar{d}$, we can put disjoint balls of radius $0.5\Delta\sqrt{\bar{d}}$ around each a_r . Thus, letting $\omega_{\bar{d}}$ be the volume of unit ball in $\mathbb{R}^{\bar{d}}$, one has

$$\omega_{\bar{d}} \left(\frac{\Delta \sqrt{\bar{d}}}{2} \right)^{\bar{d}} p_m \le \omega_{\bar{d}} \left(\frac{\Delta \sqrt{\bar{d}}}{2} \right)^{\bar{d}} \left((m+2)^{\bar{d}} - (m-1)^{\bar{d}} \right)$$

$$\Rightarrow p_m \le \left((m+2)^{\bar{d}} - (m-1)^{\bar{d}} \right)$$

$$< (m+2)^d$$

which gives

$$(2\pi\bar{\Delta}^{2})^{\frac{d}{2}} \left| (\gamma_{\bar{\Delta}} \star \nu)(x) - (\gamma_{\bar{\Delta}} \star \nu_{j})(x) \right| = \sum_{m=1}^{\infty} \sum_{r \in [k_{0}] \setminus \{j\}, \ \frac{m}{2} \le ||\frac{a_{r}}{\Delta\sqrt{d}}|| < \frac{m+1}{2}} w_{r} e^{-\frac{C_{3,2}^{2} ||a_{r}||^{2}}{2\Delta^{2}}}$$

$$\leq (ck)^{-1} \sum_{m=1}^{\infty} e^{-\frac{d(C_{3,2}^{2} m^{2} - 8 \ln(m+2))}{8}}$$

$$\leq (ck)^{-1} \sum_{m=1}^{\infty} e^{-\frac{d(C_{3,2}^{2} m^{2})}{16}}$$

We use $e^{-x} < \frac{C_{100}^{C_{100}}}{x_{c}^{C_{100}}}$ and $\sum m^{-2C_{100}} < 10$ to obtain

$$\begin{split} (2\pi\bar{\Delta}^2)^{\frac{\bar{d}}{2}} \left| (\gamma_{\bar{\Delta}} \star \nu)(x) - (\gamma_{\bar{\Delta}} \star \nu_j)(x) \right| &\leq (ck)^{-1} \sum_{m=1}^{\infty} e^{-\frac{\bar{d}C_{3,2}^2 m^2}{16}} \\ &\leq \frac{(16C_{101})^{C_{100}}}{ck\bar{d}^{C_{100}} C_{3.2}^{2C_{100}}} \sum_{m=1}^{\infty} \frac{1}{m^{2C_{100}}} \\ &\leq \frac{C_{102}}{ck\bar{d}^{C_{100}}} \end{split}$$

Note that $\gamma_{\bar{\Delta}} \star \nu_j$ is log-concave. Moreover, for any $x \in Q_l$, one has

$$(\gamma_{\bar{\Delta}} \star \nu_j)(x) = (2\pi\bar{\Delta}^2)^{-\frac{\bar{d}}{2}} w_j e^{-\frac{||x-y_j||^2}{2\bar{\Delta}^2}}$$

$$\geq \frac{c}{k(2\pi\bar{\Delta}^2)^{\frac{\bar{d}}{2}}} e^{-\frac{1.21\bar{d}}{20000C_{1.5}\ln k}}$$

$$\geq \frac{c}{k(2\pi\bar{\Delta}^2)^{\frac{\bar{d}}{2}}} e^{-\frac{1.21}{20000}}$$

so that

$$\left| \frac{(\gamma_{\bar{\Delta}} \star \nu)(x)}{(\gamma_{\bar{\Delta}} \star \nu_j)(x)} - 1 \right| \leq \frac{1}{(2\pi\bar{\Delta}^2)^{\frac{\bar{d}}{2}}} \frac{C_{102}}{ck\bar{d}^{C_{100}}} \frac{k(2\pi\bar{\Delta}^2)^{\frac{\bar{d}}{2}}}{c} e^{\frac{1.21}{20000}}$$
$$\leq \frac{C_{102}e^{\frac{1.21}{20000}}}{c^2\bar{d}^{C_{100}}}$$

This gives

$$0 \leq \log(\gamma_{\bar{\Delta}} \star \nu)(x) - \log(\gamma_{\bar{\Delta}} \star \nu_{j})(x)$$

$$= \log\left(1 + \frac{C_{102}e^{\frac{1.21}{20000}}}{c^{2}\bar{d}^{C_{100}}}\right)$$

$$\leq \frac{C_{102}e^{\frac{1.21}{20000}}}{c^{2}\bar{d}^{C_{100}}} \tag{.15}$$

Remark 5 Note that, by remark 2 and convexity of Q_{ℓ} , if

$$q_{\ell} \in B\left(y_{j}, \left(\frac{\bar{\Delta}\bar{d}}{200}\sqrt{\frac{1}{C_{1.5}\log k}}\right)\right)$$

then (with high probability) $\log(\gamma_{\bar{\Lambda}} \star \nu_j)$ is *t*-Lipschitz for

$$t \le \frac{(ck\sqrt{\ln(C_1dn)} + C_{3.2})\sqrt{C_{1.5}\log k}}{c^3}$$

The following lemma shows that every true spike of $\gamma_{\bar{\Delta}} \star \nu$ corresponding to a center gets detected by algorithm 3.

Lemma 11 If $q_{\ell} \in B\left(y_{j}, \left(\frac{\bar{\Delta}\bar{d}}{200}\sqrt{\frac{1}{C_{1.5}\log k}}\right)\right)$ for some $j \in [k_{0}]$, then

$$(\gamma_{\bar{\Delta}} \star \nu)(q_{\ell}) - k^{-C_{3.5}} \ge (\frac{w_{min}}{2})\gamma_{\bar{\Delta}}(0)$$

Proof By lemma 10 the restriction to Q_{ℓ} of $\gamma_{\bar{\Lambda}} \star \nu$ is approximately log-concave. The output q_{ℓ} of stochastic optimization algorithm \mathfrak{A}_0 satisfies

$$\left|\log m_{\ell} - \log(\gamma_{\bar{\Delta}} \star \nu)(q_{\ell})\right| \leq \frac{1}{C_{103.1}\bar{d}^{C_{100}}}$$

where $m_{\ell} := \max\{(\gamma_{\bar{\Delta}} \star \nu)(x) : x \in Q_{\ell}\}$. Equivalently,

$$m_{\ell} - (\gamma_{\bar{\Delta}} \star \nu)(q_{\ell}) \leq (\gamma_{\bar{\Delta}} \star \nu)(q_{\ell}) \left(1 - e^{-\frac{1}{C_{103.1}\bar{d}^{C_{100}}}}\right)$$

$$\leq \frac{(\gamma_{\bar{\Delta}} \star \nu)(q_{\ell})}{C_{103.1}\bar{d}^{C_{100}}}$$

$$\Rightarrow (\gamma_{\bar{\Delta}} \star \nu)(q_{\ell}) \geq m_{\ell} - \frac{(\gamma_{\bar{\Delta}} \star \nu)(q_{\ell})}{C_{103.1}\bar{d}^{C_{100}}}$$

which proves the lemma.

The next lemma shows that there are no false spikes in $\gamma_{\bar{\Delta}} \star \nu$.

Lemma 12 If $(\gamma_{\bar{\Delta}} \star \nu)(q_{\ell}) + k^{-C_{3.5}} \ge (\frac{w_{min}}{2})\gamma_{\bar{\Delta}}(0)$, then there exists some $j \in [k_0]$ such that $q_{\ell} \in B\left(y_j, \frac{\sqrt{\bar{d}}(\Delta\bar{\Delta})^{\frac{1}{2}}}{5}\right)$.

Proof The arguments are similar to that in lemma 10 above. Suppose that

$$q_{\ell} \notin \bigcup_{j \in [k_0]} B\left(y_j, \frac{\sqrt{\bar{d}}(\Delta \bar{\Delta})^{\frac{1}{2}}}{5}\right),$$

and write $a_i := y_i - q_\ell$. For $m \ge 1$, let $p_m := |S_m|$ where

$$S_m := \left(r \in [k_0]: \left(\frac{m}{2} + \frac{1}{5\sqrt{C_{3,2}}}\right)\Delta\sqrt{\bar{d}} \le ||a_r|| < \left(\frac{m+1}{2} + \frac{1}{5\sqrt{C_{3,2}}}\right)\Delta\sqrt{\bar{d}}\right)$$

One has

$$\begin{split} (\gamma_{\bar{\Delta}} \star \nu)(q_{\ell}) &= \gamma_{\bar{\Delta}}(0) \sum_{j \in [k_{0}]} w_{j} e^{-\frac{||a_{j}||^{2}}{2\bar{\Delta}^{2}}} \\ &= \gamma_{\bar{\Delta}}(0) \left(\sum_{j \in [k_{0}], \ 0 \leq ||\frac{a_{j}}{\Delta \sqrt{d}}|| - \frac{1}{5\sqrt{C_{3}}} < \frac{1}{2}} w_{r} e^{-\frac{||a_{j}||^{2}}{2\bar{\Delta}^{2}}} + \sum_{m=1}^{\infty} \sum_{j \in S_{m}} w_{r} e^{-\frac{||a_{j}||^{2}}{2\bar{\Delta}^{2}}} \right) \end{split}$$

Since $||a_r - a_s|| \ge \Delta \bar{d}$, we can put disjoint balls of radius $0.5\Delta \sqrt{\bar{d}}$ around each a_r . Thus,

$$p_m \le 2^{\bar{d}} \left(\left(\frac{m+2}{2} + \frac{1}{5\sqrt{C_{3.2}}} \right)^{\bar{d}} - \left(\frac{m-1}{2} + \frac{1}{5\sqrt{C_{3.2}}} \right)^{\bar{d}} \right)$$

$$< (m+2)^{\bar{d}}$$

which gives

$$\begin{split} (\gamma_{\bar{\Delta}} \star \nu)(q_{\ell}) &= \gamma_{\bar{\Delta}}(0) \left(\sum_{j \in [k_{0}], \ 0 \leq ||\frac{a_{j}}{\Delta \sqrt{d}}|| - \frac{1}{5\sqrt{C_{3,2}}} < \frac{1}{2}} w_{r} e^{-\frac{||a_{j}||^{2}}{2\bar{\Delta}^{2}}} + \sum_{m=1}^{\infty} \sum_{j \in S_{m}} w_{r} e^{-\frac{||a_{j}||^{2}}{2\bar{\Delta}^{2}}} \right) \\ &\leq \frac{C\gamma_{\bar{\Delta}}(0)}{k} \left(e^{-\frac{C_{3,2}\bar{d}}{50}} + \sum_{m=1}^{\infty} e^{-\frac{\bar{d}C_{3,2}m^{2}}{16}} \right) \\ &< \frac{C\gamma_{\bar{\Delta}}(0)}{k} \left(e^{-\frac{C_{3,2}\bar{d}}{50}} + \frac{2000}{\bar{d}^{2}C_{3,2}^{2}} \right) \end{split}$$

Thus, for $C_{3.2}$ sufficiently large, the inequality

$$(\gamma_{\bar{\Delta}} \star \nu)(q_\ell) + k^{-C_{3.5}} < \left(\frac{w_{min}}{2}\right) \gamma_{\bar{\Delta}}(0)$$

holds, proving the lemma.

Lemma 13 If there exists some $j \in [k_0]$ such that

$$q_{\ell} \in B\left(y_{j}, \frac{\sqrt{\bar{d}}(\Delta\bar{\Delta})^{\frac{1}{2}}}{5}\right),$$

and $|q_{\ell} - \ell| < diam(Q_{\ell})/4$, then with high probability, there exists some $j \in [k_0]$ such that $q_{\ell} \in B\left(y_j, c\bar{d}^{-\frac{5}{2}}\right)$.

Proof If
$$x \in B\left(y_j, \frac{\sqrt{\overline{d}}(\Delta \overline{\Delta})^{\frac{1}{2}}}{5}\right)$$
, by lemma 10,

$$0 \le \ln(\gamma_{\bar{\Delta}} \star \nu)(x) - \ln(\gamma_{\bar{\Delta}} \star \nu_j)(x) \le \frac{1}{K\bar{d}^5},$$

where K is an absolute constant that can be made arbitrarily large. We note that $\ln(\gamma_{\bar{\Delta}} \star \nu_j)(x) = a - \left(\frac{1}{2\bar{\Delta}^2}\right) \|x - y_j\|^2$, for some constant a. This implies that if

$$|\ln(\gamma_{\bar{\Delta}} \star \nu)(q_{\ell}) - \sup_{x} \ln(\gamma_{\bar{\Delta}} \star \nu)(x)| < \frac{2}{K\bar{d}^{5}},$$

then $q_{\ell} \in B\left(y_{j}, c\bar{\Delta}\bar{d}^{-\frac{5}{2}}\right)$. However, $|\ln(\gamma_{\bar{\Delta}} \star \nu)(q_{\ell}) - \sup_{x} \ln(\gamma_{\bar{\Delta}} \star \nu)(x)|$ is indeed less than $\frac{2}{K\bar{d}^{5}}$ by proposition 1 and lemma 5. Noting that $\bar{\Delta} < c$, this completes the proof of this lemma.

The following proposition shows that every spike extracted out of $\gamma_{\bar{\Delta}} \star \nu$ by algorithm 3, is within ϵ/k of some y_i .

Proposition 3 With probability at least $1 - \exp(-k/c)$, the following is true: The Hausdorff distance between $\{y_1, \ldots, y_{k_0}\}$ and $\{\ell_{m_1}, \ldots, \ell_{m_{k_2}}\}$ (which corresponds to the output of algorithm 1 as mentioned in algorithm 3 above) is less than ϵ/k .

Proof Consider the sequence L in algorithm 3. Note that, we know from the statements in lemma 11, lemma 12 and lemma 13 that

• If
$$q_{\ell} \in \bigcup_{j \in [k_0]} B\left(y_j, \left(\frac{\bar{\Delta}\bar{d}}{200}\sqrt{\frac{1}{C_{1.5}\log k}}\right)\right)$$
, then

$$(\nu \star \gamma_{\bar{\Delta}})(q_{\ell}) - k^{-C_{3.5}} \ge \left(\frac{w_{min}}{2}\right) \gamma_{\bar{\Delta}}(0).$$

• If $(\gamma_{\bar{\Delta}} \star \nu)(q_\ell) + k^{-C_{3.5}} \ge (\frac{w_{min}}{2})\gamma_{\bar{\Delta}}(0)$, then there exists some $j \in [k_0]$ such that

$$q_{\ell} \in B\left(y_{j}, \frac{\sqrt{\bar{d}}(\Delta\bar{\Delta})^{\frac{1}{2}}}{5}\right)$$

• If there exists some $j \in [k_0]$ such that

$$q_{\ell} \in B\left(y_{j}, \frac{\sqrt{\bar{d}}(\Delta\bar{\Delta})^{\frac{1}{2}}}{5}\right),$$

and (as is true from algorithm 3), $|q_{\ell} - \ell| < diam(Q_{\ell})/4$, then with probability at least $1 - \exp(\frac{-k}{c})$, there exists some $j \in [k_0]$ such that $q_{\ell} \in B\left(y_j, c\bar{d}^{-\frac{5}{2}}\right)$.

We have shown that L is, with high probability, contained in

$$\bigcup_{j\in[k_0]}B(y_j,c\bar{d}^{-5/2})$$

Moreover, we observe that for each $j \in [k_0]$ there must exist a q_ℓ such that $q_\ell \in B\left(y_j, c\bar{d}^{-\frac{5}{2}}\right)$, by the exhaustive choice of starting points. This proposition now follows from Theorem 4.1 of [15].

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