Gaussian mixture model decomposition of multivariate signals

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Abstract

We propose a greedy variational method for decomposing a non-negative multivariate signal as a weighted sum of Gaussians which, borrowing the terminology from statistics, we refer to as a Gaussian mixture model (GMM). Mixture components are added one at the time in two steps. In the first step, a new Gaussian atom and an amplitude are chosen based on a heuristic that aims to minimize the 2-norm of the residual. In the second step the 2-norm of the residual is further decreased by simultaneously adjusting all current Gaussians. Notably, our method has the following features: (1) It accepts multivariate signals, i.e. sampled multivariate function, histograms, time series, images, etc. as input. (2) The method can handle general (i.e. ellipsoidal) Gaussians. (3) No prior assumption on the number of mixture components is needed. To the best of our knowledge, no previous method for GMM decomposition simultaneously enjoys all these features. Since finding the optimal atom is a non-convex problem, an important point is how to initialize each new atom. We initialize the mean at the maximum of the residual. As a motivation for this initialization procedure, we prove an upper bound, which cannot be improved by a global constant, for the distance from any mode of a GMM to the set of corresponding means. For mixtures of spherical Gaussians with common variance $\sigma^2$, the bound takes the simple form $\sqrt{n}\sigma$. We evaluate our method on one- and two-dimensional signals. We also discuss the relation between clustering and signal decomposition, and compare our method to the baseline expectation maximization algorithm.

1 Introduction

Mixtures of Gaussians are often used in clustering to fit a probability distribution to some given sample points. In this work we are concerned with the related problem of approximating a non-negative but otherwise arbitrary signal by a sparse linear combination of potentially anisotropic Gaussians. Our interest in this problem stems mainly from its applications in transmission electron microscopy (TEM). The output of the TEM reconstruction procedure is a 3D voxelized structure that ideally represents the electrostatic potential of the imaged specimen. Via a process known in the TEM-community as coarse-graining, it is common to express this 3D structure as a linear combination of Gaussians [Kaw18, Jou16, JS16a, JS16b]. This speeds up post-processing tasks such as fitting an atomic model to the structure [Kaw18], but one can also use coarse-graining as a form of denoising [JS16b].

There are two classes of methods for GMM decomposition of multivariate signals in the literature. Methods of the first class are based on the expectation maximization algorithm that is commonly used for fitting a GMM to a point-cloud, and adapt it to input data in the form of multi-variate signals.

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Preprint. Under review.
The second class is the class of greedy variational methods \cite{F99,JS16a,KBGP18}. The proposed method, which belongs to the latter class, is similar to and is inspired by both \cite{KBGP18} and \cite{JS16a}. It is a continuously parameterized analogue of orthogonal matching pursuit where at each iteration the 2-norm of the error is non-increasing. It is mainly motivated by the fact that previous work on decomposition of multivariate-signals as GMMs either did not allow for arbitrary covariances, or the number of Gaussian components had to be set before-hand.

We complement our algorithm with a theorem (Theorem \ref{thm:upper_bound}) that upper-bounds the distance from a local maximum of a GMM to the set of mean vectors. This provides theoretical support for our initialization of each new mean vector at a maximum of the residual. We remark that Theorem \ref{thm:upper_bound} could also be of interest in its own right; whereas the number of modes of Gaussian mixtures have been investigated previously \cite{CP00,AEH17}, the authors of this paper are not aware of any existing quantitative bounds on the distance from a mode of a GMM to its mean vectors.

The rest of this paper is organized as follows. Section 2 contains a description of the proposed algorithm together with numerical examples. In section 3 we state and prove the afore-mentioned upper bound. Finally, in section 4 we provide a conclusion.

## 2 Proposed method

For \( x_0 \in \mathbb{R}^n \) and \( \Sigma \in \mathbb{R}^{n \times n} \) symmetric non-negative definite we define \( g(x_0, \Sigma) \) as the Gaussian density in \( n \) dimensions with mean vector \( x_0 \) and covariance matrix \( \Sigma^2 \), i.e.

\[
g(x_0, \Sigma)(x) := C_\Sigma \exp \left\{ -\frac{1}{2} (x - x_0)^T \Sigma^{-2} (x - x_0) \right\},
\]

where \( C_\Sigma \) is a normalizing factor, ensuring that \( |g(x_0, \Sigma)|_1 = 1 \). Further, by a Gaussian mixture model (GMM) we mean a linear combination of the form

\[
\sum_{m=1}^{M} a_m g(x_m, \Sigma_m), \quad a_m > 0, M > 0.
\]

The proposed method takes as input a non-negative signal \( d \in \mathbb{R}^{k_1 \times \cdots \times k_n} \), where \( k_i \) is the number of grid-points along the \( i \)-th variable. The output is a list of GMM parameters, i.e. it is a list \( (a_m^*, x_m^*, \Sigma_m^*)_{m=1}^M \) of weights, mean vectors and square roots of covariance matrices. The aim of the method is firstly that the residual

\[
r := d - \sum_{m=1}^{M} a_m^* g(x_m^*, \Sigma_m^*)
\]

should have a small 2-norm. Secondly, the approximation should be sparse, i.e. the number of Gaussians \( M \) in the sum should ideally be as small as possible given the 2-norm of the residual.

In each iteration of our algorithm, a new Gaussian is added to the GMM by a procedure that corresponds to one iteration of a continuously parametrized version of matching pursuit (MP), c.f. \cite{MZ93}. The starting guess \( x_0 \) for the mean vector is defined to be a global maximum of \( r' \), which is a smoothed version of the current residual \( r \). Likewise \( \Sigma_0 \) is set to be a square root of the matrix of second-order moments of \( r''_0 \), where \( r'' \) is \( r \) restricted to a neighborhood of \( x_0 \). The initial weight \( a_0 \) is given by projecting the Gaussian atom defined by \( (x_0, \Sigma_0) \) onto the residual, i.e. it is given as the global minimum of the convex objective \( a \rightarrow |r - a g(x_0, \Sigma_0)|_2^2, a \geq 0 \).

We found that this vanilla MP-type of approach was by itself not capable of producing a good approximation. Because of this, in our method the already obtained Gaussians are updated in a way that bears some resemblance to the projection step of orthogonal MP (OMP) \cite{PRK93}. Starting from \( (a_0, x_0, \Sigma_0) \), the parameters defining the most recently added Gaussian are updated by minimizing the 2-norm of the residual. The final step of an outer iteration is to simultaneously adjust all

\[^3\text{We do not require the GMM to be normalized, i.e. we do not require that } \sum_{m=1}^{M} a_m = 1.\]

\[^4\text{This step is not crucial for the performance of the algorithm, but was empirically found to improve the final data-fit.}\]
Gaussians in the current GMM, again by minimizing the 2-norm of the residual. We propose to use the L-BFGS-B [BLNZ95] method with non-negativity constraints on the weights for all of the three afore-mentioned minimization problems. Our algorithm runs until some user-specified stopping criterion is met and is summarized in pseudo-code in Algorithm 1.

We now assess the space- and time complexity of the proposed method in terms of the final number $M$ of Gaussians used and the dimension $n$ of the input signal. Let $N_i$ denote the number of parameters of $i$ Gaussians, so $N_i = \mathcal{O}(n^2)$. The most demanding step of a single outer iteration of the proposed algorithm is the simultaneous adjustment of all Gaussians. If this step is done using L-BFGS-B, this amounts to a cost of $\mathcal{O}(N_i)$, both in terms of space and time [BLNZ95]. Summing over the $M$ iterations we hence find the space- and time requirements of the proposed method to be $\mathcal{O}(M^2n^2)$.

### Table 1: Input GMM parameters

| Exp. 1 | Exp. 2 | Exp. 3 |
|-------|-------|-------|
| $a_m$ | $x_m$ | $\Sigma_m^2$ | $a_m$ | $x_m$ | $\Sigma_m^2$ | $a_m$ | $x_m$ | $\Sigma_m^2$ |
| 1     | 0     | 1      | 2     | (−1.5, −2.5981) | (0.7969, 1.272) | 5     | (−5, 5) | Id$_2$ |
| 8     | 0     | 4      | 2     | (−1.5, 2.5981)  | (0.7969, −1.272) | 1     | (5, −5) | Id$_2$ |
| 1     | −2    | 1      | 2     | (3, 0)          | (3, 0, 0.0625)  | 3     | (5, 5)  | Id$_2$ |
| 1     | 2     | 1      | 1     | (−1.75, −3.0311) | (1, 0)          | 4     | (−5, −5) | Id$_2$ |
| 1     | −8    | 1      | 0     | (0, 2)          | (−2, 0)         | 5     | (0, −2) | Id$_2$ |
| 1     | 8     | 1      | 5     | (0, 2)          | (0, 2)          | 5     | (0, 2)  | Id$_2$ |

### Algorithm 1

1: **procedure** GMM decomposition

   **Input:** Signal $d$, hyper-parameters $\tau_1, \tau_2 \in \mathbb{Z}_+$

   **Output:** GMM parameters $(a_m^*, x_m^*, \Sigma_m^*)_{M=1}^M$

2: $M \leftarrow 0$, $r \leftarrow d$

3: while stopping criterion is not met do

4: $M \leftarrow M + 1$

5: $r'(y) \leftarrow \frac{1}{\tau_1} \sum_{z \in A(y)} r(z)$, where $A(y) := \{ \tau_1 \text{ grid points closest to } y\}$

6: $x_0 \leftarrow \arg \max_y r'(y)$

7: $r'' \leftarrow$ restriction of $r$ to the $\tau_2$ grid points closest to $x_0$

8: $\Sigma_0 \leftarrow \text{square root of the matrix of second-order moments of } \frac{r''}{|r''|_1}$

9: $a_0 \leftarrow \arg \min_{a \geq 0} |r - ag(x, \Sigma))|^2_2$

10: $(a^*, x^*, \Sigma^*) \leftarrow \text{local minimum of } |r - ag(x, \Sigma)|^2_2, a \geq 0$

11: $(a_M^*, x_M^*, \Sigma_M^*) \leftarrow (a^*, x^*, \Sigma^*)$

12: $(a_m^*, x_m^*, \Sigma_m^*)_{M=1}^M \leftarrow (a_m^*, x_m^*, \Sigma_m^*)_{M=1}^M$

13: $(a_m^*, x_m^*, \Sigma_m^*)_{M=1}^M \leftarrow \text{local minimum of } \left| d - \sum_{m=1}^M a_m g(x_m, \Sigma_m) \right|^2_2, a_m \geq 0$

14: $r \leftarrow d - \sum_{m=1}^M a_m^* g(x_m^*, \Sigma_m^*)$

### 2.1 Main numerical results

As proof of concept for the proposed method, we ran our algorithm on small toy-examples in 1D and 2D. We refer to the examples as Experiment 1 – Experiment 3, see Figures 1–3. A
We attribute this to the greedy nature of the algorithm where a predefined number of modes is not enforced in the decomposition. As stopping criterion we used SNR where \( \epsilon \)

\[
\text{SNR} := 10 \log_{10} \frac{\text{Var}(d_{\text{clean}})}{\text{Var}(\epsilon)}.
\]

Table 2: Output GMM parameters from Exp. 1 and Exp. 2

|            | Exp. 1       | Exp. 2       |
|------------|--------------|--------------|
|            | \(a_m\) \(x_m\) \(\Sigma_m^2\) \(a_m\) \(x_m\) \(\Sigma_m^2\) |
| 5.0272     | 1.3052 2.2632 1.9833 \((-1.4937, -2.5862)\) | 0.5758 1.1181 |
| 1.0116     | -7.9756 0.9512 1.9901 \((3.0075, -9.7258 \times 10^{-4})\) | 2.982 0.0082 |
| 1.0351     | 8.0478 1.1041 2.001 \((-1.4994, 2.5924)\) | 0.7858 -1.2663 |
| 5.8708     | -1.1215 2.4119 1.0101 \((-1.7466, -3.038)\) | 0.9878 0.0126 |

Table 3: Output GMM parameters from Exp. 3

|            | \(a_m\) \(x_m\) \(\Sigma_m^2\) |
|------------|------------------|------------------|
| 4.9685     | \((9.7331 \times 10^{-4}, 2.0079)\) \((0.9781 0.0125)\) | \((0.0125 1.012)\) |
| 4.9517     | \((-4.9988, 5.0024)\) \((1.0006 0.0127)\) | \((0.0127 1.0103)\) |
| 3.9821     | \((-5.005, -4.9978)\) \((0.9999 0.0017)\) | \((0.0017 0.9731)\) |
| 2.9853     | \((4.9935, 5.0071)\) \((0.9955 -0.0308)\) | \((-0.0308 0.9976)\) |
| 5.0608     | \((-1.9916, 0.0076)\) \((1.0128 0.0154)\) | \((0.0154 0.9977)\) |
| 5.0322     | \((0.0034, -1.9952)\) \((0.9968 0.0145)\) | \((0.0145 1.0038)\) |
| 1.0048     | \((5.0158, -5.0174)\) \((1.007 0.0083)\) | \((0.0083 1.0034)\) |
| 4.9247     | \((2.0213, 0.0077)\) \((0.9743 -0.0097)\) | \((-0.0097 0.9997)\) |

clean signal \(d_{\text{clean}}\) was generated by discretizing GMMs with parameters as in Table 1 to the grids \{\(y_k = -10 + 20k/1000\)\} \(k=0\) \((1000)\) and \{\(y_k, \epsilon = (-10 + 20k/65, -10 + 20k/65)\)\} \(64\) \(\epsilon = 0\) in the one- and two-dimensional experiments respectively. From this, noisy data was then generated as \(d = d_{\text{clean}} + \epsilon\) where \(\epsilon\) is white Gaussian noise with standard deviation \(\sigma_{\text{noise}}\). The latter was chosen so that SNR = 20, where we define SNR by:

\[
\text{SNR} := 10 \log_{10} \frac{\text{Var}(d_{\text{clean}})}{\text{Var}(\epsilon)}.
\]

As stopping criterion we used \(\text{SNR}_{\text{stop}} \geq 20\), where

\[
\text{SNR}_{\text{stop}} := 10 \log_{10} \frac{\text{Var}(d_{\text{est}})}{\text{Var}(d - d_{\text{est}})},
\]

and where \(d_{\text{est}} := \sum_{m} a_{m} g(x_m^*, \Sigma_m^*)\). In all minimization sub-procedures we used the L-BFGS-B method with non-negativity constraints on the weights and ran it until convergence. Hyper-parameters \(\tau_1\) and \(\tau_2\) (introduced in line 5 and 7 in Algorithm 1) should ideally be chosen based on the amount of noise in the data, however we found that the exact values were not so important in our toy examples, and we used the ad-hoc chosen values \(\tau_1 = 10\) and \(\tau_2 = 20\). We leave a more careful sensitivity analysis with respect to these parameter to future studies. The total run-time was a few minutes on a computer with an Intel Pentium CPU running at 2.90GHz, using \(\sim 8\) GB of RAM. The final results of our experiments are tabulated in Tables 2 and 3 and are plotted in Figures 1-3. Intermediate results for the 2D experiments are plotted in Figures 4-5.

Remark 2.1. The number of modes of a GMM is not necessarily equal to the number of means. Indeed, there might be more modes than means \([\text{AEH17}]\). Alternatively, there could be fewer modes than means, for example, in Experiment 2, a low amplitude Gaussian and high amplitude Gaussian are close to each other, and there is only one mode within the vicinity of both means. Our method successfully recovered the parameters of both Gaussian. There is also a mode at the center dominantly formed by the superposition of the tails of three anisotropic Gaussians, where our algorithm did not introduce a spurious Gaussian. Similar performance is observed in Experiment 3. We attribute this to the greedy nature of the algorithm where a predefined number of modes is not enforced in the decomposition.
2.2 Clustering and comparison to expectation maximization

As one of the main techniques in unsupervised learning, clustering seeks to subdivide data into groups based on some similarity measure. A common approach in clustering is based on Gaussian mixtures. In this approach one is given a point-cloud $P \subset \mathbb{R}^n$ and the goal is to find a GMM $f$ such that the probability that $P$ is a sample from $f$ is maximal among all GMM’s with a prescribed number of components.

There are many ways of transforming a point-cloud into a signal and vice-versa. Thus one may use the method proposed in this paper for GMM-based clustering, and conversely one may use methods form clustering in order to decompose a signal into a GMM. In the below we illustrate both directions of this "problem transformation" with some numerical examples.

2.2.1 Clustering via signal decomposition

A sample point-cloud $P$ of size $10^5$ was generated from a normalized version of the GMM in Experiment 3 above. Then a signal $d$ was generated from $P$ by computing a histogram based on the 2D-grid used in the previous experiments. Results from the expectation maximization (EM) algorithm and the proposed method applied to $P$ and $d$, respectively, are shown in Figure 6. The two methods performed similarly in terms of the likelihood of $P$ given the computed GMM’s.

2.2.2 Signal decomposition via clustering

A noisy signal $d$ was generated as in Experiment 3 described in section 2.1 except that the GMM was normalized before discretization. To $d$ we then associated a point-cloud $P$ following the methodology in [Jou16], so $P$ had $|Cd(y)|$ points at grid-point $y$, where the constant $C := 10^{-5} \sum_y d(y)$ was chosen so that $P$ had roughly $10^5$ points in total. Using $P$ we estimated a GMM with the EM algorithm. The performance of EM depended on the random initialization. A typical result using EM applied to $P$, along with the result from the proposed method applied to $d$ are shown in Figure 7. We remark that is possible that a better result with EM may be obtained using some other procedure for generating the point-cloud from the given signal.
Figure 2: Results from Experiment 2. Note the faint spherical Gaussian on the upper left "leg".

3 Location of modes of Gaussian mixtures

The main contribution of our paper is Theorem 3.4, which says that a mode of a GMM cannot lie too far away from the set of means. This theorem generalizes the 1D result that any mode will lie within one standard deviation away from some mean, and provides theoretical support for our way of initializing each iteration of our method. Before turning to this theorem, we need three lemmas. In the first two lemmas we compute some integrals over the $n$-sphere of certain polynomials, and in the third lemma we provide expressions for the gradient and Hessian of a GMM.

Lemma 3.1.

\[
\int_{S^{n-1}} (x, y)^k \, dy = |x|^k C_k, \quad x \in \mathbb{R}^n, k \in \mathbb{N},
\]

where $C_k$ is constant only depending on $k$.

Proof. WLOG assume $x \neq 0$.

\[
\int_{S^{n-1}} (x, y)^k \, dy = |x|^k \int_{S^{n-1}} \left( \frac{x}{|x|}, y \right)^k \, dy = |x|^k C_k,
\]
Figure 3: Results from Experiment 3.

Figure 4: Iterations from Experiment 2.
where the constant $C_k$ is defined by $C_k := \int_{S^{n-1}} (e_1, y)^k \, dy$.

Lemma 3.2. Let $A$ be a symmetric $n \times n$ matrix. Then

$$\int_{S^{n-1}} (y, Ay) dy = Tr(A)C_2,$$

where $C_2$ is as in Lemma 3.1.
Proof. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of $A$ and take $U \in O(n)$ such that $A = U^T DU$, where $D := \text{diag}(\lambda_1, \ldots, \lambda_n)$.

\[
\int_{S^{n-1}} (y, Ay) dy = \int_{S^{n-1}} (y, U^T D U y) dy = \int_{S^{n-1}} (U y, D U y) dy
\]

\[
= \int_{S^{n-1}} (y, D y) dy = \sum_{m=1}^{n} \lambda_m \int_{S^{n-1}} (y, c_m^T y) dy
\]

\[
= \sum_{m=1}^{n} \lambda_m \int_{S^{n-1}} (c_m, y)^2 dy = C_2 \sum_{m=1}^{n} \lambda_m = C_2 \text{Tr}(A)
\]

\[\square\]

Lemma 3.3. The gradient and Hessian of a Gaussian mixture model\footnote{In the interest of readability we have abused notation and absorbed the normalizing constants $C_{\lambda_m}$ into the weights $a_m$.} are given by

\[
\nabla f = \sum_{m} a_m \left( -\Sigma_m^{-1} \right) \left( \Sigma_m^{-1} x - \Sigma_m^{-1} x_m \right) \exp \left\{ -\frac{1}{2} (x - x_m)^T \Sigma_m^{-2} (x - x_m) \right\}
\]

\[
H f = \sum_{m} a_m \left[ \left( \Sigma_m^{-2} (x - x_m) \right) \left( \Sigma_m^{-2} (x - x_m) \right)^T - \Sigma_m^{-2} \right] \exp \{ \cdots \}
\]

Proof. Since this is a standard result, we omit the straightforward proof. \[\square\]

Theorem 3.4. Consider a Gaussian mixture model in $n$ dimensions

\[
f(x) = \sum_{m} a_m \exp \left\{ -\frac{1}{2} (x - x_m)^T \Sigma_m^{-2} (x - x_m) \right\}, a_m > 0, \Sigma_m > 0.
\]

Let $\sigma_{m,\text{max}}$ and $\sigma_{m,\text{min}}$ be the maximal and minimal eigenvalues of $\Sigma_m$. Let $x'$ be a local maximum of $f$. Then there exists an index $m$ such that

\[
|x' - x_m| \leq \sqrt{n} \sigma_{m,\text{max}}^{-1} \sigma_{m,\text{min}}^{-1}\Sigma_m^{-1}.
\]

Proof. Since $x'$ is a local maximum we have $H f(x') \leq 0$, i.e. $(y, H f(x') y) \leq 0, y \in \mathbb{R}^n$. We integrate the last inequality over the unit-sphere and make use of Lemma 3.3 to conclude:

\[
\sum_{m} a_m \int_{S^{n-1}} y^T \left[ \left( \Sigma_m^{-2} (x' - x_m) \right) \left( \Sigma_m^{-2} (x' - x_m) \right)^T - \Sigma_m^{-2} \right] y dy \exp \{ \cdots \} \leq 0.
\]

The last inequality implies that there exist some index $m$ such that

\[
\int_{S^{n-1}} y^T \left[ \left( \Sigma_m^{-2} (x' - x_m) \right) \left( \Sigma_m^{-2} (x' - x_m) \right)^T - \Sigma_m^{-2} \right] y dy \leq 0,
\]

which leads to

\[
\int_{S^{n-1}} (y, \Sigma_m^{-2} (x' - x_m))^2 dy - \int_{S^{n-1}} (y, \Sigma_m^{-2} y) dy \leq 0.
\]

At this point we apply Lemma 3.1 and Lemma 3.2 and obtain:

\[
C_2 \left| \Sigma_m^{-2} (x' - x_m) \right|^2 - C_2 \text{Tr} \left( \Sigma_m^{-2} \right) \leq 0.
\]

Now $C_2 > 0$ since $C_2$ is an integral of a continuous non-negative function that is not everywhere zero. Hence

\[
\left| \Sigma_m^{-2} (x' - x_m) \right|^2 \leq \text{Tr} \left( \Sigma_m^{-2} \right).
\]
Note that
\[ \sigma_{m, \text{max}}^{-4} |x' - x_m|^2 \leq \left| \Sigma_m^{-2} (x' - x_m) \right|^2 \]
and that
\[ \text{Tr} \left( \Sigma_m^{-2} \right) \leq n \sigma_{m, \text{min}}^{-2}. \]
So
\[ \sigma_{m, \text{max}}^{-4} |x' - x_m|^2 \leq n \sigma_{m, \text{min}}^{-2}, \]
and the claim of the theorem follows.

**Corollary 3.5.** Let \( f \) be a mixture of spherical Gaussians with common variance \( \sigma^2 \), i.e.
\[ f(x) = \sum_m a_m \exp \left\{ -\frac{1}{2\sigma^2} |x - x_m|^2 \right\}, \sigma > 0, a_m > 0. \]
If \( x' \) is local maximum of \( f \), then there is an index \( m \) such that
\[ |x' - x_m| \leq \sqrt{n} \sigma. \]

**Proof.** This is an immediate consequence of Theorem 3.4.

**Proposition 3.6.** The bound in Theorem 3.4 cannot be improved by a constant, i.e. for any \( \delta > 0 \) there exist a GMM \( f \) such that some mode \( x' \) of \( f \) satisfies
\[ |x' - x_m| > \sqrt{n} \sigma^2 \sigma_{m, \text{max}}^{-1} \sigma_{m, \text{min}}^{-1} - \delta, \]
for all mean vectors \( x_m \) of \( f \).

**Proof.** We explicitly construct a family \( \{ f_\epsilon \} \) of functions that satisfy the statement of this proposition. For \( \epsilon \) such that \( \min (\delta, \sqrt{n} \sigma) > \epsilon > 0 \) let \( f_\epsilon \) be the 2n component \( n \)-dimensional spherical GMM with common variance \( \sigma^2 \), common amplitude \( a \) and with means at \( \pm (\sqrt{n} \sigma - \epsilon) e_i \), for \( i = 1, 2, \ldots, n \). We shall prove that \( f_\epsilon \) has a mode in the origin, and thus it has a mode at distance \( \sqrt{n} \sigma - \epsilon \) from the set of means of \( f_\epsilon \).

By symmetry \( \sum_m x_m = 0 \), so \( f_\epsilon \) has a critical point in the origin. Hence we are done if we prove that \( Hf_\epsilon(0) < 0 \). Again by Lemma 3.3

\[ Hf_\epsilon(0) = a \sum_m \sigma^{-4} x_m x_m^T - \sigma^{-2} I_n \exp \left\{ -\frac{1}{2\sigma^2} |x_m|^2 \right\} \]
\[ = 2a \exp \left\{ -\frac{(\sqrt{n} \sigma - \epsilon)^2}{2\sigma^2} \right\} \sum_{i=1}^n (\sigma^{-4} (\sqrt{n} \sigma - \epsilon)^2 e_i e_i^T - \sigma^{-2} I_n) \]
\[ = 2a \exp \left\{ -\frac{(\sqrt{n} \sigma - \epsilon)^2}{2\sigma^2} \right\} \sigma^{-2} (\sigma^{-2} (\sqrt{n} \sigma - \epsilon)^2 - n) I_n. \]

Hence \( Hf_\epsilon(0) < 0 \).

\(^3\)Numerical experiments suggest that \( f_\epsilon \) has a mode in the origin also for \( \epsilon = 0 \). A proof of this (if it is true) would however need an argument different from the one given here, since \( Hf_0(0) = 0 \).
4 Conclusion

Motivated primarily by applications in TEM, we have developed a new algorithm for decomposing a non-negative multivariate signal as a sum of Gaussians with full covariances. We have tested it on 1D and 2D data. Moreover, we have also proved an upper bound for the distance of a local maximum of a GMM to the set of its mean vectors. This upper bound provides motivation for a key step in our method, namely the initialization of each new Gaussian at the maximum of the residual. Finally we remark that, while we have only tested the proposed method on functions sampled on uniform grids, it is straightforward to extend the method to handle input data in the form of multivariate functions sampled on non-uniform grids.
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