Likelihood Landscape and Local Minima Structures of Gaussian Mixture Models

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Abstract
In this paper, we study the landscape of the population negative log-likelihood function of Gaussian Mixture Models with a general number of components. Due to nonconvexity, there exist multiple local minima that are not globally optimal, even when the mixture is well-separated. We show that all local minima share the same form of structure that partially identifies the component centers of the true mixture, in the sense that each local minimum involves a non-overlapping combination of fitting multiple Gaussians to a single true component and fitting a single Gaussian to multiple true components. Our results apply to the setting where the true mixture components satisfy a certain separation condition, and are valid even when the number of components is over- or under-specified. For Gaussian mixtures with three components, we obtain sharper results in terms of the scaling with the separation between the components.

1 Introduction
Mixture models, as exemplified by the Gaussian mixture model (GMM), are widely used for approximating complex multi-modal distributions. They can also be viewed as a form of latent variable models that provide a flexible approach for statistical inference with heterogeneous data. To estimate the parameters of GMM, a standard approach is via the maximum likelihood principle. When the global optimum of the likelihood function can be computed, the statistical properties of the maximum likelihood estimator is relatively well studied, including its asymptotic consistency [25] and finite-sample error rates [5, 21, 14].

Much less understood are the computational challenges associated with estimating GMMs. The negative log-likelihood function of GMM is nonconvex and in general has multiple local minima. Standard iterative algorithms, such as Expectation-Maximization (EM) [9], are only guaranteed to converge to a local minimum [27, 16]. Indeed, the work in [15] shows that for GMMs with $k_\ast \geq 3$ well-separated components, there exist spurious local minima that may be arbitrarily far from the global minimum both in distance and in likelihood values; moreover, randomly initialized EM converges to such a spurious local minimum with high probability. This result stands in sharp contrast to recent work on the special case of GMM with $k_\ast = 2$ equally weighted components, in which case the negative log-likelihood, despite being nonconvex, has no spurious local minimum, and EM converges to the global minimum from arbitrary initialization [8, 29].

Our Contributions. In this paper, we consider the problem of estimating the component centers of GMMs with a general number of equally weighted components, and aim to understand the structures of the local minima of the population negative likelihood function when fitting a mixture of $k$ Gaussians to a true mixture of $k_\ast$ Gaussians. We prove that all local minima $\beta = (\beta_1, \ldots, \beta_k)$ share the same form of structure that partially identifies the component centers $\theta^\ast = (\theta^\ast_1, \ldots, \theta^\ast_k)$ of the true mixture. Specifically, each local minimum only involves two types of configurations: either several fitted centers $\{\beta_i\}$ are close to a single true center $\theta^\ast$, or a single fitted center $\beta_i$ is close to the mean of several true centers $\{\theta^\ast_s\}$; moreover, these configurations involve disjoint sets of centers. This result remains valid even when the number $k$ of centers is mis-specified and different from the number $k_\ast$ of the true centers.
To illustrate, consider the setting with $k = 5$ and $k_* = 4$. A local minimum $\beta$ satisfies

$$\beta_1 \approx \frac{1}{2}(\theta^*_1 + \theta^*_2), \quad \beta_2 \approx \beta_3 \approx \beta_4 \approx \theta^*_3 \quad \text{and} \quad \beta_5 \approx \theta^*_4. \quad (1)$$

An illustration is given in Figure 1 below. Our main theorem shows that this is essentially the only type of local minima. In particular, in the graph theoretic terms as shown in Figure 1, each local minimum corresponds to a disjoint union of complete bipartite graphs $(S_a, S^*_a)_{a=1,2,...}$ between a subset of fitted centers $S_a$ and a subset of true centers $S^*_a$, such that at least one of $S_a$ and $S^*_a$ must be a singleton.

Figure 1: Association between fitted centers $\{\beta_i\}$ and true centers $\{\theta^*_i\}$ in a local minimum.

The above result establishes that despite the existence of spurious local minima, these minima are well structured and contain information about the global optima and the true mixture. Consequently, standard iterative algorithms such as EM and gradient descent, starting from an arbitrary initial solution (except for a set of measure zero [27, 16, 19]), converge to a solution that is informative in the above sense. Our main theorem characterizes how the approximation errors in equation (1) depend on the separation between the mixture components. For a three-component GMM, for example, the errors are exponentially small in the separation.

1.1 Related Work

In 2006 Srebro posed the question of whether the population negative log-likelihood function of GMM has spurious local minima [24]. As mentioned, this question was answered in negative in 2016 for the general case with $k_* \geq 3$ by Jin et al. [15]. Motivated by the computational considerations in estimating GMMs, recent work has been devoted to understanding on the finer properties of the likelihood function as well as those of the EM algorithm—arguably the most popular algorithm for GMMs.

One line of work focuses on the local behaviors of the likelihood in a neighborhood around the global optimum, hence pertaining to EM starting from an initial solution sufficiently close to the global optimum. The work in [2] proposes a general framework for establishing the local geometric convergence of EM, which implicitly shows that the negative log-likelihood function of a two-component GMM has no other local minima near the global minimum. Extension to multiple components is considered in the work [32]. Further work in this line studies GMMs with additional structures [33, 26, 13], EM with unknown mixture weights and covariances [4], confidence intervals constructed using EM [6], and the setting where the number of components is under-specified [12].

Another line of work aims to understand the more global properties of GMM and EM in certain restricted settings, mostly that with $k_* = 2$ (often equally-weighted) components. In this setting, the work in [8, 29] proves that EM initialized at a random solution converges to the global minimum. Their results effectively show that the negative log-likelihood function has no spurious local minimum that are not globally optimal in this case. This fact is further investigated in the work [20], which proposes a general framework for transferring the properties of the population risk to its empirical counterpart. Extensions to mixtures of two log-concave distributions [22] or two linear regressions [18] have also been considered. A more recent set of papers study the delicate behaviors of EM in the setting where the two components have small or no separation, or where the number of components is mis-specified [10, 11, 17, 28]; in this setting, EM may exhibit a slower, non-parametric statistical error rate. The above global results for $k_* = 2$, however, should be considered the exception rather than the norm: as soon as $k_* \geq 3$, spurious local minima provably exist [15]. Moreover, additional spurious local minima may arise when the mixture weights are not equal [30].
In our recent work [23], we study the related problem of optimizing the (non-smooth) k-means objective function, which can be viewed as a limit version of the log-likelihood function of GMM when the posited variance goes to zero. There we establish a qualitative similar result as in this paper: spurious local minima provably exist but possess additional hidden structures. The quantitative results in this paper is substantially sharper. The proofs here are also quite different and considerably simpler in certain aspects, taking advantage of the rich structures of the smooth log-likelihood function.

2 Problem Setup

In this section, we describe the problem setup and introduce basic notations.

Notations. For each positive integer m, let \([m] := \{1, 2, \ldots, m\}\). The Euclidean norm is denoted by \(\|\cdot\|\). We use boldface lower case letters (e.g., \(x\)) to denote fixed (column) vectors, of which \(x_i\) is the \(i\)-th element. In particular, \(e_i = (0, \ldots, 0, 1, 0, \ldots, 0)\)\(^\top\) is the \(i\)-th standard basis vector in \(\mathbb{R}^d\). We use boldface capital letters (e.g., \(X\)) to denote random variables and vectors. Denote by \(I_d\) the \(d\)-by-\(d\) identity matrix. The indicator function is denoted by \(\mathbbm{1}\{\cdot\}\). We sometimes use the big-O notations: for two quantities \(g\) and \(h\) that may depend on the problem parameters, we write \(g = \Theta(h)\) or \(h = \Omega(g)\) if \(g \leq ch\) for a universal constant \(c > 0\). Similarly, we write \(g = \Theta(h)\) if \(g = O(h)\) and \(h = O(g)\).

2.1 Gaussian Mixture Models

Let \(\phi(x \mid \mu, \sigma^2) := (\sqrt{2\pi}\sigma)^{-d} \exp\left(-\frac{\|x - \mu\|^2}{2\sigma^2}\right)\) denote the density function of the \(d\)-dimensional Gaussian distribution \(\mathcal{N}(\mu, \sigma^2 I_d)\) with mean \(\mu\) and covariance \(\sigma^2 I_d\). Consider a mixture of \(k_s\) equally weighted Gaussian distributions, with the density

\[
f^*(\cdot) = \frac{1}{k_s} \sum_{s \in [k_s]} f^*_{s}(\cdot),
\]

where \(f^*_{s}(\cdot) := \phi(\cdot \mid \theta^*_s, \sigma^2)\) is the density of the \(s\)-th mixture component, and \(\{\theta^*_s, s \in [k_s]\}\) are \(k_s\) unknown centers in \(\mathbb{R}^d\). Assuming that the variance \(\sigma^2\) is known, we fit a \(k\)-component mixture with density

\[
f(\cdot) = \frac{1}{k} \sum_{j \in [k]} f_j(\cdot),
\]

where \(f_j(\cdot) := \phi(\cdot \mid \beta_j, \sigma^2)\) and \(\{\beta_j, j \in [k]\}\) are the \(k\) fitted centers. Above we have suppressed the dependence of \(f^*\) and \(\{f^*_{s}\}\) on \(\{\theta^*_s\}\) to avoid cluttered notation; similarly for \(f\) and \(\{f_j\}\) on \(\{\beta_j\}\). Note that we allow the number of fitted components \(k\) to differ from the number of true components \(k_s\), thereby covering the exact-parametrization \((k = k_s)\), over-parametrization \((k > k_s)\) and under-parametrization \((k < k_s)\) settings.

Define the maximum and minimum component separations as

\[
\Delta_{\text{max}} := \max_{s, s' \in [k_s]} \|\theta^*_s - \theta^*_{s'}\| \quad \text{and} \quad \Delta_{\text{min}} := \min_{s, s' \in [k_s], s \neq s'} \|\theta^*_s - \theta^*_{s'}\|.
\]

We refer to the quantity \(\frac{\Delta_{\text{min}}}{\sigma}\) as the Signal-to-Noise Ratio (SNR).

We use \(E\) and \(P\) to denote the expectation and probability, respectively, under the true mixture \(f^*\). Similarly, for each \(s \in [k_s]\), we use \(E_s\) and \(P_s\) to denote the expectation and probability, respectively, under the \(s\)-th true component \(f^*_s\). Note that \(E_s = \frac{1}{k_s} \sum_{s \in [k_s]} E_s\) and \(P_s = \frac{1}{k_s} \sum_{s \in [k_s]} P_s\) by definition of the mixture model (2). We use \(E\) and \(P\) to denote generic expectation/probability when the relevant random variable and distribution is clear from the context. For clarity, in general we use \(s, s'\) to index true mixture components (e.g., \(\theta^*_s, f^*_s\)) and \(i, j\) to index the fitted components (e.g., \(\beta_i, f_j\)).
2.2 Likelihood Function

Given data $X$ from the true model $f^*$, the standard approach for fitting the model $f$ is via the maximum likelihood principle. Let $\theta^* = (\theta_1^*, \ldots, \theta_k^*) \in \mathbb{R}^{d \times k^*}$ and $\beta = (\beta_1, \ldots, \beta_k) \in \mathbb{R}^{d \times k}$ be the parameters of the true and fitted models, respectively. The population negative log-likelihood function—the infinite sample limit of the usual negative log-likelihood—is given by

$$
L(\beta) \equiv L(\beta | \theta^*) = -\mathbb{E}_* [\log f(X)] 
$$

where $D_{KL} (f^* || f) := \mathbb{E}_* [\log \frac{f^*(X)}{f(X)}]$ is the Kullback-Leibler (KL) divergence between the distributions with densities $f^*$ and $f$, and the quantity $-\mathbb{E}_* [\log f^*(X)]$ is independent of $\beta$.

**Remark 1.** It is easy to verify that the function $L$ is invariant under rotation and translation of coordinates in the following sense: for any orthonormal matrix $U \in \mathbb{R}^{d \times d}$ and vector $v \in \mathbb{R}^d$, we have

$$
L(U\beta_1 + v, \ldots, U\beta_k + v | U\theta_1^* + v, \ldots, U\theta_k^* + v) = L(\beta_1, \ldots, \beta_k | \theta_1^*, \ldots, \theta_k^*).
$$

In the analysis we frequently make use of this invariance property, which allows us to choose any convenient coordinate system.

The maximum likelihood approach involves finding the global minimizer of the negative log-likelihood $L$:

$$
\min_{\beta \in \mathbb{R}^{d \times k}} L(\beta).
$$

If $k = k^*$, from the expression (6) and the non-negativity of KL divergence, it is clear that the true centers $\theta^*$ is a global optimum of $L$. The computational challenge is that $L$ is non-convex and in general has local minima other than $\theta^*$ [15], and standard algorithms (such as EM and gradient descent) are only guaranteed to find such a local minimum.

2.3 Coefficients of Association and Optimality Conditions

Playing a crucial role in the analysis is the **coefficient of association** between a data point $x \in \mathbb{R}^d$ and a fitted center $\beta_j, j \in [k]$, defined as:

$$
\psi_j(x) := \frac{1}{f(x)} f_j(x) = \frac{\exp \left( -\frac{\|x - \beta_j\|^2}{2\sigma^2} \right)}{\sum_{\ell \in [k]} \exp \left( -\frac{\|x - \beta_\ell\|^2}{2\sigma^2} \right)}.
$$

We see that the association coefficient $\psi_j(x)$ takes the form of soft argmax and can be viewed as an approximation of the hard argmax

$$
1 \{ j = \arg \max_{\ell \in [k]} \| x - \beta_\ell \|^2 \},
$$

which indicates whether $\beta_j$ is the closest center to $x$. Our analysis makes use of this intuitive interpretation. One may also interpret $\psi_j(x)$ as the posterior probability of a data point $x$ belonging to the $j$-th fitted component, given the current center estimate $\beta$. As such, the quantity $\psi_j(x)$ appears in the E-step of the EM algorithm, as we show momentarily. For a random data point $X$ generated from the true distribution $f^*$, we define the corresponding random variable of its association coefficient as

$$
\Psi_j := \psi_j(X).
$$

With the above notation, the gradient of $L$ admits the expression

$$
\frac{\partial}{\partial \beta_j} L(\beta) = \mathbb{E}_* [\Psi_j(\beta_j - X)], \quad j \in [k];
$$

(8)
see Section 5.1 for the derivation. Consequently, $\beta$ is a stationary point of $L$ if and only if there holds the first-order stationary condition
$$E_*[\Psi_j(\beta_j - X)] = 0, \quad \forall j \in [k],$$
or equivalently
$$\beta_j = \frac{E_*[\Psi_j X]}{E_*[\Psi_j]}, \quad \forall j \in [k]. \tag{10}$$
If $\beta$ is a local minimum of $L$, then it further satisfies the second-order condition that the Hessian $\nabla^2 L(\beta)$ is positive semidefinite. See Section 5.1 for the expression of $\nabla^2 L(\beta)$.

Connection to EM. The EM algorithm is a popular iterative method for optimizing the likelihood function $L$. In the population setting, the EM update takes the form
$$\beta_j \leftarrow \frac{E_*[\Psi_j X]}{E_*[\Psi_j]} = \beta_j - \frac{1}{E_*[\Psi_j]} \cdot \frac{\partial}{\partial \beta_j} L(\beta), \quad j \in [k], \tag{11}$$
where we have combined the E-step (computing $\Psi_j$) and the M-step (computing $\beta_j$) into one update. We see that EM can be viewed as a fixed point iteration for solving the stationary condition (10), or as a gradient descent-like (or quasi-Newton) algorithm with a coordinate-dependent step size $1/E_*[\Psi_j]$ [31]. Therefore, the fixed points of EM correspond to the stationary points of $L$, and the stable fixed points of EM correspond to the local minima.

Our results in next section provide a characterization of the stationary points and local minima of $L$. These results hence apply to the solution returned by EM and more generally to other local algorithm for optimizing $L$ such as gradient descent and Newton methods.

3 Main Results

In this section, we present our main results for the likelihood landscape of Gaussian mixture models. In Section 3.1, we derive an equivalent form of the stationary condition, which immediately implies several useful properties of the stationary points of the population negative log-likelihood function $L$. This equivalent condition is also useful in subsequent proofs. In Section 3.2, we characterize the structures of all local minima of $L$ with a general number of mixture components. In Section 3.3, we consider a mixture of three Gaussian distributions and derive sharper structural results for the local minima of $L$.

3.1 Properties of Stationary Points

Our first theorem provides a sufficient and necessary condition for the stationary points of $L$.

Theorem 1 (Equivalent Stationary Condition). $\beta \in \mathbb{R}^{d \times k}$ is a stationary point of $L$ if and only if
$$\sum_{j \in [k]} \beta_j \sum_{s \in [k_*]} E_*[\Psi_j \Psi_s] = \sum_{s \in [k_*]} \theta_*^s E_*[\Psi_s], \quad \forall i \in [k]. \tag{12}$$
We prove this theorem in Section 6.1 using Stein’s identity.

The condition (12) is equivalent to the original stationary condition (10), but is often more useful as it exposes the relationship between the fitted centers $\{\beta_j\}$ and the true centers $\{\theta_*^s\}$. This result plays a key role in establishing the next two theorems. Here we present several immediate corollaries, some of which may be difficult to prove by other means.

The result in the first corollary is probably well known. It states that the weighted mean of the fitted centers in a stationary point of $L$ must equal the mean of the true centers.

Corollary 1 (Mean Consistency). If $\beta \in \mathbb{R}^{d \times k}$ is a stationary point of $L$, then we have
$$\sum_{j \in [k]} \beta_j E_*[\Psi_j] = \frac{1}{k_*} \sum_{s \in [k_*]} \theta_*^s.$$
Proof. Adding up the equivalent stationary condition (12) over \( i \in [k] \) and using the fact that \( \sum_{i \in [k]} \Psi_i = 1 \) surely, we obtain that \( \sum_{j \in [k]} \beta_j \sum_{s \in [k_j]} (\Psi_j)_s = \sum_{s \in [k_j]} (\Psi_j)_s \). Since \( \sum_{s \in [k_j]} (\Psi_j)_s = k_s E_s [\Psi_j] \), the corollary follows. Note that we can also prove this corollary using the original stationary condition (10).

The next corollary states that any stationary point of \( L \) must lie in the linear subspace spanned by the true component centers.

**Corollary 2 (Linear Span).** If \( \beta \in \mathbb{R}^{d \times k} \) is a stationary point of \( L \), then we have
\[
\beta_i \in \text{span} \{ \theta_s^*, s \in [k_s] \}, \quad i \in [k].
\]

We prove this corollary in Section 6.2. With this property, in subsequent analysis we can often restrict ourselves to the \( k_s \)-dimensional subspace \( \text{span} \{ \theta_s^* \} \).

The next corollary states that if the true mixture has one component, then this component center is the only stationary point, regardless of the number \( k \) of fitted centers.

**Corollary 3 (Fitting k Gaussians to One Gaussian).** If \( k_\cdot = 1 \), then \( L \) has a unique stationary point \( \beta \in \mathbb{R}^{d \times k} \) with
\[
\beta_i = \theta_1^*, \quad \forall i \in [k].
\]

Proof. Without loss of generality we may assume that \( \theta_1^* = 0 \) (see Remark 1). If \( \beta \) is a stationary point of \( L \), then Corollary 2 implies that \( \beta_i \in \text{span} \{ \theta_1^* \} = \{ 0 \}, \forall i \in [k] \). Conversely, if \( \beta_i = 0 \) for all \( i \), then \( \psi_i(x) = \frac{1}{k} \) for all \( x \in \mathbb{R}^d \) and it is clear that the stationary condition (10) is satisfied.

Corollary 3 is related to a recent line of work in [10, 11, 28] on the setting where the number of components in the mixture is over-specified. In particular, in the canonical over-specified setting where one fits each \( k = 2 \) Gaussians to data from a single Gaussian, they show that EM converges to the true center from random initialization (albeit with a slower convergence rate and a larger statistical error \( (d/n)^{1/4} \) than in the exact-specified setting). At the population level, Corollary 3 provides a more general result, applicable to any number \( k \) of specified components and any descent algorithms beyond EM.

Finally, as a sanity check, we consider an under-specified setting with \( k = 1 \) and \( k_\cdot \geq 1 \), that is, fitting a single Gaussian to a mixture of multiple Gaussians. In this case, we have \( \psi_i(x) = 1, \forall x \in \mathbb{R}^d \), hence equation (12) immediately implies the following result:

**Corollary 4 (Fitting One Gaussian to \( k_\cdot \) Gaussians).** If \( k = 1 \), then \( L \) has a unique stationary point \( \beta = (\beta_1) \in \mathbb{R}^{d \times 1} \) satisfying
\[
\beta_1 = \frac{1}{k_\cdot} \sum_{s \in [k_s]} \theta_s^* = E_s [X].
\]

We thus recover the elementary fact that the Maximum Likelihood Estimator of fitting a single Gaussian to a dataset is given by the mean of the data.

The last two corollaries show that when fitting multiple Gaussians to a single one, or fitting a single Gaussian to multiple ones, the population log-likelihood \( L \) has a unique stationary point that is the global optimum. As we show in the next subsection, these two settings are essentially the atomic cases of the general setting with arbitrary \( k \) and \( k_\cdot \). In particular, any local minimum of \( L \) can be decomposed into a non-overlapping collection of the above two settings (plus potentially an near-empty association setting; see Theorem 2 to follow).

### 3.2 Structures of Local Minima

For each \( i \in [k] \), define the **Voronoi set** associated with \( \beta_i \) as
\[
\mathcal{V}_i := \left\{ x \in \mathbb{R}^d : \| x - \beta_i \| \leq \| x - \beta_\ell \|, \forall \ell \in [k] \right\} = \left\{ x : \psi_i(x) \geq \psi_\ell(x), \forall \ell \in [k] \right\},
\] (13)
which is the set of points whose closest center is $\beta_i$.

We state our main theorem, which is proved in Section 7.

**Theorem 2** (Structures of Local Minima). The following holds for some universal constants $C > 1$ and $C_0 > 1$. Let $\lambda$ be an arbitrary number in $(0, \frac{1}{C_0 k_0 + k_0})$ and suppose that the SNR satisfies $\frac{\lambda}{\sigma} \geq C \frac{k_0}{\lambda}$. If $\beta$ is a local minimum of $L$, then there exist a partition $[k] = S_0^* \cup \cdots \cup S_{q_0}^* \cup S_{q_0+1}^* \cup \cdots \cup S_q^*$ of the true centers and a partition $[k] = S_0 \cup S_1 \cup \cdots \cup S_{q_0} \cup S_{q_0+1} \cup \cdots \cup S_q$ of the fitted centers, where $q \geq 1$ and $0 \leq q_0 \leq q$, such that the following are true:

- **(Near-empty association)** We have
  $$P_\ast(V_i) \leq C_0 k^3 \lambda \quad \text{and} \quad E_\ast[\Psi_i] \leq C_0 k^3 \lambda, \quad \forall i \in S_0.$$  

- **(One-fit-many)** For each $a = 1, \ldots, q_0$, we have $S_a = \{i\}$ for some $i$, $|S_a^*| \geq 1$, and
  $$\beta_i - \frac{1}{|S_a^*|} \sum_{s \in S_a^*} \theta_s^* \leq C_0 \left[ k_s k_0 \lambda \Delta_{\max} + \frac{k_s (k_s + k)}{\lambda} \sigma \right], \quad (15a)$$
  $$E_\ast[\Psi_i] \geq 1 - 4C_0 k^4 \lambda, \quad \forall s \in S_a^*, \quad (15b)$$
  $$P_\ast(V_i) \geq 1 - 4C_0 k^4 \lambda, \quad \forall s \in S_a^*. \quad (15c)$$

Moreover, we have $\beta_i \neq \beta_j, \forall j \in [k] \setminus \{i\}$.

- **(Many-fit-one)** For each $a = q_0 + 1, \ldots, q$, we have $|S_a| \geq 1$, $S_a^* = \{s\}$ for some $s$, and
  $$\|\beta_i - \theta_s^*\| \leq C_0 \frac{k_s}{\lambda} \sigma, \quad \forall i \in S_a. \quad (16)$$

Let us parse the results above. Theorem 2 states that all local minima $\beta$ of $L$ possess a similar form of structures. In particular, each of the fitted centers $\{\beta_1, \ldots, \beta_k\}$ must satisfy one of the three possibilities stated in the theorem:

- In the first possibility, equation (14) states that the association coefficient and Voronoi set of $\beta_i$ must be small. This means that most of the data points from the true mixture $f^\ast$ are far from $\beta_i$ compared to the other fitted centers $\beta_j, j \neq i$. In other words, $\beta_i$ is effectively not used to fit any of the $k_s$ components of the true mixture.

- In the second possibility, equation (15a) states that $\beta_i$ is close to the mean of several true centers indexed by $S_a^*$. Moreover, for each $s \in S_a^*$, the Voronoi set of $\beta_i$ contains most of the probability mass of the $s$-th true mixture component (equation (15c)), and the association coefficient $E_\ast[\Psi_i]$ is close to one (equation (15b)). In this case, we essentially use a single Gaussian component $N(\beta_i, \sigma^2)$ to fit a subset of components, $\{N(\theta_s^*, \sigma^2), s \in S_a^*\}$, from the true mixture (cf. Corollary 4). All other centers $\{\beta_j, j \neq i\}$ effectively do not participate in fitting these $|S_a^*|$ true components.

- In the third possibility, equation (16) states that multiple fitted centers $\{\beta_i, i \in S_a\}$ are all close to a single true center $\theta_s^*$. In this case, we essentially use $|S_a|$ Gaussian components, $\{N(\beta_i, \sigma^2), i \in S_a\}$, to fit a single true component $N(\theta_s^*, \sigma^2)$ (cf. Corollary 3).

Note that since $\{S_a\}$ and $\{S_a^*\}$ in Theorem 2 are partitions, the above three possibilities involve disjoint sets of fitted and true centers (and together they cover all these centers). Therefore, a local minimum cannot involve using multiple centers to fit multiple true centers—only one-fit-many and many-fit-one are possible. For example, when fitting $k = 3$ Gaussians to $k_s = 3$ true Gaussians, the following configuration cannot be a local minimum:

$$\beta_1 \approx \beta_2 \approx \frac{1}{2} (\theta_1^* + \theta_2^*), \quad \beta_3 \approx \theta_3^*.$$

Also note that the set $S_0$ may be empty, in which case the first possibility (near-empty association) does not occur. Moreover, if $q_0 = 0$, then the second possibility (one-fit-many) does not occur. Similarly, if $q_0 = q$, then the third possibility (many-fit-one) does not occur.
We mention that the work in [15] establishes the existence of a spurious local minimum that involves the one-fit-many and many-fit-one configurations. Theorem 2 shows that all local minima have this type of structure. In particular, while a local minimum \( \beta \) may be far from the global minimum (namely, the true centers \( \theta^* \)) both in objective value and in distance [15], it nevertheless contains partial information about the true centers, in the sense that \( \beta \) recovers a subset of the true centers (via many-fit-one) as well as the means of the other true centers (via one-fit-many).

Finally, we emphasize that Theorem 2 applies to any values of \( k \) and \( k_* \), hence covering the over-parametrization setting \( (k > k_*) \) and under-parametrization setting \( (k < k_*) \).

To better understand the quantitative bounds in Theorem 2, let us consider the setting where \( k_* = k \) and \( 1 = \Delta_{\min} = \Theta(\Delta_{\max}) \). In this case, the SNR is \( \frac{\Delta_{\min}}{\sigma} = \frac{1}{\sigma} \).

**Corollary 5.** Under the above setting, the following holds for some universal constants \( C > 1 \) and \( c > 1 \). Suppose that the SNR satisfies \( \frac{1}{\sigma} = C^2 \cdot \rho \cdot k_*^2 \), where \( \rho \geq 1 \) is an arbitrary number. If \( \beta \) is a local minimum of \( L \), then there exist a partition \( [k_*] = S_1^* \cup \cdots \cup S_q^* \) of the true centers and a partition \( [k] = S_0 \cup S_1 \cup \cdots \cup S_{q_0} \cup S_{q_0+1} \cup \cdots \cup S_q \) of the fitted centers such that the following are true:

- **(Near-empty association):** We have
  \[
P_* (V_i) \leq c \frac{1}{\sqrt{\rho}} \quad \text{and} \quad E_* [\Psi_i] \leq c \frac{1}{\sqrt{\rho}}, \quad \forall i \in S_0.
  \]

- **(One-fit-many):** For \( a = 1, \ldots, q_0 \), we have \( S_a = \{i\} \) for some \( i \), \( |S_a^*| \geq 1 \), and
  \[
  \|\beta_i - \frac{1}{|S_a^*|} \sum_{s \in S_a^*} \theta^*_s\| \leq c \frac{1}{\sqrt{\rho}}, \quad \forall i \in S_a.
  \]

- **(Many-fit-one):** For \( a = q_0 + 1, \ldots, q \) we have \( |S_a| \geq 1 \) and \( S_a^* = \{s\} \) for some \( s \), and
  \[
  \|\beta_i - \theta^*_s\| \leq c \frac{1}{\sqrt{\rho}}, \quad \forall i \in S_a.
  \]

*Proof.* Set \( \lambda = \frac{1}{c \sqrt{\rho k_*^6}} \). Note that the SNR satisfies \( \frac{1}{\sigma} = C^2 \cdot \rho \cdot k_*^2 \geq C^2 \sqrt{\rho k_*^6} = C^2 k_*^{\frac{3}{2}} \) as \( \rho \geq 1 \), so the SNR condition in Theorem 2 holds. Applying Theorem 2 and plugging in the values of \( \lambda \) and \( \frac{1}{\sigma} = C^2 \cdot \rho \cdot k_*^6 \) proves the corollary.

Corollary 5 highlights how various bounds depend on the SNR. As the SNR \( \frac{1}{\sigma} \propto \rho \) increases, all the bounds shrink at the rate \( \frac{1}{\sqrt{\rho}} \). Therefore, the aforementioned structures of the local minima become more pronounced when the SNR is larger. The result in Corollary 5 holds when the SNR satisfies \( \frac{1}{\sigma} \gtrsim \text{poly}(k_*) \) — we have not attempted to optimize the scaling with \( k_* \). We suspect that some form of SNR lower bound is necessary; otherwise, the Gaussian components of the true mixture would have a large amount of overlap, in which case local minima with a many-fit-many configuration may emerge. Finally, note that the bounds and SNR conditions in Theorem 2 and Corollary 5 are independent of the ambient dimension \( d \), thanks to Corollary 2.

### 3.3 Tighter Bounds for 3-Mixture

The error bounds in Corollary 5 are on the order of \( O(\text{SNR}^{-1/2}) \). These bounds can be sharpened to the form \( e^{-\Omega(\text{SNR}^2)} \) by a more careful analysis. We demonstrate this refined result below in the setting of three-component GMM.

Consider the setting with \( k = k_* = 3 \), \( d = 1 \) and \( \theta^* = (\theta_1^*, \theta_2^*, \theta_3^*) = (-\Delta, 0, \Delta) \), where \( \Delta > 0 \). That is, we are fitting a mixture of three one-dimensional Gaussians with exact parametrization. Note that we have \( \Delta_{\max} = 2\Delta_{\min} = 2\Delta \) in this case. The following theorem, proved in Section 8, provides a tight characterization of the local minima in this setting.
Theorem 3 (Tight Bounds for 3-Component GMM). Under the above setting, suppose that the SNR satisfies \( \frac{\Delta}{\sigma} \geq C_1 \) for some sufficiently large universal constant \( C_1 > 0 \). Then each local minimum \( \beta = (\beta_1, \beta_2, \beta_3) \) of \( L \) must satisfy (up to permutation of the component labels of \( \{\beta_i\} \) and of \( \{\theta^*_i, \theta^*_3\} \)) exactly one of the following possibilities:

1. \( |\beta_1 - \frac{1}{2}(\theta^*_1 + \theta^*_2)| \leq se^{-c\Delta^2/\sigma^2} \), \( |\beta_2 - \theta^*_3| \leq se^{-c\Delta^2/\sigma^2} \), and \( E_s[\Psi_3] \leq e^{-c\Delta^2/\sigma^2}; \)

2. \( |\beta_1 - \frac{1}{2}(\theta^*_1 + \theta^*_2)| \leq se^{-c\Delta^2/\sigma^2} \) and \( |\beta_1 - \theta^*_3| \leq se^{-c\Delta^2/\sigma^2}, i \in \{2, 3\}; \)

3. \( |\beta_1 - \theta^*_1| \leq se^{-c\Delta^2/\sigma^2}, i \in \{1, 2, 3\}. \)

Here \( c > 0 \) is a universal constant.

Theorem 3 provides tighter bounds, exponentially small in the SNR, on the approximation error and the association coefficient \( E_s[\Psi_3] \). Therefore, as the SNR increases, each fitted centers is either exponentially close to a true center (or to the mean of two), or its association coefficient (and hence its Voronoi set) becomes exponentially small. In fact, since \( L \) has no other local minima near the true centers \( \theta^* \) by existing local results on GMM [2], the errors in Case 3 above are actually zero, in which case \( \beta = \theta^* \) is the exact global minimum.

Compared to Theorem 2 and Corollary 5, the theorem above also further narrows down the possible configurations in a local minima. In particular, Theorem 3 shows that it is impossible to have one center \( \beta_1 \approx \frac{1}{2}(\theta^*_1 + \theta^*_2) \) fitting two non-adjacent true centers; the one-dimension assumption \( d = 1 \) is mainly used in excluding this possibility. Theorem 3 also eliminates the possibility that one center \( \beta_1 \approx \frac{1}{3}(\theta^*_1 + \theta^*_2 + \theta^*_3) \) fits all three true centers (and the other two centers \( \beta_2, \beta_3 \) are far away from the true centers and have near-empty-association). Such a one-fit-all configuration fails to capture the mixture structure of the data. Excluding this possibility is complicated by the issue of “local minima at infinity”. In particular, when \( \beta_2 \) and \( \beta_3 \) approach infinity and hence move away from the data, the likelihood approaches that of fitting a single Gaussian to a mixture of three. In this limiting case, \( \beta_1 = \frac{1}{3}(\theta^*_1 + \theta^*_2 + \theta^*_3) \) is indeed a local minimum (see Corollary 4). Theorem 3 above shows that any finite \( \beta \) of this one-fit-all form cannot be a local minimum. It is an interesting question whether one can further exclude Possibility 1 in Theorem 3, which involves one fitted center with near-empty association.

The proof of Theorem 3 builds off the coarse characterization in Theorem 2, which localizes the local minima of \( L \) into a small neighborhood of a few ideal solutions such as \( \beta = \theta^* \) and \( \beta = ((\theta^*_1 + \theta^*_2)/2, \theta^*_3, \theta^*_3) \). Within this neighborhood, we exploit the first-order stationary condition in a more careful manner to show that the local minima must be exponentially close to these ideal solutions. We believe that this strategy can be generalized beyond the above one-dimensional three-component setting, which we leave to future work.

The techniques used in the proof of the above result also apply to the setting where we under-specify the number of components. Recall that Corollary 4 addresses the case where one fits a single Gaussian to a mixture of three Gaussians, in which case the overall mean \( \beta_1 = \frac{1}{2}(\theta^*_1 + \theta^*_2 + \theta^*_3) \) is the only stationary point. The corollary below concerns with fitting a 2-mixture to a 3-mixture. Specifically, consider the setting with \( k = 2, n_3 = 3, d = 1 \) and \( \theta^* = (\theta^*_1, \theta^*_2, \theta^*_3) = (-\Delta, 0, \Delta) \).

Corollary 6 (Tight Bounds for Underfitting 3-Component GMM). Under the above setting, suppose that the SNR satisfies \( \frac{\Delta}{\sigma} \geq C_1 \) for some sufficiently large universal constant \( C_1 > 0 \). Then each local minimum \( \beta = (\beta_1, \beta_2) \) of \( L \) must satisfy (up to permutation of the component labels of \( \{\beta_i\} \) and of \( \{\theta^*_1, \theta^*_2\} \))

\[
|\beta_1 - \frac{1}{2}(\theta^*_1 + \theta^*_2)| \leq se^{-c\Delta^2/\sigma^2} \quad \text{and} \quad |\beta_2 - \theta^*_3| \leq se^{-c\Delta^2/\sigma^2},
\]

where \( c > 0 \) is a universal constant.

We prove Corollary 6 in Appendix C using intermediate results from the proof of Theorem 3. Corollary 6 is related to the recent work by Dwivedi et al. [12], who study a similar under-parametrization setting. There they consider fitting a symmetric 2-mixture \( \frac{1}{2}N(\beta_1, \sigma^2) + \frac{1}{2}N(-\beta_1, \sigma^2) \) to a 3-mixture of the form \( \frac{1}{5}N(\theta^*_1(1 + \alpha), \sigma^2) + \frac{1}{5}N(\theta^*_2(1 - \alpha), \sigma^2) + \frac{1}{2}N(-\theta^*_3, \sigma^2) \). They provide finite-sample convergence rates for EM assuming that EM starts from an initial solution sufficiently close to the global minimum. Note that in the setting of Corollary 6, we effectively establish that there is no other local minimum besides the global minimum around \( (\frac{1}{2}(\theta^*_1 + \theta^*_3), \theta^*_3) \), hence EM converges to this solution from arbitrary initialization.
4 Discussion

In this paper, we studied the nonconvex landscape of the population negative log-likelihood of GMM with a general number of components. We showed that all local minima have a specific form of structure that partially identifies the true components of the global minimum. It is of great interest to explore the algorithmic consequences of this structural result. For example, once we find a local minimum (e.g., using the EM algorithm) that identifies a subset of the true components, it may be possible to iteratively refine this solution and recover the remaining components by deflating the components already recovered. Over-parametrization is another promising approach for avoiding spurious local minima. In particular, when the number of fitted centers $k$ is sufficiently larger than the number of true components $k_*$, we expect that the one-fit-many configuration is unlikely, in which case all (or most) of the true components can be identified through the many-fit-one configurations. Note that a version of this idea is considered in the work [7].

An immediate future step is to transfer the population-level results in this paper to the finite-sample setting, for which the uniform concentration and localization techniques developed in [20, 10] may be immediately applicable. It is also interesting to study the low-SNR regime where the mixture components have small or even no separation, in which case the structures of the local minima may become more complicated. Finally, it would be interesting to understand whether the phenomenon of structured local minima holds more generally in other mixture and latent variable models. The recent study in [3] provides empirical evidences for the universality of this phenomenon.

5 Preliminaries

In this section, we derive several preliminary results that are useful in the proofs of our main Theorems 1–3. We focus on the setting with unit variance $\sigma^2 = 1$; results for the general setting follow easily by rescaling.

5.1 Derivatives of $L$

We begin by computing the gradient of the population negative log-likelihood function $L(\beta) := -\mathbb{E}_* [\log f(X)]$. Recall that $f_j(x) := \phi(x \mid \beta_j, 1) = \frac{1}{\sqrt{2\pi}} \exp \left( -\|x - \beta_j\|^2 / 2 \right)$, hence

$$\frac{\partial f_j(x)}{\partial \beta_j} = \frac{1}{\sqrt{2\pi}} \exp \left( -\|x - \beta_j\|^2 / 2 \right) \cdot (x - \beta_j)$$

and $\frac{\partial f_i(x)}{\partial \beta_j} = 0$ if $i \neq j$. Since $f := \frac{1}{k} \sum_{j \in [k]} f_j$, we have

$$\frac{\partial}{\partial \beta_j} L(\beta) = -\mathbb{E}_* \left[ \frac{\frac{\partial}{\partial \beta_j} f_j(X)}{f(X)} \right]$$

$$= -\mathbb{E}_* \left[ \frac{\frac{1}{k} f_j(X) \cdot (X - \beta_j)}{f(X)} \right]$$

$$= \mathbb{E}_* \left[ \psi_j \cdot (\beta_j - X) \right],$$

where the first step follows from exchanging the expectation and differentiation using the dominated convergence theorem (we ignore this argument in the sequel), the second step follows from equation (18), and the last step follows from the definition $\Psi_j := \psi_j(X) = \frac{1}{f} f_j(X) / f(X)$. This proves the gradient expression in equation (9).

To derive the Hessian of $L$, let us first compute the derivative of $\psi_j(x)$. For each $j \in [k]$, we have

$$\frac{\partial}{\partial \beta_j} \psi_j(x) = \frac{1}{k} \frac{\partial}{\partial \beta_j} f_j(x) \cdot \frac{1}{k} f_j(X) + \frac{1}{k} \frac{\partial}{\partial \beta_j} f_j(x) \cdot \frac{1}{k} f_j(X)$$

$$= \frac{1}{k^2} f_j(x) \cdot (x - \beta_j) \cdot \frac{1}{k} f_j(x) + \frac{1}{k^2} f_j(x) \cdot (x - \beta_j) \cdot \frac{1}{k} f_j(x)$$

$$= \frac{1}{k^2} \cdot \frac{-f_j(x)^2}{f(x)^2} + \frac{k f_j(x) f(x)}{f(x)^2} \cdot (x - \beta_j).$$
For each $i \neq j \in [k]$, we have
\[
\frac{\partial}{\partial \beta_i} \psi_j(x) = -\frac{1}{k} \frac{\partial}{\partial \beta_i} f_i(x) \cdot \frac{1}{k} f_j(x) + \frac{1}{k} \frac{\partial}{\partial \beta_j} f_j(x)
\]
\[
= -\frac{1}{k} f_i(x) \cdot (x - \beta_i) \cdot \frac{1}{k} f_j(x) + 0
\]
\[
= \frac{1}{k^2} \cdot (x - \beta_i) \cdot (x - \beta_i).
\]
Combining the above two equations and recalling that $\psi_i(x) = \frac{1}{k} f_i(x)/f(x)$, $\ell \in [k]$, we obtain
\[
\frac{\partial}{\partial \beta_i} \psi_j(x) = \begin{cases} (-\psi_j(x) + 1) \psi_j(x) \cdot (x - \beta_j), & i = j, \\
-\psi_i(x) \psi_j(x) \cdot (x - \beta_i), & i \neq j. \end{cases} \tag{19}
\]
It follows that the Hessian of $L$ is
\[
\frac{\partial^2}{\partial \beta_i \partial \beta_j} L(\beta) = \frac{\partial}{\partial \beta_i} E_x [\psi_j \cdot (\beta_j - X)]
\]
\[
= E_x \left[ \left( \frac{\partial}{\partial \beta_i} \psi_j \right) \cdot (\beta_j - X)^\top + \psi_j \cdot \left( \frac{\partial}{\partial \beta_i} \beta_j^\top \right) \right]
\]
\[
= \begin{cases} E_x \left[ (\psi_j - 1) \psi_j \cdot (\beta_j - X)(\beta_j - X)^\top + \psi_j \cdot I_d \right], & i = j, \\
E_x \left[ \psi_i \psi_j \cdot (\beta_i - X)(\beta_j - X)^\top \right], & i \neq j, \end{cases} \tag{20}
\]
where we use equation (19) in the last step.

### 5.2 Consequences of Local Optimality

Any local minimum $\beta$ of $L$ satisfies the first-order stationary condition (10) as well as the second-order optimality condition $\nabla^2 L(\beta) \succeq 0$, where the Hessian $\nabla^2 L$ is given explicitly in equation (20). Below we derive several consequences of this second-order condition by evaluating the Hessian along certain test directions. These results are used in the proof of our main Theorem 2.

Fix a pair $(i, j) \in [k] \times [k]$. Let $v_i, v_j \in \mathbb{R}^d$ be an arbitrary pair of vectors. If $\nabla^2 L(\beta) \succeq 0$, then any submatrix of $\nabla^2 L(\beta)$ is also positive semidefinite, hence
\[
0 \leq v_i^\top \left[ \frac{\partial^2}{\partial \beta_i \partial \beta_j} L(\beta) \right] v_i + v_j^\top \left[ \frac{\partial^2}{\partial \beta_j \partial \beta_i} L(\beta) \right] v_j + 2v_i^\top \left[ \frac{\partial^2}{\partial \beta_i \partial \beta_j} L(\beta) \right] v_j
\]
\[
= E_x \left[ (\Psi_i - 1) \Psi_i \langle \beta_i - X, v_i \rangle^2 + \Psi_i \|v_i\|^2 \right] + E_x \left[ (\Psi_j - 1) \Psi_j \langle \beta_j - X, v_j \rangle^2 + \Psi_j \|v_j\|^2 \right] + 2E_x \left[ \Psi_i \Psi_j \langle \beta_i - X, v_i \rangle \langle \beta_j - X, v_j \rangle \right]
\]
\[
\leq E_x \left[ -\Psi_j \Psi_i \langle \beta_i - X, v_i \rangle^2 + \Psi_i \|v_i\|^2 \right] + E_x \left[ -\Psi_i \Psi_j \langle \beta_j - X, v_j \rangle^2 + \Psi_j \|v_j\|^2 \right] + 2E_x \left[ \Psi_i \Psi_j \langle \beta_i - X, v_i \rangle \langle \beta_j - X, v_j \rangle \right]
\]
\[
= -E_x \left[ \Psi_i \Psi_j \langle \beta_i - X, v_i \rangle \langle \beta_j - X, v_j \rangle \right] + \|v_i\|^2 E_x [\Psi_i] + \|v_j\|^2 E_x [\Psi_j]. \tag{21}
\]
where step (i) holds because $\Psi_i - 1 \leq -\Psi_j$ and $\Psi_j - 1 \leq -\Psi_i$, both consequences of the fact that $\Psi_i \geq 0, \Psi_j \geq 0$ and $\sum_{\ell \in [k]} \Psi_\ell = 1$ surely.

We consider two specific choices of the pair $(v_i, v_j)$:

- **Let** $v_i = v_j = \frac{\beta_i - \beta_j}{\|\beta_i - \beta_j\|}$, which are unit-norm vectors. In this case, rearranging equation (21) gives
  \[
  1 \geq E_x [\Psi_i + \Psi_j] \geq E_x \left[ \Psi_i \Psi_j \langle \beta_i - \beta_j, v_i \rangle^2 \right] = \|\beta_i - \beta_j\|^2 \cdot E_x [\Psi_i \Psi_j], \quad \forall i, j \in [k]. \tag{22}
  \]
• Let \( v_i = u_{s \rightarrow i} := \frac{\beta_i - \theta_i}{\|\beta_i - \theta_i\|} \), which is unit-norm, and \( v_j = 0 \). In this case, rearranging equation (21) gives
\[
1 \geq E_s [\Psi_i] \geq E_s \left[ \Psi_i \Psi_j \langle \beta_i - X, u_{s \rightarrow i} \rangle^2 \right], \quad \forall i \in [k]. \tag{23}
\]

5.3 Voronoi Sets and Their Geometry

As can be seen above, the association coefficient \( \psi_i(x) \) plays a key role in characterizing the gradient, Hessian and optimality condition of \( L \). The quantity \( \psi_i(x) \) defines a (soft-)association between a data point \( x \in \mathbb{R}^d \) and the center \( \beta_i \), based on the relative magnitudes of the distances between \( x \) and the \( k \) centers. To understand the properties of \( \psi_i(x) \), it is useful to study the hard-association analogue thereof, where a data point is associated with the closest center among the \( k \) centers. This association induces the so-called Voronoi diagram of the space \( \mathbb{R}^d \). Below we take a closer look at this Voronoi diagram and elucidate its relationship with the association coefficients \( \psi_i(x) \). These results are used in the proof of our main Theorem 2.

Let \( \beta_{ij} := (\beta_i + \beta_j)/2 \) denote the mid point of \( \beta_i \) and \( \beta_j \). Recall the definition (13) of the (hard-)Voronoi set associated with \( \beta_i \), which has the following equivalent representation:
\[
V_i := \{ x \in \mathbb{R}^d : \|x - \beta_i\| \leq \|x - \beta_\ell\|, \forall \ell \in [k] \}
\]
\[
= \{ x : \langle x - \beta_i, \beta_i - \beta_\ell \rangle \geq 0, \forall \ell \in [k] \}
\]
\[
= \{ x : \psi_i(x) \geq \psi_\ell(x), \forall \ell \in [k] \}. 
\]

In words, \( V_i \) is the set of points whose closest center is \( \beta_i \). Also define the set of points equidistant to \( \beta_i \) and \( \beta_j \):
\[
\partial_{ij} := \{ x : \|x - \beta_i\| = \|x - \beta_j\| \}
\]
\[
= \{ x : \langle x - \beta_i, \beta_i - \beta_j \rangle = 0 \}
\]
\[
= \{ x : \psi_i(x) = \psi_j(x) \}. 
\]

The second step in the above definitions makes it clear that \( V_i \) is a polyhedron and \( \partial_{ij} \) is an affine subspace. Note that if the \( \beta_i \)'s are distinct, then so are their Voronoi sets. In this case, the Voronoi sets form a partition of the entire space \( \mathbb{R}^d \), up to the measure-zero boundaries \( V_i \cap V_j \subseteq \partial_{ij} \). On the other hand, if \( \beta_i = \beta_j \) for some pair \( i, j \in [k] \), then \( V_i = V_j \) and \( \partial_{ij} = \mathbb{R}^d \).

We also define the soft versions of the above sets: Given a parameter \( \alpha \geq 0 \), let
\[
\tilde{V}_i^\alpha := \{ x : \langle x - \beta_i, \beta_i - \beta_\ell \rangle \geq -\alpha, \forall \ell \in [k] \},
\]
\[
\tilde{\partial}_{ij}^\alpha := \{ x : -\alpha \leq \langle x - \beta_i, \beta_i - \beta_j \rangle \leq \alpha \}.
\]

The sets \( \tilde{V}_i^\alpha \) and \( \tilde{\partial}_{ij}^\alpha \) are the \( \alpha \)-enlargement of \( V_i \) and \( \partial_{ij} \), respectively, with \( \tilde{V}_i^0 = V_i \) and \( \tilde{\partial}_{ij}^0 = \partial_{ij} \). Similarly as before, \( \tilde{\partial}_{ij}^\alpha \) is a superset of the intersection \( \tilde{V}_i^\alpha \cap \tilde{V}_j^\alpha \), which can be interpreted as the soft boundary between the Voronoi sets of \( \beta_i \) and \( \beta_j \). Moreover, if \( \beta_i = \beta_j \) for some pair \( i, j \in [k] \), then \( \tilde{V}_i^\alpha = \tilde{V}_j^\alpha \) and \( \tilde{\partial}_{ij}^\alpha = \mathbb{R}^d \).

Finally, define the set
\[
\tilde{G}_{ij} := \left\{ x : \psi_i(x)\psi_j(x) \geq \frac{1}{4k^2} \right\}.
\]

The following lemma establishes the relationship between the association coefficient \( \psi_i(x) \) and the sets \( \tilde{V}_i^\alpha \), \( \tilde{\partial}_{ij}^\alpha \) and \( \tilde{G}_{ij} \).

**Lemma 1** (Soft Voronoi Sets and Boundaries). For each \( i \neq j \in [k] \) and \( c \geq 1 \), we have
\[
\tilde{V}_i^{\log c} \subseteq \left\{ x : \psi_i(x) \geq \frac{1}{ck} \right\} \subseteq \tilde{V}_i^{\log ck}; \tag{24a}
\]
consequently,
\[
\tilde{V}_i^{\log 2} \cap \tilde{V}_j^{\log 2} \subseteq \tilde{G}_{ij} \subseteq \tilde{V}_i^{2\log 2k} \cap \tilde{V}_j^{2\log 2k}. \tag{24b}
\]
We also have
\[
\tilde{\partial}_{ij}^{\log c} \cap \tilde{V}_j^{\log c} \subseteq \left\{ x : \psi_i(x)\psi_j(x) \geq \frac{1}{c^2k^2} \right\}. \tag{24c}
\]
Proof. For each \( \ell \neq i \in [k] \), recall that \( \bar{\beta}_{i\ell} := (\beta_i + \beta_\ell)/2 \). We make frequent use of the following equivalence relationship:

\[
\langle x - \bar{\beta}_{i\ell}, \beta_i - \bar{\beta}_{i\ell} \rangle \geq - \log c.
\]

\[
\iff -\|x - \beta_i\|^2/2 \geq - \log c - \|x - \beta_\ell\|^2/2
\]

\[
\iff \exp \left(-\|x - \beta_i\|^2/2\right) \geq \frac{1}{c} \exp \left(-\|x - \beta_\ell\|^2/2\right)
\]

\[
\iff f_i(x) \geq \frac{1}{c} f_\ell(x) \iff \psi_i(x) \geq \frac{1}{c} \psi_\ell(x).
\]

Below we prove the three equations in the lemma.

To prove equation (24a), we observe the implication

\[
f_i(x) \geq \frac{1}{c} f_\ell(x), \forall \ell \neq i
\]

\[
\implies \sum_{\ell \in [k]} f_\ell(x) \leq f_i(x) + c(k - 1)f_i(x) \leq ck f_i(x)
\]

\[
\implies \psi_i(x) = \frac{f_i(x)}{\sum_{\ell \in [k]} f_\ell(x)} \geq \frac{1}{ck}.
\]

Combining with equation (25), we obtain that

\[
x \in \overline{V}_{i}^{\log c} \implies \psi_i(x) \geq \frac{1}{ck},
\]

thereby proving the first inclusion in equation (24a).

Conversely, we have the implications

\[
\psi_i(x) \geq \frac{1}{ck}
\]

\[
\implies \psi_i(x) := \frac{f_i(x)}{\sum_{\ell \in [k]} f_\ell(x)} \geq \frac{1}{ck}
\]

\[
\implies f_i(x) \geq \frac{1}{ck} \sum_{\ell \in [k]} f_\ell(x) \geq \frac{1}{ck} \max_{\ell \neq i} f_\ell(x)
\]

Combining with equation (25), we obtain that

\[
\psi_i(x) \geq \frac{1}{ck} \implies x \in \overline{V}_{i}^{\log ck},
\]

thereby proving the second inclusion in equation (24a).

We next observe that

\[
\min \{\psi_i(x), \psi_j(x)\} \geq \frac{1}{2k} \implies \psi_i(x) \psi_j(x) \geq \frac{1}{4k^2} \implies \min \{\psi_i(x), \psi_j(x)\} \geq \frac{1}{4k^2}.
\]

It follows that

\[
\overline{V}_{i}^{\log 2} \cap \overline{V}_{j}^{\log 2} \subseteq G_{ij} \subseteq \overline{V}_{i}^{2\log 2k} \cap \overline{V}_{j}^{2\log 2k},
\]

which is equation (24b) in the lemma.

Finally, equation (24c) in the lemma follows from the observation that

\[
x \in \overline{\partial}_{ij}^{\log c} \cap \overline{V}_{j}^{\log c}
\]

\[
\implies \langle x - \beta_{ij}, \beta_i - \bar{\beta}_{ij} \rangle \geq - \log c, \psi_j(x) \geq \frac{1}{ck}
\]

\[
\implies \psi_i(x) \geq \frac{1}{c} \psi_j(x), \psi_j(x) \geq \frac{1}{ck}
\]

\[
\implies \psi_i(x) \psi_j(x) \geq \frac{1}{ck^2}.
\]

This completes the proof of Lemma 1.
6 Proofs of Theorem 1 and Corollary 2

In this section, we prove Theorem 1 and Corollary 2, which establish several basic properties of the stationary points of $L$.

6.1 Proof of Theorem 1

Our strategy is to apply the Stein's identity to obtain an alternative expression for the term $E_s[\Psi_i X_i]$, which appears in the stationary condition $(10)$. We make use of the following multivariate version of the Stein's identity specialized to the identity covariance setting.

**Lemma 2** (Stein’s Identity). Suppose $X \sim \mathcal{N}(\mu, \sigma^2 I_d)$ and $g : \mathbb{R}^d \to \mathbb{R}$ is a differentiable function. Then

$$E[g(X)(X - \mu)] = \sigma^2 E[\nabla g(X)].$$

To use this lemma, let us fix an index $i \in [k]$ and first compute the derivative $\nabla \psi_i(x)$ with respect to $x$. Recall from equation (7) that

$$\psi_i(x) := \sum_{s \in \mathcal{S}} e^{-\|x - \beta_i\|^2/(2\sigma^2)} = \sum_{s \in \mathcal{S}} \frac{1}{\sum_{s \in \mathcal{S}} e^{-\|x - \beta_i\|^2/(2\sigma^2)}} e^{-\|x - \beta_i\|^2/(2\sigma^2)}.$$

Taking the derivative, we have

$$\nabla \psi_i(x) = -\sum_{j \in [k]} \frac{e^{-\|x - \beta_j\|^2/(2\sigma^2)}}{\left(\sum_{s \in \mathcal{S}} e^{-\|x - \beta_j\|^2/(2\sigma^2)}\right)^2} \cdot (\beta_j - \beta_i) \cdot \sigma^{-2}$$

$$= \sigma^{-2} \sum_{j \in [k]} (\beta_i - \beta_j) \psi_i(x) \psi_j(x)$$

$$= \sigma^{-2} \left(\beta_i \psi_i(x) - \sum_{j \in [k]} \beta_j \psi_i(x) \psi_j(x)\right),$$

where the last step follows from the fact that $\sum_{j \in [k]} \psi_j(x) = 1$. Noting that $X \sim \mathcal{N}(\theta^*_s, \sigma^2 I_d)$ under $E_s$, we apply the Stein’s identity (Lemma 2) to obtain

$$E_s[\Psi_i X_i] = \theta^*_i E_s[\Psi_i] + \sigma^2 \cdot E_s[\nabla \psi_i(X)]$$

$$= \theta^*_i E_s[\Psi_i] + \beta_i E_s[\Psi_i] - \sum_{j \in [k]} \beta_j E_s[\Psi_j], \quad \forall i \in [k], s \in [k_s].$$

(26)

We are ready to prove Theorem 1. By the stationary condition $(10)$, $\beta$ is a stationary point of $L$ if and only if $\beta_i = \frac{\sum_{s \in [k_s]} E_s[\Psi_i X_i]}{\sum_{s \in [k_s]} E_s[\Psi_i]}, \forall i \in [k]$, where we use the fact that $E_s[\cdot] = \frac{1}{k_s} \sum_{s \in [k_s]} E_s[\cdot]$. Combining with the above expression (26) for $E_s[\Psi_i X_i]$, we obtain that

$$\beta_i = \frac{\sum_{s \in [k_s]} \left(\theta^*_s E_s[\Psi_i] + \beta^*_i E_s[\Psi_i] - \sum_{j \in [k]} \beta_j E_s[\Psi_j]\right)}{\sum_{s \in [k_s]} E_s[\Psi_i]}, \quad \forall i \in [k].$$

Rearranging terms gives

$$\sum_{s \in [k_s]} \sum_{j \in [k]} \beta_j E_s[\Psi_i \Psi_j] = \sum_{s \in [k_s]} \theta^*_s E_s[\Psi_i], \quad \forall i \in [k],$$

which is the equivalent stationary condition $(12)$ claimed in the theorem.
6.2 Proof of Corollary 2

Let \( \beta = (\beta_1, \ldots, \beta_k) \in \mathbb{R}^{d \times k} \) be a stationary point of \( L \). We first argue that it suffices to focus on the distinct centers in \( \{\beta_1, \ldots, \beta_k\} \) by grouping identical centers together. Indeed, suppose that the set \( \{\beta_1, \ldots, \beta_k\} \) contains \( \tilde{k} \) distinct vectors; without loss of generality assume that the first \( \tilde{k} \) vectors are distinct. Let \( \widetilde{\beta} := (\beta_1, \ldots, \beta_{\tilde{k}}) \in \mathbb{R}^{d \times \tilde{k}} \) be the distinct centers. For each \( i \in [\tilde{k}] \), define \( J_i := \{ j \in [k] : \beta_j = \beta_i \} \) and \( m_i := |J_i| \), which denote the set and number of centers identical to \( \beta_i \), respectively. Also define the grouped association coefficient

\[
\widetilde{\Psi}_i := \sum_{j \in J_i} \Psi_j = m_i \Psi_j \quad \text{for } i \in [\tilde{k}].
\]

With the above notations, the equivalent stationary condition (12) in Theorem 1 can be rewritten as

\[
\sum_{j \in [\tilde{k}]} \beta_j \sum_{s \in [k_s]} E_s \left[ \widetilde{\Psi}_i \widetilde{\Psi}_j \right] = \sum_{s \in [k_s]} \theta_s^* E_s \left[ \widetilde{\Psi}_i \right], \quad \forall i \in [\tilde{k}].
\]

Let \( \widetilde{\Psi} = (\widetilde{\Psi}_1, \ldots, \widetilde{\Psi}_\tilde{k})^\top \in \mathbb{R}^\tilde{k} \) be the vector of association coefficients. Since \( \sum_{s \in [k_s]} E_s \left[ \cdot \right] = k_s E_s \left[ \cdot \right] \), the above condition can be written compactly in matrix form as

\[
\sum_{s \in [k_s]} E_s \left[ \widetilde{\Psi} \widetilde{\Psi}^\top \right] \beta = \sum_{s \in [k_s]} E_s \left[ \widetilde{\Psi} \right] \theta_s^* \top.
\]

(27)

We claim that the \( \tilde{k} \)-by-\( \tilde{k} \) matrix \( E_s \left[ \widetilde{\Psi} \widetilde{\Psi}^\top \right] \) is invertible. Otherwise, there exists a nonzero vector \( u \in \mathbb{R}^\tilde{k} \) such that

\[
0 = u^\top E_s \left[ \widetilde{\Psi} \widetilde{\Psi}^\top \right] u = E_s \left[ \left( \widetilde{\Psi}^\top u \right)^2 \right],
\]

which means that with probability 1 (with respect to \( f^* \)):

\[
0 = \widetilde{\Psi}^\top u = \sum_{i \in [\tilde{k}]} \frac{m_i \cdot e^{-\|x - \beta_i\|_2^2 / (2\sigma^2)}}{\sum_{i \in [\tilde{k}]} e^{-\|x - \beta_i\|_2^2 / (2\sigma^2)}} \cdot u_i,
\]

or equivalently

\[
0 = \sum_{i \in [\tilde{k}]} m_i \cdot e^{-\|x - \beta_i\|_2^2 / (2\sigma^2)} \cdot u_i.
\]

Since \( m_i \geq 1 \) and \( \{\beta_i, i \in [\tilde{k}]\} \) are distinct, the \( \tilde{k} \) functions \( x \mapsto m_i \cdot e^{-\|x - \beta_i\|_2^2 / (2\sigma^2)}, i \in [\tilde{k}] \) are linearly independent, hence the above equation cannot hold, a contradiction.

Thanks to invertibility, equation (27) implies that

\[
\beta^* = \left( k_s E_s \left[ \widetilde{\Psi} \widetilde{\Psi}^\top \right] \right)^{-1} \sum_{s \in [k_s]} E_s \left[ \widetilde{\Psi} \right] \theta_s^* \top.
\]

Therefore, we find that each \( \beta_i \) is a linear combination of \( \{\theta_s^*, s \in [k_s]\} \), thereby proving Corollary 2.

7 Proof of Theorem 2

In this section we prove our main Theorem 2. Throughout this section, we fix \( \beta \) to be an arbitrary local minimizer of \( L \). We focus on the setting with unit variance \( \sigma^2 = 1 \); results for the general setting follow easily by rescaling.
7.1 Reduction to Lower Dimension

We first argue that it suffices to prove the theorem in \(k_\ast\) dimensions. Once this is established, the theorem for \(d > k_\ast\) dimensions can be deduced as follows. Suppose that \(\theta^* \in \mathbb{R}^{d \times k_\ast}\) is the ground truth solution and \(\beta \in \mathbb{R}^{d \times k_\ast}\) is a local minimum. We may choose a coordinate system such that the first \(k_\ast\) dimensions contain the subspace \(\text{span}\{\theta_1^*, \ldots, \theta_k^*\}\) (see Remark 1). This choice of coordinate implies that for each \(s \in [k_\ast]\), we have \(\theta_s^* = (\theta_s^{*,t}, 0)\) for some \(\theta_s^{*,t}\). By Corollary 2, for each \(i \in [k]\) we further have \(\beta_i = (\beta_i^{*,t}, 0)\) for some \(\beta_i^{*,t}\) \(\in \mathbb{R}^{k_\ast}\). Moreover, thanks to the rotational invariance of Gaussian distributions, the \(d\)-dimensional Gaussian mixture is a product distribution with respect to the first \(k_\ast\) dimensions and the last \(d - k_\ast\) dimensions, where the first \(k_\ast\)-dimensional margin is itself a Gaussian mixture. Indeed, for any \(x = (x', z) \in \mathbb{R}^d\) with \(x' \in \mathbb{R}^{k_\ast}\) and \(z \in \mathbb{R}^{d - k_\ast}\), the density of the Gaussian mixture factorizes:

\[
\begin{align*}
    f^*(x) &\propto \frac{1}{k_\ast} \sum_{s=1}^{k_\ast} \exp \left( - \frac{|x - \beta_s^*|^2}{2} \right) \\
&= \frac{1}{k_\ast} \sum_{s=1}^{k_\ast} \exp \left( - \frac{|(x', z) - (\beta_s^{*,t}, 0)|^2}{2} \right) \\
&= \left[ \frac{1}{k_\ast} \sum_{s=1}^{k_\ast} \exp \left( - \frac{|x' - \beta_s^{*,t}|^2}{2} \right) \right] \cdot \exp \left( - \frac{|z|^2}{2} \right).
\end{align*}
\]

Now, since \(\beta\) is a local minimum of \(L\), \(\beta'\) is also a local minimum of \(L\) restricted to the first \(k_\ast\) dimensions. Applying the theorem with dimension \(k_\ast\), we obtain bounds on the quantities \(||\beta' - \theta_s^*||_d\), \(||\beta' - \lambda^{-1} \sum_{s \in S} \theta_s^*||_d\) and \(\mathbb{P}_s(\mathcal{V}_i(\beta'))\). We claim that these three quantities are equal to \(||\beta - \theta_s^*||_d\), \(||\beta - \lambda^{-1} \sum_{s \in S} \theta_s^*||_d\) and \(\mathbb{P}_s(\mathcal{V}_i(\beta))\), respectively. Indeed, the first two equalities are immediate under our coordinate system; the last equality holds because the Gaussian mixture factorizes (shown above) and so do the Voronoi sets: \(\mathcal{V}_i(\beta) = \mathcal{V}_i(\beta') \times \mathbb{R}^{d - k_\ast}\). A similar argument applies to the quantity \(\mathbb{E}_s[\psi_i]\). We conclude that the same collection of bounds hold in dimension \(d\) as well. In the rest of the proof, we can safely assume that \(d \leq k_\ast\).

7.2 Structural Properties

The proof of Theorem 2 relies on three key propositions that establish several structural properties of the local minimizer \(\beta\). Before we state these propositions, it is useful to recall the concepts and properties of (hard/soft-)Voronoi sets discussed in Section 5.3. In particular, equations (24b) and (24c) in Lemma 1 say that the soft boundary between the Voronoi sets of (hard/soft-)Voronoi sets discussed in Section 5.3. In particular, equations (24b) and (24c) in Lemma 1 say that the soft boundary between the Voronoi sets of \(\beta_i\) and \(\beta_j\) are roughly the set of points for which the product \(\psi_i(x)\psi_j(x)\) is large. Consequently, the expected value \(\mathbb{E}_s[\psi_i \psi_j]\) can be viewed as a measure of the size of this boundary, with respect to the density \(f^*_s\) of the \(s\)-th mixture component. The propositions below characterize the relationship between the fitted centers \(\{\beta_j\}\) and the true centers \(\{\theta_s^*\}\) depending on whether \(\mathbb{E}_s[\psi_i \psi_j]\) is large or small.

For each \(i, j \in [k]\), recall that \(\beta_{ij} := (\beta_i + \beta_j)/2\) and define

\[
d_{ij} := \|\beta_i - \beta_j\| = 2 \|\beta_i - \bar{\beta}_{ij}\| = 2 \|\beta_j - \bar{\beta}_{ij}\|.
\]

The first proposition states that if \(\mathbb{E}_s[\psi_j \psi_{\ell}]\) is large for some \(j, \ell\), then \(\beta_j\) and \(\beta_\ell\) must be both close to the true center \(\theta_s^*\).

**Proposition 1** (Large Boundary). Let \(\lambda \in (0, 1]\) be a fixed number. For each \((s, j, \ell) \in [k_\ast] \times [k] \times [k]\), if \(\max \{1, d_{j\ell}\} \mathbb{E}_s[\psi_j \psi_{\ell}] \geq \lambda\), then

\[
    \|\beta_j - \theta_s^*\| + \|\beta_\ell - \theta_s^*\| \leq C_0 \frac{k_\ast}{\lambda},
\]

where \(C_0 > 1\) is a universal constant. If in addition \(\theta_s^* \in \mathcal{V}_i\) for some \(i \in [k]\), then \(\|\beta_i - \theta_s^*\| \leq C_0 \frac{k_\ast}{\lambda}\).

We prove this proposition in Section 7.4.

Let \(\text{int}\mathcal{V}_j\) denote the interior of the Voronoi set \(\mathcal{V}_j\). The second proposition states that if \(\theta_s^* \notin \text{int}\mathcal{V}_j\) and \(\mathbb{E}_s[\psi_j \psi_{\ell}]\) is small for all \(\ell\), then \(\beta_j\) must have a small Voronoi set and a small association coefficient under \(f^*_s\).
Proposition 2 (Small Boundary, I). Let $\lambda \in (0, 1]$ be a fixed number. For each $(s, j) \in [k_\ast] \times [k]$ such that $\theta_s^* \notin \text{int} \mathcal{V}_j$, if $\max \{1, d_{jt}\} E_s[\Psi_j \Psi_t] < \lambda$ for all $t \in [k] \setminus \{j\}$, then

$$
P_s (\mathcal{V}_j) \leq C_0 k^3 \lambda,
E_s[\Psi_j] \leq 4C_0 k^3 \lambda,$$

where $C_0 > 1$ is a universal constant.

We prove this proposition in Section 7.5.

To state the third proposition, we need some additional notations. For each $s \in [k_\ast]$, define the index set

$$H_s := \left\{ i \in [k] : \max_{\ell \in [k] \setminus \{i\}} \max \{1, d_{it}\} E_s[\Psi_i \Psi_t] \geq \lambda \right\}.$$  

For each $i \in [k]$, let $A_i := \{ s \in [k_\ast] : \theta_s^* \in \mathcal{V}_i \}$ index the true centers that are in the Voronoi set of $\beta_i$, and $A_i^c$ be the complement of $A_i$. We then define two subsets of $A_i$ and $A_i^c$:

$$\hat{A}_i := \{ s \in A_i : H_s = \emptyset \} = \left\{ s \in A_i : \max_{j \in [k], j \neq \ell} \max \{1, d_{it}\} E_s[\Psi_j \Psi_t] < \lambda \right\},$$
$$\hat{A}_i^c := \{ s \in A_i^c : H_s \notin i \} = \left\{ s \in A_i^c : \max_{\ell \in [k] \setminus \{i\}} \max \{1, d_{it}\} E_s[\Psi_i \Psi_t] < \lambda \right\}.$$

Proposition 3 (Small Boundary, II). Let $\lambda \in (0, 1/k_\ast \lambda^2)$ be a fixed number, and suppose that the SNR satisfies $\Delta_{\min} \geq C k_\ast^2 \lambda$, where $C > 1$ is a sufficiently large universal constant. For each $i \in [k]$, if $|\hat{A}_i| \geq 1$, then we have

$$\beta_i \neq \beta_j, \quad \forall j \in [k] \setminus \{i\},$$
$$E_s[\Psi_i] \geq 1 - 4C_0 k^3 \lambda, \quad \forall s \in \hat{A}_i, \quad (28a)$$
$$P_s (\mathcal{V}_j) \geq 1 - C_0 k^3 \lambda, \quad \forall s \in \hat{A}_i, \quad (28b)$$
$$\left\| \beta_i - \frac{1}{|\hat{A}_i|} \sum_{s \in \hat{A}_i} \theta_s^* \right\| \leq C_0 k_\ast k^3 \lambda \Delta_{\max} + C_0 \frac{k_\ast (k_\ast + k)}{\lambda}, \quad (28c)$$

where $C_0 \geq 1$ is a universal constant.

We prove this proposition in Section 7.6. The definition of the sets $\hat{A}_i, \hat{A}_i^c$ and the statement of Proposition 3 are somewhat complicated. As shall become clear momentarily, this complication is needed to ensure disjointness of the sets $\{S_\ast_a\}$ and $\{S_a\}$ as promised by Theorem 2.

7.3 Completing the Proof of Theorem 2

With Propositions 1–3, we are ready to construct the sets $\{S_\ast_a\}$ and $\{S_a\}$ that satisfy the properties stated in Theorem 2. We do so via a procedure with a combinatorial flavor.

Step 1 (one-fit-many): For each $i \in [k]$ with $|\hat{A}_i| \geq 1$, construct the pair of sets

$$S_a = \{ i \}, \quad S_a^\ast = \hat{A}_i.$$  

Proposition 3 ensures that $\beta_i \neq \beta_j, \forall j \in [k] \setminus \{i\}$, and that equation (15) in Theorem 2 holds. Let $(S_a, S_a^\ast), a = 1, \ldots, q_0$ be the sets constructed in this step.

Step 2 (many-fit-one): For each $s$ with $|H_s| \geq 1$, construct the pair of sets

$$S_a = H_s \cup \{ i \in [k] : \mathcal{V}_i \ni \theta_s^* \} \setminus \bigcup_{b=1}^{q_0} S_b, \quad S_a^\ast = \{ s \}.$$
Proposition 1 ensures that equation (16) in Theorem 2 holds. Let \((S_a, S_a^*)\), \(a = q_0 + 1, \ldots, q\) be the sets constructed in this step.

**Step 3 (near-empty):** We are left with the fitted centers

\[
S_0 := [k] \setminus \bigcup_{a=1}^q S_a.
\] (29)

For each \(i \in S_0\), we have \(\hat{A}_i = \emptyset\) (otherwise, \(i\) would be covered in step 1), which further implies that \(A_i = \emptyset\) (otherwise, there exists some \(s \in A_i = A_i \setminus \hat{A}_i\) with \(H_s \neq \emptyset\), in which case \(V_i \ni \theta_s^*\) and hence \(i\) would be covered in step 2); moreover, we have

\[
\max \{1, d_{ij}\} \mathbb{E}_s[\Psi_i \Psi_j] < \lambda, \quad \forall s \in [k], j \in [k] \setminus \{i\},
\]

(otherwise, \(i\) would be covered in step 2). Note that \(A_i = \emptyset\) means that

\[
\theta_s^* \notin V_i, \quad \forall s \in [k].
\]

When the last two display equations hold, Proposition 2 ensures that

\[
\mathbb{P}_s(V_i) \leq C_0 k^3 \lambda \quad \text{and} \quad \mathbb{E}_s[\Psi_i] \leq 4C_0 k^3 \lambda, \quad \forall s \in [k].
\]

Since \(\mathbb{P}_s = \frac{1}{k_s} \sum_{s \in [k_s]} \mathbb{P}_s\) and \(\mathbb{E}_s = \frac{1}{k_s} \sum_{s \in [k_s]} \mathbb{E}_s\), equation (14) in Theorem 2 follows.

With the three steps above, we have constructed two collection of sets \(\{S_a\}\) and \(\{S_a^*\}\) that satisfy the bounds (14), (15) and (16) in Theorem 2.

It remains to prove that \(\{S_a\}\) and \(\{S_a^*\}\) are partitions. We first show that \(\{S_a\}\) forms a cover of \([k]\) and \(\{S_a^*\}\) forms a cover of \([k_s]\):

- By equation (29) it is clear that \(\bigcup_{a=0}^q S_a = [k]\).
- We claim that \(\bigcup_{a=0}^q S_a^* = \{s\} \). To see this, take any \(s \in [k_s]\). Since the Voronoi sets cover the entire space \(\mathbb{R}^d\), we must have \(s \in A_i\) for some \(i \in [k] \setminus S_0\). If \(H_s = \emptyset\), then \(s \in \hat{A}_i \subseteq \bigcup_{a=0}^q S_a^*\). Otherwise, we have \(|H_s| \geq 1\), in which case \(s \in \bigcup_{a=q_0+1}^q S_a^*\). Note that this claim implies that \(q \geq 1\).

We next show that \(\{S_a\}\) are disjoint sets and so are \(\{S_a^*\}\):

- By construction, the three sets \(S_0, \bigcup_{a=1}^q S_a\) and \(\bigcup_{a=q_0+1}^q S_a\) are disjoint. Also by construction, the sets \(S_a, a = 1, \ldots, q_0\) are disjoint. We claim that \(S_a, a = q_0 + 1, \ldots, q\) are disjoint. Otherwise, there exists \(i \in S_a \cap S_b\) for some \(q_0 + 1 \leq a < b \leq q\), where \(S_a^* = \{s\}\) and \(S_b^* = \{s'\}\) for some \(s \neq s' \in [k_s]\). By equation (16), we have

\[
||\theta_s^* - \theta_{s'}^*|| \leq ||\theta_s^* - \beta_s|| + ||\theta_{s'}^* - \beta_s|| \leq C_0 \frac{k_s}{\lambda}
\]

contradicting the separation assumption \(\Delta_{\min} \geq C \frac{k_s}{\lambda}\) in Theorem 2.

- The sets \(S_a^*, a = q_0 + 1, \ldots, q\) are disjoint by construction. We claim that the sets \(S_a^*, a = 1, \ldots, q_0\) are disjoint. Otherwise, there exists \(s \in \hat{A}_i \cap \hat{A}_j\) for some \(i \neq j \in \bigcup_{a=1}^{q_0} S_a\). By equation (15b) and the assumption \(\lambda < \frac{1}{4C_0}\) of Theorem 2, we have \(\mathbb{E}_s[\Psi_i] > 1/2\) and \(\mathbb{E}_s[\Psi_j] > 1/2\), which contradicts the fact that \(\mathbb{E}_s[\Psi_i + \Psi_j] \leq 1\). It remains to verify that the two sets \(\bigcup_{a=1}^{q_0} S_a^*\) and \(\bigcup_{a=q_0+1}^q S_a^*\) are also disjoint. Indeed, each \(s\) in the first set satisfies \(H_s = \emptyset\), and each \(s'\) in the second set satisfies \(H_s \neq \emptyset\), so they cannot overlap.

Combining pieces, we conclude that \(\{S_a\}\) forms a partition of \([k]\) and \(\{S_a^*\}\) forms a partition of \([k_s]\), thereby completing the proof of Theorem 2.
7.4 Proof of Proposition 1

In the proof, we frequently make use of the fact that for any non-negative random variable \( Z \equiv Z(X) \), there holds the crude lower bound \( \mathbb{E}_s[ Z ] = \frac{1}{k_s} \sum_{k \in [k_s]} \mathbb{E}_s[Z] \geq \frac{1}{k_s} \mathbb{E}_s[ \cdot ], \forall s \in [k_s]. \)

Let \( \kappa \in \{0, 1\} \) be such that \((d_{j\ell})^\kappa \mathbb{E}_s[\Psi_j \Psi_\ell] \geq \lambda \) as assumed. By equation (22)—a consequence of the second-order optimality condition—we obtain that

\[
1 \geq d_{j\ell}^\kappa \mathbb{E}_s[\Psi_j \Psi_\ell] \\
\geq (d_{j\ell})^2 \kappa \cdot (d_{j\ell})^\kappa \frac{1}{k_s} \mathbb{E}_s[\Psi_j \Psi_\ell] \\
\geq (d_{j\ell})^2 \kappa \cdot \frac{\lambda}{k_s}.
\]

Rearranging the above inequality gives

\[
d_{j\ell} \leq \left( \frac{k_s}{\lambda} \right)^{\frac{1}{\kappa}}.
\]

On the other hand, recalling the notation \( u_{s \rightarrow j} := \frac{\beta_j - \theta^*_s}{\|\beta_j - \theta^*_s\|} \), we have for each \( x \in \mathbb{R}^d \):

\[
\|\beta_j - \theta^*_s\|^2 = (\beta_j - \theta^*_s, u_{s \rightarrow j})^2 \leq 2 (\beta_j - x, u_{s \rightarrow j})^2 + 2 (x - \theta^*_s, u_{s \rightarrow j})^2.
\]

Combining with equation (23)—another consequence of the second-order optimality condition—we obtain that

\[
1 \geq \mathbb{E}_s[\Psi_j \Psi_\ell \langle \beta_j - X, u_{s \rightarrow j} \rangle^2] \\
\geq \frac{1}{k_s} \mathbb{E}_s[\Psi_j \Psi_\ell \langle \beta_j - X, u_{s \rightarrow j} \rangle^2] \\
\geq \frac{1}{k_s} \mathbb{E}_s[\Psi_j \Psi_\ell \left( \frac{1}{2} \|\beta_j - \theta^*_s\|^2 - \langle X - \theta^*_s, u_{s \rightarrow j} \rangle^2 \right)] \\
= \frac{1}{2k_s} \|\beta_j - \theta^*_s\|^2 \mathbb{E}_s[\Psi_j \Psi_\ell] - \frac{1}{k_s} \mathbb{E}_s[\Psi_j \Psi_\ell \langle X - \theta^*_s, u_{s \rightarrow j} \rangle^2].
\]

Note that under the distribution \( f_{s}^\ast \), we have \( Z := \langle X - \theta^*_s, u_{s \rightarrow j} \rangle \sim \mathcal{N}(0, 1) \), hence \( \mathbb{E}_s[\Psi_j \Psi_\ell \langle X - \theta^*_s, u_{s \rightarrow j} \rangle^2] \leq \mathbb{E}_s[Z^2] = 1 \). Combining with the last display equation and rearranging terms, we obtain

\[
4k_s \geq \|\beta_j - \theta^*_s\|^2 \mathbb{E}_s[\Psi_j \Psi_\ell] \\
\geq (i) \|\beta_j - \theta^*_s\|^2 \cdot \left( \frac{1}{d_{j\ell}} \right)^\kappa \lambda \\
\geq (ii) \|\beta_j - \theta^*_s\|^2 \left( \frac{\lambda}{k_s} \right)^{\frac{1}{\kappa}} \lambda,
\]

where step (i) follows from the assumption \((d_{j\ell})^\kappa \mathbb{E}_s[\Psi_j \Psi_\ell] \geq \lambda \) and step (ii) follows from the bound (30). Rearranging terms gives

\[
\|\beta_j - \theta^*_s\| \leq C_0 \sqrt{\left( \frac{k_s}{\lambda} \right)^{\frac{1}{2\kappa}} \frac{k_s}{\lambda}} = C_0 \left( \frac{k_s}{\lambda} \right)^{\frac{1}{2\kappa}} \frac{k_s}{\lambda} \leq C_0 \frac{k_s}{\lambda},
\]

where \( C_0 \geq 1 \) is a universal constant, and the last step holds because \( \lambda \leq 1 \) by assumption. Swapping the roles of \( j \) and \( \ell \), we can similarly prove that \( \|\beta_\ell - \theta^*_s\| \leq C_0 \frac{k_s}{\lambda} \). This establishes the first part of Proposition 1.

If in addition \( \theta^*_s \in V_i \), then by definition of the Voronoi set \( V_i \), we have

\[
\|\beta_\ell - \theta^*_s\| \leq \|\beta_j - \theta^*_s\| \leq C_0 \frac{k_s}{\lambda},
\]

thereby establishing the second part of Proposition 1.
Figure 2: Illustration for the proof of Lemma 3. The figure shows the polyhedral Voronoi set $V_j$ and the direction $v = e_1$ that defines the separating hyperplane between $V_j$ and $0$. For each point $x = (x_1, x_2^d)^\top \in \text{int} V_j$, the half line $\{ x - be_1, b \geq 0 \}$ intersects a facet $F$ of $V_j$ at a unique point $y = y(x_2^d)$, where $F \subseteq \partial_j \ell$ for some $\ell = \ell(x_2^d) \in [k]$. The set $L_j$ indexes the Voronoi boundaries colored in blue and green.

7.5 Proof of Proposition 2

Our proof relies on the following geometric lemma.

Lemma 3 (Controlling Volume by Intersection). Suppose that $\theta^*_s \notin \text{int} V_j$. With $\alpha = \log 2$, we have

$$\mathbb{P}_s(V_j) \leq \sum_{\ell \in [k] \setminus \{j\}} C \max \left\{ 1, \frac{d_{j\ell}}{\alpha} \right\} \cdot \mathbb{P}_s\left( V_j \cap \partial_j \ell \right),$$

where $C > 0$ is a universal constant.

Proof. With $\alpha = \log 2$ fixed, we introduce the shorthands $\tilde{V}_j \equiv \tilde{V}_j^\alpha$ and $\tilde{\partial}_j \ell \equiv \tilde{\partial}_j^\alpha \ell$. Without loss of generality assume that $\theta^*_s = 0$. Since $\theta^*_s \notin \text{int} V_j$ and $V_j$ is convex, the Separating Hyperplane Theorem ensures that there exists some $v \in \mathbb{R}^d$ such that $\langle v, x \rangle \geq 0$ for all $x \in V_j$. Because the Gaussian distribution is rotation invariant, we may assume that $v = e_1$. For each point $x \in \text{int} V_j$, the half line $\{ x - be_1, b \geq 0 \}$ intersects a facet $F$ of the polyhedron $V_j$ at a unique point $y$, where $F \subseteq \partial_j \ell$ for some $\ell \in [k]$ with $\beta_\ell \neq \beta_j$ (if there are multiple such $\ell$‘s, we pick the smallest one). It is clear that $y$ and $\ell$ are independent of the value of $x_1$, hence we can write $y = y(x_2^d)$ and $\ell = \ell(x_2^d)$, where $x_2^d := (x_2, \ldots, x_d)^\top \in \mathbb{R}^{d-1}$. Consequently, each $x \in \text{int} V_j$ can be written as $x = x_1 y_1(x_2^d) + be_1$ for some $b \geq 0$. Note that by construction and the separating hyperplane property, it holds that $x_1 \geq y_1(x_2^d) = \langle e_1, y(x_2^d) \rangle \geq 0$. Let $L_j := \{ \ell \in [k] \setminus \{j\} : \ell = \ell(x_2^d) \}$ for some $x \in \text{int} V_j$. See Figure 2 for an illustration of these notations.

With a slight overloading of notation, for any $d' \geq 1$ and $z \in \mathbb{R}^{d'}$, let $\phi(z) = (\sqrt{2\pi})^{-d'} e^{-\|z\|^2/2}$ denote the density of the standard Gaussian distribution in dimension $d'$. With the notations above, we can write the probability of interest as an iterated integral as follows:

$$\mathbb{P}_s(V_j) = \int_{\mathbb{R}^d} \mathbf{1} \{ x \in V_j \} \phi(x)dx$$

$$= \sum_{\ell \in L_j} \int_{\mathbb{R}^d} \mathbf{1} \{ x \in V_j, \ell(x_2^d) = \ell \} \phi(x)dx$$

$$= \sum_{\ell \in L_j} \int_{\mathbb{R}^{d-1}} \left[ \int_{y_1(x_2^d)}^\infty \mathbf{1} \{ x \in V_j \} \phi(x_1)dx_1 \right] \mathbf{1} \{ \ell(x_2^d) = \ell \} \phi(x_2^d)dx_2.$$ 

Define the quantity $U(x_2^d) := \max \{ x_1 : (x_1, x_2^d)^\top \in V_j \} \in [0, \infty]$, with the convention that $y_1(x_2^d) = U(x_2^d) = 0$ if $\{(x_1, x_2^d)^\top : x_1 \in \mathbb{R}\} \cap V_j = \emptyset$. Continuing from the last display equation, we have

$$\mathbb{P}_s(V_j) = \sum_{\ell \in L_j} \int_{\mathbb{R}^{d-1}} \left[ \int_{y_1(x_2^d)}^{U(x_2^d)} \phi(x_1)dx_1 \right] \mathbf{1} \{ \ell(x_2^d) = \ell \} \phi(x_2^d)dx_2. \quad (32)$$
On the other hand, for each index $\ell \in \mathcal{L}_j$, by a similar argument we may write

\[
P_x \left( \tilde{V}_j \cap \tilde{\partial}_{j\ell} \right) \geq P_x \left( V_j \cap \tilde{\partial}_{j\ell} \right)
\]

\[
= \sum_{\ell' \in \mathcal{L}_j} \int_{\mathbb{R}^{d-1}} \left[ \int_{y_1(x_2^j)} U(x_2^j) \right] \mathbb{1} \{ x \in \tilde{\partial}_{j\ell} \} \phi(x_1) \, dx_1 \mathbb{1} \{ \ell(x_2^j) = \ell' \} \phi(x_2^d) \, dx_2^d
\]

\[
\geq \int_{\mathbb{R}^{d-1}} \left[ \int_{y_1(x_2^j)} U(x_2^j) \right] \mathbb{1} \{ x \in \tilde{\partial}_{j\ell} \} \phi(x_1) \, dx_1 \mathbb{1} \{ \ell(x_2^j) = \ell \} \phi(x_2^d) \, dx_2^d.
\]

We claim that for each $\ell \in \mathcal{L}_j$, there holds the implication

\[
\ell(x_2^j) = \ell \quad \text{and} \quad 0 \leq x_1 - y_1(x_2^j) \leq \frac{\alpha}{d_{j\ell}} \implies x \in \tilde{\partial}_{j\ell}. \tag{33}
\]

Proof of claim: Fix an $x$ with $\ell(x_2^j) = \ell$ and $0 \leq x_1 - y_1(x_2^j) \leq \frac{\alpha}{d_{j\ell}}$. Since $y(x_2^j) \in \partial_{j\ell}$ and $x_2^j = y_2^j(x_2^j)$, we have $\langle y(x_2^j) - \beta_{j\ell}, \beta_{j\ell} \rangle = 0$ and hence

\[
|\langle x - \beta_{j\ell}, \beta_j - \beta_{j\ell}, \beta_{j\ell} \rangle| = |\langle x - y(x_2^j), \beta_j - \beta_{j\ell} \rangle| \\
\leq \| x - y(x_2^j) \| \| \beta_j - \beta_{j\ell} \| \\
= |x_1 - y_1(x_2^j)| \| \beta_j - \beta_{j\ell} \| \\
\leq \frac{\alpha}{d_{j\ell}} \frac{d_{j\ell}}{2} \leq \alpha.
\]

The above equation implies that $x \in \tilde{\partial}_{j\ell}$ by definition of $\tilde{\partial}_{j\ell}$, so the claim holds. By the implication (33), we have

\[
\mathbb{1} \{ x_1 \leq y_1(x_2^j) + \frac{\alpha}{d_{j\ell}} \}, \mathbb{1} \{ \ell(x_2^j) = \ell \} \leq \mathbb{1} \{ x \in \tilde{\partial}_{j\ell} \}, \mathbb{1} \{ \ell(x_2^j) = \ell \},
\]

hence

\[
P_x \left( \tilde{V}_j \cap \tilde{\partial}_{j\ell} \right) \geq \int_{\mathbb{R}^{d-1}} \left[ \int_{y_1(x_2^j)} U(x_2^j) \right] \mathbb{1} \{ x_1 \leq y_1(x_2^j) + \frac{\alpha}{d_{j\ell}} \} \phi(x_1) \, dx_1 \mathbb{1} \{ \ell(x_2^j) = \ell \} \phi(x_2^d) \, dx_2^d. \tag{34}
\]

In view of the inequalities (32) and (34), the desired inequality (31) in the lemma is implied by

\[
\sum_{\ell \in \mathcal{L}_j} \int_{\mathbb{R}^{d-1}} \left[ \int_{y_1(x_2^j)} U(x_2^j) \right] \mathbb{1} \{ \ell(x_2^j) = \ell \} \phi(x_2^d) \, dx_2^d
\]

\[
\leq \sum_{\ell \in \mathcal{L}_j} C \max \left\{ 1, \frac{\sigma_{j\ell}}{\alpha} \right\} \int_{\mathbb{R}^{d-1}} \left[ \int_{y_1(x_2^j)} U(x_2^j) \right] \mathbb{1} \{ x_1 \leq y_1(x_2^j) + \frac{\alpha}{d_{j\ell}} \} \phi(x_1) \, dx_1 \mathbb{1} \{ \ell(x_2^j) = \ell \} \phi(x_2^d) \, dx_2^d,
\]

which is further implied by the following pointwise inequality for the integrand:

\[
\int_{y_1(x_2^j)} U(x_2^j) \phi(x_1) \, dx_1 \leq C \max \left\{ 1, \frac{d_{j\ell}}{\alpha} \right\} \int_{y_1(x_2^j)} U(x_2^j) \mathbb{1} \{ x_1 \leq y_1(x_2^j) + \frac{\alpha}{d_{j\ell}} \} \phi(x_1) \, dx_1, \quad \forall \ell \in \mathcal{L}_j, \forall x_2^d \in \mathbb{R}^{d-1}. \tag{35}
\]

To proceed, we make use of a simple technical lemma for Gaussian, which is proved in Appendix A.

**Lemma 4.** There exists a universal constant $C > 0$ for which the following holds: for any $0 \leq L \leq U \leq \infty$ and $w > 0$, we have

\[
\int_L^U \phi(z) \, dz \leq C \max \left\{ 1, \frac{1}{w} \right\} \int_L^U \mathbb{1} \{ z \leq L + w \} \phi(z) \, dz.
\]

Applying the Lemma 4, we see that the desired inequality (35) holds, thereby completing the proof of Lemma 3. \hfill \square
Given Lemma 3, Proposition 2 follows easily. In particular, we have

\[ \mathbb{P}_s(\mathcal{V}_j) \overset{(i)}{\leq} C \sum_{\ell \in [k] \setminus j} \max \left\{ \frac{d_{j\ell}}{\alpha} \right\} \cdot \mathbb{P}_s(\tilde{\mathcal{V}}_j \cap \tilde{\mathcal{V}}_{j\ell}) = C \cdot 8k^2 \sum_{\ell \in [k] \setminus j} \max \left\{ \frac{d_{j\ell}}{\alpha} \right\} \cdot \mathbb{E}_s \left[ \frac{1}{8k^2} \mathbb{1} \left\{ \tilde{\mathcal{V}}_j \cap \tilde{\mathcal{V}}_{j\ell} \right\} \right] \overset{(ii)}{\leq} C \cdot 8k^2 \cdot \sum_{\ell \in [k] \setminus j} \max \left\{ \frac{d_{j\ell}}{\alpha} \right\} \cdot \mathbb{E}_s [\Psi_j \Psi_{j\ell}] \overset{(iii)}{\leq} C \cdot 8k^2 \cdot k \cdot \frac{3}{2} \lambda, \]

where step (i) follows from Lemma 3, step (ii) follows from equation (24c) in Lemma 1 with \( c = 2 \), and step (iii) follows from \( \frac{1}{\alpha} = \frac{1}{\log 2} \leq \frac{3}{2} \) and the assumption of Proposition 2. Setting \( C_0 = 12C \) proves the first inequality in Proposition 2.

By assumption of the proposition, we have the inequalities \( \mathbb{E}_s [\Psi_j \Psi_{j\ell}] < \lambda, \forall \ell \in [k] \setminus \{j\} \). Summing these inequalities over \( \ell \in [k] \setminus \{j\} \), we obtain that

\[ k \lambda > \mathbb{E}_s [\Psi_j (1 - \Psi_j)] = \mathbb{E}_s [\Psi_j \mathbb{1} \{ \mathcal{V}_j \}] - \mathbb{E}_s [\Psi_j^2 \mathbb{1} \{ \mathcal{V}_j \}] + \mathbb{E}_s [\Psi_j (1 - \Psi_j) \mathbb{1} \{ \mathcal{V}_j^c \}] \overset{(i)}{\geq} \frac{1}{2} \mathbb{E}_s [\Psi_j \mathbb{1} \{ \mathcal{V}_j \}] - \mathbb{P}_s (\mathcal{V}_j) + \frac{1}{2} \mathbb{E}_s [\Psi_j \mathbb{1} \{ \mathcal{V}_j^c \}] = \frac{1}{2} \mathbb{E}_s [\Psi_j] - \mathbb{P}_s (\mathcal{V}_j) \overset{(ii)}{\geq} \frac{1}{2} \mathbb{E}_s [\Psi_j] - C_0 k^3 \lambda, \]

where step (i) holds because \( x \in \mathcal{V}_j \) implies \( \psi_j(x) < \frac{1}{\alpha} \), and step (ii) follows from the first inequality in the proposition we just proved. Rearranging terms gives the second inequality in Proposition 2.

### 7.6 Proof of Proposition 3

As in the proof of Proposition 2, we use the shorthand \( \tilde{\mathcal{V}}_j \equiv \tilde{\mathcal{V}}_j^\alpha \), where \( \alpha = \log 2 \).

Fix an index \( i \in [k] \) that satisfies \( |\hat{A}_i| \geq 1 \). Define the set \( I := \{ \ell \in [k] : \beta_\ell = \beta_i \} \), which is non-empty. For each \( s \in \hat{A}_i \) and \( j \in I^c \), we have

\[ \mathbf{\theta}_s^* \notin \text{int} \mathcal{V}_j \quad \text{and} \quad \max_{\ell \in [k] \setminus \{j\}} \max \left\{ 1, \frac{d_{j\ell}}{\alpha} \right\} \mathbb{E}_s [\Psi_j \Psi_{j\ell}] < \lambda \] \hspace{1cm} (36)

by definition of \( \hat{A}_i \). Applying Proposition 2, we obtain that \( \mathbb{E}_s [\Psi_j] \leq 4C_0 k^3 \lambda \), whence

\[ \mathbb{E}_s [\Psi_i] = \frac{1}{|I|} \sum_{\ell \in I} \mathbb{E}_s [\Psi_i] = \frac{1}{|I|} \left( 1 - \sum_{j \in I^c} \mathbb{E}_s [\Psi_j] \right) \geq \frac{1}{|I|} \left( 1 - 4C_0 k^4 \lambda \right). \] \hspace{1cm} (37)

The inequality (37) implies in particular that \( \mathbb{E}_s [\Psi_i] \geq \frac{3}{4} \), since \( |I| \leq k \) and \( \lambda < 1/(Ck^4) \) by assumption of Proposition 3. If there exists some \( \ell \in I \) with \( \ell \neq i \), then we have

\[ \mathbb{E}_s [\Psi_i \Psi_{i\ell}] = \mathbb{E}_s [\Psi_i^2] \geq \left( \mathbb{E}_s [\Psi_i] \right)^2 \geq \frac{9}{16k^2} \geq \lambda, \]

which contradicts the assumption that \( s \in \hat{A}_i \). Therefore, we must have \( I = \{i\} \), proving equation (28a) in Proposition 3. In this case, equation (37) proves equation (28b) in Proposition 3.
Since equation (36) holds for all \( j \in [k] \setminus \{i\} \), applying Proposition 2 again gives that \( \mathbb{P}_s(\mathcal{V}_j) \leq C_0k^3\lambda \). Combining with the observation that \( \mathcal{V}_i^c \subseteq \bigcup_{j \in [k] \setminus \{i\}} \mathcal{V}_j \), we obtain

\[
\mathbb{P}_s\left(\mathcal{V}_i^c\right) \leq \mathbb{P}_s(\mathcal{V}_i^c) \leq \sum_{j \in [k] \setminus \{i\}} \mathbb{P}_s(\mathcal{V}_j) \leq C_0k^4\lambda < 1, \quad \forall s \in \hat{A}_i,
\]

where the last step holds under the assumption on \( \lambda \). The inequality (38) implies equation (28c) in Proposition 3.

It remains to prove the last equation (28d) in Proposition 3. Observe that for each \( s \in \hat{A}_i^c \), we have \( \theta_s^* \notin \mathcal{V}_i \) and \( \max\{1, d_{i\ell}\} \mathbb{E}_s[\Psi_i\Psi_\ell] < \lambda \) for all \( \ell \in [k] \setminus \{i\} \) by definition of \( \hat{A}_i^c \). Hence

\[
\mathbb{E}_s[\Psi_i(1 - \Psi_i)] = \sum_{\ell \in [k] \setminus \{i\}} \mathbb{E}_s[\Psi_i\Psi_\ell] < k\lambda,
\]

where we use the fact that \( \sum_{\ell \in [k]} \Psi_\ell = 1 \) surely. Moreover, Proposition 2 ensures that \( \mathbb{P}_s(\mathcal{V}_i) \leq C_0k^3\lambda \). Combining the last two inequalities gives

\[
\mathbb{E}_s[\Psi_i] = \mathbb{E}_s\left[\Psi_i 1\left\{\Psi_i > \frac{1}{2}\right\}\right] + \mathbb{E}_s\left[\Psi_i 1\left\{\Psi_i < \frac{1}{2}\right\}\right]
\]

\[
\leq \mathbb{E}_s[\Psi_i 1\{X \in \mathcal{V}_i\}] + \mathbb{E}_s\left[\Psi_i 1\left\{1 - \Psi_i > \frac{1}{2}\right\}\right] \quad \psi_i(x) \geq \frac{1}{2} \implies x \in \mathcal{V}_i
\]

\[
\leq \mathbb{P}_s(\mathcal{V}_i) + 2\mathbb{E}_s\left[\Psi_i(1 - \Psi_i) 1\left\{1 - \Psi_i > \frac{1}{2}\right\}\right]
\]

\[
\leq C_0k^3\lambda + 2k\lambda \leq 3C_0k^3\lambda, \quad \forall s \in \hat{A}_i^c.
\]

We are ready to prove equation (28d) in Proposition 3. Let us choose a coordinate system such that \( \frac{1}{|\hat{A}_i|} \sum_{s \in \hat{A}_i} \mathbb{E}_s[X] = \frac{1}{|\hat{A}_i|} \sum_{s \in \hat{A}_i} \theta_s^* = 0 \), hence the quantity of interest, \( \beta_i - \frac{1}{|\hat{A}_i|} \sum_{s \in \hat{A}_i} \theta_s^* \), is equal to \( \beta_i \). Since \( \beta \) is a local minimum, by the stationary condition in equation (10) we have

\[
\beta_i = \frac{\mathbb{E}_s[\Psi_i X]}{\mathbb{E}_s[\Psi_i]} = \frac{\sum_{s \in [k]} \mathbb{E}_s[\Psi_i X]}{\sum_{s \in [k]} \mathbb{E}_s[\Psi_i]}.
\]

For the denominator, using equation (28b) in Proposition 3 proved above as well as equation (39), we have

\[
\sum_{s \in [k]} \mathbb{E}_s[\Psi_i] = |\hat{A}_i| + \sum_{s \in \hat{A}_i} \mathbb{E}_s[\Psi_i] - 1 + \sum_{s \in \hat{A}_i^c} \mathbb{E}_s[\Psi_i] + \sum_{s \notin \hat{A}_i \cup \hat{A}_i^c} \mathbb{E}_s[\Psi_i]
\]

\[
\geq |\hat{A}_i| - |\hat{A}_i^c| \cdot C_0k^4\lambda - k_\ast \cdot C_0k^3\lambda + \sum_{s \notin \hat{A}_i \cup \hat{A}_i^c} \mathbb{E}_s[\Psi_i]
\]

\[
\geq \frac{1}{2} + \sum_{s \notin \hat{A}_i \cup \hat{A}_i^c} \mathbb{E}_s[\Psi_i],
\]

where the last step holds under the assumption that \( |\hat{A}_i| \geq 1 \) and \( \lambda \leq \frac{1}{Ck^4(k + k_\ast)} \). For the numerator, we
have the decomposition
\[
\left\| \sum_{s \in \mathcal{X}} \mathbb{E}_s [\Psi_i X] \right\| = \left\| \sum_{s \in \mathcal{X}} \mathbb{E}_s [\Psi_i X] - \sum_{s \in \mathcal{A}_i} \mathbb{E}_s [X] \right\|.
\]
\[
\leq \left\| \sum_{s \in \mathcal{A}_i} \mathbb{E}_s [(\Psi_i - 1)X] + \sum_{s \in \mathcal{A}_i} \mathbb{E}_s [\Psi_i X] + \sum_{s \notin \mathcal{A}_i \cup \mathcal{A}_i^c} \mathbb{E}_s [\Psi_i X] \right\|
\leq \sum_{s \in \mathcal{A}_i} \|\mathbb{E}_s [(\Psi_i - 1)X]\| + \sum_{s \in \mathcal{A}_i^c} \|\mathbb{E}_s [\Psi_i X]\| + \sum_{s \notin \mathcal{A}_i \cup \mathcal{A}_i^c} \mathbb{E}_s [\Psi_i X] \right\|.
\]
It follows that
\[
\|\beta_i\| \leq 2T_1 + 2T_2 + \frac{T_3}{2} + \sum_{s \notin \mathcal{A}_i \cup \mathcal{A}_i^c} \mathbb{E}_s [\Psi_i] \right\|.
\]
(40)

Let us bound each of the three terms on the right hand side, making use of the following simple lemma.

**Lemma 5.** Let \( Y \) be a scalar random variable taking value in \([0, 1]\), and \( X \sim N(u, I_d) \). Then we have \( \|\mathbb{E} [Y X]\| \leq \mathbb{E} [Y] \|u\| + \sqrt{d} \).

**Proof.** Letting \( Z := X - u \), we have
\[
\|\mathbb{E} [Y X]\| \leq \|\mathbb{E} [Y u]\| + \|\mathbb{E} [Y Z]\|
\leq \mathbb{E} [Y] \|u\| + \|\mathbb{E} [Y Z]\| \leq \mathbb{E} [Y] \|u\| + \sqrt{d},
\]
where step (i) follows from Jensen’s inequality and the fact that \( Y \in [0, 1] \).

Using Lemma 5, the fact that \( d \leq k_s + k \) (see Section 7.1) and equation (28b) in Proposition 3, we have, for some universal constant \( C_1 > 0 \),
\[
T_1 \leq \sum_{s \in \mathcal{A}_i} \left( \mathbb{E}_s [1 - \Psi_i] \|\theta_i\| + \sqrt{k_s + k} \right)
\leq C_1 k_s \left( k^4 \lambda \Delta_{\max} + \sqrt{k_s + k} \right) \leq C_1 [k_s k^4 \lambda \Delta_{\max} + k_s (k_s + k)],
\]
where in step (i) we use the fact that \( \max_{s \in [k_s]} \|\theta_i\| \leq \max_{s \in [k_s]} \|\theta_i - \theta_i\| = \Delta_{\max} \) since the point \( 0 = \sum_{s \in \mathcal{A}_i} \theta_i \) lies in the convex hull of \( \{\theta_i\} \). Similarly, by Lemma 5, the fact that \( d \leq k_s + k \) and equation (39), we have
\[
T_2 \leq \sum_{s \in \mathcal{A}_i^c} \left( \mathbb{E}_s [\Psi_i] \|\theta_i\| + \sqrt{k_s + k} \right)
\leq C_1 k_s \left( k^3 \lambda \Delta_{\max} + \sqrt{k_s + k} \right) \leq C_1 [k_s k^4 \lambda \Delta_{\max} + k_s (k_s + k)].
\]

Turning to the third term in equation (40), we claim that \( \left| \left( \mathcal{A}_i \cup \mathcal{A}_i^c \right)^c \right| \leq 1 \).

**Proof of Claim.** For each \( s \notin \mathcal{A}_i \cup \mathcal{A}_i^c \), the definition of these sets implies that one of the following two statements must be true:
\[
\bullet \ s \in \mathcal{A}_i \text{ and } H_s \neq \emptyset; \text{ that is, } \theta_i \in \mathcal{V}_i \text{ and } \max_{\ell \in [k] \setminus \{j\}} \max \{1, d_{j\ell}\} \mathbb{E}_s [\Psi_j \Psi_{\ell}] \geq \lambda \text{ for some } j \in [k].
\]
\[
\bullet \ s \in \mathcal{A}_i^c \text{ and } H_s \ni i; \text{ that is, } \theta_i \not\in \mathcal{V}_i \text{ and } \max_{\ell \in [k] \setminus \{i\}} \max \{1, d_{i\ell}\} \mathbb{E}_s [\Psi_i \Psi_{\ell}] \geq \lambda.
\]
In either case, Proposition 1 ensures that \( \|\beta_i - \theta_i^*\| \leq C_1 \frac{k_s}{\lambda} \). If the claim is false and there exit two distinct indices \( s, s' \notin \hat{A}_i \cup \hat{A}_i^c \), then

\[
\Delta_{\min} \leq \|\theta_i^* - \theta_s^*\| \leq \|\beta_i - \theta_i^*\| + \|\beta_i - \theta_s^*\| \leq 2C_1 \frac{k_s}{\lambda},
\]

which contradicts the SNR assumption \( \Delta_{\min} \geq C \frac{k_s}{\lambda} \) in Proposition 3. \( \square \)

Now, if \( (\hat{A}_i \cup \hat{A}_i^c)^c = \emptyset \), then \( T_3 = 0 \). Otherwise, the above claim implies that \( (\hat{A}_i \cup \hat{A}_i^c)^c = \{s_0\} \) for some \( s_0 \in [k_s] \). In this case we have

\[
T_3 = \|\beta_i E_{s_0} [\Psi_i] + (\theta_{s_0}^* - \beta_i) E_{s_0} [\Psi_i] + E_{s_0} [\Psi_i (X - \theta_{s_0}^*)]\|
\leq \|\beta_i\| E_{s_0} [\Psi_i] + C_1 \frac{k_s}{\lambda} + \sqrt{k_s + k},
\]

where the last step follows from Lemma 5.

Plugging the above bounds for \( T_1 \), \( T_2 \) and \( T_3 \) into equation (40), we obtain that for some universal constant \( C_2 \geq 1 \):

\[
\|\beta_i\| \leq C_2 k_s k^4 \lambda \Delta_{\max} + C_2 k_s (k_s + k) + \frac{\|\beta_i\| E_{s_0} [\Psi_i] + C_1 \frac{k_s}{\lambda} + (k_s + k)}{1 + E_{s_0} [\Psi_i]}
\leq C_2 k_s k^4 \lambda \Delta_{\max} + 5C_2 \frac{k_s (k_s + k)}{\lambda} + \frac{\|\beta_i\| E_{s_0} [\Psi_i]}{1 + E_{s_0} [\Psi_i]}
\leq C_2 k_s k^4 \lambda \Delta_{\max} + 5C_2 \frac{k_s (k_s + k)}{\lambda} + \frac{2}{3} \|\beta_i\|,
\]

where step (i) holds because \( \lambda \leq 1 \) and step (ii) holds because \( E_{s_0} [\Psi_i] \leq 1 \). Rearranging terms, we obtain

\[
\|\beta_i\| \leq 3C_2 k_s k^4 \lambda \Delta_{\max} + 15C_2 \frac{k_s (k_s + k)}{\lambda},
\]

thereby proving the last inequality (28d) in Proposition 3.

8 Proof of Theorem 3

By rescaling, we may assume unit variance \( \sigma^2 = 1 \). When \( k = k_s = 3 \), the value \( q \) and the sets \( \{S_a\} \) and \( \{S_a^*\} \) in Theorem 2 can only have, up to permutation of component labels, the following possibilities:

1. \( q = 1; S_0 = \{2, 3\}; S_1 = \{1\}, S_1^* = \{1, 2, 3\} \).
2. \( q = 2; S_0 = \{3\}; \)
   (a) \( S_1 = \{1\}, S_1^* = \{1, 2\}, S_2 = \{2\}, S_2^* = \{3\} \);
   (b) \( S_1 = \{1\}, S_1^* = \{1, 3\}, S_2 = \{2\}, S_2^* = \{2\} \).
3. \( q = 2; S_0 = \emptyset \);
   (a) \( S_1 = \{1\}, S_1^* = \{1, 2\}, S_2 = \{2, 3\}, S_2^* = \{3\} \);
   (b) \( S_1 = \{1\}, S_1^* = \{1, 3\}, S_2 = \{2, 3\}, S_2^* = \{2\} \).
4. \( q = 3; S_0 = \emptyset; S_1 = \{1\}, S_1^* = \{1\}, S_2 = \{2\}, S_2^* = \{2\}, S_3 = \{3\}, S_3^* = \{3\} \).

Moreover, when \( \lambda = \frac{1}{\sqrt{k_s}} \) and the SNR satisfies \( \Delta \geq C_1 \) for some constant \( C_1 \), the bounds (14) in Theorem 2 becomes \( \mathbb{P}_s (V_i) \leq \epsilon, E_s [\Psi_i] \leq \epsilon \), the bounds (15) become \( \|\beta_i - |S_a^*|^{-1} \sum_{s \in S_a^*} \theta_s^*\| \leq \epsilon \Delta, E_s [\Psi_i] \geq 1 - \epsilon, \mathbb{P}_s (V_i) \geq 1 - \epsilon \), and the bound (16) becomes \( |\beta_i - \theta_i^*| \leq \epsilon \Delta \). Here \( \epsilon > 0 \) can be make arbitrarily small as long as \( C_1 \) is sufficiently large.
We claim that Case 2b above, where \( \beta_1 \) fits two non-adjacent centers \( \{\theta_1^*, \theta_2^*\} \), is impossible. Otherwise, we must have \( \beta_1 \neq \beta_2 \) by Theorem 2; say \( \beta_1 < \beta_2 \). In this case, it holds that \( \mathcal{V}_1 \subset (-\infty, \beta_2) \subset (-\infty, \theta_2^*], \) where the last inclusion holds since \( |\beta_2 - \theta_2^*| \leq \epsilon \Delta \). It follows that \( \mathbb{P}_3(\mathcal{V}_1) \leq \mathbb{P}_3((-\infty, \theta_2^*)) = \frac{1}{2} \), contradicting the inequality \( \mathbb{P}_3(\mathcal{V}_1) \geq 1 - \epsilon \) in equation (15c). By a similar argument, Case 3b above is impossible.

We are left with the Cases 1, 2a, 3a and 4. We analyze each of these cases separately after stating some technical lemmas.

### 8.1 Technical Lemmas

We frequently make use of the following two lemmas. The first lemma is proved in Appendix B.1.

**Lemma 6 (Exponential Association).** For each \( s \in [k] \) and \( (i, j) \in [k] \times [k] \), if \( |\beta_j - \theta_i^*| \geq |\beta_i - \theta_j^*| + \frac{5}{6} D \) with \( D \geq 35 \), then \( \mathbb{E}_s[\Psi_j] \leq e^{-D^2/33} \).

Lemma 6 says that if \( \beta_j \) is dominated by some other \( \beta_i \) in terms of closeness to a true center \( \theta_i^* \), then the association coefficient of \( \beta_j \) with \( \theta_i^* \) must be exponentially small.

The second lemma is proved in Appendix B.2.

**Lemma 7 (Exponential Accuracy).** Under the setting of Theorem 3, suppose that \( \beta \) is a stationary point of \( L \). For each \( i \in [3] \) and \( \emptyset \neq S_i \subset [3] \), if it holds that

\[
\begin{align*}
|\beta_j - \theta_i^*| &\geq |\beta_i - \theta_j^*| + C \Delta, \quad \forall j \in [3] \setminus \{i\}, s \in S_i, \tag{41a} \\
|\beta_i - \theta_j^*| &\geq \min_{j \in [3]} |\beta_j - \theta_i^*| + C \Delta, \forall s \in [3] \setminus S_i, \tag{41b}
\end{align*}
\]

for some universal constant \( C > 0 \), then \( |\beta_i - \frac{1}{|S_i|} \sum_{s \in |S_i|} \theta_i^*| \leq e^{-c \Delta^2} \), where \( c > 0 \) is an universal constant.

Lemma 7 says that if \( \beta_i \) dominates all other \( \beta_j \)’s in terms of closeness to a set of true centers and at the same time is dominated in terms closeness to all other true centers, then \( \beta_i \) must be exponentially close to the mean of this set of true centers.

We also record the following elementary inequality for exponential orderings: if \( c_0, c_1 \) are positive constants and \( \Delta \geq C_1 \) for a sufficiently large constant \( C_1 > 0 \), then

\[
c_0 \Delta e^{-\Delta^2/c_1} = e^{-(\Delta^2/c_1 - 2 \log c_0 - \log \Delta)} \leq e^{-\Delta^2/(c_1 - 1)}.
\]

### 8.2 Case 1

We first make a simple observation.

**Claim.** \( |\beta_i - \theta_i^*| > |\beta_1 - \theta_1^*|, \forall i \in \{2, 3\}, s \in [3] \).

**Proof of Claim.** Suppose that the claim is false and hence \( |\beta_i - \theta_i^*| \leq |\beta_1 - \theta_1^*| \). In this case, we would have \( \mathcal{V}_2 \cup \mathcal{V}_3 \supseteq \{\theta_i^*, \infty\} \) or \( \mathcal{V}_2 \cup \mathcal{V}_3 \supseteq (\infty, \theta_i^*] \), hence \( \mathbb{P}_s(\mathcal{V}_2 \cup \mathcal{V}_3) \geq \frac{1}{2} \). But equation (14) ensures that \( \mathbb{P}_s(\mathcal{V}_2 \cup \mathcal{V}_3) \leq 2 \epsilon \), whence

\[
\mathbb{P}_s(\mathcal{V}_2 \cup \mathcal{V}_3) \leq \sum_{s' \in [3]} \mathbb{P}_{s'}(\mathcal{V}_2 \cup \mathcal{V}_3) = 3 \cdot \mathbb{P}_s(\mathcal{V}_2 \cup \mathcal{V}_3) \leq 3 \cdot 2 \epsilon,
\]

which is a contradiction. \( \square \)

In view of the above claim and the inequality \( |\beta_1 - \theta_2^*| \leq \epsilon \Delta \) guaranteed by Theorem 2, we see that \( \{\beta_2, \beta_3\} \) must lie outside the interval \( [\theta_1^*, \theta_2^*] \). In what follows, we assume that \( \beta_2 \) and \( \beta_3 \) are on the same side of this interval; say \( \theta_2^* \leq \beta_2 \leq \beta_3 \). (The opposite-side case can be analyzed in a similar manner.) Note that by Corollary 1, we have \( 0 = \frac{1}{3} \sum_{s \in [3]} \theta_i^* = \sum_{i \in [3]} \beta_i \mathbb{E}_s[\Psi_i] \). It follows that \( \beta_1 = -\frac{1}{3 \mathbb{E}_s[\Psi_1]} \sum_{i \in [3]} \beta_i \mathbb{E}_s[\Psi_i] < 0 \) since \( \beta_3 \geq \beta_2 \geq \theta_2^* > 0 \). We illustrate this case in the plot below.

\[
\begin{array}{c}
|\theta_1^*| = -\Delta & |\theta_2^*| = 0 & |\theta_3^*| = \Delta \\
\beta_1 & \beta_2 & \beta_3
\end{array}
\]
Let us first lower bound the second RHS term. It is easy to verify that
\[ 0 = 3 \cdot E_s[\psi_i(\beta_i - X)] = \sum_{s \in [3]} E_s[\psi_i(\beta_i - X)], \quad \forall i \in \{2, 3\}. \]
Summing up these two equations gives
\[
0 = \sum_{i \in \{2, 3\}} E_1[\psi_i(\beta_i - X)] + \sum_{s \in \{2, 3\}} \left( E_s[\psi_2(\beta_2 - X)] + E_s[\psi_3(\beta_3 - X)] \right)
\geq \sum_{i \in \{2, 3\}} E_1[\psi_i(\beta_i - X)] + \sum_{s \in \{2, 3\}} E_s[(\psi_2 + \psi_3)(\beta_2 - X)],
\]
where the last step holds since \(\beta_3 \geq \beta_2\). Rewriting the first term in the RHS above using the Stein’s identity, as done in equation (26), we obtain that
\[
0 \geq \sum_{i \in \{2, 3\}} \left( -\theta_i^* E_1[\psi_i] + \sum_{j \in [3]} \beta_j E_1[\psi_i \psi_j] \right) + \sum_{s \in \{2, 3\}} E_s[(\psi_2 + \psi_3)(\beta_2 - X)]
\geq \sum_{s \in \{2, 3\}} E_s[(\psi_2 + \psi_3)(\beta_2 - X)],
\]
where the last step holds since \(\beta_j \geq \theta_i^*, \forall j \in [3]\) and \(E_1[\psi_i] = \sum_{j \in [3]} E_1[\psi_i \psi_j]\).

For each \(i \in \{2, 3\}\), define \(\tilde{\psi}_i = \tilde{\psi}_i(X) := e^{-(X-\beta_i)^2/2}/(\sqrt{2\pi} e^{-(X-\beta_i)^2/2} + \sqrt{2\pi} e^{-(X-\beta_j)^2/2})\), which is the association coefficient of \(\beta_i\) if there were only two fitted centers \(\beta_i\) and \(\beta_1\). Continuing from the last display equation, we have
\[
0 \geq \sum_{s \in \{2, 3\}} E_s[\tilde{\psi}_2(\beta_2 - X)] + \sum_{s \in \{2, 3\}} E_s[(\psi_2 + \psi_3 - \tilde{\psi}_2)(\beta_2 - X)].
\]
Let us first lower bound the second RHS term. It is easy to verify that \(\psi_2 + \psi_3 - \tilde{\psi}_2 \geq 0\) surely by definition, hence for \(s \in \{2, 3\}\):
\[
E_s[(\psi_2 + \psi_3 - \tilde{\psi}_2)(\beta_2 - X)] \geq E_s[(\psi_2 + \psi_3 - \tilde{\psi}_2)(\beta_2 - X)1\{\beta_2 - X \leq 0\}]
\geq -E_s[(\beta_2 - X)1\{X \geq \beta_2\}] \quad \left| \psi_2 + \psi_3 - \tilde{\psi}_2 \right| \leq 1
\geq -E_s[(\beta_2 - X^*)1\{X \geq \beta_2\}] \quad \beta_2 \geq \theta_s^*, s \in \{2, 3\}
= -\int_{\beta_2 - \theta_s^*}^\infty \frac{1}{\sqrt{2\pi}} e^{-z^2/2} dz
= -\frac{1}{\sqrt{2\pi}} e^{-(\beta_2 - \theta_s^*)^2/2}.
\]
It follows that
\[
0 \geq \sum_{s \in \{2, 3\}} E_s[\tilde{\psi}_2(\beta_2 - X)] - \sum_{s \in \{2, 3\}} \frac{1}{\sqrt{2\pi}} e^{-(\beta_2 - \theta_s^*)^2/2}.
\]
The first RHS term can be controlled using the following lemma, which is proved in Appendix B.3.

**Lemma 8.** If \(\beta_i - \theta_s^* \geq \theta_s^* - \beta_1 > 0\), then
\[
E_s[\tilde{\psi}_i(\beta_i - X)] \geq (\beta_i - \theta_s^*) \cdot E_s[\tilde{\psi}_i(\tilde{\psi}_i - \tilde{\psi}_1)] \geq (\beta_i - \theta_s^*) \cdot \frac{1}{8} \Phi^c \left( \frac{\beta_i + \beta_1}{2} - \theta_s^* + \frac{1}{\theta_s^* - \beta_1} \right),
\]
where \(\tilde{\psi}_1 := 1 - \tilde{\psi}_i\) and \(\Phi^c\) is the complementary cumulative distribution function of the standard normal distribution.
Applying the Lemma 8 with \( i = 2 \), we obtain

\[
0 \geq \sum_{s \in \{2,3\}} \frac{1}{8} (\beta_2 - \theta_s^*) \Phi^c \left( \frac{\beta_2 + \beta_1}{2} - \theta_s^* + \frac{1}{\theta_s^* - \beta_1} \right) - \sum_{s \in \{2,3\}} \frac{1}{\sqrt{2\pi}} e^{-\frac{(\beta_2 - \theta_s^*)^2}{2}} \\
\quad \quad \geq \frac{1}{8} \Phi^c \left( \frac{\beta_2 + \beta_1}{2} - \theta_3^* + \frac{1}{\theta_3^* - \beta_1} \right) - e^{-\frac{(\beta_2 - \theta_3^*)^2}{2}} \\
\quad = \frac{1}{8} \Phi^c (t) - e^{-\frac{(\beta_2 - \theta_3^*)^2}{2}},
\]

where step (i) holds since \( \beta_2 - \theta_3^* \geq \Delta \geq 1 \) and \( \beta_2 \geq \theta_3^* > \theta_2^* \), and in the last step we introduce the shorthand \( t := \frac{\beta_2 + \beta_1}{2} - \theta_3^* + \frac{1}{\theta_3^* - \beta_1} \geq 0 \). The first term above can be controlled using a standard Gaussian tail bound (see Lemma 11):

\[
\frac{1}{8} \Phi^c (t) \geq \frac{1}{8} \cdot \frac{1}{\sqrt{2\pi}} \cdot \frac{1}{t+1} e^{-t^2/2} \geq \frac{1}{8\sqrt{2\pi}} e^{-t} \cdot e^{-t^2/2} \geq \frac{1}{8\sqrt{2\pi}} e^{-\frac{(t+1)^2}{2}}.
\]

Recall that \( \beta_2 - \theta_3^* \geq \theta_3^* - \beta_1 \geq \Delta \). Therefore, the exponent on the RHS of equation (44) satisfies

\[
t + 1 \leq \frac{\beta_2 + \beta_1}{2} - \theta_3^* + 2 = (\beta_2 - \theta_3^*) - \frac{\beta_2 - \beta_1}{2} + 2 \leq (\beta_2 - \theta_3^*) - \Delta + 2,
\]

where \( \Delta \geq C_1 \) with a sufficiently large constant \( C_1 \) by assumption. It follows that \( \frac{1}{8} \Phi^c (t) > e^{-\frac{(\beta_2 - \theta_3^*)^2}{2}} \), which contradicts equation (43). We conclude that Case 1 cannot happen.

### 8.3 Cases 2a and 3a

We discuss these two cases together. In both cases, Theorem 2 ensures that \( |\beta_1 - \frac{1}{2}(\theta_1^* + \theta_2^*)| \leq \epsilon \Delta \) and \( |\beta_2 - \theta_3^*| \leq \epsilon \Delta \) for a small constant \( \epsilon > 0 \). Moreover, by an argument similar to that in the beginning of Section 8.2, we have \( |\beta_3 - \theta_2^*| \geq |\beta_1 - \theta_1^*|, \forall s \in \{1,2\} \). For \( \beta_3 \), there are four possible subcases:

1. \( \beta_3 < \theta_1^* - (\frac{1}{2} - \epsilon) \Delta \).
2. \( \theta_2^* + (\frac{1}{2} - \epsilon) \Delta < \beta_3 < \theta_2^* - 2\epsilon \Delta \).
3. \( \theta_2^* - 2\epsilon \Delta \leq \beta_3 \leq \theta_3^* + 2\epsilon \Delta \).
4. \( \beta_3 > \theta_3^* + 2\epsilon \Delta \).

We discuss each of these subcases below.

#### 8.3.1 Subcase i): \( \beta_3 < \theta_1^* - (\frac{1}{2} - \epsilon) \Delta \)

This case is illustrated below.

\[
\begin{array}{ccccc}
\beta_3 & \bullet & \beta_1 & \bullet & \beta_2 \\
\end{array}
\]

Rearranging terms in the equivalent stationary condition (12) with \( i = 3 \), we have

\[
\beta_2 \mathbb{E}_1 [\Psi_3 \Psi_2] - \theta_1^* \mathbb{E}_1 [\Psi_3 \Psi_2] + \sum_{j \in \{3\}} \beta_j \sum_{s \in \{2,3\}} \mathbb{E}_s [\Psi_3 \Psi_j] - \sum_{s \in \{2,3\}} \theta_s^* \mathbb{E}_s [\Psi_3] \\
\quad = - \beta_3 \mathbb{E}_1 [\Psi_3^2] - \beta_1 \mathbb{E}_1 [\Psi_3 \Psi_1] + \theta_1^* \mathbb{E}_1 [\Psi_3 (\Psi_3 + \Psi_1)].
\]

Note that \( |\beta_2 - \theta_1^*| \geq |\beta_1 - \theta_1^*| + \Delta \). Using Lemma 6 and inequality (42), we obtain that

\[
|\beta_2 \mathbb{E}_1 [\Psi_3 \Psi_2] - \theta_1^* \mathbb{E}_1 [\Psi_3 \Psi_2]| \leq |\beta_2 - \theta_1^*| \mathbb{E}_1 [\Psi_2] \leq 2 \Delta \epsilon^{-\Delta^2/33} \leq \epsilon^{-3/34}.
\]
Similarly, for each $s \in \{2, 3\}$ we have
\[
\left| \sum_{j \in [3]} \beta_j E_s [\Psi_3 \Psi_j] - \theta^*_s E_s [\Psi_3] \right| = \left| \sum_{j \in [3]} (\beta_j - \theta^*_s) E_s [\Psi_3 \Psi_j] \right| \\
\leq \sum_{j \in [3]} |\beta_j - \theta^*_s| E_s [\Psi_3]
\]
\[
\left( \sum_{j \in [3]} |\beta_j - \theta^*_s| E_s [\Psi_3] \right)^{1/3} (2) \leq 3 (\Delta + |\beta_3 - \beta_1|) \cdot e^{-7/2} \leq e^{-\Delta^2/34},
\]
where the step (i) holds by Lemma 6 and step (ii) holds since $|\beta_3 - \beta_1| \geq |\beta_1 - \theta^*_1| \geq (2 \Delta^2 - 2 \epsilon^2 \Delta \geq 0.9 \Delta$. Combining the last three display equations, we obtain that
\[
2 e^{-\Delta^2/34} \geq -\beta_3 E_1 [\Psi_3^2] - \beta_1 E_1 [\Psi_3 \Psi_1] + \theta^*_1 E_1 [\Psi_3 (\Psi_3 + \Psi_1)]
\]
\[
= (\theta^*_1 - \beta_3) E_1 [\Psi_3^2] - (\beta_1 - \theta^*_1) E_1 [\Psi_3 \Psi_1]
\]
\[
\geq (\theta^*_1 - \beta_3) E_1 [\Psi_3 (\Psi_3 - \Psi_1)],
\]
where the last step holds since $\beta_1 - \theta^*_1 \leq \theta^*_1 - \beta_3$. Define $\tilde{\Psi}_3$ as in Section 8.2 and note that $\Psi_1 \leq \tilde{\Psi}_1 := 1 - \tilde{\Psi}_3$ surely. We thus have
\[
E_1 [\tilde{\Psi}_3 (\Psi_3 - \Psi_1)] \geq E_1 \left[ \tilde{\Psi}_3 (\Psi_3 - \tilde{\Psi}_1) \right]
\]
\[
= E_1 \left[ \tilde{\Psi}_3 \tilde{\Psi}_3 - \tilde{\Psi}_1 \right] - E_1 \left[ \tilde{\Psi}_3 (\tilde{\Psi}_3 - \tilde{\Psi}_1) - \tilde{\Psi}_3 (\Psi_3 - \tilde{\Psi}_1) \right]
\]
\[
= E_1 \left[ \tilde{\Psi}_3 (\tilde{\Psi}_3 - \tilde{\Psi}_1) \right] - E_1 \left[ (\tilde{\Psi}_3 + \Psi_3 - \tilde{\Psi}_1) (\tilde{\Psi}_3 - \Psi_3) \right]
\]
\[
\geq E_1 \left[ \tilde{\Psi}_3 (\tilde{\Psi}_3 - \tilde{\Psi}_1) \right] - 2 E_1 \left[ \tilde{\Psi}_3 - \Psi_3 \right].
\]

But
\[
E_1 \left[ \tilde{\Psi}_3 - \Psi_3 \right] \leq E_1 \left[ e^{-\frac{(X-\beta_3)^2}{2}} - e^{-\frac{(X-\beta_1)^2}{2}} \right]
\]
\[
\leq E_1 \left[ e^{-\frac{(X-\beta_3)^2}{2}} + e^{-\frac{(X-\beta_1)^2}{2}} \right]
\]
\[
\geq E_1 \left[ \tilde{\Psi}_3 \right] \leq e^{-\Delta^2/33},
\]
where the last step follows from noting that $|\beta_3 - \theta^*_1| \geq |\beta_1 - \theta^*_1| + \Delta$ and applying Lemma 6. Moreover, note that $\theta^*_1 - \beta_3 \geq \beta_1 - \theta^*_1 > 0$. Applying inequality (b) in Lemma 8 and noting the change of sign, we obtain
\[
E_1 \left[ \tilde{\Psi}_3 (\tilde{\Psi}_3 - \tilde{\Psi}_1) \right] \geq \frac{1}{8} \Phi^e \left( \theta^*_1 - \frac{\beta_1 + \beta_1}{2} + \frac{1}{\beta_1 - \theta^*_1} \right)
\]
\[
\geq \frac{1}{8} \Phi^e \left( \theta^*_1 - \frac{\beta_1 + \beta_1}{2} + 1 \right) \geq \frac{1}{8} e^{-\frac{(\theta^*_1 - \beta_3 - \beta_1 + \beta_1 + 1)^2}{2}},
\]
where the last step follows from the same argument as in equation (44). Plugging the last three inequalities into equation (45), we obtain that
\[
4 e^{-\Delta^2/34} \geq \frac{1}{8} \Phi^e \left( \theta^*_1 - \beta_3 \right) e^{-\frac{(\theta^*_1 - \beta_3 + \beta_1 + 1)^2}{2}} \geq \frac{1}{8} e^{-\frac{(\theta^*_1 - \beta_3 + \beta_1 + 1)^2}{2}},
\]
where the last step holds since $\theta^*_1 - \beta_3 \geq \frac{1}{2} (\sqrt{2} \epsilon - \Delta \geq 2 \sqrt{2} \epsilon \geq 2 \sqrt{2} \epsilon \geq 0.9 \Delta$. It follows that $\theta^*_1 - \frac{\beta_3 + \beta_1}{2} + 2 \geq \frac{\Delta}{\sqrt{18}} \geq \frac{\Delta}{\sqrt{18}} + 2$, which in turns implies $|\beta_3 - \theta^*_1| \geq |\beta_1 - \theta^*_1| + \frac{\Delta}{\sqrt{18}}$. Since we also have $|\beta_3 - \theta^*_1| \geq |\beta_1 - \theta^*_1| + \frac{\Delta}{\sqrt{18}}$ for $s \in \{2, 3\}$, applying Lemma 6 proves that
\[
E_s [\Psi_3] = \frac{1}{3} \sum_{s \in \{2, 3\}} E_s [\Psi_3] \leq e^{-\frac{\epsilon^2 \Delta^2}{2}},
\]
where \( c > 0 \) is a universal constant. Moreover, applying Lemma 7 with \( i = 1 \) and \( S_* = \{1, 2\} \) proves that

\[
\left| \beta_1 - \frac{1}{2}(\theta_1^* + \theta_2^*) \right| \leq e^{-c\Delta^2}.
\]

Applying the same lemma with \( i = 2 \) and \( S_* = \{3\} \) proves that

\[
|\beta_2 - \theta_3^*| \leq e^{-c\Delta^2}.
\]

With the last three bounds, we conclude that Possibility 1 in Theorem 3 holds.

### 8.3.2 Subcase ii): \( \theta_2^* + (\frac{1}{2} - \epsilon)\Delta < \beta_3 < \theta_3^* - 2\epsilon\Delta \)

This case is illustrated below.

In this case, \( \beta_1 \) fits \( \{\theta_1^*, \theta_2^*\} \), \( \beta_2 \) fits \( \theta_3^* \), and \( |\beta_3 - \theta_3^*| \geq |\beta_2 - \theta_3^*| + \Omega(\Delta) \). By a similar argument as in subcase i) above, we can show that \( |\beta_3 - \theta_3^*| \geq |\beta_1 - \theta_3^*| + \Omega(\Delta), \forall s \in \{1, 2\} \) and hence Possibility 1 in Theorem 3 holds.

### 8.3.3 Subcase iii): \( \theta_3^* - 2\epsilon\Delta \leq \beta_3 \leq \theta_3^* + 2\epsilon\Delta \)

This case is illustrated below.

Under the case assumption, we can apply Lemma 7 with \( i = 1 \) and \( S_* = \{1, 2\} \) to obtain that

\[
\left| \beta_1 - \frac{1}{2}(\theta_1^* + \theta_2^*) \right| \leq e^{-c\Delta^2},
\]

where \( c > 0 \) is a universal constant. We claim that

\[
\max_{i \in \{2, 3\}} |\beta_i - \theta_3^*| \leq e^{-c\Delta^2}.
\]

Once this is established, together with the bound (46) for \( \beta_1 \) we conclude that Possibility 2 in Theorem 3 holds.

It remains to prove equation (47). By translation of coordinates, we may assume that \( \theta_3^* = 0 \) (see Remark 1). Define \( \Psi_i \equiv \Psi_i(X) := e^{-(X - \beta_3)^2/2} e^{-\epsilon(X - \beta_3)^2/2} e^{-(X - \beta_3)^2/2} \) for \( i \in \{2, 3\} \), which are the association coefficients if there were only two fitted centers \( \beta_2 \) and \( \beta_3 \).

For \( \beta_3 \), the stationary condition (10) implies that

\[
0 = 3E_* [\Psi_3(X - \beta_3)] = E_3 [\Psi_3(X - \beta_3)] + E_3 [\Psi_3(X - \beta_3)] + \sum_{s \in \{1, 2\}} E_s [\Psi_3(X - \beta_3)].
\]

We bound the last two RHS terms. Note that

\[
E_3 \left[ (\Psi_3 - \Psi_3)^2 \right] = E_3 \left[ \left( e^{-(X - \beta_3)^2/2} e^{-\epsilon(X - \beta_3)^2/2} e^{-(X - \beta_3)^2/2} \right)^2 \right]
\]

\[
\leq E_3 \left[ \min \left\{ \Psi_1^2, \Psi_3^2 \right\} \right]
\]

\[
\leq \min \left\{ E_3 [\Psi_1], E_3 [\Psi_3] \right\}
\]

\[
\leq \min \left\{ 33 e^{-\Delta^2/3}, e^{-(\beta_3 - \epsilon\Delta)^2} e^{-(\beta_3 - \epsilon\Delta) \geq 35} \right\}
\]

\[
= \exp \left( -\frac{1}{33} \max \left\{ \Delta^2, (\beta_3 - \epsilon\Delta)^2 \right\} \{ \beta_3 - \epsilon\Delta \geq 35 \} \right)
\]
where step (i) holds by Lemma 6. Observe that since $\beta_3 \geq -2\epsilon\Delta$ under the case assumption, we have $\max \{\Delta^2, (\beta_3 - \epsilon\Delta)^2 \mathbb{I} \{\beta_3 - \epsilon\Delta \geq 35\} \} \geq \frac{1}{2}(\Delta^2 + \beta_3^2)$, hence

$$
\mathbb{E}_3 \left[ (\Psi_3 - \Psi)^2 \right] \leq \frac{1}{\beta_3^2 + \Delta^2} e^{-(\Delta^2 + \beta_3^2)/67} \leq \frac{1}{\beta_3^2 + 1} e^{-\Delta^2/67}
$$

by inequality (42). Also note that $\mathbb{E}_3 \left[ (X - \beta_3)^2 \right] = \mathbb{E}_3 \left[ X^2 \right] + \beta_3^2 \leq 1 + \beta_3^2$. With the last two bounds, it follows that

$$
|\mathbb{E}_3 [(\Psi_3 - \Psi)(X - \beta_3)]| \leq \frac{1}{\beta_3^2 + 1} e^{-\Delta^2/67} \cdot (1 + \beta_3^2) = e^{-\Delta^2/134}.
$$

On the other hand, for each $s \in \{1, 2\}$ a similar argument as above shows that $|\mathbb{E}_s [\Psi_3(X - \beta_3)]| \leq e^{-\Delta^2/134}$. Plugging the last two inequalities into equation (48) gives

$$
|\mathbb{E}_3 [\Psi_3(\beta_3 - X)]| \leq 3e^{-\Delta^2/134} \leq e^{-\Delta^2/135},
$$

where the last step follows from inequality (42). Rewriting the above LHS using Stein’s identity, as done in equation (26), we obtain that

$$
e^{-\Delta^2/135} \geq \left| \beta_3 \mathbb{E}_3 [\Psi_3^2] + \beta_2 \mathbb{E}_3 [\Psi_3 \Psi_2] \right| = \left| \beta_3 \mathbb{E}_3 [(1 - \Psi_2)^2] + \beta_2 \mathbb{E}_3 [\Psi_2 (1 - \Psi_2)] \right|.
$$

Using the stationary condition (10) for $\beta_2$ and running a similar argument as above, we obtain that

$$
e^{-\Delta^2/135} \geq \left| \beta_2 \mathbb{E}_3 [\Psi_2^2] + \beta_3 \mathbb{E}_3 [\Psi_2^2] \right| = \left| \beta_2 \mathbb{E}_3 [(1 - \Psi_2)^2] + \beta_3 \mathbb{E}_3 [\Psi_2 (1 - \Psi_2)] \right|.
$$

To proceed, we observe that $-A \cdot \mathbb{E}_3 [\Psi_2^2] + B \cdot \mathbb{E}_3 [1 - \Psi_2] = (\beta_2 - \beta_3) \cdot (\mathbb{E}_3 [\Psi_2^2] - \mathbb{E}_3 [\Psi_2]^2)$. Combining with equations (49) and (50), we obtain that

$$
e^{-\Delta^2/135} \geq |\beta_2 - \beta_3| \cdot \left( \mathbb{E}_3 [\Psi_2^2] - \mathbb{E}_3 [\Psi_2]^2 \right) = |\beta_2 - \beta_3| \cdot \text{Var}_3(\Psi_2),
$$

where $\text{Var}_3(\cdot)$ denotes the variance under the distribution $f_3$, which is $\mathcal{N}(0, 1)$ since we have assumed that $\theta_3^* = 0$. Note the alternative expression $\overline{\Psi}_2 = \frac{1}{1 + e^{-\Delta} - \beta_2 - \beta_3}$. To lower bound $\text{Var}_3(\Psi_2)$, we make use of the following lemma, whose proof is given in Appendix B.4.

**Lemma 9** (Variance Lower Bound). Let $a$ and $w$ be two fixed numbers. Suppose that $X \sim \mathcal{N}(0, 1)$ and $Y := \frac{1}{1 + e^{-(x-a)w}}$. We have

$$
\text{Var}(Y) \geq \frac{|w|^5}{48} e^{-4(|w|+2|a|)^2}.
$$

Applying Lemma 9, we obtain that $\text{Var}_3(\Psi_2) \geq \frac{1}{48} |\beta_2 - \beta_3|^5 e^{-4(|\beta_2 - \beta_3| + |\beta_2 + \beta_3|)^2}$. Combining with equation (51) gives

$$
\frac{1}{48} |\beta_2 - \beta_3|^6 e^{-4(|\beta_2 - \beta_3| + |\beta_2 + \beta_3|)^2} \leq e^{-\Delta^2/135}.
$$

Under the case assumption, we have $4 \left| (\beta_2 - \beta_3) + |\beta_2 + \beta_3| \right|^2 \leq \frac{1}{2} \Delta^2_{135}$. It follows that

$$
|\beta_2 - \beta_3| \leq \left( \frac{48e^{-\Delta^2/135}}{e^{-\Delta^2/(2\cdot135)}} \right)^{1/6} \leq e^{-c'\Delta^2},
$$

where the last step holds by inequality (42) and $c' > 0$ is a universal constant.
Finally, adding up equations (49) and (50) gives \(2e^{-\Delta^2/135} \geq |(\beta_2 - \beta_3)E_3[\Psi_2] + \beta_3|\). It follows that

\[ |\beta_3 - \theta_*^3| = |\beta_3| \leq \left(2e^{-\Delta^2/135} + |\beta_2 - \beta_3| \cdot 1 \right) \leq e^{-c \Delta^2}, \]

where the last step follows from the bound \( |\beta_2 - \beta_3| = e^{-c' \Delta^2} \) proved above, and \( c > 0 \) is a universal constant. These bounds imply that \(|\beta_2 - \theta_*^3| \leq e^{-c \Delta^2}\) as well, so equation (47) holds as desired.

8.3.4 Subcase iv): \( \beta_3 > \theta_*^3 + 2\epsilon \Delta \)

This case is illustrated below.

In this case, applying Lemma 6 shows that \(E_*[\Psi_3] = \frac{1}{2} \sum_{s \in [3]} E_s[\Psi_3] \leq e^{-c \Delta^2}\), where \( c > 0 \) is a universal constant. Applying Lemma 7 with \( i = 1 \) and \( S_* = \{1, 2\} \) proves that \(|\beta_1 - \frac{1}{2}(\theta_*^1 + \theta_*^2)| \leq e^{-c \Delta^2}\). Applying Lemma 7 with \( i = 2 \) and \( S_* = \{3\} \) proves that \(|\beta_2 - \theta_*^3| \leq e^{-c \Delta^2}\). We have established that Possibility 1 in Theorem 3 holds.

8.4 Case 4

By Theorem 2, we know that \(|\beta_i - \theta_*^i| \leq \epsilon \Delta, \forall i \in [3]\) for a small constant \( \epsilon > 0 \). For each \( i \in [3]\), applying Lemma 7 with \( S_* = \{i\} \) proves that \(|\beta_i - \theta_*^i| \leq e^{-c \Delta^2}\), where \( c > 0 \) is a universal constant. We conclude that Possibility 3 in Theorem 3 holds.

We have completed the proof of Theorem 3.

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Appendices

A Proof of Lemma 4

If \( U \leq L + w \), we have

\[
\int_U^L \phi(z)dz \leq C \max \left\{1, \frac{1}{w}\right\} \int_L^U \phi(z)dz = C \max \left\{1, \frac{1}{w}\right\} \int_L^U 1 \{z \leq L + w\} \phi(z)dz
\]

as claimed. Below we assume that \( U > L + w \). Consider two cases:

- \( w \geq 1 \).
  In this case, we have
  
  \[
  \int_{L+w}^U \phi(z)dz \leq \sqrt{2\pi} \cdot \phi(L + w) \leq (C - 1)w \cdot \phi(L + w) \leq (C - 1) \int_{L}^{L+w} \phi(z)dz.
  \]
  
  \( \phi \) is non-increasing on \([L, L + w]\).
It follows that

\[ \int_{L}^{U} \phi(z)dz = \int_{L}^{L+w} \phi(z)dz + \int_{L+w}^{U} \phi(z)dz \]
\[ \leq \int_{L}^{L+w} \phi(z)dz + (C-1) \int_{L}^{L+w} \phi(z)dz \]
\[ = C \int_{L}^{U} \mathbb{1} \{ z \leq L + w \} \phi(z)dz \]
\[ \leq C \max \left\{ 1, \frac{w}{L+w} \right\} \int_{L}^{U} \mathbb{1} \{ z \leq L + w \} \phi(z)dz, \]

hence the desired inequality holds.

- \( w < 1 \). In this case, we have

\[ \int_{L+w}^{\infty} \phi(z)dz \leq \sqrt{2\pi} \cdot \phi(L+w) \]
\[ \leq \phi(L+w) \cdot (C-w) \]
\[ \leq \left( \frac{C}{w} - 1 \right) \int_{L+w}^{\infty} \phi(z)dz. \]

It is non-increasing on \([L, L+w]\).

It follows that

\[ \int_{L}^{U} \phi(z)dz \leq \int_{L}^{L+w} \phi(z)dz + \int_{L+w}^{\infty} \phi(z)dz \leq C \int_{L}^{L+w} \phi(z)dz. \]

which implies the desired inequality since \( U > L + w \).

## B Proofs for Section 8

In this section, we prove the technical lemmas used in the proof of Theorem 3, which concerns fitting a one-dimensional, three-component GMM.

### B.1 Proof of Lemma 6

We write

\[ E_s [\Psi_j] = E_s \left[ \Psi_j \mathbb{1} \left\{ |X - \theta_s^*| > \frac{D}{4} \right\} \right] + E_s \left[ \Psi_j \mathbb{1} \left\{ |X - \theta_s^*| \leq \frac{D}{4} \right\} \right]. \]

We bound each of the two RHS terms. For the first term, using the fact that \( \Psi_j \leq 1 \) and \( X \sim N(\theta_s^*, 1) \), we have \( E_s \left[ \Psi_j \mathbb{1} \left\{ |X - \theta_s^*| > \frac{D}{4} \right\} \right] \leq \mathbb{P}_s \left( |X - \theta_s^*| > \frac{D}{4} \right) \leq 2e^{-\left(\frac{D}{4}\right)^2/2} \). Turning to the second term, when \( |X - \theta_s^*| \leq \frac{D}{4} \), and under the assumption that \( |\beta_j - \theta_s^*| - |\beta_i - \theta_s^*| \geq \frac{D}{6} \), we have

\[ |\beta_j - X| = (|\beta_j - X| + |X - \theta_s^*|) + (|\beta_i - \theta_s^*| + |X - \theta_s^*|) + (|\beta_j - \theta_s^*| - |\beta_i - \theta_s^*|) - 2|X - \theta_s^*| - |\beta_j - \theta_s^*| \]
\[ \geq |\beta_j - \theta_s^*| + |\beta_i - X| + \frac{5}{6}D - 2 \cdot \frac{1}{4}D - |\beta_j - \theta_s^*| \]
\[ = |\beta_i - X| + \frac{1}{3}D, \]

whence

\[ \Psi_j = \frac{e^{-|X-\beta_j|^2/2}}{e^{-|X-\beta_j|^2/2} + e^{-|X-\beta_i|^2/2} + \sum_{\ell \in \{k\} \setminus \{j, i\}} e^{-|X-\beta_\ell|^2/2}} \]
\[ \leq e^{-|X-\beta_j|^2/2} \]
\[ \leq e^{-((|X-\beta_i|+\frac{1}{3}D)^2/2 + |X-\beta_i|^2)/2} \leq e^{-D/3)^2/2}. \]
It follows that $\mathbb{E}_s [\Psi_j 1 \{ |X - \theta_s^*| \leq \frac{D}{4} \}] \leq e^{-(D/4)^2/2}$. Combining pieces, we obtain that

$$\mathbb{E}_s [\Psi_j] \leq 2e^{-(D/4)^2/2} + e^{-(D/3)^2/2} \leq 3e^{-(D/4)^2/2} \leq e^{-D^2/33}$$

as claimed, where the last step holds when $D \geq 35$.

**B.2 Proof of Lemma 7**

We first record an elementary inequality.

**Lemma 10** (Fraction Approximation). Let $a, b, \epsilon_1, \epsilon_2$ be real numbers satisfying $\frac{b}{a} \geq |\epsilon_2|$. Then

$$\frac{a + \epsilon_1}{b + \epsilon_2} - \frac{a}{b} \leq 2\frac{|\epsilon_1|}{b} + \frac{2|a||\epsilon_2|}{b^2}. \quad (\text{Fraction Approximation})$$

**Proof.** We have

$$\left| \frac{a + \epsilon_1}{b + \epsilon_2} - \frac{a}{b} \right| = \left| \frac{\frac{a}{b} + \frac{\epsilon_1}{b} + \frac{\epsilon_2}{b}}{b + \epsilon_2} - \frac{a}{b} \right| = \left| \frac{\frac{\epsilon_1}{b} + \frac{\epsilon_2}{b}}{b + \epsilon_2} \right| \leq \frac{|\epsilon_1|}{b} + \frac{|\epsilon_2|}{b^2},$$

where the last step follows from the assumption that $\frac{b}{a} \geq |\epsilon_2|$. $\square$

We now prove Lemma 7. Without loss of generality, assume that $\frac{1}{|S_e|} \sum_{s \in S_e} \theta_s^* = 0$ (see Remark 1). Note that

$$\mathbb{E}_s [X^2] = \mathbb{E}_s [(X - \theta_s^*)^2] + (\theta_s^*)^2 \leq 1 + (2\Delta)^2 \leq 5\Delta^2, \quad \forall s \in [3].$$

Below we introduce the shorthand $S_e^c := [3] \setminus S_e$ and $I^c := [3] \setminus \{i\}$, and use $c_1, c_2, \ldots$ to denote positive universal constants. When equation (41a) holds, applying Lemma 6 shows that for each $s \in S_e$ and $j \in I^c$, it holds that $\mathbb{E}_s [\Psi_j] \leq e^{-c_1 \Delta^2}$, whence

$$|\mathbb{E}_s [\Psi_j X]| \leq \sqrt{\mathbb{E}_s [\Psi_j^2] \mathbb{E}_s [X^2]} \leq \sqrt{\mathbb{E}_s [\Psi_j] \mathbb{E}_s [X^2]} \leq e^{-c_1 \Delta^2} \cdot 5\Delta^2 \leq e^{-c_3 \Delta^2}, \quad \forall s \in S_e, j \in I^c, \quad (52)$$

where in the last step we use inequality (42). When equation (41b) holds, applying a similar argument as above shows that for each $s \in S_e$, it holds that $\mathbb{E}_s [\Psi_i] \leq e^{-c_1 \Delta^2}$, whence

$$|\mathbb{E}_s [\Psi_i X]| \leq e^{-c_3 \Delta^2}, \quad \forall s \in S_e^c. \quad (53)$$

We are ready to control the quantity $\beta_i - \frac{1}{|S_e|} \sum_{s \in S_e} \theta_s^*$ of interest. Observe that

$$\left| \beta_i - \frac{1}{|S_e|} \sum_{s \in S_e} \theta_s^* \right| = \left| \frac{\sum_{s \in [3]} \mathbb{E}_s [\Psi_j X] - \sum_{s \in S_e} \mathbb{E}_s [X]}{\sum_{s \in [3]} \mathbb{E}_s [\Psi_j] - \sum_{s \in S_e} \mathbb{E}_s [X]} \right| \leq$$

$$\leq \frac{\sum_{s \in S_e} \mathbb{E}_s [X] - \sum_{s \in [3]} \sum_{j \in I^c} \mathbb{E}_s [\Psi_j X] + \sum_{s \in S_e^c} \mathbb{E}_s [\Psi_i X]}{\sum_{s \in S_e} \mathbb{E}_s [X]} \leq 2 \cdot \frac{\sum_{s \in S_e^c} \mathbb{E}_s [\Psi_j X]}{|S_e|} + 2 \cdot \frac{\sum_{s \in S_e^c} \mathbb{E}_s [\Psi_i X]}{|S_e^c|},$$

where step (i) holds since $\sum_{j \in [3]} \mathbb{E}_s [\Psi_j] = 0$ surely, and step (ii) holds by Lemma 10 and the fact that $\sum_{s \in S_e} \mathbb{E}_s [X] = \sum_{s \in S_e} \theta_s^* = 0$. Plugging in the inequalities (52) and (53), we obtain that

$$\left| \beta_i - \frac{1}{|S_e|} \sum_{s \in S_e} \theta_s^* \right| \leq 18e^{-c_2 \Delta^2} \leq e^{-c_3 \Delta^2},$$

where in the last step we use inequality (42). This completes the proof of Lemma 7.
B.3 Proof of Lemma 8

Without loss of generality, assume that $\theta^* = 0$. Recall $\tilde{\Psi}_1 := 1 - \tilde{\Psi}_i$. Applying equation (26), we obtain

$$E_s\left[\tilde{\Psi}_i(\beta_i - X)\right] = \beta_i E_s\left[\tilde{\Psi}_i^2\right] + \beta_1 E_s\left[\tilde{\Psi}_i \tilde{\Psi}_1\right] \geq \beta_i E_s\left[\tilde{\Psi}_i(1 - \tilde{\Psi}_1)\right],$$

where the last step holds since $\beta_i \geq -\beta_1$ by assumption. This proves inequality (a) in Lemma 8.

Let $\beta := (\beta_i + \beta_1)/2$ and $\delta := (\beta - \beta_1)/2$. We write $\psi_i(x) \left(\psi_i(x) - \tilde{\psi}_3(x)\right) = e^{-(x-\beta)/2} \cdot g(x)$, where

$$g(x) := \frac{e^{-(x-\beta)/2} - e^{-(x-\beta_1)/2}}{\left(1 + e^{-(x-\beta_1)/2}\right)} \cdot g(y) \cdot e^{-y/2} \cdot e^{-y/2} dx \cdot e^{-y/2} dy.\]$$

Note that the function $g(\cdot)$ is odd around $\beta$. By a change of variable $y = x - \beta$, we have

$$E_s\left[\tilde{\Psi}_i(\tilde{\Psi}_i - \tilde{\Psi}_1)\right] \geq \frac{1}{\sqrt{2\pi}} \int_{-\beta_1}^{\beta_1} g(y + \beta) \left[\frac{1}{h_1(y)} \left(\frac{1}{h_2(y)} \right)\right] dy,$$

where the last step follows from the oddness of $g$ around $\beta$. Note that $h_1(x) = e^{-2\beta_1 y} \geq 1, \forall y \geq 0$ since $\beta_1 < 0$ by assumption. It follows that

$$E_s\left[\tilde{\Psi}_i(\tilde{\Psi}_i - \tilde{\Psi}_1)\right] \geq \frac{1}{\sqrt{2\pi}} \int_{-\beta_1}^{\beta_1} g(y + \beta) \left[\frac{1}{h_1(y)} \left(\frac{1}{h_2(y)} \right)\right] dy.$$

When $y \geq \frac{1}{\beta_1} \geq \frac{1}{2}$, we have

$$g(y + \beta) = \frac{e^{y/2} - e^{-y/2}}{\left(1 + e^{-(y-\beta)/2}\right)} \cdot e^{-(y-\beta)/2} \geq \frac{e - e^{-1}}{2e^{-(y-\beta)^2/2}} \geq \frac{e}{4} e^{-(y-\beta)^2/2}$$

and $h_1(x) \geq e^{-2\beta_1} > 2$, whence

$$E_s\left[\tilde{\Psi}_i(\tilde{\Psi}_i - \tilde{\Psi}_1)\right] \geq \frac{1}{\sqrt{2\pi}} \int_{-\beta_1}^{\beta_1} \frac{1}{4} \left(\frac{1}{h_1(y)} \left(\frac{1}{h_2(y)} \right)\right) dy.$$

This proves inequality (b) in Lemma 8.

B.4 Proof of Lemma 9

We first consider the case with $a \geq 0$ and $w \geq 0$. Let $\mu := E[Y]$. Observe that

$$\sqrt{2\pi} \text{Var}(Y) = \sqrt{2\pi} E\left[(Y - \mu)^2\right] \geq \int_{a}^{\infty} \left(\frac{1}{1 + e^{-(x-a)w} - \mu}\right)^2 e^{-x^2/2} dx + \int_{-\infty}^{a} \left(\frac{1}{1 + e^{-(x-a)w} - \mu}\right)^2 e^{-x^2/2} dx \geq \int_{a}^{\infty} \left(\frac{1}{1 + e^{-(x-a)w} - \mu}\right)^2 \left(\frac{1}{1 + e^{(x+a)w} - \mu}\right)^2 e^{-x^2/2} dx.$$
Using the elementary inequality \( u^2 + v^2 \geq \frac{1}{2}(u - v)^2, \forall u, v, \) we obtain that
\[
\sqrt{2\pi} \text{Var}(Y) \geq \frac{1}{2} \int_{a}^{\infty} \left(1 + e^{-(x-a)^2} - \frac{1}{1 + e^{(x-a)^2}}\right)^2 e^{-x^2/2} \, dx.
\]
\[
= \frac{1}{2} \int_{a}^{\infty} (e^{xw} - e^{-xw})^2 \left(1 + e^{xw}\right)^2 e^{-x^2/2} \, dx.
\]
\[
\geq \frac{1}{4} \int_{a+w}^{a+2w} \left(\frac{xw}{1 + e^{xw}} - 1\right)^2 e^{-x^2/2} \, dx,
\]
where step (i) holds since \( e^{-xw} \leq e^{-aw} = 1 \) and \( e^{xw} \geq 1 \) for all \( x \geq a \geq 0 \). When \( x \in [a+w, a+2w] \), we have
\[
\frac{xw}{1 + e^{xw}} - 1 \geq \frac{e^{(2a+w)w} - 1}{e^{2(a+w)w} + 1} \geq \frac{w^2}{2e^{(w+2a)^2}}
\]
since \( \frac{e^{xw}}{1 + e^{xw}} \) is non-decreasing in \( x \), and \( e^{-x^2/2} \geq e^{-(w+a)^2}/2 \). It follows that
\[
\sqrt{2\pi} \text{Var}(Y) \geq \frac{1}{4} \left(\frac{w^2}{2e^{(w+2a)^2}}\right)^2 e^{-(w+a)^2/2} \cdot w \geq \frac{w^5}{16} e^{-4(w+2a)^2}.
\]
Dividing both sides by \( \sqrt{2\pi} \) and noting that \( 16\sqrt{2\pi} \leq 48 \), we prove the desired variance bound.

In the case where \( a \geq 0 \) and \( w \leq 0 \), we observe that \( Y = 1 - \frac{1}{1 + e^{-(x-a)(-w)}} \) and hence \( \text{Var}(Y) = \text{Var}\left(\frac{1}{1 + e^{-(x-a)(-w)}}\right) \). Since \( -w \geq 0 \), applying the bound proved above establishes the desired variance bound.

Finally, in the case where \( a \leq 0 \), \( w \leq 0 \) or \( a \leq 0 \), \( w \geq 0 \), we write \( Y = 1 - \frac{1}{1 + e^{-(x-a)(-w)}} \) and observe that \( -X \) has the same distribution as \( X \). Applying the bound for the above two cases establishes the desired variance bound.

### C Proof of Corollary 6

The proof follows the same lines as in the proof of Theorem 3 in Section 8. By rescaling, we may assume unit variance \( \sigma^2 = 1 \). When \( k_r = 3 \) and \( k = 2 \), the value \( q \) and the sets \( \{S_0\} \) and \( \{S^*_0\} \) in Theorem 2 can only have, up to permutation of component labels, the following possibilities:

1. \( q = 1; S_0 = \{2\}; S_1 = \{1\}, S^*_1 = \{1, 2, 3\} \).
2. \( q = 2; S_0 = \emptyset \);
   a. \( S_1 = \{1\}, S^*_1 = \{1, 2\}; S_2 = \{2\}, S^*_2 = \{3\} \);
   b. \( S_1 = \{1\}, S^*_1 = \{1, 3\}; S_2 = \{2\}, S^*_2 = \{2\} \).

We claim that Case 2b above, where \( \beta_1 \) fits two non-adjacent centers \( \{\theta_1^*, \theta_3^*\} \), is impossible. Otherwise, we must have \( \beta_1 \neq \beta_2 \) by Theorem 2; say \( \beta_1 < \beta_2 \). In this case, it holds that \( V_1 \subset (-\infty, \beta_2) \subset (-\infty, \theta_3^*) \), where the last inclusion holds since \( \beta_2 - \theta_3^* \leq \epsilon \Delta \) for a sufficiently small constant \( \epsilon > 0 \) by Theorem 2. It follows that \( P_3(V_1) \leq P_3((-\infty, \theta_3^*)) = \frac{1}{3} \), contradicting the inequality \( P_3(V_1) \geq 1 - \epsilon \) in equation (15c).

In Case 1 above, \( \beta_1 \) fits all three true centers and \( \beta_2 \) has near-empty association. This case is impossible by an argument similar to Case 1 in the proof of Theorem 3 (Section 8.2).

In Case 2a above, \( \beta_1 \) fits \( \{\theta_1^*, \theta_2^*\} \) and \( \beta_2 \) fits \( \theta_3^* \). By an argument similar to subcase iv) in the proof of Theorem 3 (Section 8.3.4), we find that the exponential error bounds in equation (17) of Corollary 6 must hold.

We have completed the proof of Corollary 6.
Lemma 11 (Gaussian Tail Bounds). If $Z \sim N(0,1)$ and $\phi$ is the density function of $Z$, then for each $t \geq 0$,
\[
\frac{1}{t+1} \phi(t) \leq \frac{1}{t + \sqrt{t^2 + 4}} \sqrt{\frac{2}{\pi}} e^{-t^2/2} \leq P(Z \geq t) \leq e^{-t^2/2} = \sqrt{2\pi} \phi(t).
\]

Proof. The upper bound is standard. The lower bound can be found in [1, Formula 7.1.13].

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