Multivariate, Heteroscedastic Empirical Bayes via Nonparametric Maximum Likelihood

Jake A. Soloff\textsuperscript{1}, Adityanand Guntuboyina\textsuperscript{1,1}, and Bodhisattva Sen\textsuperscript{1,2}

\textsuperscript{1}Department of Statistics, University of California, Berkeley
\textsuperscript{2}Department of Statistics, Columbia University

September 9, 2021

Abstract

Multivariate, heteroscedastic errors complicate statistical inference in many large-scale denoising problems. Empirical Bayes is attractive in such settings, but standard parametric approaches rest on assumptions about the form of the prior distribution which can be hard to justify and which introduce unnecessary tuning parameters. We extend the nonparametric maximum likelihood estimator (NPMLE) for Gaussian location mixture densities to allow for multivariate, heteroscedastic errors. NPMLEs estimate an arbitrary prior by solving an infinite-dimensional, convex optimization problem; we show that this convex optimization problem can be tractably approximated by a finite-dimensional version. We introduce a dual mixture density whose modes contain the atoms of every NPMLE, and we leverage the dual both to show non-uniqueness in multivariate settings as well as to construct explicit bounds on the support of the NPMLE.

The empirical Bayes posterior means based on an NPMLE have low regret, meaning they closely target the oracle posterior means one would compute with the true prior in hand. We prove an oracle inequality implying that the empirical Bayes estimator performs at nearly the optimal level (up to logarithmic factors) for denoising without prior knowledge. We provide finite-sample bounds on the average Hellinger accuracy of an NPMLE for estimating the marginal densities of the observations. We also demonstrate the adaptive and nearly-optimal properties of NPMLEs for deconvolution. We apply the method to two astronomy datasets, constructing a fully data-driven color-magnitude diagram of 1.4 million stars in the Milky Way and investigating the distribution of chemical abundance ratios for 27 thousand stars in the red clump.

MSC 2010 subject classifications: 62C12, 62G05, 62P35.
Key words: Adaptive estimation, empirical Bayes, Gaussian mixture model, $g$-modeling, heteroscedasticity, Kiefer-Wolfowitz estimator.

1 Introduction

Consider a $d$-dimensional ($d \geq 1$), heteroscedastic normal observation model

\[
X_i \mid \theta^*_i \overset{\text{ind}}{\sim} \mathcal{N}(\theta^*_i, \Sigma_i), \quad \text{with} \quad \theta^*_i \overset{\text{ind}}{\sim} G^*, \quad \text{for } i \in \{1, \ldots, n\},
\]

where $(\Sigma_i)_{i=1}^n$ is a known sequence of $d \times d$ positive-definite covariance matrices, and the underlying mean vectors $(\theta^*_i)_{i=1}^n$ are additionally assumed to be drawn from a common prior $G^*$, where $G^*$ belongs to the collection $\mathcal{P}(\mathbb{R}^d)$ of all probability measures on $\mathbb{R}^d$. In settings where $G^*$ is known, model (1) fully specifies a Bayesian model; this paper studies the common empirical Bayes setting where $G^*$ must be estimated. The main goal of the paper is to nonparametrically estimate $G^*$ and the sequence $(\theta^*_i)_{i=1}^n$ from the observed data $(X_i, \Sigma_i)_{i=1}^n$.

Empirical Bayes methods for the normal sequence model (1) have been studied extensively in the univariate, homoscedastic setting where $d = 1$ and $\Sigma_i \equiv \sigma^2$ (see, e.g., James and Stein (1961);

*Supported by NSF Grant DMS-2023505 and by the Office of Naval Research under the Vannevar Bush Fellowship
†Supported by NSF CAREER Grant DMS-16-54589
‡Supported by NSF Grant DMS-2015376
Efron and Morris (1972a,b, 1973a,b); Morris (1983); Efron (2012, 2014) as well as Johnstone (2019) for a manuscript on estimation in Gaussian sequence models). Numerous methods extend empirical Bayes to the univariate, heteroscedastic case (see Jiang et al., 2011; Xie et al., 2012; Tan, 2016; Weinstein et al., 2018; Jiang, 2020; Banerjee et al., 2021, and references therein). Relatively little attention has been given to the general case of the present paper.

Model (1) naturally arises in the analysis of astronomy data, where often a calibrated measurement error distribution comes attached to each observation, and typically these errors are heteroscedastic (Kelly, 2012); also see e.g. Akritas and Bershady (1996), Hogg et al. (2010), Anderson et al. (2018). The first part of model (1) indicates that the target sequence \( (\theta^*)_{i=1}^n \) has, due to measurement error, been corrupted by additive, zero-mean Gaussian noise, i.e.

\[
X_i = \theta^*_i + \epsilon_i, \quad \text{where} \quad \epsilon_i \overset{\text{ind}}{\sim} \mathcal{N}(0, \Sigma_i), \quad \text{for} \ i = 1, \ldots, n.
\]

Interestingly, the \( \Sigma_i \)'s above, which typically differ across \( i \), are known in many applications where the measurement process is well-characterized. In many situations it is assumed that \( \theta^*_i \) is itself random and independent of \( \epsilon_i \) for all \( i \). Although each observation has a different error distribution, the \( n \) observations are tied together by the assumption that the \( \theta^*_i \)'s are i.i.d. from some distribution \( G^* \), yielding model (1). By allowing for arbitrary prior distributions \( G^* \in \mathcal{P}(\mathbb{R}^d) \), model (1) captures a range of important structural assumptions on the underlying sequence \( (\theta^*_i)_{i=1}^n \); for instance, the clustering problem (where the terms of \( (\theta^*_i)_{i=1}^n \) take on at most \( k^* \) distinct values) corresponds to discrete \( G^* \), and sparse modeling (where most of the \( (\theta^*_i)_{i=1}^n \) are zero) corresponds to \( G^*(\{0\}) \approx 1 \). The model also accommodates more complex manifold-like structures (see e.g. Figure 1) as well as substantially more heterogeneous sequences (e.g. \( G^* \) heavy tailed).

Our motivating example for model (1) involves the construction of a precise stellar color-magnitude diagram. A color-magnitude diagram (CMD) is a scatter plot of stars, displaying their absolute magnitude (luminosity) versus color (surface temperature) to provide a cross-sectional view of stellar evolution. The continued expansion of available stellar measurements has made purely statistical models such as model (1) increasingly attractive for denoising. One common approach, known as Extreme Deconvolution (XD) (Bovy et al., 2011), assumes

\[
G^* = \sum_{j=1}^K \alpha_j^* \mathcal{N}(\mu_j^*, V_j^*)
\]

and estimates the parameters \( (\alpha_j^*, \mu_j^*, V_j^*)_{j=1}^K \) via the Expectation-Maximization (EM) algorithm with split-and-merge operations designed to avoid local optima. For instance, Anderson et al. (2018) applied XD to build a low-noise CMD with \( n \approx 1.4 \) million de-reddened stars from the Gaia TGAS catalogue. The XD assumption (2) that the prior \( G^* \) is itself a mixture of \( K \)-Gaussians has a number of drawbacks. Although the class of Gaussian location-scale mixtures is flexible for large \( K \), the choice of \( K \) requires tuning; violations of assumption (2) for fixed \( K \) induce bias in the estimation. To our knowledge, no theoretical results for the statistical properties of XD are available, making it difficult to quantify the misspecification error. Moreover, the class of all probability distributions of the form (2) is non-convex for finite \( K \), so even split-and-merge techniques employed within EM do not guarantee convergence to the global maximizer of the likelihood.

To avoid these difficulties, we extend the Kiefer and Wolfowitz (1956) nonparametric maximum likelihood estimator (NPME) to incorporate multivariate and heteroscedastic errors. An NPME is any \( \hat{G}_n \in \mathcal{P}(\mathbb{R}^d) \) which maximizes the marginal likelihood of the observations \( (X_i)_{i=1}^n \). Marginally, the observations are independent, and the \( i^{th} \) observation \( X_i \) is distributed according to a Gaussian location mixture with density

\[
f_{G^*, \Sigma_i}(x) := \int \varphi_{\Sigma_i}(x - \theta) \, dG^*(\theta), \quad \text{for} \ x \in \mathbb{R}^d,
\]

where \( \varphi_{\Sigma_i}(x) := \frac{1}{\sqrt{\det(2\pi \Sigma_i)}} \exp\left(-\frac{1}{2}x^T \Sigma_i^{-1}x\right) \) denotes the density of \( \mathcal{N}(0, \Sigma_i) \). Hence an NPME is any maximizer

\[
\hat{G}_n \in \operatorname{argmax}_{G \in \mathcal{P}(\mathbb{R}^d)} \frac{1}{n} \sum_{i=1}^n \log f_{G, \Sigma_i}(X_i).
\]
Figure 1: A noisy color-magnitude diagram (CMD) corresponding to the observations $X_i$ in model (1), with corresponding fully-nonparametric denoised estimates $\hat{\theta}_i$ in the right panel. To avoid overplotting, we display a subsample of $n = 10^5$ stars.

In contrast to the parametric model used in XD, the nonparametric domain $\mathcal{P}(\mathbb{R}^d)$ is convex, so $\hat{G}_n$ solves a convex optimization problem, and tools from convex optimization may be leveraged to find principled approximations to $\hat{G}_n$ (Koenker and Mizera, 2014; Kim et al., 2020).

Given an estimate $\hat{G}_n$ of the prior $G^*$, empirical Bayes imitates the optimal Bayes analysis, known as the oracle (Efron, 2019). If $G^*$ were known, optimal denoising of $\theta^*_i$ would be achieved through the posterior distribution $\theta^*_i \mid X_i$. It is well known, for instance, that the oracle posterior mean

$$\hat{\theta}^*_i := \mathbb{E}_{G^*}[\theta^*_i \mid X_i], \quad \text{where } \theta^*_i \sim G^* \quad \text{and} \quad X_i \mid \theta^*_i \sim \mathcal{N}(\theta^*_i, \Sigma_i)$$

(5)

minimizes the squared error Bayes risk

$$\mathbb{E}_{G^*}\|\hat{\theta}_i(X_i) - \theta^*_i\|^2_2$$

over all measurable functions $\hat{\theta}_i : \mathbb{R}^d \to \mathbb{R}^d$. The NPMLE (4) yields a fully data-driven, empirical Bayes estimate of the oracle posterior mean via

$$\hat{\theta}_i := \mathbb{E}_{\hat{G}_n}[\theta^*_i \mid X_i], \quad \text{where } \theta^*_i \sim \hat{G}_n \quad \text{and} \quad X_i \mid \theta^*_i \sim \mathcal{N}(\theta^*_i, \Sigma_i).$$

(6)

Figure 1 shows the $d = 2$ dimensional dataset of Anderson et al. (2018), where each observation has a known error distribution and may be modeled as multivariate normal after a suitable transformation. The noise in the raw CMD of Figure 1 obscures many known features of stellar evolution, rendering the raw CMD unreliable for downstream parallax inference. The right panel of Figure 1 displays the empirical Bayes posterior means $(\hat{\theta}_i)_{i=1}^n$ based on the NPMLE. The substantial shrinkage of our method reveals many recognizable features of the CMD, such as the red clump and a narrow red giant branch in the upper-right region of the plot, as well as the binary sequence tail distinct from the main sequence tail in the bottom-center region. The NPMLE $\hat{G}_n$ and corresponding posterior means $(\hat{\theta}_i)_{i=1}^n$ offer a powerful approach to shrinkage estimation under minimal assumptions.

The idea of using the NPMLE to estimate a prior distribution, due to Robbins (1950), has seen a resurgence in recent years (Jiang and Zhang, 2009, 2010; Koenker and Mizera, 2014; Dicker and Zhao, 2016; Gu and Koenker, 2016; Koenker and Gu, 2017; Feng and Dicker, 2018; Kim et al., 2019; Efron, 2019; Saha and Guntuboyina, 2020a; Jiang, 2020; Polyanskiy and Wu, 2020; Deb et al., 2021). These advancements, taken together, have begun to establish the NPMLE as a formidable approach to shrinkage estimation both in theory and in practice. All this prior work has focused on either the univariate setting $d = 1$ or the homoscedastic setting $\Sigma_i \equiv \Sigma$, however. Our work
extends the NPMLE to the practically important and more general setting of multivariate and heteroscedastic errors, uncovering a number of important differences.

Basic properties of the NPMLE that are well-understood in the univariate, homoscedastic setting (Lindsay, 1995) have not received careful attention in more complex settings. We verify in Lemma 1 that a solution \( G_n \) exists for every instance of the optimization problem (4), and we record the first-order optimality conditions characterizing the solution set. Similar to the univariate, homoscedastic setting, there exists a solution \( G_n \) which is discrete with at most \( n \) atoms, and the sequence of fitted values \( \hat{L} \equiv (\hat{L}_1, \ldots, \hat{L}_n) = (f_{G_n, \Sigma}(X_i))_{i=1}^n \) is unique, i.e. every solution \( G_n \) has the same sequence of fitted likelihood values \( \hat{L} \).

An important contribution of Lemma 1 is our reinterpretation of the characterizing system of inequalities in terms of a natural ‘dual’ mixture density \( \hat{\psi}_n \). Specifically, \( \hat{\psi}_n \) is a heteroscedastic, \( n \)-component mixture density—a convex combination of Gaussian bumps centered at the data-points \( N(X_i, \Sigma) \) with weights inversely proportional to \( \hat{L}_i \) for \( i = 1, \ldots, n \)—such that the support of every NPMLE \( G_n \) is contained in the set of the global maximizers of \( \hat{\psi}_n \). This observation has a number of important consequences that we explore in detail in Section 2; in particular, tools from algebraic statistics for studying the modes of Gaussian mixtures (Ray and Lindsay, 2005; Améndola et al., 2020) translate directly into results on the support set. We leverage this connection to establish that \( G_n \) is not necessarily unique when \( d > 1 \), even in the homoscedastic case. This finding is distinctive from the univariate, homoscedastic case where it is known that (4) has a unique solution for every problem instance (Lindsay and Roeder, 1993). Our counterexample in Lemma 2 appears to be new and seems to invalidate prior claims of strict concavity of the log-likelihood (Marriott, 2002; Koenker and Gu, 2017). Whereas the fitted values \( \hat{L} \) are always unique, our counterexample also demonstrates that the empirical Bayes posterior means \( \hat{\theta}_i \);\( i=1 \) are not necessarily unique. In light of the non-uniqueness of \( G_n \), a natural question is whether there exist non-discrete solutions: we rule out this possibility in Corollary 3, however, showing every solution is indeed discrete with a finite number of atoms.

The problem of computing a solution \( G_n \) is complicated by the presence of multivariate, heteroscedastic errors. The main difficulty in general is that the NPMLE solves an infinite-dimensional optimization problem. Since \( G_n \) may be taken to be discrete with at most \( n \) atoms, a solution can in principle be found with a finite mixture model. In particular, defining the set of discrete distributions with at most \( k \geq 1 \) atoms,

\[
P_k(\mathbb{R}^d) = \left\{ \sum_{j=1}^k w_j \delta_{a_j} : \sum_j w_j = 1, w \geq 0, a_j \in \mathbb{R}^d, j = 1, \ldots, k \right\},
\]

maximum likelihood solutions over \( P_n(\mathbb{R}^d) \) are also NPMLEs. Hence, the EM algorithm can be applied to optimize \( (w_j, a_j)_{j=1}^m \), as first observed by Laird (1978), though EM over discrete distributions is prohibitively slow for moderately large \( n \) and suffers from the same non-convexity issue as XD. Many algorithms (Böhning, 1985; Lesperance and Kalbfleisch, 1992; Wang, 2007; Liu and Zhu, 2007) have been proposed for finding approximate solutions to the optimization problem (4): Koenker and Mizera (2014) identified a convex, finite-dimensional, highly scalable approximation. Instead of maximizing the log-likelihood of the data \( \frac{1}{n} \sum_{i=1}^n \log f_{G_n, \Sigma}(X_i) \) over \( G \in P_n(\mathbb{R}^d) \), the idea is to maximize the log-likelihood over \( P(A) \), the collection of all probability measures supported on a finite set \( A \subset \mathbb{R}^d \). If \( A \) has \( m > 0 \) elements, then \( P(A) \) is isometric to the \( m-1 \) dimensional simplex \( \Delta_{m-1} = \{ w \in \mathbb{R}^m_+ : \sum_j w_j = 1 \} \), and maximizing the likelihood corresponds to optimizing over the mixing proportions \( w \), which is a convex optimization problem. When \( d = 1 \), it is straightforward to see that \( G_n \) is supported on the range of the data \( \{ X_{(1)}, X_{(n)} \} \), so Koenker and Mizera (2014) proposed taking \( A \) to discretize this range. Jiang and Zhang (2009, Proposition 5) bounded the discretization error in \( d = 1 \) dimension, establishing that optimizing the weights \( w \) via EM can lead to a good approximation once \( m > (\log n) \sqrt{n} \). Dicker and Zhao (2016) further justified the discretization scheme in \( d = 1 \) dimension by showing the discretized NPMLE is statistically indistinguishable from \( G_n \) once the analyst uses at least \( m = \lceil \sqrt{n} \rceil \) atoms.

The discretization approach naturally extends to multivariate, heteroscedastic settings, but to our knowledge, no principled recommendations are available for choosing \( A \subset \mathbb{R}^d \) in general. Feng and Dicker (2018) recommended taking \( A \) to be a grid over a compact region containing the data. We address the key questions of how to choose this compact region and how the discretization error depends on the fineness of the grid. For choosing a compact region to discretize, a natural desideratum is that the region should contain the support of \( G_n \). To this end, in Corollary 3 we
present compact support bounds on the NPMLE in terms of the data \((X_i, \Sigma_i)_{i=1}^n\). When \(d = 1\) our support bounds reduce to the range of the data, reaffirming the original suggestion of Koenker and Mizera (2014), and when \(d > 1\) but the errors are homoscedastic, it suffices to discretize the convex hull of \((X_i)_{i=1}^n\). Interestingly, with multivariate and heteroscedastic errors, the support of the NPMLE can lie outside the convex hull of \((X_i)_{i=1}^n\), so a different region known as the ridgeline manifold \(M\) of \((X_i, \Sigma_i)_{i=1}^n\) is needed. Fortunately, this region \(M \subset \mathbb{R}^d\) is compact, and the NPMLE over \(\mathcal{P}(M)\) agrees with the NPMLE over \(\mathcal{P}(\mathbb{R}^d)\). This justifies the choice of \(\mathcal{A}\) as a \(\delta > 0\) cover of \(M\), and in Proposition 5, we verify that as \(\delta \downarrow 0\), the log-likelihood of the discretized NPMLE approaches that of the NPMLE. We prove a quantitative bound on the gap for fixed \(\delta\), providing some guidance on how the discretization error depends on the fineness of the grid.

Our principled and efficient method of computation facilitates simulation studies assessing the performance of the empirical Bayes estimate \(\hat{\theta}_i\) in a setting where we can actually compare to the oracle Bayes estimate \(\theta_i^*\). Figure 2 illustrates the method on simulated data. The means \(\theta_i^*\) were drawn i.i.d. from a circle of radius two, and the data \(X_i \mid \theta_i^*\) were drawn according to (1) using a variety of diagonal covariance matrices \(\Sigma_i = \begin{bmatrix} \sigma_{1,1}^2 & 0 \\ 0 & \sigma_{2,2}^2 \end{bmatrix}\), taking each \(\sigma_{j,i}^2 \in (1/2, 3/4)\). Visually, it is clear that the empirical Bayes estimates improve upon the observations by shrinking towards the underlying circle; the corresponding mean squared errors were \(\frac{1}{n} \sum_{i=1}^n \| \theta_i - \theta_i^* \|_2^2 = 0.87\) and \(\frac{1}{n} \sum_{i=1}^n \| X_i - \theta_i^* \|_2^2 = 1.46\), respectively. The oracle, which minimizes the mean squared error in expectation, attained an error of \(\frac{1}{n} \sum_{i=1}^n \| \theta_i^* - \theta_i^* \|_2^2 = 0.84\). While the oracle cannot be computed in practice because \(G^*\) is unknown, this value sets a benchmark in simulations to which we may compare the performance of bona fide estimators. The empirical Bayes estimates not only track well with this benchmark; the individual estimates also track remarkably well with the oracle. In our simulation, the regret—defined as the mean squared error between the estimator \((\hat{\theta}_i)_{i=1}^n\) and the oracle \((\theta_i^*)_{i=1}^n\)—was \(\frac{1}{n} \sum_{i=1}^n \| \theta_i - \theta_i^* \|_2^2 = 0.03\). Whereas \(\hat{\theta}_i\) is a function of the observed data, the oracle \(\theta_i^*\) makes optimal use of the unknown prior \(G^*\), making the similarity striking between the two especially striking.

This striking similarity between \(\hat{\theta}_i\) and \(\theta_i^*\) affirms the empirical Bayes adage that “large data sets of parallel situations carry within them their own Bayesian information” (Efron and Hastie, 2016). However, the setting of Figure 2 is complicated by the fact the situations are not directly parallel, in that each observation \(X_i\) has a distinct error distribution. Even in heteroscedastic settings, the extent to which we glean prior information for the purpose of denoising is captured by the empirical Bayes regret \(\frac{1}{n} \sum_{i=1}^n \| \theta_i - \theta_i^* \|_2^2\). Theorem 8 develops a detailed profile of the finite-sample regret properties of the NPMLE for denoising. We show that under certain tail conditions on \(G^*\) the regret is bounded by a rate that is nearly parametric in \(n\), i.e., \(\frac{1}{n}\) up to logarithmic multiplicative factors. The regret still converges at a slower, nonparametric rate under less structured conditions, where \(G^*\) may have heavy tails. Furthermore, when \(G^*\) possesses finer structure, such as the clustering problem where \(G^*\) is a discrete measure with \(k^*\) atoms, we prove that the regret is bounded from above by \(\frac{\log k^*}{n}\) up to logarithmic multiplicative factors in \(n\). The clustering case is particularly remarkable, as the NPMLE is completely tuning-free, with no knowledge of \(k^*\), yet \(\hat{G}_n\) performs essentially as well as any estimator which knows the number of clusters \(k^*\). Thus, Theorem 8 demonstrates that the NPMLE effectively discovers structure when available and also effectively learns when structure is unavailable. Theorem 8 generalizes the regret bounds of Saha and Guntheboyina (2020a) and Jiang (2020) who analyzed the homoscedastic \(\Sigma_i \equiv \Sigma\) setting and the univariate \(d = 1\) setting, respectively. These papers in turn built upon Jiang and Zhang (2009) who studied the univariate, homoscedastic setting.

A key ingredient in the analysis of the regret is a more explicit representation of the estimator \((\hat{\theta}_i)_{i=1}^n\) and oracle \((\theta_i^*)_{i=1}^n\). The oracle posterior mean (5) has the following alternative expression, known as Tweedie’s formula (Dyson, 1926; Robbins, 1956; Efron, 2011; Banerjee et al., 2021):

\[
\hat{\theta}_i^* = X_i + \Sigma_i \nabla f_{G^*, \Sigma_i} (X_i) / f_{G^*, \Sigma_i} (X_i)
\]

Similarly, our plug-in estimate can be written as

\[
\hat{\theta}_i = X_i + \Sigma_i \nabla f_{\hat{G}_n, \Sigma_i} (X_i) / f_{\hat{G}_n, \Sigma_i} (X_i)
\]
Figure 2: Toy data of size $n = 1,000$ and $d = 2$. Top: observations $X_i$ (left) were generated by adding heteroscedastic Gaussian errors to the underlying means $\theta_i^* \overset{iid}{\sim} G^*$ (right), generated IID uniformly from a circle of radius 2. Our discrete estimate $\hat{G}_n$ of the prior is shown in red over the prior $G^*$ in black. Bottom: a comparison of oracle Bayes $\hat{\theta}_i^*$ (left) based on knowledge of the prior distribution $G^*$ and empirical Bayes $\hat{\theta}_i$ (right), a function of the observed data.

Tweedie’s formula clarifies that under model (1) the posterior means only depend on the prior $G^*$ via the marginal likelihood $f_{G^*,\Sigma_i}(X_i)$ and its gradient. Jiang and Zhang (2009) first leveraged this observation to relate the empirical Bayes regret to the problem of estimating the marginal density. In heteroscedastic problems, there are $n$ different marginal densities, $(f_{G^*,\Sigma_i})_{i=1}^n$, to estimate, and corresponding estimators $(f_{\hat{G}_n,\Sigma_i})_{i=1}^n$. We show in Theorem 6 and Corollary 7 that the NPMLE achieves similar adaptive rates in the density estimation problem under an appropriate average Hellinger distance across all $i = 1, \ldots, n$ estimands $(f_{\hat{G}_n,\Sigma_i})_{i=1}^n$.

Whereas most recent work has focused on properties of $\hat{G}_n$ for density estimation and denoising, the NPMLE is potentially much more generally applicable as a plug-in estimate of the prior. To expand our understanding of its applicability, we present the first analysis of the deconvolution error for the NPMLE. Whereas density estimation captures the problem of describing the observations $(X_i)_{i=1}^n$, deconvolution is the equally natural problem of interpreting the infinite-dimensional parameter $G^*$. We study the accuracy of the NPMLE under a Wasserstein distance $W_2(\hat{G}_n, G^*)$. The Wasserstein distance is particularly useful for this problem since $\hat{G}_n$ and $G^*$ are typically mutually singular; in particular, $G^*$ may be absolutely continuous whereas $\hat{G}_n$ is always discrete. The Wasserstein distance will be discussed in detail in Section 4. We show in Theorem 10 that $\hat{G}_n$ attains the minimax rate of deconvolution, which happens to be a very slow, logarithmic
rate $\frac{1}{\log n}$. Inspired by the richness of the density estimation and denoising results, we hint at some of the adaptation properties of the NPMLE under the Wasserstein loss; Theorem 12 shows that when $G^* = \delta_\mu$ is a point mass distribution, the Wasserstein rate improves dramatically to $n^{-1/3}$ up to logarithmic factors.

The rest of the paper is organized as follows: Section 2 systematically addresses basic properties of the NPMLE, including existence, discreteness, and non-uniqueness. Section 3 gives a full account of the approximate computation of NPMLEs. Section 4 establishes finite-sample risk bounds on the accuracy of $\hat{G}_n$ as an estimator of $G^*$ for the purposes of density estimation, denoising and deconvolution. In Section 5, we apply the method to astronomy data to construct a fully data driven color-magnitude diagram of 1 million stars and compare our method to extreme deconvolution where it has previously been applied (Anderson et al., 2018). We also apply the method to chemical abundance data for a smaller subset of stars that has previously been analyzed by Ratcliffe et al. (2020). Section 6 concludes with some discussion of future work. The proofs are in the appendix.

2 Characterization and basic properties

In this section, we establish some basic properties of solutions to the nonparametric maximum likelihood problem (4), including existence, non-uniqueness, discreteness of solutions $\hat{G}_n$, invariance under certain transformations, and bounds on the support. These results provide a foundation both for computing $\hat{G}_n$ (Section 3) and for understanding its statistical properties (Section 4). Our first result extends the well-known characterization of $\hat{G}_n$ for univariate, homoscedastic errors (Lindsay, 1995, Theorems 18-21) to our more general setting.

Lemma 1. Problem (4) attains its maximum: there exists a discrete solution $\hat{G}_n$ with at most $n$ atoms, and the vector $\hat{L} \equiv (\hat{L}_1, \ldots, \hat{L}_n) = (f_{\hat{G}_n, \Sigma_i}(X_i))_{i=1}^n$ of fitted likelihood values is unique. Moreover, $\hat{G}_n \in P(\mathbb{R}^d)$ solves (4) if and only if

$$D(\hat{G}_n, \vartheta) \leq 0 \text{ for all } \vartheta \in \mathbb{R}^d, \text{ where } D(G, \vartheta) := \frac{1}{n} \sum_{i=1}^n \varphi_{\Sigma_i}(X_i - \vartheta) - 1.$$ 

The support of any $\hat{G}_n$ is contained in the zero set $Z := \{\vartheta : D(\hat{G}_n, \vartheta) = 0\}$; the zero set $Z$ is equal to the set of global maximizers of the $n$-component, heteroscedastic dual mixture density

$$\tilde{\psi}_n(\vartheta) := \sum_{i=1}^n \left( \frac{\hat{L}_i^{-1}}{\sum_{i=1}^n \hat{L}_i^{-1}} \right) \varphi_{\Sigma_i}(X_i - \vartheta).$$

We prove Lemma 1, along with all results in this section, in Appendix A. The first statement of the lemma guarantees the existence of a discrete solution, which we typically write as $\hat{G}_n = \sum_{j=1}^k \tilde{w}_j \delta_{\tilde{a}_j}$ (here $\tilde{w}_j \geq 0$, $\sum_j \tilde{w}_j = 1$ and $\tilde{a}_j \in \mathbb{R}^d$), with $k \leq n$ providing an upper bound on the complexity of at least one solution. This implies that $\hat{G}_n$ may be taken to be the maximum likelihood solution to a $k$-component, heteroscedastic Gaussian mixture model where $k$ is selected in a data dependent manner. Since finite mixture models are nested by the number of components and $k \leq n$, we may also say in general that $\hat{G}_n$ is the maximum likelihood solution to an $n$-component, heteroscedastic Gaussian mixture model.

The bound $k \leq n$ is tight: for each $n \geq 1$, there are sequences of observations $(X_i)_{i=1}^n$ and covariances $(\Sigma_i)_{i=1}^n$ such that the smallest number of components $k$ of any solution $\hat{G}_n$ to (4) is precisely $n$ (see, e.g., Lindsay, 1995, p. 116). However, in practice, the number of components is typically much smaller than $n$. For instance, in the univariate, homoscedastic case, Polanskiy and Wu (2020) established a much stronger bound of $k = O_P(\log n)$ under certain conditions on the prior distribution $G^*$.

The last part of Lemma 1 states that the atoms of $\hat{G}_n$ occur at the global maximizers of the $n$-component Gaussian mixture $\tilde{\psi}_n$, which has component distributions of the form $\mathcal{N}(X_i, \Sigma_i)$ for $i = 1, \ldots, n$ with weights inversely proportional to fitted likelihoods $\hat{L}$. Results on the modes of Gaussian mixtures (e.g. Ray and Lindsay, 2005; Dytso et al., 2019; Améndola et al., 2020) thus provide information about the support of the NPMLE; in particular, our next two results exploit this connection to yield novel results on the NPMLE.

In the univariate $d = 1$ and homoscedastic setting $\Sigma_i \equiv \sigma_i^2$, it is additionally known that (4) has a unique solution $\hat{G}_n$ for all observations $X_1, \ldots, X_n$ (Lindsay and Roeder, 1993). This means
that, for every dataset $X_1, \ldots, X_n$ and every variance level $\sigma^2 > 0$, there is a unique probability measure $\hat{G}_n \in \mathcal{P}(\mathbb{R}^2)$ such that $L_i = f_{\hat{G}_n, \sigma^2}(X_i)$ for all $i$, where $\hat{L}$ is the unique vector of optimal likelihoods from Lemma 1. We observe, however, that uniqueness of the solution $\hat{G}_n$ may not hold when $d > 1$, even with isotropic covariances $\Sigma = \sigma^2 I_d$.

**Lemma 2.** Let $d = 2$, $n = 3$ and $X_1 = (0, 1)$, $X_2 = (\sqrt{2}/2, -1/2)$, $X_3 = (-\sqrt{2}/2, -1/2)$. Then (4) with data $(X_i)_{i=1}^3$, covariances $\Sigma_i \equiv \sigma^2 I_2$ and $\sigma^2 = 3/(\log 256)$ has infinitely many solutions of the form

$$\hat{G}_n = \alpha \delta_0 + (1 - \alpha) \frac{1}{3} \sum_{i=1}^3 \delta_{X_i/2},$$

where $\alpha \in [0, 1]$.

Figure 3 illustrates the counterexample given in Lemma 2. A key observation in the proof of Lemma 2 is that, for every dataset $X_1, \ldots, X_n$ such that, for every dataset $X_1, \ldots, X_n$ and every variance level $\sigma^2 > 0$, there is a unique probability measure $\hat{G}_n \in \mathcal{P}(\mathbb{R}^2)$ such that $L_i = f_{\hat{G}_n, \sigma^2}(X_i)$ for all $i$, where $\hat{L}$ is the unique vector of optimal likelihoods from Lemma 1. We observe, however, that uniqueness of the solution $\hat{G}_n$ may not hold when $d > 1$, even with isotropic covariances $\Sigma = \sigma^2 I_d$.

**Lemma 2.** Let $d = 2$, $n = 3$ and $X_1 = (0, 1)$, $X_2 = (\sqrt{2}/2, -1/2)$, $X_3 = (-\sqrt{2}/2, -1/2)$. Then (4) with data $(X_i)_{i=1}^3$, covariances $\Sigma_i \equiv \sigma^2 I_2$ and $\sigma^2 = 3/(\log 256)$ has infinitely many solutions of the form

$$\hat{G}_n = \alpha \delta_0 + (1 - \alpha) \frac{1}{3} \sum_{i=1}^3 \delta_{X_i/2},$$

where $\alpha \in [0, 1]$.

Figure 3 illustrates the counterexample given in Lemma 2. A key observation in the proof of Lemma 2 is that the dual mixture $\hat{\psi}_n = f_{\hat{G}_n, \sigma^2 I_2}$ can be written explicitly as a homoscedastic mixture with uniform mixing distribution $H = \frac{1}{4} \sum_{i=1}^3 \delta_{X_i}$ over the observations $(X_i)_{i=1}^3$. This set-up closely follows a construction, due to Duistermaat (see Améndola et al., 2020), exhibiting an isotropic, homoscedastic Gaussian mixture with more modes than components. Duistermaat used the same component locations $X_i$ but took $\sigma^2 = 0.53$ to obtain an example of a three-component mixture of isotropic, homoscedastic Gaussians such that the mixture has four modes. By specifically choosing $\sigma^2 = \frac{3}{\log 256} = 0.54$, the height of the mixture $\hat{\psi}_n = f_{\hat{G}_n, \sigma^2 I_2}$ is equal at all four modes, i.e. all four modes are global maximizers, and the modes are located at $\{X_1/2, X_2/2, X_3/2, 0\}$. By Lemma 1 any NPMLE must be supported on these modes. Representing the fitted values $\hat{L} = (f_{\hat{G}_n, \sigma^2 I_2}(X_i))_{i=1}^3$ by a probability measure $\hat{G}_n = \sum_{j=1}^3 \hat{w}_j \delta_{X_j/2} + \hat{w}_4 \delta_0$ supported on the global modes is equivalent to finding a set of weights $\hat{w} \in \mathbb{R}_+^4$ such that $\sum_{j=1}^4 \hat{w}_j = 1$ and $\hat{w}$ solves the under-determined linear system $\hat{L} = A \hat{w}$, where $A$ is a $3 \times 4$ matrix given by

$$A_{ij} = \begin{cases} \varphi_{\sigma^2 I_2}(X_i - X_j/2) & j \leq 3 \\ \varphi_{\sigma^2 I_2}(X_i) & j = 4. \end{cases}$$

Finally, we also note that although the fitted likelihoods $f_{\hat{G}_n, \sigma^2 I_2}(X_i)$ are unique, the posterior means $\hat{\theta}_i$ in this example differ for the solutions $\hat{G}_n$ given in Lemma 2.

![Figure 3](image_url)

**Figure 3:** Level sets of the dual mixture density $\hat{\psi}_n = f_{\hat{G}_n, \sigma^2 I_2}$ where $n = 3$ and $H = \frac{1}{4} \sum_{i=1}^3 \delta_{X_i}$ is uniform over the vertices of the larger equilateral triangle $\Delta X_1 X_2 X_3$.

With $\sigma^2 = \frac{3}{\log 256}$, the dual mixture density $\hat{\psi}_n$ has four global modes.

Although the NPMLE searches over all probability measures $G \in \mathcal{P}(\mathbb{R}^d)$ supported on $\mathbb{R}^d$, it is useful algorithmically to reduce the search space to probability measures supported on a
compact subset of \( \mathbb{R}^d \). By Lemma 1, to restrict the support of the NPMLE it suffices to bound the maximizers \( Z \) of the \( n \)-component Gaussian mixture \( \tilde{\psi}_n \). Ray and Lindsay (2005, Theorem 1) showed that all critical points of a Gaussian mixture \( \tilde{\psi}_n(\vartheta) = \sum_{i=1}^n \left( \frac{L_{ii}^{-1}}{\sum_{i=1}^n L_{ii}^{-1}} \right) \varphi_{\Sigma_i}(X_i - \vartheta) \) belong to the ridgeline manifold

\[
\mathcal{M} := \left\{ x^*(\alpha) : \alpha \in \mathbb{R}^n_+, \sum_{i=1}^n \alpha_i = 1 \right\},
\]

where

\[
x^*(\alpha) := \left( \sum_{i=1}^n \alpha_i \Sigma_i^{-1} \right)^{-1} \sum_{i=1}^n \alpha_i \Sigma_i^{-1} X_i.
\]

(9)

In general, the ridgeline manifold \( \mathcal{M} \) is a compact subset of \( \mathbb{R}^d \) which does not depend on the weights \( \left( \frac{L_{ii}^{-1}}{\sum_{i=1}^n L_{ii}^{-1}} \right)_{i=1}^n \). In the univariate case \( d = 1 \), the ridgeline manifold \( \mathcal{M} = [X(1), X(n)] \) is simply the range of the data, so the univariate NPMLE is constrained to be supported on this range. In the multivariate setting, we may further simplify \( \mathcal{M} \) depending on certain shape restrictions on the covariance matrices.

**Corollary 3.** Every solution to (4) is discrete with a finite number of atoms, supported on the ridgeline manifold \( \mathcal{M} \) defined in (9). Depending on the values of \( (\Sigma_i) \) we further bound the support as follows:

(i) (Homoscedastic) If \( \Sigma_i = \Sigma \) for all \( i \), or if \( \Sigma_i = c_i \Sigma \) are proportional up to a sequence \( (c_i) \) of positive scalars, the ridgeline manifold \( \mathcal{M} \) is the convex hull of the data \( \text{conv}(\{X_1, \ldots, X_n\}) \).

(ii) (Diagonal Covariances) If \( \Sigma_i \) is a diagonal matrix for every \( i \), the ridgeline manifold \( \mathcal{M} \) is contained in the axis-aligned minimum bounding box of the data

\[
\prod_{j=1}^d \left[ \min_{k \in \{1, \ldots, n\}} X_{ij}, \max_{n \in \{1, \ldots, n\}} X_{ij} \right],
\]

where \( X_i = (X_{i1}, \ldots, X_{id}) \) for all \( i \).

(iii) (General Covariances) Let \( \kappa \geq k > 0 \) be chosen such that \( k I_d \leq \Sigma_i \leq \kappa I_d \) for all \( i \), where \( A \preceq B \) means \( B - A \) is a symmetric positive semidefinite matrix. Choose \( r > 0 \) and \( x_0 \in \mathbb{R}^d \) such that \( \|X_i - x_0\|_2 \leq r \) for all \( i \). Then the ridgeline manifold \( \mathcal{M} \) is contained in the ball

\[
\mathbb{B}_{kr}(x_0) := \{ y \in \mathbb{R}^d : \|y - x_0\|_2 \leq kr \}
\]

where \( \kappa = k/k \).

The first part of Corollary 3 in general gives the smallest possible convex body over which the support of \( \tilde{G}_n \) can be constrained independently of \( \{\Sigma_i\} \). To see that the first part is tight, consider a fixed set of observations \( \{X_i\}_{i=1}^n \), and isotropic covariance matrices \( \Sigma = \sigma^2 I_d \); as \( \sigma \) is made arbitrarily small, the support of \( \tilde{G}_n \) approaches the set of observations \( \{X_i\}_{i=1}^n \) (Lindsay, 1995). Therefore, in general the convex hull is the smallest convex body containing the support in the homoscedastic setting and more generally the setting of proportional covariance matrices. By contrast, the convex hull of the data is in general too small to capture the support of \( \tilde{G}_n \) in the heteroscedastic setting. Figure 4 presents one example with diagonal covariances where the support of \( \tilde{G}_n \) is pushed towards the corners of the minimum axis-aligned bounding box of the data. Thus, the above discussion and Figure 4 indicate that both parts (i) and (ii) of Corollary 3 give the tightest possible convex support bounds in their respective special cases.

We close this section with a brief discussion on how the NPMLE behaves under certain simple transformations of the data \( (X_i, \Sigma_i)_{i=1}^n \). Given a map \( T : \mathbb{R}^d \to \mathbb{R}^d \), let \( T_{#} G \in \mathcal{P}(\mathbb{R}^d) \) denote the pushforward of \( G \in \mathcal{P}(\mathbb{R}^d) \) given by \( T_{#} G(B) = G(T^{-1}(B)) \), for any Borel set \( B \subseteq \mathbb{R}^d \). In other words, if \( V \sim G \), then \( T_{#} G \) is the distribution of \( T(V) \).

**Lemma 4.** Fix a dataset \( (X_i, \Sigma_i)_{i=1}^n \), a point \( x_0 \in \mathbb{R}^d \) and a \( d \times d \) orthogonal matrix \( U_0 \). Consider the transformed dataset \( (X'_i, \Sigma'_i)_{i=1}^n \) where \( \Sigma'_i = U_0 \Sigma_i U_0^T \) and \( X'_i = T(X_i) \) for \( i = 1, \ldots, n \), with \( T(x) = U_0 x + x_0 \). Then

\[
T_{#} f_{G_{\Sigma}, \Sigma_i}(X_i) = f_{G_{\Sigma'}, \Sigma'_i}(X'_i)
\]

for all \( i = 1, \ldots, n \) and all \( G \in \mathcal{P}(\mathbb{R}^d) \).
Figure 4: Left: An example of observations $X_1 = (0, 1)$, $X_2 = (0, -1)$, $X_3 = (1, 0)$, and $X_4 = (-1, 0)$ (blue points) with diagonal covariances $\Sigma_1 = \Sigma_2 = \begin{bmatrix} 0 & 0.05 \\ 0 & 0.05 \end{bmatrix}$ (dashed ellipses), where the NPMLE is supported on atoms $a_1, \ldots, a_4$ (red points) well outside the convex hull of the data, and near the corners of the minimum axis-aligned bounding box. Right: The mixture $\hat{\psi}_n(\theta) = \frac{1}{4} \sum_{i=1}^{4} \varphi_{\Sigma_i}(X_i - \theta)$ only has modes at the atoms $a_1, \ldots, a_4$, so no NPMLE is supported within the convex hull of the data.

Lemma 4 is a straightforward consequence of the change of variables formula, but it has a number of useful corollaries. In particular, if $\hat{G}_n \in \mathcal{P}(\mathbb{R}^d)$ is an NPMLE for the dataset $(X_i, \Sigma_i)_{i=1}^{n}$, then $T_{x_0} \hat{G}_n$ is an NPMLE for the modified dataset $(X_i', \Sigma_i')_{i=1}^{n}$, and the fitted likelihood values are the same, i.e.

$$f_{T_{x_0} \hat{G}_n, \Sigma_i'}(X_i') = f_{\hat{G}_n, \Sigma_i}(X_i),$$

for all $i = 1, \ldots, n$. Thus, an NPMLE $\hat{G}_n = \sum_{j=1}^{k} \bar{w}_j \delta_{a_j}$ is equivariant under translations $T(y) = y + x_0$: if every observation is shifted by some fixed $x_0 \in \mathbb{R}^d$, then the modified NPMLE $T_{x_0} \hat{G}_n = \sum_{j=1}^{k} \bar{w}_j \delta_{a_j + x_0}$ simply shifts every atom by $x_0$. Similarly, the NPMLE is equivariant under orthogonal transformations, which explains why the fitted likelihood values are all equal in the rotationally symmetric toy datasets presented in Figure 3 and Figure 4.

3 Computation

The NPMLE solves a convex optimization problem (4) that is infinite-dimensional in the sense that the decision variable $G$ ranges over all probability measures on $\mathbb{R}^d$. Many numerical methods for approximately computing the NPMLE have been considered—including EM (Laird, 1978), vertex direction and exchange methods (Böhning, 1985), semi-infinite methods (Lesperance and Kalbfleisch, 1992), constrained-Newton methods (Wang, 2007), and hybrid methods (Liu and Zhu, 2007; Böhning, 2003)—typically described for the special case of univariate and homoscedastic errors. In this section, we discuss our strategy for computing the NPMLE as well as the challenges of scaling the computation to large datasets.

We follow the approach of Koenker and Mizera (2014), who approximated the infinite-dimensional problem by constraining the support of $G$ to a large finite set. For a non-empty, closed set $\mathcal{A} \subseteq \mathbb{R}^d$, define a support-constrained NPMLE as any solution $\hat{G}_n^{\mathcal{A}} \in \mathcal{P}(\mathcal{A})$.

$$\hat{G}_n^{\mathcal{A}} \in \arg\max_{G \in \mathcal{P}(\mathcal{A})} \frac{1}{n} \sum_{i=1}^{n} \log f_{G, \Sigma_i}(X_i),$$

where $\mathcal{P}(\mathcal{A})$ denotes the set of probability measures supported on $\mathcal{A}$. In particular, $\hat{G}_n = \hat{G}_n^{\mathbb{R}^d}$ by definition, and by Corollary 3 we may write $\hat{G}_n = \hat{G}_n^{\mathcal{M}}$ for a compact subset $\mathcal{M}$ defined explicitly in terms of the data.
We now describe our strategy for choosing the discretization set $\mathcal{A}$. Let $\mathcal{M}$ denote a covering of $\mathcal{M}$ by closed hypercubes of width $\delta$, i.e. $\mathcal{H} = \{x_j + [-\delta/2, \delta/2]^d : j \in \{1, \ldots, J\}\}$ for some set of points $x_1, \ldots, x_J \in \mathbb{R}^d$ that $\mathcal{M} \subseteq \bigcup_{j=1}^J \{x_j + [-\delta/2, \delta/2]^d\}$. Now define the discretized support $\mathcal{A}$ to be the set of corners of hypercubes in $\mathcal{H}$: specifically, for each hypercube $x_j + [-\delta/2, \delta/2]^d$ in $\mathcal{H}$, the point $x_j + \frac{\delta}{2}v \in \mathcal{A}$ for every $v \in \{-1, 1\}^d$. Because $\mathcal{M}$ is compact, $\mathcal{A}$ is a finite set which we denote by $\{a_{ij}\}_{i,j=1}^m$. Constraining the NPMLE to this finite set of atoms $a_1, \ldots, a_m$ yields a finite-dimensional convex optimization problem over the mixing proportions. That is, the solution to (10) can be written as $\hat{G}_n^A = \sum_{j=1}^m \hat{w}_j a_{ij}$, where

$$
\hat{w} \in \arg\max_{\hat{w} \in \Delta_{m-1}} \frac{1}{n} \sum_{i=1}^n \log \left( \sum_{j=1}^m L_{ij} w_j \right),
$$

and $L_{ij} = \phi_{ij}(x_i - a_j)$ encodes an $n \times m$ kernel matrix. The EM algorithm (Dempster et al., 1977) can be used to optimize directly over the mixing proportions $\hat{w}$. While this approach was advocated by Lashkari and Golland (2008) and Jiang and Zhang (2009), EM can be prohibitively slow (Redner and Walker, 1984; Koenker and Mizera, 2014). A crucial observation made by Koenker and Mizera (2014) is that (11) is a (finite-dimensional) convex optimization problem, enabling the use of a wide array of tools from modern convex optimization; they proposed solving the dual to (11) using an interior point solver, and Gu and Koenker (2017) provided an R implementation to solve univariate problems. Kim et al. (2020) proposed sequential quadratic programming to solve a variant of the primal problem directly, demonstrating superior scalability with the sample size $n$. Our implementation uses the MOSEK library (MOSEK ApS, 2019) for Python.

To justify the grid approximation, some consideration of the discretization error is warranted. Our next result shows that as $\delta \downarrow 0$, the log-likelihood of the discretized NPMLE approaches that of the (unconstrained) NPMLE; moreover, the bound on the gap depends on known quantities, so it can be used to guide a suitable choice of $\delta$.

**Proposition 5.** Let $\mathcal{M} \subseteq \mathbb{R}^d$ denote any compact set such that every solution (4) is supported on $\mathcal{M}$. Suppose the diameter of the set $\mathcal{M}$ is at most $D$, the minimum eigenvalue of each $\Sigma_i$ is at least $k$, and fix $\delta \in \left(0, \sqrt{\frac{3}{2mL}}D^{-1}\right)$. Let $\mathcal{H}$ denote a cover of $\mathcal{M}$ by closed hypercubes of width $\delta$, and let $\mathcal{A}$ denote the set of corners of hypercubes in $\mathcal{H}$. Every approximate NPMLE $\hat{G}_n^A$ satisfies

$$
\sup_{G \in \mathcal{P}(\mathbb{R}^d)} \frac{1}{n} \sum_{i=1}^n \log f_{G, \Sigma_i}(X_i) - \frac{1}{n} \sum_{i=1}^n \log f_{\hat{G}_n^A, \Sigma_i}(X_i) \leq dk^{-2} \left(2D^2 + \frac{1}{2}\right)\delta^2.
$$

We prove Proposition 5 in Appendix A. Proposition 5 shows that we can tractably approximate the NPMLE via a finite-dimensional, convex optimization problem. As we show in Section 4, our theoretical results on the statistical properties of the NPMLE hold for any approximate solution $\hat{G}_n^A$, which places nearly as high likelihood on the observations as the global optimizer, in the sense of (12). Hence for $\delta$ sufficiently small we can guarantee that the discretization error is negligible.

Dicker and Zhao (2016) showed in the univariate, homoscedastic case that a finely discretized NPMLE is statistically indistinguishable from the NPMLE for the purpose of density estimation. However, their analysis of the discretization error makes use of the modeling assumptions (1) and is statistical in nature, so their theoretical results provide little guidance on how much error is incurred due to discretization for a fixed dataset. Our result aligns more closely with and in fact essentially generalizes Jiang and Zhang (2009, Proposition 5), which bounded the optimality gap for a particular algorithm, discretization scheme and fixed dataset. The main difference between our result and Jiang and Zhang (2009, Proposition 5) is that the latter analyzed the EM algorithm for the mixing proportions (11), whereas by using a black-box, second-order optimization method to solve for the mixing proportions $\hat{w}$, we can solve for the discretized NPMLE $\hat{G}_n^A$ much more accurately.

## 4 Statistical properties

The NPMLE $\hat{G}_n$ applies as a plug-in estimator of the prior distribution $G^*$ for many purposes. The traditional statistical setting is density estimation, where working in a Gaussian mixture model greatly simplifies the problem of estimating the marginal density of each observation $X_i$. In...
particular, \( f_{G^\ast, \Sigma_i} \) is a natural, tuning-free estimate of the true marginal density \( f_{G^\ast, \Sigma_i} \). Another problem setting—at the heart of empirical Bayes methodology—is to imitate the Bayesian inference we would conduct if we knew \( G^\ast \). Denoising, using \( (\hat{\theta}_i^n)_{i=1}^n \) as plug-in estimators of the true posterior means \( (\hat{\theta}_{i}^\ast)_{i=1}^n \), represents the most basic instantiation. Finally, often we wish to compare \( \hat{G}_n \) to the prior \( G^\ast \) directly. Since we are estimating the prior given observations from a convolution model \( X_i \overset{iid}{\sim} f_{G^\ast, \Sigma_i} \), deconvolution refers to the problem of estimating \( G^\ast \).

In this section, we establish that the NPMLE is well-suited for all three disparate targets of estimation: the marginal densities \( (f_{G^\ast, \Sigma_i})_{i=1}^n \), the oracle posterior means \( (\hat{\theta}_i^\ast)_{i=1}^n \) and the prior \( G^\ast \). In this section, we allow for the possibility that \( \hat{G}_n \) is an approximate NPMLE, with the exact conditions being given in each theorem. Throughout this section, we use the standard notation \( X \leq_{p,q} Y \) to mean \( X \leq C_{p,q} Y \) for some positive constant \( C_{p,q} > 0 \) depending only on problem parameters \( p, q \).

4.1 Density estimation: average Hellinger accuracy

As the distribution of \( X_i \) varies with \( i \), we consider the density estimation quality of the NPMLE (4) in terms of the average squared Hellinger distance, i.e. for \( G, H \in \mathcal{P}(\mathbb{R}^d) \),

\[
\overline{h}^2(f_G, f_H) := \frac{1}{n} \sum_{i=1}^n h^2(f_G, f_H),
\]

where \( h^2(f, g) = \frac{1}{2} \int (\sqrt{f} - \sqrt{g})^2 \) denotes the usual squared Hellinger distance between a pair of densities \( f, g \). In the homoscedastic case where \( \Sigma_i = \Sigma \), our proposed loss function \( h^2(f_G, f_H) = h^2(f_{G, \Sigma}, f_{H, \Sigma}) \) agrees with the usual squared Hellinger distance. Our first result bounds the average squared Hellinger accuracy \( \overline{h}^2(f_{\hat{G}_n}, f_{G^\ast}) \) of the NPMLE. In order to accommodate general heteroscedastic \( \Sigma_i \), we state our results in terms of uniform upper and lower bounds on the spectra of all of the matrices, i.e. \( k_{Id} - \Sigma_i \leq \overline{\Sigma}Id_{kd} \) for all \( i \). To state the result, some additional notation is needed. We fix a positive scalar \( M \geq \sqrt{16k} \log n \) and a non-empty compact set \( S \subset \mathbb{R}^d \). Define the rate function controlling the squared Hellinger distance

\[
\varepsilon_n^2(M, S, G^\ast) := \text{Vol}(S^{1/2}) \frac{M^d}{n} \left( \log n \right)^{d+1} + \inf_{\vartheta \in S} \left( \frac{2\mu_q}{M} \right)^q \log n,
\]

where \( \mu_q \) denotes the \( q \)-th-moment of \( \mathcal{D}_S(\vartheta) := \inf_{s \in S} \| \vartheta - s \|_2 \), \( S^a := \{ \vartheta \in \mathcal{D}_S(\vartheta) \} \) denotes the \( a \)-enlargement of the set \( S \). Note that we have suppressed the dependence of \( \varepsilon_n^2 \) on the upper bound \( R \).

The following result states that \( \varepsilon_n^2(M, S, G^\ast) \) bounds the rate in average Hellinger accuracy both with high probability and in expectation. The scalar \( M \geq \sqrt{16k} \log n \) and compact set \( S \neq \emptyset \) are free parameters. Note that the first term on the right-hand side of (13) is increasing in \( M \) and \( S \), whereas the second is decreasing in each. In principle, then, we may tune the values of \( M \) and \( S \) to optimize the rate function \( \varepsilon_n^2(M, S, G^\ast) \). Later in this section, we discuss a number of special cases where a more explicit rate can be obtained.

**Theorem 6.** Suppose \( X_i \overset{iid}{\sim} f_{G, \Sigma_i} \), where \( k_{Id} \leq \Sigma_i \leq \overline{\Sigma}Id_{kd} \) for all \( i \). Any (approximate) solution \( \hat{G}_n \in \mathcal{P}(\mathbb{R}^d) \) of (4) satisfying

\[
\sup_{G \in \mathcal{P}(\mathbb{R}^d)} \frac{1}{n} \sum_{i=1}^n \log f_{G, \Sigma_i}(X_i) - \frac{1}{n} \sum_{i=1}^n \log f_{\hat{G}_n, \Sigma_i}(X_i) \leq d \overline{\Sigma} \varepsilon_n^2(M, S, G^\ast)
\]

satisfies

\[
\mathbb{E} \left( h^2(f_{\hat{G}_n, \Sigma_i}, f_{G^\ast}) \right) \leq d \overline{\Sigma} \varepsilon_n^2(M, S, G^\ast),
\]

for all \( t \geq 1 \), provided \( n \geq \max(ek^{-d/2}/(2\pi)^{d/2}) \). Moreover,

\[
\mathbb{E} \left( h^2(f_{\hat{G}_n, \Sigma_i}, f_{G^\ast}) \right) \leq d \overline{\Sigma} \varepsilon_n^2(M, S, G^\ast).
\]
We prove Theorem 6 in Appendix B. Our proof extends Theorem 2.1 of Saha and Guntuboyina (2020a) on the multivariate, homoscedastic case \( \Sigma_i = I_d \) and Theorem 4 of Jiang (2020) on the univariate, heteroscedastic case \( d = 1 \), which in turn build upon Theorem 1 of Zhang (2009) on the univariate, homoscedastic case. The general theory on rates of convergence for maximum likelihood estimators (Wong and Shen, 1995; van de Geer, 2000) can in principle be used to bound \( \hat{h}^2(f_{\hat{G}_n,\cdot}, f_{G^*,\cdot}). \) Our proof technique deviates from the general theory by directly bounding the likelihood \( f_{\hat{G}_n,\Sigma_i}(x) \) for \( x \) outside some pre-specified domain (controlled by the choice of set \( S \)), and then covering the set of densities \( \{f_{\hat{G}_n \cdot} : G \in \mathcal{P}(\mathbb{R}^d)\} \) within the domain in the \( L_\infty \) metric.

Theorem 6 provides a sharp bound in many special cases of \( G^* \). For a given \( G^* \) we need to optimize over the choices of \( M \geq \sqrt{10\log n} \) and the nonempty compact set \( S \subset \mathbb{R}^d \) to obtain the smallest value of the rate function \( \varepsilon_n^2(M,S,G^*) \). Our next result performs this calculation for various assumptions on the prior \( G^* \).

**Corollary 7.** Suppose \( X_i \overset{iid}{\sim} f_{G^*,\Sigma_i} \) where \( kI_d \preceq \Sigma_i \preceq \overline{k}I_d \) for all \( i \). Suppose \( \hat{G}_n \in \mathcal{P}(\mathbb{R}^d) \) is any approximate NPMLE such that
\[
\sup_{G \in \mathcal{P}(\mathbb{R}^d)} \frac{1}{n} \sum_{i=1}^{n} \log f_{G,\Sigma_i}(X_i) = \frac{1}{n} \sum_{i=1}^{n} \log f_{\hat{G}_n,\Sigma_i}(X_i) \lesssim_{d,K,d} \frac{(\log n)^{d+1}}{n}.
\]

(i) (Discrete support) If \( G^* = \sum_j \omega_j^* \delta_{a_j^*} \), then
\[
\mathbb{E}h^2(f_{\hat{G}_n,\cdot}, f_{G^*,\cdot}) \lesssim_{d,K,d} \frac{k^*}{n} (\log n)^{d+1}.
\]

(ii) (Compact support) If \( G^* \) has compact support \( S^* \), then
\[
\mathbb{E}h^2(f_{\hat{G}_n,\cdot}, f_{G^*,\cdot}) \lesssim_{d,K,d} \frac{\text{Vol}(S^* + \mathbb{B}_2^{1/2}(0))}{n} (\log n)^{d+1},
\]
where \( \mathbb{B}_r(x) = \{ y : \|x - y\|_2 \leq r \} \) denotes the \( d \)-dimensional ball of radius \( r \) centered at \( x \).

(iii) (Simultaneous moment control) Suppose that there is a compact \( S^* \subset \mathbb{R}^d \) and \( \alpha \in (0,2] \), \( K \geq 1 \) such that \( \mu_q = \mathbb{E}_{\theta \sim G^*} [\|\theta - \theta(S)\|_2]^{1/q} \leq K q^{1/\alpha} \) for all \( q \geq 1 \) (recall \( \theta(S) = \inf_{S \subset S} \|\theta - s\|_2 \) as above). Then
\[
\mathbb{E}h^2(f_{\hat{G}_n,\cdot}, f_{G^*,\cdot}) \lesssim_{d,K,d} \frac{\text{Vol}(S^* + \mathbb{B}_2^{1/2}(0))}{n} (\log n)^{\frac{2\alpha}{2 + \alpha}d+1}.
\]

(iv) (Finite \( q \)th moment) Suppose that there is a compact \( S^* \subset \mathbb{R}^d \) and \( \mu, q > 0 \) such that \( \mu_q \leq \mu \). Then
\[
\mathbb{E}h^2(f_{\hat{G}_n,\cdot}, f_{G^*,\cdot}) \lesssim_{d,K,d} \frac{\text{Vol}(S^* + \mathbb{B}_2^{1/2}(0))}{n} (\log n)^{\frac{q}{2 + q}d+1}.
\]

Given the general result in Theorem 6, Corollary 7 follows directly from the calculations of Saha and Guntuboyina (2020a) in Corollary 2.2 and Theorem 2.3. Corollary 7 captures an important adaptation property of the NPMLE. The cases (i) - (iv) described in the result are nested in the sense that (i) implies (ii), (ii) implies (iii), and (iii) implies (iv); consequently the rates get progressively worse as our assumptions weaken. This means that the NPMLE, despite searching over all probability measures \( \mathcal{P}(\mathbb{R}^d) \), obtains better rates when structure is present in the prior \( G^* \).

Most strikingly, when \( G^* \) has discrete support with \( k^* \) support points, the rate in (i) is \( \frac{k^*}{n} \) up to logarithmic factors without assuming any knowledge of \( k^* \). This rate matches the minimax rate over all discrete distributions with at most \( k^* \) support points (Saha and Guntuboyina, 2020a), meaning we could not expect to do much better even if \( k^* \) were known. In the extreme case where \( k^* = 1 \), the observations actually come from a simple Gaussian, i.e. \( f_{G^*,\Sigma_i}(x) = \phi_{\Sigma_i}(x - a_i^*) \) with common mean \( a_i^* \in \mathbb{R}^d \), so our result says we don’t lose much in the rate when we model the density with a mixture even when it turns out to be a simple Gaussian. Similarly, in (ii), the rate adapts to the size of the support \( S^* \) without prior knowledge of this support or even a bound on its size. Up through simultaneous moment control (iii), the dimension \( d \) only affects the rate.
as a function of $n$ through the logarithmic factor. Hence, the NPMLE avoids the usual curse of dimensionality to some extent, while still achieving consistency in the heavier tailed setting (iv). The logarithmic factors in our bounds might be reduced slightly but cannot be eliminated as they are present in the minimax lower bounds (Kim and Guntuboyina, 2020).

4.1.1 Implications for the Discretization Rate

Theorem 6 establishes that up to a multiplicative constant (depending only on the dimension $d$ and bounds $k, \tilde{k}$ on the eigenvalues of the covariance matrices) the quantity $\varepsilon_n^2(M, S, G^*)$ controls the average Hellinger accuracy $\mathbb{E}[h^2(f_{\hat{G}_n,*}, f_{G^*,*})]$ of the NPMLE. This also holds for approximate solutions to the optimization problem (4) that, in accordance with (14), place nearly as much likelihood on the data as does a global maximizer. It is natural to compare the requirement (14) with our computational guarantee on the discretization error (12) from Proposition 5. The free parameter which controls the discretization error is the resolution $\delta > 0$, which represents the width of the hypercubes we use to cover the ridgeline manifold $\mathcal{M}$ or any of its outer-approximations from Corollary 3. Thus, in order to satisfy the main requirement of Theorem 6, we need to take $\delta$ such that

$$
\varepsilon_n^2(M, S, G^*) \geq d,k k^{-2} \left(2D^2 + \frac{1}{2}\right) \delta^2.
$$

Observe from the definition of $\varepsilon_n^2$ that $\varepsilon_n^2(M, S, G^*) \geq d,k k^{-2} \frac{\log(n)^{d+1}}{n}$ for all $M \geq \sqrt{10k}\log(n)$ and all compact $S$. Absorbing additional terms depending on $d,k$, and $\tilde{k}$ and assuming for simplicity that $D > \frac{1}{2}$, choosing $\delta$ such that

$$
D^2 \delta^2 \leq d,k k^{-2} \frac{\log(n)^{d+1}}{n}
$$

(18)
suffices for the discretized NPMLE to be statistically indistinguishable from a global maximizer.

The inequality (18) gives a preliminary bound on the rate at which the discretization level $\delta$ should decrease with $n$. Still, recall from Proposition 5 that $D$ denotes the diameter of the ridgeline manifold $\mathcal{M}$, so $D$ does depend on $n$. To sketch the dependence, let us consider a representative example where $G^*$ has sub-Gaussian tails and all of the $\Sigma_i$’s are diagonal. In this case, by Corollary 3 part (ii), the ridgeline manifold $\mathcal{M}$ is contained in the axis-aligned minimum bounding box of the data

$$
\prod_{j=1}^d \left[ \min_{i \in \{1, \ldots, n\}} X_{ij}, \max_{i \in \{1, \ldots, n\}} X_{ij} \right].
$$

Due to the tail condition, the length of each side of this hyper-rectangle grows like $\sqrt{\log(n)}$ with high probability up to multiplicative factors depending on $\tilde{k}$; hence, the diameter $D$ also scales like $\sqrt{\log(n)}$ with high probability up to multiplicative factors depending on $\tilde{k}$ and $d$. We have thus shown that it suffices to discretize at a resolution of $\delta \simeq \sqrt{\frac{\log(n)^2}{n}}$. The number of points in our covering $\mathcal{A}$ is of order $m \simeq \left(\frac{n}{\log(n)^d}\right)^{d/2}$. In the univariate case $d = 1$, this slightly improves the finding of Theorem 2 of Dicker and Zhao (2016), who showed that an $m = \sqrt{n}$-discretization of the range of the data $[X_{(1)}, X_{(n)}]$ suffices for the same rate in Hellinger distance. Their bound on the large-deviation probability is also logarithmic, i.e. $O\left(\frac{1}{\log(n)}\right)$ whereas our equation (15) is polynomial in $n$. Our analysis also clarifies that the sense in which we need approximate NPMLE (14) is through the likelihood of the observations, relative to the global optimum, which could be useful for comparing alternative approaches to approximating the NPMLE.

4.2 Denoising: an oracle inequality

In this section we turn to the problem of estimating the oracle posterior means $(\hat{\theta}_i^*)_{i=1}^n$; see (5). We evaluate the performance of $(\hat{\theta}_i)_{i=1}^n$ (see (6)) as an estimator for $(\hat{\theta}_i^*)_{i=1}^n$ using the mean squared error risk measure

$$
\frac{1}{n} \sum_{i=1}^n \mathbb{E}[\|\hat{\theta}_i - \hat{\theta}_i^*\|_2^2].
$$

Since $\hat{\theta}_i^*$ is the optimal estimator of $\theta_i^*$ given model (1), the above mean squared error quantifies the price of misspecifying $G^*$ with the data-driven estimator $\hat{G}_n$. Hence, this loss is also known as the per-instance empirical Bayes regret.
Our next result states that the rate function $\varepsilon^2_n(M, S, G^*)$ governing the Hellinger accuracy (see (13)) also upper bounds the regret, up to additional logarithmic factors. We provide the same special cases of the rate as those stated in Corollary 7.

**Theorem 8.** Suppose $X_i \sim f_{G^*, \Sigma_i}$ where $k_{I_d} \leq \Sigma_i \leq \overline{k}_{I_d}$ for all $i$. Let $\hat{G}_n$ denote any approximate NPMLE satisfying (17). Fix some $M \geq \sqrt{10k\log n}$ and a nonempty, compact set $S \subset \mathbb{R}^d$. Define $\varepsilon^2_n(M, S, G^*)$ as in (13). For all $n \geq \varepsilon_n^{d/2} + (2\pi)^{d/2},$

$$\frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[ \| \hat{\theta}_i - \theta^*_i \|_2^2 \right] \leq \varepsilon_n^{2} (M, S, G^*) (\log n)^{(d/2-1)\nu^3}.$$  

(19)

In particular, consider the following special cases for $G^*$:

(i) (Discrete support) If $G^* = \sum_{j=1}^{k^*_n} w^*_j \delta_{a^*_j}$, then

$$\frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[ \| \hat{\theta}_i - \theta^*_i \|_2^2 \right] \leq \frac{k^*_n}{n} (\log n)^{d+(d/2)\nu^4}.$$

(ii) (Compact support) If $G^*$ has compact support $S^*$, then

$$\frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[ \| \hat{\theta}_i - \theta^*_i \|_2^2 \right] \leq \frac{\text{Vol}\left(S^* + \overline{B}_{\varepsilon_2/2}(0)\right)}{n} (\log n)^{d+(d/2)\nu^4}.$$

(iii) (Simultaneous moment control) Suppose that there is a compact $S^* \subset \mathbb{R}^d$ and $\alpha \in (0, 2]$, $K \geq 1$ such that $\mu_q := \mathbb{E}_{\theta \sim \Sigma^*} [\theta^q(\theta, S^*)]^{1/\alpha} \leq K q^\alpha$ for all $q \geq 1$. Then

$$\frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[ \| \hat{\theta}_i - \theta^*_i \|_2^2 \right] \leq \frac{\text{Vol}\left(S^* + \overline{B}_{\varepsilon_2/2}(0)\right)}{n} (\log n)^{\frac{d}{\alpha} + d+(d/2)\nu^4}.$$

(iv) (Finite $q^{th}$ moment) Suppose that there exists a compact $S^* \subset \mathbb{R}^d$ and $\mu, q > 0$ such that $\mu q \leq \mu$. Then

$$\frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[ \| \hat{\theta}_i - \theta^*_i \|_2^2 \right] \leq \frac{\text{Vol}\left(S^* + \overline{B}_{\varepsilon_2/2}(0)\right)}{n} (\log n)^{\frac{d}{\alpha q} + d+(d/2)\nu^4}.$$

Theorem 8 shows that the denoising problem shares the adaptation features as the density estimation problem. Since we have assumed $k_{I_d} \leq \Sigma_i \leq \overline{k}_{I_d}$ for all $i = 1, \ldots, n$, the same set of results also hold for the scaled regret $\frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[ \| \hat{\theta}_i - \theta^*_i \|_2^2 \right] \Sigma^{-1}_i (\hat{\theta}_i - \theta^*_i)$.

**Remark 9.** (On the proof of Theorem 8 in Appendix C) Our proof extends Theorem 3.1 of Saha and Gantumur (2020a) on the multivariate, homoscedastic case $\Sigma_i = I_d$ and Theorem 1 of Jiang (2020) on the univariate, heteroscedastic case $d = 1$, which in turn build upon Theorem 5 of Jiang and Zhang (2009) on the univariate, homoscedastic case. Jiang and Zhang (2009) and Jiang (2020) used a related notion of regret

$$\sqrt{\frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[ \| \hat{\theta}_i - \theta^*_i \|_2^2 \right]} - \sqrt{\frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[ \| \hat{\theta}_i - \theta^*_i \|_2^2 \right]}.$$

Tweedie’s formula relates the oracle (7) and empirical Bayes (8) posterior means to the corresponding marginal likelihoods, so the density estimation results of the previous section turn out to be useful for proving Theorem 8 as well. In particular, we consider Bayes rules for priors in a covering of the Hellinger ball

$$\left\{ G \in \mathcal{P}(\mathbb{R}^d) : k^2(f_{G, \Sigma_*}, f_{G', \Sigma_*}) \leq d\pi \frac{\ell^2 \varepsilon_n^2 (M, S, G^*)}{n} \right\},$$

which, by Theorem 6, contains $\hat{G}_n$ with high probability. For a fixed prior $G$, the denominator in the correction factor of Tweedie’s formula

$$X_i + \Sigma_n \frac{\nabla f_{G, \Sigma_*}(X_i)}{f_{G, \Sigma}(X_i)},$$

15
namely \( f_{G_i}(X_i) \), can be small. To avoid dividing by near-zero quantities, we regularize the above Bayes rule by replacing the denominator with \( \max(f_{G_i}(X_i), \rho) \) for a small positive \( \rho \). To handle heteroscedastic errors, we show that Tweedie’s formula, even its regularized form, is equivariant under scale transformations.

4.3 Deconvolution: estimating the prior

We turn to the fundamental question of how well \( \hat{G}_n \) estimates \( G^* \). This is known as the deconvolution problem and has received much attention in the statistical literature (Meister, 2009). Indeed, the original consistency results (Kiefer and Wolfowitz, 1956; Pfanzagl, 1988) for the NPMLE focused on weak convergence of \( \hat{G}_n \) to \( G^* \) as \( n \to \infty \). While most prior work on deconvolution has focused on deconvolution with homoscedastic error distributions, Delaigle and Meister (2008) allowed for heteroscedastic errors but relied on kernel estimators which contain additional smoothing parameters. By contrast, the NPMLE provides a tuning-free estimate of the mixing distribution \( G^* \), yet to our knowledge, non-asymptotic bounds on the rate of convergence for \( \hat{G}_n \) in the deconvolution problem are not known.

In practice, the true prior \( G^* \) may not be discrete even though \( \hat{G}_n \) always is, and even if both distributions are discrete, their supports will typically differ. Our loss function must allow for comparisons of probability measures with potentially disjoint supports. Nguyen (2013) established that a natural loss for this problem is the Wasserstein distance from the theory of optimal transport

\[
W_2^2(G, H) = \min_{(U,V) \in \Pi_{G,H}} \mathbb{E} \|U - V\|_2^2,
\]

where \( G, H \in \mathcal{P}(\mathbb{R}^d) \) are two probability measures and \( \Pi_{G,H} \) denotes the set of couplings of \( G \) and \( H \), i.e. joint distributions over \( (U, V) \in \mathbb{R}^{2d} \) such that \( U \sim G \) and \( V \sim H \). Indeed, even the likelihood criterion is intimately related to the Wasserstein distance: in the homoscedastic case \( \Sigma_i \equiv \sigma^2 I_d \), it is known that the NPMLE (4) equivalently solves an entropic-regularized optimal transport problem (Rigollet and Weed, 2018).

Nguyen (2013) connected the deconvolution error \( W_2^2(G, H) \) to the density estimation error between the mixtures, i.e. \( h^\ast(f_{G_i}, f_{H_i}) \) in a homoscedastic Gaussian deconvolution setting. By leveraging similar techniques as well as the support bounds of Corollary 3, we arrive at the following upper bound on the deconvolution error.

**Theorem 10.** Suppose \( X_i \sim f_{G_i, \Sigma_i} \) where \( k_i I_d \leq \Sigma_i \leq \bar{k}_i I_d \) and \( \Sigma_i \) is a diagonal matrix for each \( i \). Suppose further that \( G^*([L, L]^d) = 1 \) for some \( L \geq 0 \). Let \( \hat{G}_n \) denote any approximate NPMLE supported on the minimum axis-aligned bounding box of the data satisfying (17). Then there is a function \( n(d, \bar{k}, k_\ast, L) \) such that, for all sample sizes \( n \) with \( n \geq n(d, \bar{k}, k_\ast, L) \),

\[
W_2^2(G^*, \hat{G}_n) \leq n(d, \bar{k}, k_\ast, L) \frac{1}{\log n},
\]

with probability at least \( 1 - \frac{4}{n^2 d} \).

Theorem 10 (proved in Appendix D) upper bounds the rate of convergence under the Wasserstein distance by the extremely slow logarithmic rate \( \frac{1}{\log n} \). It is well known that the smoothness of the Gaussian errors makes the deconvolution more difficult; in fact, the logarithmic rate is minimax optimal (Dedecker and Michel, 2013).

**Remark 11.** (On Theorem 10) To our knowledge, Theorem 10 is novel, and the rate of convergence for the NPMLE under a Wasserstein distance has not been studied previously. The structure of the proof follows the proof of Theorem 2 of Nguyen (2013). To deal with the fact that \( \hat{G}_n \) and \( G^* \) are typically singular, we convolve each with a distribution with full support but low variance. Compared to our results on the density estimation and denoising problems, Theorem 10 makes additional assumptions on the problem structure, specifically that the covariance matrices are diagonal and that \( G^* \) is compactly supported. Many practical applications satisfy the diagonal covariances restriction, including both of our applications in Section 5.

A common feature to our results on density estimation and denoising have been that the NPMLE adapts to the complexity of \( G^* \). It is reasonable to conjecture, then, that in the deconvolution problem, \( \hat{G}_n \) will also enjoy some adaptation properties under the Wasserstein distance. We close this section with a sharper result on the Wasserstein rate in the special case where the observations are drawn from Gaussian distributions with common mean \( \mu \in \mathbb{R}^d \).
Theorem 12. Suppose \( X_i \sim \mathcal{N}(\mu, \Sigma_i) \), i.e. \( X_i \sim f_{G^*, \Sigma_i} \) where \( G^* = \delta_\mu \) and \( kI_d \preceq \Sigma_i \preceq kI_d \) for all \( i = 1, \ldots, n \). Let \( \hat{G}_n \) denote any approximate NPMLE satisfying (17) and supported on \( \mathbb{B}_{\kappa r}(X) \) where \( \kappa = k/k_r, r = \max \|X_i - X\|_2 \), and \( X = \frac{1}{n} \sum_{i=1}^{n} X_i \). Then
\[
W_2(\hat{G}_n, G^*) \lesssim_d \frac{\sqrt{\log n}}{n^{1/4}}
\]
with probability at least \( 1 - 3n^{-2} \) for all \( t \geq 1 \).

If the approximate NPMLE \( \hat{G}_n \) of Theorem 12 is selected according to the strategy described in Section 3, then by Corollary 3 part (iii) its support will be contained within the ball \( \mathbb{B}_{\kappa r}(X) \). This additional assumption on the support of the approximate NPMLE is needed to have some control over the moments of \( \hat{G}_n \).

Up to logarithmic factors, the \( n^{1/4} \)-rate in Theorem 12 agrees with Corollary 4.1 of Ho and Nguyen (2016) for the MLE of an overfitted mixture. Specifically, their result compared the MLE of \( k \)-component finite Gaussian mixture to a true mixing distribution \( G^* \) with \( k^* < k \) components. Wu and Yang (2020) and Doss et al. (2020) also derived the \( n^{1/2} \)-rate for a different estimator under a different Wasserstein metric. All of these previous results were restricted to the homoscedastic setting. In our setting, \( k^* = 1 \) and \( k = k^* \) is the data-dependent order of the NPMLE. The best known bound on \( k \) is logarithmic in \( n \) (Polyanskiy and Wu, 2020), whereas Ho and Nguyen (2016) required \( k \) to be fixed as \( n \to \infty \). When \( k^* \) is known, a faster \( n^{1/2} \)-rate is possible (Heinrich and Kahn, 2018) and is achieved by the MLE in a well-specified finite mixture model, i.e. setting \( k = k^* \) (Ho and Nguyen, 2016).

While the slower \( n^{1/4} \)-rate appears to be the price of flexibility of the NPMLE, Theorem 12 establishes that the NPMLE indeed adapts to structure in \( G^* \). Our analysis is greatly simplified by the assumption \( G^* = \delta_\mu \), since there is only one coupling between \( \hat{G}_n \) and \( G^* \). We leave for future work the important question of the extent to which \( \hat{G}_n \) adapts to more general distributions \( G^* \).

5 Applications

5.1 Color-magnitude diagram

In this section, we continue our discussion of denoising the color-magnitude diagram (CMD) from Section 1. Our modeling strategy is closely related to the work of Anderson et al. (2018). To compare our method to extreme deconvolution (Bovy et al., 2011), we use the same stellar sample, relaxing only their assumption that the prior \( G^* \) is a mixture of Gaussians; by contrast, we allow \( G^* \) to be an arbitrary probability measure. Specifically, we assume that after a suitable transformation of the color and magnitude measurements, the pair, denoted \( X_i \in \mathbb{R}^2 \), come from a two-dimensional Gaussian mixture \( f_{G^*, \Sigma_i} \) with known covariance \( \Sigma_i \).

Figure 1 in Section 1 shows the plot of the observed data \( X_i \) (left) and estimated posterior means \( \hat{\theta}_i \) (right), the latter constituting the denoised CMD. Contrasting our CMD with theirs (Anderson et al., 2018, Figure 7), which we do not depict here, it appears that ours performs more shrinkage overall. Our CMD has rather sharp tails in the bottom of the plot (i.e. the main sequence) and the top right (i.e. the tip of the red-giant branch) as well as a definitive cluster in the center-right (i.e. the red clump).

There are also important differences between the NPMLE and extreme deconvolution in the estimated prior \( \hat{G}_n \). Figure 5 shows the initial and final iterates in the computation of the NPMLE. It is clear that we are using a discrete distribution to model the prior, and since all of the covariance matrices \( \Sigma_i \) are diagonal, by Corollary 3 we have restricted the support points to lie in the minimum axis-aligned bounding box of the data. By contrast, extreme deconvolution models the prior as itself a Gaussian mixture, so the estimated prior (Anderson et al., 2018, Figure 4) actually is supported on all of \( \mathbb{R}^2 \).

5.2 Chemical abundance ratios

Our second data set is taken from the Apache Point Observatory Galactic Evolution Experiment survey (APOGEE); see Majewski et al. (2017), Abolfathi et al. (2018). We examine chemical abundance ratios for the red clump (RC) stars given in the DR14 APOGEE red clump catalog; see Ratcliffe et al. (2020) where this data set has been studied. Following the pre-processing in
Figure 5: Initial grid (left) of $m = 10^4$ support points and estimated prior $\hat{G}_n$ (right) where the area of each atom is proportional to its weight.

Ratcliffe et al. (2020) to remove the outliers with anomalous abundance measurements, the data set contains $n = 27,238$ observations. We pick $d = 2$ features from the 19 dimensions, namely, [Si/Fe]-[Mg/Fe].

In Figure 6 we plot the observed data (top left) and estimated posterior means using Gaussian denoising under the estimated prior $\hat{G}_n$ (top right). The initial grid (bottom left) of $m = 10^4$ support points and estimated prior $\hat{G}_n$ (bottom right), where the area of each atom is proportional to its weight, is also provided. The denoised data reveals a very interesting structure — it shows that the variables [Si/Fe] and [Mg/Fe] are strongly correlated, especially, the observations for the upper right cluster of stars could be lying on one dimensional manifold; something that is not at all visible when plotting the original data.

6 Concluding remarks

In this paper we study the NPMLE $\hat{G}_n$ as an estimator of a prior distribution $G^*$ in the presence of multivariate, heteroscedastic measurement errors. We resolve a number of basic questions on the existence, uniqueness, discreteness, and support of the NPMLE, where in several cases the answers differ significantly from the traditional univariate, homoscedastic setting. Our analysis identifies a dual mixture density $\hat{\psi}_n$ with Gaussian $\mathcal{N}(X_i, \Sigma_i)$ components at each observation, whose modes contain the atoms of the NPMLE. Our characterization implies that the NPMLE is supported on the ridgeline manifold $M$, which is a compact subset of $\mathbb{R}^d$ defined in terms of the observations $(X_i)_{i=1}^n$ and corresponding covariance matrices $(\Sigma_i)_{i=1}^n$. This support reduction allows us to approximate the NPMLE by a finite-dimensional convex optimization over the mixing proportions, and we develop a novel approach to bounding the discretization error, justifying the gridding scheme proposed by Koenker and Mizera (2014). Our real data applications show that this approach is viable for practical astronomy problems. Our theoretical results in Section 4 provide strong justification for using the NPMLE in a variety of contexts—estimating the prior, marginal densities, and oracle posterior means.

We conclude by outlining some possible future research directions. Computation remains an important barrier for large-scale applications. Specifically, for problems with a large number of samples, e.g. $n \gg 10^6$, some additional forms of approximation are warranted, such as stochastic optimization or binning via coresets (see also Ritchie and Murray (2019) on approaches for scaling Extreme Deconvolution to large datasets). Further, our result on the discretization error suggests that discretization becomes infeasible in moderate-dimensions, where the number of atoms needs to grow roughly like a polynomial in the number of dimensions, e.g. $m = O(\delta^{-d})$. This limitation, which is common to many forms of discretization across applied mathematics, highlights the need
Figure 6: Top: Observed data (left) and estimated posterior means (right); Bottom: Initial grid (left) of $m = 10^4$ support points and estimated prior $\hat{G}_n$ (right) where the area of each atom is proportional to its weight.

for grid-free methods for computation of the NPMLE in high-dimensions. The connection to entropic-regularized optimal transport established by Rigollet and Weed (2018) represents one possible direction for grid-free methods.

Next, while our framework allows the prior $G^*$ to be arbitrary, the underlying assumption—that the means $(\theta^*_i)$ are identically distributed—can sometimes be difficult to justify for heteroscedastic observations. The IID assumption reflects the belief that the observation covariance $\Sigma_i$ is uninformative for the corresponding mean $\theta^*_i$. This assumption led to reasonable results in our applications but may be problematic in other settings. In the univariate, heteroscedastic case, Weinstein et al. (2018) proposed grouping observations with similar variances and applying a spherically symmetric estimator separately within each group. Their approach is capable of capturing dependence between $\theta_i$ and $\sigma_i^2$, at the expense of not sharing information across groups. Furthermore, to our knowledge, the grouping approach has not been extended to multivariate settings where binning the set of covariance matrices is more difficult. Thus, in multivariate settings there remains the important problem of how to model the relationship between $\theta_i$ and $\Sigma_i$.

Finally, there remain a number of open statistical questions for future work. Our analysis of the denoising problem focuses on estimating the posterior mean based on the unknown prior $G^*$, but there are numerous inferential goals one could target with an approximate prior. The analyst might
summarize the empirical posteriors using a different functional, such as the posterior median or the posterior mean of some transformed parameter. This question warrants a more general analysis evaluating the quality of the empirical posterior distributions for the true, unknown posteriors.

Acknowledgement

We would like to thank Bridget L. Ratcliffe for providing both datasets. Jake A. Soloff would like to thank Jacob Steinhardt and Serena Wang for their valuable feedback on an early draft.

A Proofs of Results in Sections 2 and 3

A.1 Proof of Lemma 1

The following uses similar techniques as Section 5.2 of Lindsay (1995), which contains a subset of our result in the homoscedastic case.

Proof of Lemma 1. By convexity, the first-order optimality condition for $\widehat{G}_n$ is

$$D(\widehat{G}_n, G) \leq 0$$

for all $G \in \mathcal{P}(\mathbb{R}^d)$.

where

$$D(\widehat{G}_n, G) := \lim_{\alpha \downarrow 0} \frac{1}{\alpha} \sum_{i=1}^n \left[ \log f_{(1-\alpha)\widehat{G}_n+\alpha G, \Sigma_i}(X_i) - \log f_{\widehat{G}_n, \Sigma_i}(X_i) \right]$$

$$= \frac{1}{n} \sum_{i=1}^n \left( f_{G, \Sigma_i}(X_i) - f_{\widehat{G}_n, \Sigma_i}(X_i) \right) = \frac{1}{n} \sum_{i=1}^n \int f_{G, \Sigma_i}(X_i) d\Phi_i - 1$$

When $G = \delta_\theta$ is a point mass we write $D(\widehat{G}_n, \theta)$ instead of $D(\widehat{G}_n, G)$. It suffices to check $D(\widehat{G}_n, \theta) \leq 0$ for all $\theta \in \mathbb{R}^d$ because $D(\widehat{G}_n, G) = \int D(\widehat{G}_n, \theta) d\mathcal{G}[\theta]$.

For the first part of the Lemma, define $\mathcal{C} := \{(f_{G, \Sigma_i}(X_i))_{i=1}^n : G \in \mathcal{P}(\mathbb{R}^d) \cup \{0\}$. Observe that $\mathcal{C} = \text{conv}(\mathcal{L})$, where $\mathcal{L} := \{(\varphi_{\Sigma_i}(X_i - \theta))_{i=1}^n : \theta \in \mathbb{R}^d \cup \{0\}. \}$

Since $\theta \mapsto (\varphi_{\Sigma_i}(X_i - \theta))_{i=1}^n$ is continuous and $\lim_{\|\theta\| \to \infty} (\varphi_{\Sigma_i}(X_i - \theta))_{i=1}^n = 0$, the set $\mathcal{L}$ is closed, and by boundedness of the Gaussian likelihood, $\mathcal{L}$ is compact. Hence $\mathcal{C} \subset \mathbb{R}^n$ is convex and compact, and $f(L) = \frac{1}{n} \sum_{i=1}^n \log L_i$ is strictly concave over $\mathcal{C}$. Thus, $f$ attains its maximum at a unique (non-zero) boundary point $\hat{L} \in \partial \mathcal{C}$. Observe $\mathcal{C} = \text{conv} \{(\varphi_{\Sigma_i}(X_i - \theta))_{i=1}^n : \theta \in \mathbb{R}^d \}$: by Carathéodory’s theorem, any boundary point $\hat{L} \in \partial \mathcal{C}$ can be written as $\hat{L}_i = \sum_{j=1}^{k} \hat{w}_{ij} \varphi_{\Sigma_i}(X_i - \tilde{\alpha}_j)$ for some $k \leq n$.

Suppose $B \subset \text{supp}(\widehat{G}_n)$ is contained in the support of the NPMLE. Given $\widehat{G}_n(B) > 0$, define a new probability measure $\widehat{G}_n^B$ via $\widehat{G}_n^B(A) = \frac{\widehat{G}_n(A \cap B)}{\widehat{G}_n(B)}$. Since $\widehat{G}_n = \alpha_0 \widehat{G}_n + (1-\alpha_0) \widehat{G}_n^B$ for $\alpha_0 = \widehat{G}_n(B)$, the mixture

$G_{\alpha} = (1-\alpha)\widehat{G}_n + \alpha \widehat{G}_n^B$

remains a valid probability measure for $\alpha \geq \frac{\alpha_0}{1-\alpha_0}$. Since $\alpha = 0$ maximizes the log-likelihood of $G_{\alpha}$ over a range $\alpha \in [-\frac{\alpha_0}{1-\alpha_0}, 1]$ including both negative and positive values, the derivative of the log-likelihood is zero at $\alpha = 0$, i.e.

$0 = D(\widehat{G}_n, \widehat{G}_n^B) = \int D(\widehat{G}_n, \theta) d\widehat{G}_n^B[\theta]$,

so $\widehat{G}_n^B(Z) = 1$ for all $B \subset \text{supp}(\widehat{G}_n)$ such that $\widehat{G}_n(B) > 0$. This implies $\widehat{G}_n(B \cap Z) = \widehat{G}_n(B)$ for all measurable $B$, from which we may conclude $Z \supset \text{supp}(\widehat{G}_n)$. Finally, observe that

$$D(\widehat{G}_n, \theta) = \frac{1}{n} \sum_{i=1}^n \hat{L}_i^{-1} \varphi_{\Sigma_i}(X_i - \theta) - 1 = \left( \frac{1}{n} \sum_{i=1}^n \hat{L}_i^{-1} \right) \widehat{\psi}_n(\theta) - 1,$$

so $D(\widehat{G}_n, \theta) \leq 0$ is equivalent to $\widehat{\psi}_n(\theta) \leq \left( \frac{1}{n} \sum_{i=1}^n \hat{L}_i^{-1} \right)^{-1}$. This proves the last statement of the Lemma, that $Z$ is equal to the set of global maximizers of $\widehat{\psi}_n$. $\diamondsuit$
A.2 Proof of Lemma 2

Proof of Lemma 2. By Lemma 4, the fitted values $\hat{L}_1 = \hat{L}_2 = \hat{L}_3$ are equal. By Lemma 1, the atoms of $\widehat{G}_n$ occur at the global modes of $\hat{\psi}_n = f_{H, \sigma^2, \delta_2}$, where $H = \frac{1}{3} \sum_{i=1}^{\delta X_i}$. Since $\hat{L}_1 = \hat{L}_2 = \hat{L}_3$, the fitted values are also equal to the global maximum of $\hat{\psi}_n$, i.e.

$$\hat{L}_i = \max_x f_{H, \sigma^2, \delta_2}(x) = \frac{2^{2/3} \log 2}{3\pi}$$

for each $i = 1, 2, 3$. Note that $\hat{L}_i = f_{\delta_0, \sigma^2, \delta_2}(X_i)$ for all $X_i$, so $\widehat{G}_n = \delta_0$ is an NPMLE. Now let $\widehat{G}'_n = \frac{1}{3} \sum_{i=1}^{\delta X_i/2}$. It suffices to check the fitted values of $\widehat{G}_n'$ at the observations. For $i = 1$,

$$f_{\widehat{G}_n', \sigma^2, \delta_2}(X_1) = \frac{1}{3} \sum_{i=1}^{\delta X_i} \phi_{\sigma^2, \delta_2}(X_1 - X_i/2) = \frac{4 \log 2}{9\pi} (2^{-4/3}(1/4) + 2^{-4/3}(7/4) + 2^{-4/3}(7/4)) \approx \frac{22/3 \log 2}{3\pi} = \hat{L}_1.$$

Similarly, for $i = 2$,

$$f_{\widehat{G}_n', \sigma^2, \delta_2}(X_2) = \frac{1}{3} \sum_{i=1}^{\delta X_i} \phi_{\sigma^2, \delta_2}(X_2 - X_i/2) = \frac{4 \log 2}{9\pi} (2^{-4/3}(7/4) + 2^{-4/3}(1/4) + 2^{-4/3}(7/4)) \approx \frac{22/3 \log 2}{3\pi} = \hat{L}_2,$$

and, for $i = 3$,

$$f_{\widehat{G}_n', \sigma^2, \delta_2}(X_3) = \frac{1}{3} \sum_{i=1}^{\delta X_i} \phi_{\sigma^2, \delta_2}(X_3 - X_i/2) = \frac{4 \log 2}{9\pi} (2^{-4/3}(7/4) + 2^{-4/3}(7/4) + 2^{-4/3}(1/4)) \approx \frac{22/3 \log 2}{3\pi} = \hat{L}_3.$$

This verifies that $\widehat{G}_n' = \frac{1}{3} \sum_{i=1}^{\delta X_i/2}$ is also an NPMLE, so every convex combination $\alpha \widehat{G}_n + (1 - \alpha) \widehat{G}_n'$ is an NPMLE.

A.3 Proof of Corollary 3

Proof of Corollary 3. We have already observed that $\mathcal{Z} \subset \mathcal{M}$ (Ray and Lindsay, 2005). Observe that $\mathcal{M}$ is compact as it is the continuous image of the simplex, a compact set. Since any real-analytic function has a finite number of zeros, $\mathcal{Z}$ is finite. Hence any NPMLE $\widehat{G}_n$ is discrete with a finite number of atoms.

In the proportional covariances case $\Sigma_i = c_i \Sigma$, we have

$$x^*(\alpha) = \left( \sum_{i=1}^{n} \alpha_i \Sigma_i^{-1} \right)^{-1} \sum_{i=1}^{n} \alpha_i \Sigma_i^{-1} X_i$$

$$= \sum_{i=1}^{n} \frac{\alpha_i}{c_i} \Sigma_i^{-1} X_i$$

As $\alpha$ ranges over the simplex, so does $\left( \frac{\alpha_i/c_i}{\Sigma_i^{-1}} \right)^{n}$ for each $i$. Thus $\mathcal{M} = \text{conv} \{ (X_1, \ldots, X_n) \}$, proving (i).

If each $\Sigma_i$ is diagonal, letting $x^*_j(\alpha)$ denote the $j$th coordinate of $x^*(\alpha) \in \mathbb{R}^d$,

$$x^*_j(\alpha) = \sum_{i=1}^{n} \frac{\alpha_i (\Sigma_i)_{jj}}{\sum_{i=1}^{n} \alpha_i (\Sigma_i)_{jj}} X_{ij} \in \left[ \min_{i=1}^{n} X_{ij}, \max_{i=1}^{n} X_{ij} \right],$$

proving (ii). For (iii), using concavity of the minimum eigenvalue,

$$\|x^*(\alpha) - x\|_2 = \left\| \sum_{i=1}^{n} \alpha_i \Sigma_i^{-1} \left( \sum_{i=1}^{n} \alpha_i \Sigma_i^{-1} (X_i - x) \right) \right\|_2$$

$$\leq \left\| \sum_{i=1}^{n} \alpha_i \Sigma_i^{-1} \right\|_2 \left\| \sum_{i=1}^{n} \alpha_i \Sigma_i^{-1} (X_i - x) \right\|_2$$

$$\leq \left( \sum_{i=1}^{n} \alpha_i k^{-1} \right) \left( \sum_{i=1}^{n} \alpha_i k^{-1} \right) \| X_i - x \|_2 \leq kr$$

so $\mathcal{M} \subseteq \mathbb{B}_{kr}(x)$.
A.4 Proof of Lemma 4

Proof of Lemma 4. By the change of variables formula,

\[ f_{T_{\#}G} \Sigma_i'(X_i') = \int \varphi_{U_{\#} G} U_{\#} \varphi(U_0 X_i + x_0 - \theta) \, dT_{\#} G(\theta) = \int \varphi_{U_{\#} G} U_{\#} \varphi(U_0 X_i + x_0 - T(\theta)) \, dG(\theta) = \int \varphi_{\Sigma_i} (X_i - \theta) \, dG(\theta) = f_{G, \Sigma_i}(X_i), \]

completing the proof.

A.5 Proof of Proposition 5

Proof of Proposition 5. Write \( \tilde{G}_n = \sum_{j=1}^{\hat{k}} \tilde{w}_j \delta_{a_j} \), and for each \( j \in [\hat{k}] \), let \( C_j \in \mathcal{H} \) such that \( \tilde{a}_j \in C_j \).

Next, define a positive measure \( H_j \) supported on the corners of \( C_j \) such that \( H_j(C_j) = \tilde{w}_j \) and

\[ \int_{C_j} u \, dH_j(u) = \tilde{w}_j \tilde{a}_j = \int_{C_j} u \, d\tilde{G}_n(u), \tag{20} \]

where \( \tilde{G}_n \) := \( \tilde{w}_j \delta_{a_j} \). Now fix \( u \in C_j \) and \( i \in [n] \), and let \( x_j = \Sigma_i^{-1/2}(X_i - \tilde{a}_j) \) and \( t = \Sigma_i^{-1/2}(u - \tilde{a}_j) \).

By the moment identity (20) and by Jiang and Zhang (2009, A.27),

\[ \int_{C_j} \varphi_{\Sigma_i}(X_i - u) \, d\tilde{G}_n^i(u) - \int_{C_j} \varphi_{\Sigma_i}(X_i - u) \, dH_j(u) \leq \int_{C_j} (x_j, t)^2 \varphi_{\Sigma_i}(X_i - u) \, d\tilde{G}_n^i(u) + \int_{C_j} (e^{b/2} - 1) \varphi_{\Sigma_i}(X_i - u) \, dH_j(u) \leq k^{-2} D^2 d^2 \int_{C_j} \varphi_{\Sigma_i}(X_i - u) \, d\tilde{G}_n^i(u) + \left(e^{b/2} - 1\right) \int_{C_j} \varphi_{\Sigma_i}(X_i - u) \, dH_j(u). \]

Let \( H = \Sigma_j H_j \). Summing the above inequality over \( j \),

\[ f_{\tilde{G}_n, \Sigma_i}(X_i) - f_{H, \Sigma_i}(X_i) \leq k^{-2} D^2 d^2 f_{\tilde{G}_n, \Sigma_i}(X_i) + \left(e^{b/2} - 1\right) f_{H, \Sigma_i}(X_i). \]

Since \( H \) is supported on \( A \), by optimality of \( \tilde{G}_n^A \),

\[ \prod_{i=1}^n f_{\tilde{G}_n, \Sigma_i}(X_i) \geq \prod_{i=1}^n f_{H, \Sigma_i}(X_i). \]

Combining our findings,

\[ \prod_{i=1}^n f_{\tilde{G}_n^A, \Sigma_i}(X_i) \geq e^{-\frac{nk^{-2} d^2 b}{2}} \left(1 - k^{-2} D^2 d^2\right)^n \prod_{i=1}^n f_{\tilde{G}_n, \Sigma_i}(X_i). \]

Using the elementary inequality \( 1 - x \geq e^{-2x} \) for \( x \leq 3/4 \), we obtain

\[ \prod_{i=1}^n f_{\tilde{G}_n^A, \Sigma_i}(X_i) \geq \exp \left(-n k^{-2} d^2 b^2 / 2 - 2nk^{-2} D^2 d^2\right) \prod_{i=1}^n f_{\tilde{G}_n, \Sigma_i}(X_i). \]

for \( \delta \leq \sqrt{\frac{3}{2}} k^{-1} D^{-1} \).

B Proof of Theorem 6

The following notation will be used throughout this section:

1. \( \mathbb{B}_r(x) = \{ y \in \mathbb{R}^d : \|x - y\| \leq r \} \) denotes a closed ball in \( \mathbb{R}^d \).

2. For a positive integer \( m \), let \([m] = \{1, \ldots, m\}\).
3. Given a pseudo-metric space \((M, \rho)\) and \(\varepsilon > 0\), let \(N(\varepsilon, M, \rho)\) denote the \(\varepsilon\)-covering number, i.e. the smallest positive integer \(N\) such that there exist \(x_1, \ldots, x_N \in M\) such that

\[
M \subseteq \bigcup_{i=1}^{N} \{y : \rho(y, x_i) \leq \varepsilon\}.
\]

Any such a set \(\{x_i\}_{i=1}^{N}\) is known as an \(\varepsilon\)-net or \(\varepsilon\)-cover of \(M\) under the pseudo-metric \(\rho\). When \(M\) is a subset of Euclidean space we write \(N(\varepsilon, M)\) instead of \(N(\varepsilon, M, \| \cdot \|_2)\).

4. We use the shorthand \(f_{G, \cdot} = (f_{G, \Sigma_i})_{i=1}^n\), the matrices \(\Sigma_1, \ldots, \Sigma_n\) being viewed as fixed. Let

\[
\mathbb{F} = \{ f_{G, \cdot} : G \in \mathcal{P}(\mathbb{R}^d) \}.
\]

5. For \(S \subseteq \mathbb{R}^d\) and \(M > 0\), let \(S^M\) denote the \(M\)-enlargement \(S^M = \{ x \in \mathbb{R}^d : \partial_S(x) \leq M \}\).

6. Define the semi-norm

\[
\| f_{G, \cdot} - f_{H, \cdot} \|_{\infty, S^M} := \max_{1 \leq i \leq n} \sup_{x \in S^M} | f_{G, \Sigma_i}(x) - f_{H, \Sigma_i}(x) |.
\]

Similarly, define

\[
\| f_{G, \cdot} - f_{H, \cdot} \|_{\nabla, S^M} := \max_{1 \leq i \leq n} \sup_{x \in S^M} | \nabla f_{G, \Sigma_i}(x) - \nabla f_{H, \Sigma_i}(x) |.
\]

Our proof generalizes and builds upon prior techniques for analyzing the Hellinger accuracy of the NPMLE (Zhang, 2009; Saha and Guntuboyina, 2020a; Jiang, 2020). The basic structure of our argument is to recognize, given the approximation (14) in the likelihood, that we may trivially rewrite the large deviation probability for the NPMLE as a joint probability

\[
\mathbb{P}\left( \tilde{h}(f_{G_n, \cdot}, f_{G^*, \cdot}) \geq d_{\mathbb{R}^d} t \varepsilon_n \right) = \mathbb{P}\left( \tilde{h}(f_{G_n, \cdot}, f_{G^*, \cdot}) \geq d_{\mathbb{R}^d} t \varepsilon_n, \prod_{i=1}^n \frac{f_{G_n, \Sigma_i}(X_i)}{f_{G^*, \Sigma_i}(X_i)} \geq \exp\left(-c_{d, \mathbb{R}^d} n \varepsilon_n^2\right) \right).
\]

If \(\tilde{G}_n\) were a fixed probability measure \(G_0\) such that \(\tilde{h}(f_{G_n, \cdot}, f_{G^*, \cdot}) \geq d_{\mathbb{R}^d} t \varepsilon_n\), the right-hand side of the last display similarly simplifies as

\[
\mathbb{P}\left( \tilde{h}(f_{G_n, \cdot}, f_{G^*, \cdot}) \geq d_{\mathbb{R}^d} t \varepsilon_n, \prod_{i=1}^n \frac{f_{G_n, \Sigma_i}(X_i)}{f_{G^*, \Sigma_i}(X_i)} \geq \exp\left(-c_{d, \mathbb{R}^d} n \varepsilon_n^2\right) \right) = \mathbb{P}\left( \prod_{i=1}^n \frac{f_{G_n, \Sigma_i}(X_i)}{f_{G^*, \Sigma_i}(X_i)} \geq \exp\left(-c_{d, \mathbb{R}^d} n \varepsilon_n^2\right) \right).
\]

Since \(\tilde{G}_n\) is not fixed, we first approximate it using a covering argument, and then bound the right-hand side of the previous display using Markov’s inequality.

**Proof of Theorem 6.** Suppose for some \(\gamma_n\) the NPMLE satisfies

\[
\prod_{i=1}^n \frac{f_{\hat{G}_n, \Sigma_i}(X_i)}{f_{G^*, \Sigma_i}(X_i)} \geq \exp\left( (\beta - \alpha) n \gamma_n^2 \right) \text{ for some } 0 < \beta < \alpha < 1.
\]

We bound the probability

\[
\mathbb{P}\left( \tilde{h}(f_{\hat{G}_n, \cdot}, f_{G^*, \cdot}) \geq t \gamma_n \right)
\]

for \(t > 1\).

Take \(\{f_{H_j, \cdot}\}_{j=1}^N \subseteq \mathbb{F}\) to be an \(\eta\)-net of \(\mathbb{F}\) under \(\| \cdot \|_{\infty, S^M}\). For each \(j\), let \(H_{0,j}\) be a distribution satisfying

\[
\| f_{H_{0,j}, \cdot} - f_{H_j, \cdot} \|_{\infty, S^M} \leq \eta \quad \text{and} \quad \tilde{h}(f_{H_{0,j}, \cdot}, f_{G^*, \cdot}) \geq t \gamma_n
\]

and \(J = \{ j \in [N] : H_{0,j} \text{ exists} \}\). By construction of the \(\eta\)-net, there is \(j^* \in [N]\) such that

\[
\| f_{H_{j^*}, \cdot} - f_{\hat{G}_n, \cdot} \|_{\infty, S^M} \leq \eta.
\]

On the event \(\{ \tilde{h}(f_{\hat{G}_n, \cdot}, f_{G^*, \cdot}) \geq t \gamma_n \}\), the NPMLE \(\hat{G}_n\) acts as a witness that \(j^* \in J\), so by the triangle inequality

\[
\| f_{H_{0,j^*}, \cdot} - f_{\hat{G}_n, \cdot} \|_{\infty, S^M} \leq 2 \eta.
\]
This gives
\[ f_{\bar{G}_n, \Sigma_i}(x) \leq \begin{cases} f_{H_{0,j}, \Sigma_i}(x) + 2\eta, & \text{if } x \in S^M \\ \frac{1}{(2\pi)^{d/2} |\Sigma_i|} & \text{otherwise.} \end{cases} \]

Defining \( v(x) = \eta 1_{x \not\in S^M} + \eta \left( \frac{M}{\delta_v(x)} \right)^{d+1} 1_{x \in S^M} \), we have
\[ \exp((\beta - \alpha)nt^2\gamma_n^2) \leq \max_{j \in J} \left[ \prod_{i=1}^{n} \frac{f_{H_{0,j}, \Sigma_i}(X_i) + 2v(X_i)}{f_{G^*, \Sigma_i}(X_i)} \right] \left[ \prod_{i \notin X, i \not\in S^M} \frac{1}{\sqrt{(2\pi)^{d/2} |\Sigma_i|} 2v(X_i)} \right] \quad (22) \]
on the event \( \{ h(f_{\bar{G}_n, \cdot}, f_{G^*, \cdot}) \geq t\gamma_n \} \). Hence
\[ P(h(f_{\bar{G}_n, \cdot}, f_{G^*, \cdot}) \geq t\gamma_n) \leq P \left( \max_{j \in J} \prod_{i=1}^{n} f_{H_{0,j}, \Sigma_i}(X_i) + 2v(X_i) \right) \geq \exp(-\alpha nt^2\gamma_n^2) \]
\[ + \mathbb{P} \left( \prod_{i \notin X, i \not\in S^M} \frac{1}{\sqrt{(2\pi)^{d/2} |\Sigma_i|} 2v(X_i)} \right) \geq \exp(\beta nt^2\gamma_n^2) \quad (25) \]

By a union bound and Markov's inequality, the first term (24) is bounded by
\[ e^{\alpha nt^2\gamma_n^2} \sum_{j \in J} \prod_{i=1}^{n} \mathbb{E} \left[ \frac{f_{H_{0,j}, \Sigma_i}(X_i) + 2v(X_i)}{f_{G^*, \Sigma_i}(X_i)} \right] \leq \exp \left( -\frac{nt^2\gamma_n^2}{2} + n \int \sqrt{v} \right) \quad (26) \]

Writing out the expectation,
\[ \prod_{i=1}^{n} \mathbb{E} \left[ \frac{f_{H_{0,i}, \Sigma_i}(X_i) + 2v(X_i)}{f_{G^*, \Sigma_i}(X_i)} \right] = \exp \left( \sum_{i=1}^{n} \log \mathbb{E} \left[ \frac{f_{H_{0,i}, \Sigma_i}(X_i) + 2v(X_i)}{f_{G^*, \Sigma_i}(X_i)} \right] \right) \]
\[ \leq \exp \left( \sum_{i=1}^{n} \left( \int \sqrt{f_{H_{0,i}, \Sigma_i} + 2v/f_{G^*, \Sigma_i} - 1} \right) \right) \]
\[ \leq \exp \left( -\frac{nt^2\gamma_n^2}{2} + n \int \sqrt{v} \right) \]

Putting together the pieces, the first term (24) is bounded by
\[ P \left( \max_{j \in J} \prod_{i=1}^{n} f_{H_{0,j}, \Sigma_i}(X_i) + 2v(X_i) \right) \geq e^{-\alpha nt^2\gamma_n^2} \]
\[ \leq \exp \left( -\frac{nt^2\gamma_n^2}{2} + n \int \sqrt{v} \right) \quad (27) \]

For the second term (25), observe by Markov’s inequality
\[ \mathbb{P} \left( \prod_{i \notin X, i \not\in S^M} \frac{1}{\sqrt{(2\pi)^{d/2} |\Sigma_i|} 2v(X_i)} \right) \geq \exp(\beta nt^2\gamma_n^2) \]
\[ \leq \exp \left( -\frac{\beta nt^2\gamma_n^2}{2\log n} \right) \mathbb{E} \left( \prod_{i \notin X, i \not\in S^M} \frac{1}{\sqrt{(2\pi)^{d/2} |\Sigma_i|} 2v(X_i)} \right)^{1/2\log n} \]
\[ = \exp \left( -\frac{\beta nt^2\gamma_n^2}{2\log n} \right) \mathbb{E} \left( \prod_{i=1}^{n} \left( \frac{\delta_{\Sigma_i}(X_i)}{\sqrt{2\pi \Sigma_i}} \right) \right)^{1/2\log n} \left( \frac{d+1/2}{M} \right)^{(d+1)/2\log n} \left( \frac{d+1/2}{\delta_{\Sigma_i}(X_i) \cdot |\Sigma_i|} \right)^{1/2\log n} \right) \]

To reduce clutter write \( a = \frac{1}{\delta_v(x) + \eta (d+1)^M} \) and \( \lambda = \frac{d+1}{2\log n} \). The above expectation is further upper
bounded by
\[
E\left( \prod_{i=1}^{n} (a \vartheta_{S}(X_i))^1_{\vartheta_{S}(X_i) \geq M} \right)^{\lambda} = \prod_{i=1}^{n} E (a \vartheta_{S}(X_i))^1_{\vartheta_{S}(X_i) \geq M}^\lambda \\
\leq \prod_{i=1}^{n} \left( 1 + a^\lambda E \left[ \vartheta_{S}(X_i)^1_{\vartheta_{S}(X_i) \geq M} \right] \right) \\
\leq \exp \left( a^\lambda \sum_{i=1}^{n} E \left[ \vartheta_{S}(X_i)^1_{\vartheta_{S}(X_i) \geq M} \right] \right) \\
\leq \exp \left( na^\lambda \left( C_d M^{d+\lambda-2} k^{1-d/2} e^{-M^2/(8K)} + M^{\lambda} \left( \frac{2\mu_q}{M} \right)^q \right) \right)
\]

The last inequality follows from Lemma 13. Note we need
\[
\frac{d+1}{2(1 \land q)} \leq \log n,
\]
to ensure \( \lambda \leq 1 \land q \). Taking \( M \geq \sqrt{8K \log n} \), we have \( e^{-M^2/(8K)} \leq \frac{1}{n} \), so
\[
E\left( \prod_{i=1}^{n} (a \vartheta_{S}(X_i))^1_{\vartheta_{S}(X_i) \geq M} \right)^{\lambda} \leq \exp \left( (aM)^\lambda \left[ C_d M^{d-2} k^{1-d/2} + n \left( \frac{2\mu_q}{M} \right)^q \right] \right)
\]
Noting \((aM)^\lambda = (K^{d/2} \eta)^{-1/(2 \log n)}\), choose \( \eta = \frac{n^{2}}{dK^{d/2}} \), so \((aM)^\lambda = e\). We directly apply Lemma A.7 of Saha and Guntuboyina (2020b) for the integral
\[
\int v \leq C_d \text{Vol}(S^M).
\]
To bound the metric entropy, i.e. \( \log N \) where \( N \) denotes the size of our \( \eta \)-net \( \{f_{H_j, \bullet}\}_{j=1}^{N} \subset F \), we apply Lemma 16
\[
\log N = \log N \left( \eta, F, \| \cdot \|_{\infty, S^M} \right) \leq C_d N \left( u, (S^M)^u \right) \left( \log \frac{C_d \nu K}{\eta} \right)^2,
\]
where the scalar \( u \) in the above display corresponds to \( a \) used in the lemma. Assuming \( 4n \geq (2\pi)^{d/2} \),
\[
u = \sqrt{-\frac{2K \log \left( ((2\pi K)^{d/2} 2)^2 \right)}{4}} \geq \sqrt{2K \log n}
\]
Similarly \( u \leq \sqrt{6K \log n} \), so
\[
N \left( u, (S^M)^u \right) \leq N \left( \sqrt{2K \log n}, (S^M)^{\sqrt{6K \log n}} \right) \leq C_d \text{Vol}(S^{2M})(\log n)^{-d/2}
\]
Combining our findings,
\[
P \left( h(f_{G_n, \bullet}, f_{G^*, \bullet}) \geq t \nu_n \right) \\
\leq \exp \left( - (1 - \alpha) \frac{mt_n^2}{2} + C_d K \left( \log n \right)^{d/2 + 1} \text{Vol}(S^{2M}) + C_d \sqrt{K} - d/2 \text{Vol}(S^M) \right) \\
+ \exp \left( - \frac{\beta}{\log n} \frac{mt_n^2}{2} + C_d M^{d-2} k^{1-d/2} + c n \inf_{q \in (d+1)/(2 \log n)} \left( \frac{2\mu_q}{M} \right)^q \right)
\]
for any \( t > 1 \). Absorbing the dependence on \( d, K \) and \( K \) into constants, take \( \nu_n^2 = \nu_n^2(M, S, G^*) \) such that
\[
\max \left\{ (\log n)^{d/2 + 1} \text{Vol}(S^{2M}), \sqrt{\text{Vol}(S^M)}, M^{d-2}, c n \inf_{q \in (d+1)/(2 \log n)} \left( \frac{2\mu_q}{M} \right)^q \right\} \leq C_d K \nu_n^2(M, S, G^*)
\]
25
If we then take $\gamma_n^2 = \frac{C_d \varepsilon^2 (M,S,G^*)}{4 \min(1,\alpha,\beta)}$, 
\[
P \left( \frac{\mathcal{h}(\tilde{G}_n, \bullet) - f_{G^*} \| \gamma_n^2}{\gamma_n^2} \right) \leq 2 \exp \left( -\frac{(1-\alpha) \wedge \beta}{4 \log n} n t \gamma_n^2 \right)
\]
This proves (15). To prove (16), integrate the tail from (15),
\[
E \left[ \frac{\mathcal{h}^2(\tilde{G}_n, \bullet) - f_{G^*} \| \gamma_n^2}{\gamma_n^2} \right] \leq 1 + \int_1^{\infty} P \left( \frac{\mathcal{h}^2(\tilde{G}_n, G^*) \| \gamma_n^2}{\gamma_n^2} \geq s \right) ds \\
\leq 1 + \int_1^{\infty} 4tn^{-t^2} dt = 1 + \frac{2}{n \log n} \leq 3
\]
for $n > 1$, completing the proof.

We now state and prove the lemmas needed in the proof of Theorem 6.

**Lemma 13.** Let $\theta^* \sim G^*$ and $Z \sim \mathcal{N}(0, I_d)$ independently, and $Y = \theta^* + \Sigma^{1/2} Z$, where $kI_d \leq \Sigma \leq kI_d$.
Then
\[
E \left[ \vartheta_S(Y)^{\lambda} 1_{\vartheta_S(Y) \geq M} \right] \leq C_d M^{d+\lambda} - 2k^{1-d/2} e^{-M^2/(s \tilde{\gamma})} + M^\lambda \left( \frac{2\mu_q}{M} \right)^q
\]
for any $\lambda \in (0, 1 \wedge q]$, where $\mu_q$ is the $q^{th}$-moment of $\vartheta_S(\theta^*)$ under $\theta^* \sim G^*$.

**Proof.** Since distance $\vartheta_S$ is 1-Lipschitz,
\[
E \left[ \vartheta_S(Y)^{\lambda} 1_{\vartheta_S(Y) \geq M} \right] \leq E \left[ (2\|\Sigma^{1/2} Z\|_2)^{\lambda} 1_{\Sigma^{1/2} Z \geq M} \right] + E \left[ (2\vartheta_S(\theta^*))^{\lambda} 1_{2\vartheta_S(\theta^*) \geq M} \right]
\]
For the first term on the RHS of (28),
\[
E \left[ (2\|\Sigma^{1/2} Z\|_2)^{\lambda} 1_{\Sigma^{1/2} Z \geq M} \right] \leq M^\lambda E \left[ \left( \frac{\|\Sigma^{1/2} Z\|_2}{M/2} \right)^\lambda 1_{\Sigma^{1/2} Z \geq M/2} \right]
\leq 2M^{\lambda-1} E \left[ \|\Sigma^{1/2} Z\|_2 1_{\Sigma^{1/2} Z \geq M/2} \right]
\leq 2M^{\lambda-1} k^{1/2} E \left[ \|Z\|_2 1_{Z \geq M/(2k^{1/2})} \right]
\leq 2C_d M^{\lambda-1} k^{1/2} \left( \frac{M}{k^{1/2}} \right)^{d-1} e^{-M^2/(s \tilde{\gamma})}
= C_d M^{d+\lambda} - 2k^{1-d/2} e^{-M^2/(s \tilde{\gamma})}
\]
The penultimate inequality uses $\|\Sigma^{1/2} Z\|_2 \leq k^{1/2} \|Z\|_2$, and the last inequality directly uses Lemma A.6 of Saha and Guntuboyina (2020b).

Since $\lambda < q$, applying Hölder to the second term on the RHS of (28) yields
\[
E \left[ (2\vartheta_S(\theta^*))^{\lambda} 1_{2\vartheta_S(\theta^*) \geq M} \right] \leq M^\lambda \left( \frac{2\mu_q}{M} \right)^q
\]
**Lemma 14.** (Moment matching, part i) Let $G, H \in \mathcal{P}(R^d)$. Suppose $A \subset \mathbb{R}^d$ is such that
\[
B_d(x) \subset A \subset B_{cd}(x)
\]
for some $c \geq 1$, and that
\[
\int_A \theta_1^{k_1} \ldots \theta_d^{k_d} dG(\theta) = \int_A \theta_1^{k_1} \ldots \theta_d^{k_d} dH(\theta), \; \text{for } k_1, \ldots, k_d \in [2m+1],
\]
for some $m \geq 1$. Then
\[
\max_{1 \leq i \leq n} |f_{G, \Sigma_i}(x) - f_{H, \Sigma_i}(x)| \leq \frac{1}{(2\pi k)^{d/2}} \left( \frac{ec^2a^2}{2k(m+1)} \right)^{m+1} + \frac{e^{-a^2/(2\tilde{\gamma})}}{(2\pi k)^{d/2}}.
\]

26
Proof. For each \( i \in [n] \), write
\[
f_{G, \Sigma_i}(x) - f_{H, \Sigma_i}(x) = \int_A \varphi_{\Sigma_i}(x - \theta)(dG(\theta) - dH(\theta)) + \int_{A^c} \varphi_{\Sigma_i}(x - \theta)(dG(\theta) - dH(\theta))
\]
on \( A^c \), \( \|x - \theta\|_2 \geq a \), so
\[
\varphi_{\Sigma_i}(x - \theta) \leq \frac{e^{-\frac{a^2}{2(2\pi k)}}}{(2\pi k)^{d/2}}.
\]
Write the pdf as \( \varphi_{\Sigma_i}(z) = P_i(z) + R_i(z) \) where \( P_i \) is a polynomial of degree \( 2m \) and the remainder \( R_i \) satisfies
\[
|R_i(z)| \leq \left( \frac{e\|z\|^2}{2k(m + 1)} \right)^{m+1}
\]
By hypothesis, \( f_{A^c} P_i(x - \theta)(dG(\theta) - dH(\theta)) \), so
\[
\left| \int_A \varphi_{\Sigma_i}(x - \theta)(dG(\theta) - dH(\theta)) \right| \leq \left| \int_A R_i(x - \theta)(dG(\theta) - dH(\theta)) \right| \leq \frac{1}{(2\pi k)^{d/2}} \left( \frac{e\|a\|^2}{2k(m + 1)} \right)^{m+1}
\]
completing the proof. \( \Box \)

Lemma 15. (Moment matching, part ii) For any \( G \in \mathcal{P}(\mathbb{R}^d) \), there is a discrete distribution \( H \) supported on \( S^a \) with at most
\[
l := (2[13.5a^2/F] + 2)^d N(a, S^a) + 1
\]
atoms such that
\[
\|f_G - f_H\|_{\infty, S^a} \leq \left( 1 + \frac{1}{\sqrt{2\pi}} \right) (2\pi k)^{-d/2} e^{-a^2/(2F)}.
\]
Proof. The idea is to choose \( H \) to match moments, and then apply the previous lemma. The proof is identical to Lemma D.3 of Saha and Guntuboyina (2020b), except that we take \( m := \lfloor 27a^2 \rfloor \). \( \Box \)

Lemma 16. There exists positive constants \( C_d \) and \( c_{d,F,k} \) depending on \( d, F, k \) alone such that for every compact set \( S \subset \mathbb{R}^d \), \( M > 0 \) and \( \eta \in (0, e^{-1} \wedge 4(2\pi k)^{-d/2}) \), we have
\[
\log N(\eta, F, \| \cdot \|_{\infty, S}) \leq C_d N(a, S^a) \left( \frac{\log \frac{c_{d,F,k}}{\eta}}{c_{d,F,k}} \right)^{d+1}
\]
Proof. The idea here is to take \( f_G \in \mathcal{P}(\mathbb{R}^d) \) (induced by some \( G \in \mathcal{P}(\mathbb{R}^d) \)), approximate \( G \) by a discrete distribution \( H \), and then further approximate that discrete distribution with another discrete distribution over a fixed set of atoms and weights. So let \( G \in \mathcal{P}(\mathbb{R}^d) \), and apply the previous Lemma to obtain a discrete distribution \( H \) supported on \( S^a \) with at most \( l \) atoms such that
\[
\|f_G - f_H\|_{\infty, S^a} \leq \left( 1 + \frac{1}{\sqrt{2\pi}} \right) (2\pi k)^{-d/2} e^{-a^2/(2F)}.
\]
Let \( \mathcal{C} \) denote a minimal \( \zeta \)-net of \( S^a \), and let \( H' \) approximate each atom of \( H \) with its closest element from \( \mathcal{C} \). Writing \( H = \sum_j w_j \delta_{a_j} \) and \( H' = \sum_j w_j \delta_{b_j} \), we have
\[
\|f_H - f_{H'}\|_{\infty, S^a} = \max_{i \in [n]} \max_{x \in S^a} |f_{H, \Sigma_i}(x) - f_{H', \Sigma_i}(x)|
\]
\[
\leq \max_{i \in [n]} \max_{x \in S^a} \sum_j w_j |\varphi_{\Sigma_i}(x - a_j) - \varphi_{\Sigma_i}(x - b_j)|
\]
\[
\leq \zeta \max_{i \in [n]} \max_{z \in S^a} \| \nabla \varphi_{\Sigma_i}(z) \|_2 = \zeta \max_{i \in [n]} \max_{z \in S^a} \| \Sigma_i^{-1} z \|_2
\]
\[
\leq \zeta \max_{i \in [n]} \max_{z \in S^a} \exp \left( -\frac{t^2}{2k} \right) t
\]
\[
\leq \zeta \max_{i \in [n]} \max_{z \in S^a} \exp \left( -\frac{t^2}{2k} \right) t
\]
27
Let $\mathcal{D}$ denote a minimal $\xi$-net of $\Delta^{l-1}$ in the $\ell_1$ norm, and approximate the weights $w$ by their closest element $v \in \mathcal{D}$. Writing $H'' = \sum v_j \delta_{b_j}$,
\[
\|H'' - f_H\|_{\infty,S} = \max_{i \in [n]} \sup_{x \in S} |f_H(x) - f_H(\Sigma_i(x))| \\
\leq \max_{i \in [n]} \sum_{j} |w_j - v_j\|_{\Sigma_i(x) - b_j} \leq (2\pi k)^{-d/2} \xi.
\]

Applying triangle inequality to the past three displays,
\[
\|f_G - f_H\|_{\infty,S} \leq (2\pi k)^{-d/2} \left[ 2e^{-a^2/(2\xi)} + \xi k^{-1}(\xi/e)^{1/2} + 2 \right] 
\]

Letting $\xi = (2\pi k)^{-d/2} a/4$, $\zeta = \xi k/(\xi/e)^{-1/2}$, and $a = \sqrt{2k} \log \xi^{-1}$ yields $\|f_G - f_H\|_{\infty,S} \leq \eta$. In order to take $a$ as such we need $\xi < 1$, or equivalently $\eta < 4(2\pi k)^{-d/2}$.

The number of possible $H''$ is
\[
|\mathcal{D}| = N(\xi, \Delta^{l-1}) \left( \frac{N(\xi, S^n)}{l} \right)^l \leq \left( \frac{1 + \frac{2}{\xi}} {l} \right) N(\xi, S^n)^l 
\]

From the previous Lemma, $l \geq N(a, S^n)/\pi d$, so
\[
N(\xi, S^n)/\pi d \leq \frac{\zeta}{\kappa} N(\xi, S^n)/\pi d \leq \kappa (\frac{1 + \frac{2}{\xi}} {\xi})^d \leq \kappa^d (\frac{1}{\xi})^d \leq C_d \left( \frac{\kappa^d}{\xi^{d/2}} \right)^{3p/2} 
\]

Thus,
\[
\log N(\eta, F, \|\cdot\|_{\infty, S}) \leq C_d N(a, S^n) \log \left( \frac{1}{\kappa^{d/2}} \left( \frac{\kappa^{d/2}}{\xi^{d/2}} \right)^{3p/2} \right) 
\]

\section{Proof of Theorem 8}

Throughout the proof we will group sequences of the form $\theta_1, \ldots, \theta_n$ into $n \times d$ matrices $\theta$, so that, for instance, the regret $\frac{1}{n} \sum_{i=1}^n \mathbb{E} \|\hat{\theta}_i - \theta_i\|_2^2$ in the statement of the theorem may be rewritten as the expected squared Frobenius norm $\frac{1}{n} \mathbb{E} \|\hat{\theta} - \hat{\theta}^*\|_F^2$, where $\|\theta\|_F^2 = \sum_{i=1}^n \sum_{j=1}^d \theta_{ij}^2$. Additionally, we use the same notation introduced at the start of Appendix B.

\subsection{Regularizing the Bayes rule}

In evaluating $\hat{\theta}$, an apparent difficulty is that the denominator in Tweedie’s formula can be arbitrarily small. However, since $\hat{G}_n$ is an approximate NPMLE, we show that the likelihood is lower bounded at each of the observations. In accordance with (17), we write that
\[
\frac{1}{n} \sum_{i=1}^n \log f_{\hat{G}_n, \Sigma_i}(X_i) - \sup_{G \in \mathcal{P}(R^d)} \frac{1}{n} \sum_{i=1}^n \log f_{G, \Sigma_i}(X_i) \geq q, 
\]

for some $q > 0$. Following (Jiang and Zhang, 2009, Proof of Proposition 2), for a fixed $j \in [n]$ choose $G = n^{-1} \delta_{X_j} + (1 - n^{-1}) \hat{G}_n$. Then by the previous display,
\[
\prod_{i=1}^n f_{\hat{G}_n, \Sigma_i}(X_i) \geq e^{-nq} \prod_{i=1}^n f_{G, \Sigma_i}(X_i) \\
\geq e^{-nq} \varphi_{\Sigma_i}(0)(1 - n^{-1})^{n-1} \prod_{i \neq j} f_{\hat{G}_n, \Sigma_i}(X_i). 
\]

Cancelling terms for $i \in [n] \setminus \{j\}$, we conclude
\[
f_{\hat{G}_n, \Sigma_j}(X_j) \geq e^{-nq - \log n} \frac{1}{c \sqrt{2\pi \Sigma_j^2}}. 
\]
Given this, it is natural to define the regularized empirical Bayes and oracle Bayes rules

\[
\hat{\theta}_{\rho,i} = X_i + \Sigma_i \frac{\nabla f_{G^*,\Sigma_i}(X_i)}{f_{G^*,\Sigma_i}(X_i) \vee (\rho/\sqrt{\Sigma_i})}
\]

(33)

\[
\hat{\theta}^*_{\rho,i} = X_i + \Sigma_i \frac{\nabla f_{G^*,\Sigma_i}(X_i)}{f_{G^*,\Sigma_i}(X_i) \vee (\rho/\sqrt{\Sigma_i})}
\]

(34)

By the lower bound (32) we know that \(\hat{\theta}_\rho = \hat{\theta}\) when \(\rho \leq \rho_0 := e^{-nq - \log n} \frac{1}{c(2\pi)^{n/2}}\). In particular,

\[
\|\hat{\theta} - \hat{\theta}^*\|_F = \|\hat{\theta}_\rho - \hat{\theta}^*\|_F \leq \|\hat{\theta}_\rho - \hat{\theta}_\rho^*\|_F + \|\hat{\theta}_\rho^* - \hat{\theta}^*\|_F.
\]

(35)

The first term \(\|\hat{\theta}_\rho - \hat{\theta}_\rho^*\|_F\) represents the regret between regularized rules, which prevents the denominator in Tweedie’s formula from blowing up. The second term represents the cost of introducing a small amount of regularization in the oracle Bayes rule.

### C.2 Regularization error of oracle Bayes

Let us first consider the second term \(\|\hat{\theta}_\rho - \hat{\theta}^*\|_F\) on the RHS of the bound (35). Fixing \(i \in [n]\), let \(G_i^\ast\) denote the distribution of \(\xi_i = \Sigma_i^{-1/2} \theta_i^*\) where \(\theta_i^* \sim G^\ast\). Then we may write \(X_i = \Sigma_i^{1/2} X_i\) where \(X_i \sim G_i^\ast, I_d\). Note how the scale change affects the terms in Tweedie’s formula:

\[
f_{G^\ast,\Sigma}(X_i) = \mathbb{E}_{\xi_i \sim G^\ast} \left[ \frac{1}{\sqrt{2\pi \Sigma_i}} \exp \left( -\frac{1}{2} (X_i - \theta_i)^\top \Sigma_i^{-1} (X_i - \theta_i) \right) \right]
\]

(36)

\[
= \frac{1}{\sqrt{\Sigma_i}} \mathbb{E}_{\xi_i \sim G_i^\ast} \left[ \varphi_{I_d}(\Sigma_i^{-1/2} X_i - \xi_i) \right] = \frac{1}{\sqrt{\Sigma_i}} f_{G_i^\ast, I_d}(X_i)
\]

\[
\nabla f_{G^\ast,\Sigma}(X_i) = \mathbb{E}_{\xi_i \sim G^\ast} \left[ \Sigma_i^{1/2} \nabla \varphi_{I_d}(\Sigma_i^{-1/2} X_i - \xi_i) \right] = \frac{1}{\sqrt{\Sigma_i}} \Sigma_i^{-1/2} \nabla f_{G_i^\ast, I_d}(X_i)
\]

In particular, Tweedie’s formula, even in its regularized form, is scale equivariant:

\[
\hat{\theta}^*_{\rho,i} = \Sigma_i^{1/2} \left( X_i + \frac{\nabla f_{G_i^\ast, I_d}(X_i)}{f_{G_i^\ast, I_d}(X_i) \vee \rho} \right)
\]

(37)

In this form, Saha and Guntuboyina (2020a, Lemma 4.3) directly applies. Specifically, defining

\[
\Delta(G, \rho) := \int \left( 1 - \frac{f_{G_i^\ast, I_d}}{f_{G_i^\ast, I_d} \vee \rho} \right)^2 \frac{\|\nabla f_{G_i^\ast, I_d}\|_2^2}{f_{G_i^\ast, I_d}}
\]

for any \(\rho \leq \rho_0\) and for all compact sets \(S_1, \ldots, S_n \subset \mathbb{R}^d\),

\[
\mathbb{E}\|\hat{\theta}_\rho - \hat{\theta}^*\|_F^2 = \sum_{i=1}^n \mathbb{E}\|\hat{\theta}^*_{\rho,i} - \hat{\theta}^*_i\|_2^2 \leq k \sum_{i=1}^n \Delta(G_i^\ast, \rho)
\]

\[
\leq k \sum_{i=1}^n \left\{ C_d N \left( \frac{4}{L(\rho)}, S_i \right) L(\rho) \rho + d G_i^\ast(S_i) \right\},
\]

(38)

where \(L(\rho) := \sqrt{-\log((2\pi)^d \rho^2)}\) and \(N\) denotes the usual covering number in the Euclidean norm.

Choosing \(\rho = (2\pi)^{-d/2} n\) and \(S_i = \Sigma_i^{-1/2} S^M\),

\[
\mathbb{E}\|\hat{\theta}_\rho - \hat{\theta}^*\|_F^2 \leq k n \left\{ C_d N \left( \frac{4}{\sqrt{\log n}}, \Sigma_i^{-1/2} S^M \right) \frac{(\log n)^{d/2}}{n} + d G_i^\ast((S^M)^\ast) \right\}.
\]

Let \(x_1, \ldots, x_m\) denote a \(t\)-net of \(S^M\). Let \(y \in S_i\) and \(x = \Sigma_i^{1/2} y\). There is some \(j\) s.t. \(\|x_j - x\|_2 \leq t\).

Let \(y_j = \Sigma_i^{-1/2} x_j\). Then

\[
I^2 \geq (x_j - x)^\top (x_j - x) = (y_j - y)^\top \Sigma_i (y_j - y) \geq k \|y_j - y\|_2^2
\]
so \(y_1, \ldots, y_m\) is a \(t/k^{1/2}\)-net of \(S_1\). This shows \(N(t/k^{1/2}, S_1) \leq N(t, S^M)\). By Saha and Guntuboyina (2020b, Lemma F.6) and Markov’s inequality,

\[
\mathbb{E}\|\hat{\theta}_\rho - \hat{\theta}_{\rho}^*\|^2 \leq C_d k^d \left( k^{-d/2} \text{Vol}(S^1) M^d \left( \frac{\log n}{n} \right)^d + \inf_{\|g\|_1 \leq (d+1)/2 \log n} \left( \frac{2\mu_g}{M} \right)^q \right). \tag{39}
\]

### C.3 Regret of regularized rules

Now we consider the first term \(\|\hat{\theta}_\rho - \hat{\theta}_{\rho}^*\|_F\) on the RHS of the bound (35). First, we will introduce some additional notation. For \(\delta > 0\) let \(A_\delta = \{ h^2(f_{G, \eta, \bullet}, f_{G^*, \bullet}) \leq \delta \}\). Given a compact set \(S \subset \mathbb{R}^d\), define another metric

\[
m^S(G, G') = \max_{w \in [n]} \sup_{x \in S(x) \in M} \left\| \frac{\Sigma_i \nabla f_{G, \Sigma_i} (x)}{f_{G, \Sigma_i} (x) \vee (\rho/\sqrt{|\Sigma_i|})} - \frac{\Sigma_i \nabla f_{G', \Sigma_i} (x)}{f_{G', \Sigma_i} (x) \vee (\rho/\sqrt{|\Sigma_i|})} \right\|_2.
\]

Let \(G^{(1)}, \ldots, G^{(N)}\) denote a minimal \(\eta^*\)-covering of \(\{ G : h^2(f_{G, \bullet}, f_{G^*, \bullet}) \leq \delta \}\) in the metric \(m^S\). For \(j \in [N]\) similarly define an \(n \times d\) matrix \(\hat{\theta}_\rho^{(j)}\) where the \(i^{th}\) row is given by \(X_i + \Sigma_i \frac{\nabla f_{G^{(j)}}, \Sigma_i (X_i)}{f_{G^{(j)}}, \Sigma_i (X_i) \vee (\rho/\sqrt{|\Sigma_i|})}\).

We bound the regret as \(\|\hat{\theta}_\rho - \hat{\theta}_{\rho}^*\|_F \leq \sum_{i=1}^n \zeta_i\), where

\[
\begin{align*}
\zeta_1 &:= \|\hat{\theta}_\rho - \hat{\theta}_{\rho}^*\|_F 1_{A_\delta}, \\
\zeta_2 &:= \left( \|\hat{\theta}_\rho - \hat{\theta}_{\rho}^*\|_F - \max_{j \in [N]} \|\hat{\theta}_\rho^{(j)} - \hat{\theta}_{\rho}^*\|_F \right)_+, \\
\zeta_3 &:= \max_{j \in [N]} \left( \|\hat{\theta}_\rho^{(j)} - \hat{\theta}_{\rho}^*\|_F - \mathbb{E}\|\hat{\theta}_\rho^{(j)} - \hat{\theta}_{\rho}^*\|_F \right)_+, \\
\zeta_4 &:= \max_{j \in [N]} \mathbb{E}\|\hat{\theta}_\rho^{(j)} - \hat{\theta}_{\rho}^*\|_F.
\end{align*}
\]

We will control the second moment of each \(\zeta_i\). Here’s our rough overview. \(\zeta_1\) uses Theorem 6 to show the NPMLE places small probability on \(A_\delta\); \(\zeta_2\) uses the fact that (on \(A_\delta\)) the cover \(\{ G^{(j)} \}\) must have some element that is close to the NPMLE in \(m^S\); \(\zeta_3\) follows from Gaussian concentration of measure; and \(\zeta_4\) bounds each expectation individually and uses closeness in Hellinger.

#### C.3.1 Bounding \(\mathbb{E}\zeta_1^2\)

By the scaled Tweedie’s formula (37)

\[
\|\hat{\theta}_{\rho,i} - \hat{\theta}_{\rho,i}^*\|_2^2 \leq k \left\| \frac{\nabla f_{G, \Sigma_i} (X_i)}{f_{G, \Sigma_i} (X_i) \vee \rho} - \frac{\nabla f_{G^*, \Sigma_i} (X_i)}{f_{G^*, \Sigma_i} (X_i) \vee \rho} \right\|_2^2.
\]

Saha and Guntuboyina (2020b, Lemma F.1) provides

\[
\mathbb{E}\zeta_1^2 \leq 4k n \log \left( \frac{(2\pi)^d}{\rho^2} \right) P(A_\delta^c). \tag{41}
\]

By Theorem 6, there is a constant \(C_{d, k, k} > 0\) such that \(\delta = C_{d, k, k} \varepsilon_k^2 (M, S, G^*)\) satisfies \(P(A_\delta^c) \leq 2/n\). Hence

\[
\mathbb{E}\zeta_1^2 \leq 48k n \log (n). \tag{42}
\]

#### C.3.2 Bounding \(\mathbb{E}\zeta_2^2\)

Observe

\[
\begin{align*}
\zeta_2^2 &\leq 1_{A_\delta} \min_{j \in [N]} \left\| \hat{\theta}_\rho - \hat{\theta}_\rho^{(j)} \right\|_F^2, \\
&= 1_{A_\delta} \min_{j \in [N]} \sum_{i=1}^n \left\| \frac{\Sigma_i \nabla f_{G, \Sigma_i} (X_i)}{f_{G, \Sigma_i} (X_i) \vee (\rho/\sqrt{|\Sigma_i|})} - \frac{\Sigma_i \nabla f_{G^{(j)}, \Sigma_i} (X_i)}{f_{G^{(j)}, \Sigma_i} (X_i) \vee (\rho/\sqrt{|\Sigma_i|})} \right\|_2^2.
\end{align*}
\]
On $A_3$, we may take $j$ such that $m^S(G_{n},G^{(j)}) \leq \eta^*$. For each $i$, consider two cases, where $X_i \in S^M$ and where $X_i \notin S^M$. When $X_i \in S^M$ bound the above $\| \cdot \|_2$ by the supremum over all $x \in S^M$. When $X_i \notin S^M$ bound the regularized rules as before. This yields

$$
\zeta_2^2 \leq 1_{A_3}\left( \#(i : X_i \in S^M)(\eta^*)^2 + \#(i : X_i \notin S^M)4k \log\left(\frac{(2\pi)^d}{\rho^2}\right) \right)
$$

(43)

so in particular

$$
\mathbb{E} \zeta_2^2 \leq n(\eta^*)^2 + 4k \log\left(\frac{(2\pi)^d}{\rho^2}\right)\sum_{i=1}^{n} \mathbb{P}(\mathcal{D}_S(X_i) \geq M).
$$

(44)

To bound the probabilities on the RHS, write $X_i = \theta_i + \Sigma^{1/2}Z_i$. By Lemma 13, taking $\lambda \downarrow 0$,

$$
\mathbb{E} \zeta_2^2/n \leq (\eta^*)^2 + 4k \log\left(\frac{(2\pi)^d}{\rho^2}\right) \left( C_d M^{d-2} n^{-1/2} \inf_{q \in (d+1)/2} \log n \left( \frac{2M}{M} \right)^d \right).
$$

(45)

C.3.3  Bounding $\mathbb{E} \zeta_3^2$

Fix $j \in [N]$. Let $Z_i \overset{\text{iid}}{\sim} \mathcal{N}(0,I_d)$ and $\xi^*_i \sim G^*_i$ and $\xi^{(j)}_i \sim G^{(j)}_i$, where $G^{(j)}_i$ denotes the scale change of $G^{(j)}_i$ by $\Sigma_i^{-1/2}$. In accordance with (37), we write

$$
\| \hat{\theta}^{(j)}_{\rho} - \hat{\theta}^{*}_{\rho} \|_F
$$

$$
= \left( \sum_{i=1}^{n} \left( \xi^{(j)}_i + Z_i + \frac{\nabla f_{G^{(j)}_i,I_d}(\xi^{(j)}_i + Z_i)}{f_{G^{(j)}_i,I_d}(\xi^{(j)}_i + Z_i) \vee \rho} \right) - \xi^{*}_i + Z_i + \frac{\nabla f_{G^{*}_i,I_d}(\xi^{*}_i + Z_i)}{f_{G^{*}_i,I_d}(\xi^{*}_i + Z_i) \vee \rho} \right)^2 \right)^{1/2}
$$

Call the RHS above $F(Z)$. Then

$$
|F(Z) - F(Z')| = \| \hat{\theta}^{(j)}_{\rho}(Z) - \hat{\theta}^{*}_{\rho}(Z) \|_F - \| \hat{\theta}^{(j)}_{\rho}(Z') - \hat{\theta}^{*}_{\rho}(Z') \|_F
$$

$$
\leq \| \theta^{(j)}_{\rho}(Z) - \theta^{(j)}_{\rho}(Z') \|_F + \| \theta^{*}_{\rho}(Z) - \theta^{*}_{\rho}(Z') \|_F
$$

Focusing on the second term on the RHS,

$$
\| \hat{\theta}^{*}_{\rho}(Z) - \hat{\theta}^{*}_{\rho}(Z') \|_F
$$

$$
\leq \bar{k}^{1/2} \left( \sum_{i=1}^{n} \left( \xi^{*}_i + Z_i + \frac{\nabla f_{G^{*}_i,I_d}(\xi^{*}_i + Z_i)}{f_{G^{*}_i,I_d}(\xi^{*}_i + Z_i) \vee \rho} \right) - \xi^{*}_i + Z_i + \frac{\nabla f_{G^{*}_i,I_d}(\xi^{*}_i + Z_i)}{f_{G^{*}_i,I_d}(\xi^{*}_i + Z_i) \vee \rho} \right)^2
$$

$$
\leq \bar{k}^{1/2} \left( \sum_{i=1}^{n} \left( Z_i + \frac{\nabla f_{G^{*}_i,I_d}(Z_i)}{f_{G^{*}_i,I_d}(Z_i) \vee \rho} \right) - \left( Z_i + \frac{\nabla f_{G^{*}_i,I_d}(Z_i)}{f_{G^{*}_i,I_d}(Z_i) \vee \rho} \right) \right)^2
$$

Saha and Guntuboyina (2020b), Proof of Lemma F.3 then gives

$$
\| \hat{\theta}^{*}_{\rho}(Z) - \hat{\theta}^{*}_{\rho}(Z') \|_F \leq \bar{k}^{1/2} L^2(\rho) \| Z - Z' \|_F,
$$

where as before $L(\rho) = \sqrt{-\log((2\pi)^d e^2)^d}$. The same argument applies to $\| \hat{\theta}^{(j)}_{\rho}(Z) - \hat{\theta}^{(j)}_{\rho}(Z') \|_F$. Hence $F$ is $2kL^2(\rho)$-Lipschitz. By concentration of Lipschitz functions of Gaussians and a union bound

$$
\mathbb{P}(\zeta_3^{*} \geq x) \leq N \exp\left( - \frac{x^2}{8kL^4(\rho)} \right).
$$

Integrating the tail gives

$$
\mathbb{E} \zeta_3^2 \leq 8kL^4(\rho) \log(eN).
$$

(46)
C.3.4 Bounding $\mathbb{E} \zeta^2$

Again by the scaled Tweedie’s formula (37),

$$
\mathbb{E} \left| \hat{\theta}^{(j)} - \hat{\theta}^n \right|_F \leq \sqrt{\mathbb{E} \left| \hat{\theta}^{(j)} - \hat{\theta}^n \right|_F^2} \leq \sqrt{\sum_{i=1}^{n} \mathbb{E}_{X_i \sim f \mathcal{G}^{(j)}_i} \left[ \frac{\nabla f \mathcal{G}^{(j)}_i(x)}{f \mathcal{G}^{(j)}_i(x) \vee \rho} - \frac{\nabla f \mathcal{G}^{(j)}_i(x)}{f \mathcal{G}^{(j)}_i(x) \vee \rho} \right]^2}.
$$

Saha and Guntuboyina (2020a, Lemma E.1) bounds the above expectation, yielding

$$
\left( \mathbb{E} \left| \hat{\theta}^{(j)} - \hat{\theta}^n \right|_F \right)^2 \leq C_d k \sum_{i=1}^{n} \max \left\{ \left( \log n \right)^3, -\log h_i \right\} h_i^2.
$$

By a change of variables,

$$
h^2 \left( f \mathcal{G}^{(j)}_i, f \mathcal{G}^{(j)}_i \right) = h^2 \left( f \mathcal{G}^{(j)}_i, f \mathcal{G}^{(j)}_i \right).
$$

Using the shorthand $h^2_i = h^2 \left( f \mathcal{G}^{(j)}_i, f \mathcal{G}^{(j)}_i \right)$ and using $\rho = (2\pi)^{-d/2}/n$,

$$
\left( \mathbb{E} \left| \hat{\theta}^{(j)} - \hat{\theta}^n \right|_F \right)^2 \leq C_d k \sum_{i=1}^{n} \max \left\{ \left( \log n \right)^3, -\log h_i \right\} h_i^2
$$

$$
= C_d k \left( \sum_{i: \left( \log n \right)^3 \leq -\log h_i} \left( \log n \right)^3 h_i^2 + \sum_{i: \left( \log n \right)^3 < -\log h_i} -\left( \log h_i \right) h_i^2 \right) \leq C_d k \left( n \left( \log n \right)^3 \delta + \sum_{i: \left( \log n \right)^3 \leq \log h_i^{-1}} \left( \log h_i^{-1} \right) h_i^2 \right).
$$

where in the last step we used $\frac{1}{2} \sum_{i=1}^{n} h_i^2 = h^2 \left( f \mathcal{G}^{(j)}_i, f \mathcal{G}^{(j)}_i \right) \leq \delta$. To bound the second term, note for $n \geq 6$, $(\log n)^3 \geq 3 \log n$, implying $h_i \leq n^{-3}$ for all $i$ such that $(\log n)^3 < \log h_i^{-1}$. Since $h_i \log h_i^{-1} \leq \epsilon^{-1}$ all $h_i \in [0, 1]$,

$$
\sum_{i: \left( \log n \right)^3 \leq \log h_i^{-1}} \left( \log h_i^{-1} \right) h_i^2 \leq \sum_{i: \left( \log n \right)^3 \leq \log h_i^{-1}} \frac{1}{\epsilon n^2} \leq \frac{1}{\epsilon n^2}.
$$

The first term dominates, so

$$
\mathbb{E} \zeta^2 \leq C_d k n (\log n)^3 \delta.
$$

C.3.5 Bounding the metric entropy $\log N$

We will actually bound the larger covering number $\log N(\eta^*, \mathcal{P}(\mathbb{R}^d), m^S)$ of the space of all probability measures $\mathcal{P}(\mathbb{R}^d)$ in the metric $m^S$. For any measure $G$ we let $G_i$ denote the measure scaled by $\Sigma_i^{-1/2}$ as in the scaled Tweedie formula. For $G, H \in \mathcal{P}(\mathbb{R}^d)$,

$$
m^S(G, H) = \max_{i \in [n]} \sup_{x: \mathcal{G}_i(x) \in \mathcal{M}} \left\| \Sigma_i \nabla f \mathcal{G}_i(x) - \Sigma_i \nabla f H, \Sigma_i(x) \right\|_2
$$

$$
\leq \max_{i \in [n]} \sup_{x: \mathcal{G}_i(x) \in \mathcal{M}} \left\| \Sigma_i \nabla f \mathcal{G}_i(x) - \Sigma_i \nabla f H, \Sigma_i(x) \right\|_2
$$

$$
+ \max_{i \in [n]} \sup_{x: \mathcal{G}_i(x) \in \mathcal{M}} \left\| \Sigma_i \nabla f \mathcal{G}_i(x) - \Sigma_i \nabla f H, \Sigma_i(x) \right\|_2
$$

$$
\leq \max_{i \in [n]} \sup_{x: \mathcal{G}_i(x) \in \mathcal{M}} \left\| \Sigma_i \nabla f \mathcal{G}_i(x) - \Sigma_i \nabla f H, \Sigma_i(x) \right\|_2
$$

$$
+ \max_{i \in [n]} \sup_{x: \mathcal{G}_i(x) \in \mathcal{M}} \left\| \Sigma_i \nabla f \mathcal{G}_i(x) - \Sigma_i \nabla f H, \Sigma_i(x) \right\|_2
$$

$$
\leq \max_{i \in [n]} \sup_{x: \mathcal{G}_i(x) \in \mathcal{M}} \left\| \Sigma_i \nabla f \mathcal{G}_i(x) - \Sigma_i \nabla f H, \Sigma_i(x) \right\|_2
$$

$$
+ \max_{i \in [n]} \sup_{x: \mathcal{G}_i(x) \in \mathcal{M}} \left\| \Sigma_i \nabla f \mathcal{G}_i(x) - \Sigma_i \nabla f H, \Sigma_i(x) \right\|_2
$$

$$
\leq \max_{i \in [n]} \sup_{x: \mathcal{G}_i(x) \in \mathcal{M}} \left\| \Sigma_i \nabla f \mathcal{G}_i(x) - \Sigma_i \nabla f H, \Sigma_i(x) \right\|_2
$$

$$
+ \max_{i \in [n]} \sup_{x: \mathcal{G}_i(x) \in \mathcal{M}} \left\| \Sigma_i \nabla f \mathcal{G}_i(x) - \Sigma_i \nabla f H, \Sigma_i(x) \right\|_2
$$

32
For the first term, by Saha and Guntuboyina (2020b, Lemma F.1),
\[
\left\| \frac{\Sigma_1 \nabla f_{G, \Sigma_1}(x)}{f_{G, \Sigma_1}(x) \vee (\rho/\sqrt{|\Sigma_1|})} \right\|_2 \leq \kappa^{1/2} L(\rho).
\]
Replacing \( f \vee (\rho/\sqrt{|\Sigma_1|}) \) with \( \rho/\sqrt{|\Sigma_1|} \) in the denominator can only make the denominator smaller, so
\[
m^S(G, H) \leq \kappa^{1/2} \rho^{-1} L(\rho) \max_{i \in [n]} \sup_{x \in \partial^S(x) \subseteq M} \sqrt{|\Sigma_i|} \| f_{G, \Sigma_i}(x) - f_{H, \Sigma_i}(x) \|_2 + \rho^{-1} \max_{i \in [n]} \sup_{x \in \partial^S(x) \subseteq M} \sqrt{|\Sigma_i|} \| \nabla f_{G, \Sigma_i}(x) - \nabla f_{H, \Sigma_i}(x) \|_2 \]
\[
\leq \kappa^{d/2+1/2} \rho^{-1} L(\rho) \| f_{G, \cdot} - f_{H, \cdot} \|_{\infty, S^M} + \kappa^{d/2+1} \rho^{-1} \| f_{G, \cdot} - f_{H, \cdot} \|_{\psi, S^M}
\]
In particular, letting
\[
\eta^* = (\kappa^{d/2+1/2} L(\rho) + \kappa^{d/2+1}) \frac{\eta}{\rho}
\]
we have
\[
\log N(\eta^*, \mathcal{P}([d]), m^S) \leq \log N(\eta/2, \mathbb{F}, \| \cdot \|_{\infty, S^M}) + \log N(\eta/2, \mathbb{F}, \| \cdot \|_{\psi, S^M}).
\]
We already have a bound on \( \log N(\eta/2, \mathbb{F}, \| \cdot \|_{\infty, S^M}) \) in Lemma 16, and we bound the other term similarly in Lemma 17 below. Combining these bounds,
\[
\log N(\eta^*, \mathcal{P}([d]), m^S) \leq C_d N(a, S^{M+a}) \left( \log \frac{c_{d,k}}{\eta} \right)^{d+1},
\]
where \( a = \sqrt{-2k \log \left( \frac{\sqrt{k} \max \{ 1, (2\pi)^{d/2} \} \eta }{ 5 } \right)} \). Take \( \eta = \rho/n = (2\pi)^{-d/2}/n^2 \).
\[
a = \sqrt{4k \log n + 2k \log \left( \frac{5}{\sqrt{k} \max \{ 1, (2\pi)^{d/2} \} \eta } \right) \in \left[ \sqrt{2k \log n}, \sqrt{6k \log n} \right],}
\]
provided \( 1/n \leq \frac{5}{\sqrt{k} \max \{ 1, (2\pi)^{d/2} \} \eta } \leq n \). Hence by Saha and Guntuboyina (2020b, Lemma F.6) (see the argument on page 6) gives
\[
\log N \leq c_{d,k} (\log n)^{1+d/2} \text{Vol}(S^{2M}).
\]
Lemma 17. For all compact \( S \subseteq [d], M > 0 \) and \( \eta > 0 \) sufficiently small,
\[
\log N(\eta, \mathbb{F}, \| \cdot \|_{\psi, S^M}) \leq C_d N(a, S^n) \left( \log \frac{c_{d,k}}{\eta} \right)^{d+1}
\]
where \( a = \sqrt{2k \log \frac{c_{d,k}}{\eta}} \).
Proof. Fix \( G \in \mathcal{P}([d]) \). By Lemma 15, there is a discrete measure \( H \) supported on \( S^n \) with at most
\[
l \leq \left( 2 \left[ 13.5a^2/\kappa \right] + 2 \right)^d N(a, S^n) + 1
\]
atoms such that
\[
\| f_{G, \cdot} - f_{H, \cdot} \|_{\psi, S^n} \leq a \left( 1 + \frac{3}{\sqrt{2\pi}} \right) (2\pi)^{-d/2} e^{-a^2/(2k)}
\]
Now let \( C \) denote a minimal \( \alpha \)-net of \( S^n \). Write \( H = \sum_j w_j \delta_{a_j} \), and define \( H' = \sum_j w_j \delta_{b_j} \) where \( b_j \in C \) is the closest element to \( a_j \). Then
\[
\| \nabla f_{H, \Sigma_i}(x) - \nabla f_{H', \Sigma_i}(x) \|_2 \leq \sum_j w_j \| \nabla \varphi_{S_i}(x) - \nabla \varphi_{S_i}(x - a_j) \|_2 \]
\[
\leq \kappa^{-1/2} |\Sigma_i|^{-1/2} \sum_j w_j \left\| \nabla \left( \Sigma_i^{-1/2} (x - a_j) \right) - \nabla \left( \Sigma_i^{-1/2} (x - b_j) \right) \right\|_2 \]
\[
\leq \kappa^{-d/2-1/2} \frac{\alpha}{(2\pi)^{d/2}} \left[ 1 + \frac{2}{e} + \frac{\alpha}{\sqrt{ke}} \right]
\]
Now let $\mathcal{D}$ denote a minimal $\beta$-net of $\Delta_{\ell-1}$ under $\| \cdot \|_1$. Let $H'' = \sum_{j} w''_{j} \delta_{j}$ where $\| w' - w'' \|_1 \leq \beta$.

Then

$$\| \nabla f_{H'\Sigma}(x) - \nabla f_{H''\Sigma}(x) \|_{2} \leq \beta \sup_{u} \| \nabla \varphi_{\Sigma}(u) \|_{2} \leq \frac{k^{-d/2-1/2} \beta}{(2\pi)^{d/2} \sqrt{e}}.$$  

By triangle inequality,

$$\| f_{G^{\bullet}, \bullet} - f_{H'' \Sigma, \bullet} \|_{\psi, S\mu} \leq (2\pi k)^{-d/2} \left[ \left( 1 + \frac{3}{\sqrt{2\pi}} \right) ae^{-a^2/(2k)} + \frac{\alpha}{\sqrt{k}} \left[ 1 + \frac{2}{e} + \frac{\alpha}{\sqrt{ke}} \right] + \frac{\beta}{\sqrt{ke}} \right].$$

Taking $a = \sqrt{2k \log \alpha^{-1}} \geq 1$ and $\alpha = \beta = \sqrt{k \wedge 1} (2\pi k)^{d/2} \eta$, \n
$$\| f_{G^{\bullet}, \bullet} - f_{H'' \Sigma, \bullet} \|_{\psi, S\mu} \leq \frac{5\alpha a}{\sqrt{k \wedge 1}} (2\pi k)^{-d/2} = a\eta$$

The proof is completed following same steps as the proof of Lemma 5.

\section*{C.4 Putting together the pieces}

Combining (39), (42), (45), (46), and (49) and pulling out any constants depending on $d, k$, or $\bar{\delta}$,

$$\mathbb{E}[\| \hat{\theta} - \hat{\theta}^* \|_F^2/n \leq (5/n) \left[ \mathbb{E}[\| \hat{\theta}_p - \hat{\theta}^*_p \|^2_F + \sum_{i=1}^d E_i^2] \right] \leq c_{d,k}\left( \varepsilon_n^2(M,S,G^*) (\sqrt{\log n})^{d-2} + \frac{\log n}{n} + (\eta^*)^2 + \varepsilon_n^2(M,S,G^*) \right. \left. + \log(eN) \left( \frac{\log n}{n} \right)^2 \right) + \varepsilon_n^2(M,S,G^*) (\sqrt{\log n})^{(d-2)\nu} \right.$$

This completes the proof of Theorem 8.

\section*{D Proofs of Theorems 10 and 12}

\textbf{Proof of Theorem 10.} We will relate the Wasserstein distance to the average Hellinger distance, so we rely on the tools of Nguyen (2013, proof of theorem 2). Fix a symmetric density $K$ whose Fourier transform $\tilde{K}$ is bounded with support on $[-1,1]^d$. For any $\delta > 0$ define the scaled kernel $K_\delta(x) = \frac{1}{\delta^d} K(x/\delta)$. By the triangle inequality,

$$W_2(G^*, \tilde{G}_n) \leq W_2(G^*, G^* * K_\delta) + W_2(G^* * K_\delta, \tilde{G}_n * K_\delta) + W_2(\tilde{G}_n * K_\delta, \tilde{G}_n).$$

For the first and third terms, bound the minimum over all couplings by the strong coupling:

$$W_2^2(G, G * K_\delta) = \min_{\theta : \tilde{G} = \phi * \tilde{G}, \tilde{G} \sim \hat{K}} \mathbb{E}[\| \theta - (\theta' + \delta \varepsilon) \|_2 \leq \delta^2 \mathbb{E}_{\tilde{G} \sim \hat{K}} \| \varepsilon \|_2^2,$$

where the inequality follows from choosing the coupling where $\theta = \theta'$ almost surely. Letting $m_2(K) = E_{\tilde{G} \sim \hat{K}} \| \varepsilon \|_2^2$ denote the second moment of the (unscaled) kernel, we have

$$W_2(G^*, \tilde{G}_n) \leq 2\sqrt{m_2(K)}\delta + W_2(G^* * K_\delta, \tilde{G}_n * K_\delta).$$

For the second term, Villani (2008, Theorem 6.15) yields

$$W_2^2(G^* * K_\delta, \tilde{G}_n * K_\delta) \leq 2 \int \| x \|_2 \psi d\| G^* * K_\delta - \tilde{G}_n * K_\delta \|_2(x)$$

34
By Nguyen (2013, Lemma 6), for any $s > 2$ such that $m_s(K) = \mathbb{E} \| \varepsilon \|_2^s < \infty$,

$$W_2^s(G^* \ast K_\delta, \widehat{G}_n \ast K_\delta) \leq 4 \left\| G^* \ast K_\delta - \widehat{G}_n \ast K_\delta \right\|_{L_2}^{(s-2)/2} R^{2/s}$$

$$= 4 \cdot 2^{(s-2)/s} \mathbb{E} \left[ (\text{Vol}(B_1))^s R^{d+2s} \left\| G^* \ast K_\delta - \widehat{G}_n \ast K_\delta \right\|_{L_2}^{2(s-2)/(s+2d)} \right]^{(s-2)/s} R^{2/s}$$

$$\leq 8 \mathbb{E} \left[ (\text{Vol}(B_1))^s R^{d+2s} \left\| G^* \ast K_\delta - \widehat{G}_n \ast K_\delta \right\|_{L_2}^{2(s-2)/(s+2d)} \right]^{(s-2)/s} R^{2/s}$$

where $R = \mathbb{E}_{\theta^* \sim G^*, \varepsilon \sim K} \| \theta^* + \delta \varepsilon \|_2^s + \mathbb{E}_{\theta \sim G, \varepsilon \sim K} \| \theta + \delta \varepsilon \|_2^s$.

For moments in the term $R$, use $\mathbb{E}(\| \theta + \delta \varepsilon \|_2^s) \leq 2^s (\mathbb{E}(\| \theta \|_2^s + \delta \varepsilon \|_2^s m_s(K)))$, so

$$R \leq 2^s (m_s(G^*) + m_s(\widehat{G}_n) + 2 \delta m_s(K)).$$

The quantity $m_s(K)$ is regarded as a constant depending only on $s > 2$ and $d$. By assumption, the support of $\widehat{G}_n$ is contained in the minimum bounding box of the observations, which is further contained in $[-U, U]^d$ where $U = \max_{i,j} |X_{ij}| \leq L + \max_{i,j} |X_{ij} - \theta^*_{ij}|$. Since $X_{ij} - \theta^*_{ij} \sim \mathcal{N}(0, (\Sigma_i)_{jj})$, we have by a standard concentration argument that

$$U \leq L + 4\sqrt{k \log n}$$

with probability at least $1 - \frac{2d}{n^s}$. Hence, with the same probability

$$m_s(\widehat{G}_n) = \mathbb{E}_{\widehat{G}_n} \| \theta \|_2^s \leq 4^{d/2} \mathbb{E}_{\widehat{G}_n} \| \theta \|_2^s \leq 4^{d/2} \left( L + 4\sqrt{k \log n} \right)^s.$$

This same bound holds for $m_s(G^*)$.

For the $\| \cdot \|_{L_2}$ norm $\| G^* \ast K_\delta - \widehat{G}_n \ast K_\delta \|_{L_2}$, let $g^{(i)}_\delta$ denote the inverse Fourier transform of $K_\delta/\hat{\Sigma}_i$, so that $G^* \ast K_\delta = f \ast G \ast \Sigma_i \ast g^{(i)}_\delta$. Hence, by Proposition 8.49 of Folland (1999), we have for each $i = 1, \ldots, n$,

$$\| G^* \ast K_\delta - \widehat{G}_n \ast K_\delta \|_{L_2} \leq 2d_{TV}(f \ast G \ast \Sigma_i, f \hat{\Sigma}_i, g^{(i)}_\delta) \| g^{(i)}_\delta \|_{L_2}.$$

Using Plancherel’s theorem and the fact that $\hat{K}$ is bounded on its support of $[-1, 1]^d$,

$$\| g^{(i)}_\delta \|_{L_2}^2 = \int_{[-1, 1]^d} \hat{K}(\omega) \hat{\Sigma}_i(\omega)^2 \hat{g}^{(i)}_\delta(\omega)^2 d\omega \leq C_d \int_{[-1,1]^d} \hat{\Sigma}_i(\omega)^2 \hat{g}^{(i)}_\delta(\omega)^2 d\omega$$

$$= C_d \int_{[-1,1]^d} \exp(\omega^T \Sigma_i \omega) d\omega = C_d \prod_{j=1}^d \int_{-1}^1 \exp(\Sigma_{jj} \omega_j^2) d\omega_j$$

$$\leq C_d \prod_{j=1}^d \left( \int_{-1}^1 \exp(-\Sigma_{jj} \omega_j^2) d\omega_j \right)^{1/2} \leq C_d \left( \frac{n}{k} \right)^{d/2} e^{2\sqrt{d}}. $$

Averaging over $i = 1, \ldots, n$,

$$\| G^* \ast K_\delta - \widehat{G}_n \ast K_\delta \|_{L_2} \leq C_d \left( \frac{n}{k} \right)^{d/2} e^{2\sqrt{d} \delta^s} \cdot \frac{1}{n} \sum_{i=1}^n d_{TV}(f \ast G \ast \Sigma_i, f \hat{\Sigma}_i, g^{(i)}_\delta) \| g^{(i)}_\delta \|_{L_2}.$$

Combining our calculations following (54), we have

$$W_2(G^*, \widehat{G}_n) \leq C_d s \inf_{\delta \in (0,1)} \left\{ \delta + \left( \frac{2^s}{d^{1/2}} \left( L + 4\sqrt{k \log n} \right)^s + 2 \delta^{\ast} m_s(K) \right) \right\}^{3d/(2d+4s)}$$

$$\times \left( \frac{n}{k} \right)^{d/2} e^{2\sqrt{d} \delta^s} \hat{h}(G^*, \widehat{G}_n) \left( \frac{s-2}{(d+2s)} \right).$$

Assume $n$ is large enough that $4\sqrt{k \log n} \geq L$ and $2^s \left( 4\sqrt{k \log n} \right)^s \geq 2m_s(K)$, so

$$W_2(G^*, \widehat{G}_n) \leq C_d s \inf_{\delta \in (0,1)} \left\{ \delta + \left( \frac{n}{k} \log n \right)^{3d/(4d+2s)} \left( \frac{n}{k} \right)^{d/2} e^{2\sqrt{d} \delta^s} \hat{h}(G^*, \widehat{G}_n) \left( \frac{s-2}{(d+2s)} \right) \right\}. $$

(56)
Choosing $\delta^{-2} = -\frac{1}{8kd} \log h(G^*, \widehat{G}_n)$ (provided $\delta < 1$) and $s = d + 2$ yields

$$W_2^2(G^*, \widehat{G}_n) \leq C_d \left\{ \frac{\bar{K}d}{-\log h(G^*, \widehat{G}_n)} + (\bar{K} \log n)^{d/2} \left( \frac{1}{h^2(G^*, \widehat{G}_n)} \right)^{1/12} \right\}. \tag{57}$$

$\varepsilon_n^2(M, S, G^*)$ defined in (13), with $S = [-L, L]^d$ and $M = \sqrt{10K \log n}$ gives

$$\varepsilon_n^2 = \left( \frac{4\sqrt{10}(L^2 \sqrt{n})}{n} \right)^d (\log n)^{d+1}.$$  

By Theorem 6,

$$W_2^2(G^*, \widehat{G}_n) \leq C_d \left\{ \frac{\bar{K}d}{\log n - \log C_{d, \bar{K}_i} t^2 (\log n)^{d+1}} + (\bar{K} \log n)^{d/2} \left( C_{d, \bar{K}_i} t \log n \right)^{d+1} \right\},$$

with probability at least $1 - 2n^{-t^2}$. Take $t^2 = 8$. For $n$ sufficiently large the first term dominates, $\delta < 1$, and $\log n - \log C_{d, \bar{K}_i} t 8(\log n)^{d+1} \geq (\log n)/2$. 

**Proof of Theorem 12.** Take $\mu = 0$ by location equivariance (see Lemma 4). Write $\widehat{G}_n = \sum_{j=1}^k \hat{w}_j \hat{a}_j$. Since $G^* = \delta_0$ is a point mass,

$$W_2^2(\widehat{G}_n, G^*) = \mathbb{E}_{\delta_0, \widehat{G}_n} \| \theta \|_2^2 = \sum_{j=1}^k \hat{w}_j \| \hat{a}_j \|_2^2.$$  

We relate this to the marginal density $f_{\widehat{G}_n, \bullet}$ via

$$\int f_{\widehat{G}_n, \Sigma_i}(x) \| x \|_2^2 \, dx = \sum_{j=1}^k \hat{w}_j \int \varphi_{\Sigma_i}(x - \hat{a}_j) \| x \|_2^2 \, dx$$

$$= \sum_{j=1}^k \hat{w}_j \int \varphi_{\Sigma_i}(x) (\| x \|_2^2 + \| \hat{a}_j \|_2^2 + 2(x, \hat{a}_j)) \, dx$$

$$= \int f_{G^*, \Sigma_i}(x) \| x \|_2^2 \, dx + W_2^2(\widehat{G}_n, G^*).$$

Hence for any $i \in \{1, \ldots, n\}$,

$$W_2^2(\widehat{G}_n, G^*) = \int (f_{\widehat{G}_n, \Sigma_i}(x) - f_{G^*, \Sigma_i}(x)) \| x \|_2^2 \, dx$$

$$\leq 2h(f_{\widehat{G}_n, \Sigma_i}, f_{G^*, \Sigma_i}) \left( \int (f_{\widehat{G}_n, \Sigma_i}(x) + f_{G^*, \Sigma_i}(x)) \| x \|_2^2 \, dx \right)^{1/2}.$$  

Averaging over $i \in \{1, \ldots, n\}$,

$$W_2^2(\widehat{G}_n, G^*) \leq 2h(\widehat{G}_n, \bullet, G^*, \bullet) \max_{i=1}^n \left( \int (f_{\widehat{G}_n, \Sigma_i}(x) + f_{G^*, \Sigma_i}(x)) \| x \|_2^2 \, dx \right)^{1/2}.$$  

Applying Theorem 6 with $S = \{0\}$ and $M = \sqrt{10K \log n}$,

$$\bar{h}^2(f_{\widehat{G}_n, \bullet}, f_{G^*, \bullet}) \leq d_{\bar{K}_i} t^2 (\log n)^{d+1}$$

with probability at least $1 - 2n^{-t^2}$ for all $t \geq 1$.

For the remaining terms,

$$\int f_{G^*, \Sigma_i}(x) \| x \|_2^4 \, dx = \mathbb{E} \| X_i \|_2^4 = \mathbb{E}_{Z \sim \mathcal{N}(0, A_d)} \Sigma_i^{1/2} Z \|_2^4 \leq \bar{K}^2 \mathbb{E} A \cdot \chi_2 A^2 = \bar{K}^2 d(d+2)$$

and

$$\int f_{\widehat{G}_n, \Sigma_i}(x) \| x \|_2^4 \, dx = \sum_j \hat{w}_j \int \varphi_{\Sigma_i}(x) \| x \|_2^4 + \| \hat{a}_j \|_2^4 \, dx$$

$$\leq 8 \sum_j \hat{w}_j \int \varphi_{\Sigma_i}(x) \| x \|_2^4 + \| \hat{a}_j \|_2^4 \, dx$$

$$\leq 8 \bar{K}^2 d(d+2) + 8 \sum_j \hat{w}_j \| \hat{a}_j \|_2^4.$$  

36
By our assumption on the support that each \( \hat{a}_j \in B_{\kappa^*}(\bar{X}) \), each \( \hat{a}_j \) equivalently satisfies
\[
\|\hat{a}_j - \bar{X}\|^2 \leq \left( \frac{k}{d} \right)^4 \max_i \|X_i - \bar{X}\|^2.
\]
Noting that \( X_i - \bar{X} \sim \mathcal{N}(0, (1 - 2n^{-1}) \Sigma_i + n^{-1} \Sigma) \) with \( \Sigma = n^{-1} \sum_{j=1}^n \Sigma_j \), we bound
\[
\sum_j \hat{w}_j \|\hat{a}_j\|^2 \leq s \left( \|\bar{X}\|^2 + \max_j \|\hat{a}_j - \bar{X}\|^2 \right)
\leq s \left( \|\bar{X}\|^2 + \kappa^4 \max_{i\in[n]} \|X_i - \bar{X}\|^2 \right)
\leq \kappa s  \left( n^{-2} A_i^2 + \kappa^4 \max_{i\in[n]} A_i^2 \right)
\leq 16 \frac{k^6}{\kappa^4} \max_i A_i^2,
\]
where \( A_0, A_1, \ldots, A_n \sim \chi^2_k \) are possibly dependent, and \( \leq_{st} \) denotes stochastic inequality.

For \( t \geq 1 \), we use the following tail bound (see Laurent and Massart, 2000, Lemma 1)
\[
P\left( \max_{i=0:n} A_i^2 \geq 60 t^2 (\log n)^2 \right) \leq n^{-t^2},
\]
where we have used the assumption in Theorem 6 that \( n \geq (2\pi)^{d/2} \) to eliminate the dependence on \( d \). We have thus shown that
\[
\max_{i=1:n} \left( \int (f_{\mathcal{G}_n, \Sigma_i}(x) + f_{\mathcal{G}^*, \Sigma}(x)) \|x\|_d^2 \, dx \right)^{1/2} \leq \left( 9 k^2 d (d + 2) + 400 \frac{k^6}{\kappa^4} (\log n)^2 \right)^{1/2} \leq \frac{k}{\kappa} t (\log n)
\]
with probability at least \( 1 - n^{-t^2} \). Combining with a union bound over our earlier estimate,
\[
W_2(\bar{G}_n, G^*) \leq d \frac{k}{\kappa} t^{3/2} (\log n)^{d+3/4} \frac{1}{n^{1/4}}
\]
with probability at least \( 1 - 3n^{-t^2} \) for all \( t \geq 1 \).

\section*{References}

Bela Abolfathi, DS Aguado, Gabriela Aguilar, Carlos Allende Prieto, Andres Almeida, Tonina Tasnim Ananna, Friedrich Anders, Scott F Anderson, Brett H Andrews, Borja Anguiano, et al. The fourteenth data release of the Sloan Digital Sky Survey: first spectroscopic data from the extended Baryon Oscillation Spectroscopic Survey and from the second phase of the Apache Point Observatory Galactic Evolution Experiment. The Astrophysical Journal Supplement Series, 235 (2):42, 2018.

Michael G Akritas and Matthew A Bershady. Linear regression for astronomical data with measurement errors and intrinsic scatter. The Astronomical Journal, 470(2):706, 1996.

Carlos Améndola, Alexander Engström, and Christian Haase. Maximum number of modes of Gaussian mixtures. Information and Inference: A Journal of the IMA, 9(3):587–600, 2020.

Lauren Anderson, David W Hogg, Boris Leistedt, Adrian M Price-Whelan, and Jo Bovy. Improving Gaia parallax precision with a data-driven model of stars. The Astronomical Journal, 156(4):145, 2018.

Trambak Banerjee, Luella J Fu, Gareth M James, and Wenguang Sun. Nonparametric empirical Bayes estimation on heterogeneous data. 2021. URL http://faculty.marshall.usc.edu/gareth-james/Research/Nest%20Biometrika.pdf.

Dankmar Böhning. Numerical estimation of a probability measure. Journal of statistical planning and inference, 11(1):57–69, 1985.
Dankmar Böning. The EM algorithm with gradient function update for discrete mixtures with known (fixed) number of components. *Statistics and Computing*, 13(3):257–265, 2003.

Jo Bovy, David W Hogg, and Sam T Roweis. Extreme deconvolution: Inferring complete distribution functions from noisy, heterogeneous and incomplete observations. *Annals of Applied Statistics*, 5(2B):1657–1677, 2011.

Nabarun Deb, Sujayam Saha, Adityanand Guntuboyina, and Bodhisattva Sen. Two-component mixture model in the presence of covariates. *Journal of the American Statistical Association*, pages 1–15, 2021.

Jérôme Dedecker and Bertrand Michel. Minimax rates of convergence for Wasserstein deconvolution with supersmooth errors in any dimension. *Journal of Multivariate Analysis*, 122:278–291, 2013.

Aurore Delaigle and Alexander Meister. Density estimation with heteroscedastic error. *Bernoulli*, 14(2):562–579, 2008.

Arthur P Dempster, Nan M Laird, and Donald B Rubin. Maximum likelihood from incomplete data via the EM algorithm. *Journal of the Royal Statistical Society: Series B (Methodological)*, 39(1):1–22, 1977.

Lee H Dicker and Sihai D Zhao. High-dimensional classification via nonparametric empirical Bayes and maximum likelihood inference. *Biometrika*, 103(1):21–34, 2016.

Natalie Doss, Yihong Wu, Pengkun Yang, and Harrison H Zhou. Optimal estimation of high-dimensional Gaussian mixtures. *arXiv preprint arXiv:2002.05818*, 2020.

Frank Dyson. A method for correcting series of parallax observations. *Monthly Notices of the Royal Astronomical Society*, 86:686, 1926.

Alex Dytso, Semih Yagli, H Vincent Poor, and Shlomo Shamai Shitz. The capacity achieving distribution for the amplitude constrained additive Gaussian channel: An upper bound on the number of mass points. *IEEE Transactions on Information Theory*, 66(4):2006–2022, 2019.

Bradley Efron. Tweedie’s formula and selection bias. *Journal of the American Statistical Association*, 106(496):1602–1614, 2011.

Bradley Efron. *Large-scale inference: empirical Bayes methods for estimation, testing, and prediction*, volume 1. Cambridge University Press, 2012.

Bradley Efron. Two modeling strategies for empirical Bayes estimation. *Statistical Science*, 29(2):285, 2014.

Bradley Efron. Bayes, oracle Bayes and empirical Bayes. *Statistical Science*, 34(2):177–201, 2019.

Bradley Efron and Trevor Hastie. *Computer age statistical inference*, volume 5. Cambridge University Press, 2016.

Bradley Efron and Carl Morris. Empirical Bayes on vector observations: An extension of Stein’s method. *Biometrika*, 59(2):335–347, 1972a.

Bradley Efron and Carl Morris. Limiting the risk of Bayes and empirical Bayes estimators—Part II: The empirical Bayes case. *Journal of the American Statistical Association*, 67(337):130–139, 1972b.

Bradley Efron and Carl Morris. Combining possibly related estimation problems. *Journal of the Royal Statistical Society: Series B (Methodological)*, 35(3):379–402, 1973a.

Bradley Efron and Carl Morris. Stein’s estimation rule and its competitors—an empirical Bayes approach. *Journal of the American Statistical Association*, 68(341):117–130, 1973b.

Long Feng and Lee H Dicker. Approximate nonparametric maximum likelihood for mixture models: A convex optimization approach to fitting arbitrary multivariate mixing distributions. *Computational Statistics & Data Analysis*, 122:80–91, 2018.
Gerald B Folland. *Real analysis: modern techniques and their applications*, volume 40. John Wiley & Sons, 1999.

Jiaying Gu and Roger Koenker. On a problem of Robbins. *International Statistical Review*, 84(2):224–244, 2016.

Jiaying Gu and Roger Koenker. Rebayes: an R package for empirical Bayes mixture methods. Technical report, cemmap working paper, 2017.

Philippe Heinrich and Jonas Kahn. Strong identifiability and optimal minimax rates for finite mixture estimation. *Annals of Statistics*, 46(6A):2844–2870, 2018.

Nhat Ho and XuanLong Nguyen. On strong identifiability and convergence rates of parameter estimation in finite mixtures. *Electronic Journal of Statistics*, 10(1):271–307, 2016.

David W Hogg, Adam D Myers, and Jo Bovy. Inferring the eccentricity distribution. *The Astrophysical Journal*, 725(2):2166, 2010.

W. James and Charles Stein. Estimation with quadratic loss. In *Proceedings of the Fourth Berkeley Symposium on Mathematical Statistics and Probability, Volume 1: Contributions to the Theory of Statistics*, pages 361–379, Berkeley, Calif., 1961. University of California Press. URL https://projecteuclid.org/euclid.bsmsp/1200512173.

Jiming Jiang, Thuan Nguyen, and J Sunil Rao. Best predictive small area estimation. *Journal of the American Statistical Association*, 106(494):732–745, 2011.

Wenhua Jiang. On general maximum likelihood empirical Bayes estimation of heteroscedastic IID normal means. *Electronic Journal of Statistics*, 14(1):2272–2297, 2020.

Wenhua Jiang and Cum-Hui Zhang. General maximum likelihood empirical Bayes estimation of normal means. *The Annals of Statistics*, 37(4):1647–1684, 2009.

Wenhua Jiang and Cum-Hui Zhang. Empirical Bayes in-season prediction of baseball batting averages. In *Borrowing Strength: Theory Powering Applications—A Festschrift for Lawrence D. Brown*, pages 263–273. Institute of Mathematical Statistics, 2010.

Iain M Johnstone. Gaussian estimation: Sequence and wavelet models. 2019. URL http://www-stat.stanford.edu/~imj/.

Brandon C Kelly. Measurement error models in astronomy. In *Statistical challenges in modern astronomy V*, pages 147–162. Springer, 2012.

Jack Kiefer and Jacob Wolfowitz. Consistency of the maximum likelihood estimator in the presence of infinitely many incidental parameters. *The Annals of Mathematical Statistics*, pages 887–906, 1956.

Arlene KH Kim and Adityanand Guntuboyina. Minimax bounds for estimating multivariate Gaussian location mixtures. *arXiv preprint arXiv:2012.00444*, 2020.

Youngseok Kim, Peter Carbonetto, Matthew Stephens, and Mihai Anitescu. A fast algorithm for maximum likelihood estimation of mixture proportions using sequential quadratic programming. *Journal of Computational and Graphical Statistics*, (just-accepted):1–34, 2019.

Youngseok Kim, Peter Carbonetto, Matthew Stephens, and Mihai Anitescu. A fast algorithm for maximum likelihood estimation of mixture proportions using sequential quadratic programming. *Journal of Computational and Graphical Statistics*, 29(2):261–273, 2020.

Roger Koenker and Jiaying Gu. REBayes: Empirical Bayes mixture methods in R. *Journal of Statistical Software*, 82(8):1–26, 2017.

Roger Koenker and Ivan Mizera. Convex optimization, shape constraints, compound decisions, and empirical Bayes rules. *Journal of the American Statistical Association*, 109(506):674–685, 2014.
Nan Laird. Nonparametric maximum likelihood estimation of a mixing distribution. *Journal of the American Statistical Association*, 73(364):805–811, 1978.

Danial Lashkari and Polina Golland. Convex clustering with exemplar-based models. In *Advances in neural information processing systems*, pages 825–832, 2008.

Beatrice Laurent and Pascal Massart. Adaptive estimation of a quadratic functional by model selection. *Annals of Statistics*, pages 1302–1338, 2000.

Mary L Lesperance and John D Kalbfleisch. An algorithm for computing the nonparametric MLE of a mixing distribution. *Journal of the American Statistical Association*, 87(417):120–126, 1992.

Bruce G Lindsay. Mixture models: theory, geometry and applications. In *NSF-CBMS regional conference series in probability and statistics*. JSTOR, 1995.

Bruce G Lindsay and Kathryn Roeder. Uniqueness of estimation and identifiability in mixture models. *Canadian Journal of Statistics*, 21(2):139–147, 1993.

Lei Liu and Yu Zhu. Partially projected gradient algorithms for computing nonparametric maximum likelihood estimates of mixing distributions. *Journal of Statistical Planning and Inference*, 137(7):2509–2522, 2007.

Steven R Majewski, Ricardo P Schiavon, Peter M Frinchaboy, Carlos Allende Prieto, Robert Barkhouser, Dmitry Bizyaev, Basil Blank, Sophia Brunner, Adam Burton, Ricardo Carrera, et al. The Apache Point Observatory Galactic Evolution Experiment (APOGEE). *The Astronomical Journal*, 154(3):94, 2017.

Paul Marriott. On the local geometry of mixture models. *Biometrika*, 89(1):77–93, 2002.

Alexander Meister. *Deconvolution problems in nonparametric statistics*, volume 193. Springer Science & Business Media, 2009.

Carl N Morris. Parametric empirical Bayes inference: theory and applications. *Journal of the American statistical Association*, 78(381):47–55, 1983.

MOSEK ApS. Mosek optimization suite. 2019. URL http://docs.mosek.com/9.0/intro.pdf.

XuanLong Nguyen. Convergence of latent mixing measures in finite and infinite mixture models. *The Annals of Statistics*, 41(1):370–400, 2013.

Johann Pfanzagl. Consistency of maximum likelihood estimators for certain nonparametric families, in particular: mixtures. *Journal of Statistical Planning and Inference*, 19(2):137–158, 1988.

Yury Polyanskiy and Yihong Wu. Self-regularizing property of nonparametric maximum likelihood estimator in mixture models. *arXiv preprint arXiv:2008.08244*, 2020.

Bridget L Ratcliffe, Melissa K Ness, Kathryn V Johnston, and Bodhisattva Sen. Tracing the assembly of the Milky Way’s disk through abundance clustering. *The Astrophysical Journal*, 900(2):165, 2020.

Surajit Ray and Bruce G Lindsay. The topography of multivariate normal mixtures. *The Annals of Statistics*, 33(5):2042–2065, 2005.

Richard A Redner and Homer F Walker. Mixture densities, maximum likelihood and the EM algorithm. *SIAM review*, 26(2):195–239, 1984.

Philippe Rigollet and Jonathan Weed. Entropic optimal transport is maximum-likelihood deconvolution. *Comptes Rendus Mathematique*, 356(11-12):1228–1235, 2018.

James A Ritchie and Iain Murray. Scalable extreme deconvolution. *arXiv preprint arXiv:1911.11665*, 2019.

Herbert Robbins. A generalization of the method of maximum likelihood-estimating a mixing distribution. In *Annals of Mathematical Statistics*, volume 21, pages 314–315, 1950.
Herbert Robbins. An empirical Bayes approach to statistics. *Proceedings of the Third Berkeley Symposium on Mathematical Statistics and Probability*, 1:157–163, 1956.

Sujayam Saha and Adityanand Guntuboyina. On the nonparametric maximum likelihood estimator for Gaussian location mixture densities with application to Gaussian denoising. *Annals of Statistics*, 48(2):738–762, 2020a.

Sujayam Saha and Adityanand Guntuboyina. Supplement to “On the nonparametric maximum likelihood estimator for Gaussian location mixture densities with application to Gaussian denoising”. 2020b. URL https://doi.org/10.1214/19-AOS1817SUPP.

Zhiqiang Tan. Steinized empirical Bayes estimation for heteroscedastic data. *Statistica Sinica*, pages 1219–1248, 2016.

Sara van de Geer. *Empirical Processes in M-estimation*, volume 6. Cambridge university press, 2000.

Cédric Villani. *Optimal transport: old and new*, volume 338. Springer Science & Business Media, 2008.

Yong Wang. On fast computation of the non-parametric maximum likelihood estimate of a mixing distribution. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 69(2): 185–198, 2007.

Asaf Weinstein, Zhuang Ma, Lawrence D Brown, and Cun-Hui Zhang. Group-linear empirical Bayes estimates for a heteroscedastic normal mean. *Journal of the American Statistical Association*, 113(522):698–710, 2018.

Wing Hung Wong and Xiaotong Shen. Probability inequalities for likelihood ratios and convergence rates of sieve MLEs. *The Annals of Statistics*, 23(2):339–362, 1995.

Yihong Wu and Pengkun Yang. Optimal estimation of Gaussian mixtures via denoised method of moments. *The Annals of Statistics*, 48(4):1981–2007, 2020.

Xianchao Xie, SC Kou, and Lawrence D Brown. SURE estimates for a heteroscedastic hierarchical model. *Journal of the American Statistical Association*, 107(500):1465–1479, 2012.

Cun-Hui Zhang. Generalized maximum likelihood estimation of normal mixture densities. *Statistica Sinica*, pages 1297–1318, 2009.