Nonparametric Finite Mixture Models with Possible Shape Constraints: A Cubic Newton Approach

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Abstract

We explore computational aspects of maximum likelihood estimation of the mixture proportions of a nonparametric finite mixture model—a convex optimization problem with old roots in statistics and a key member of the modern data analysis toolkit. Motivated by problems in shape constrained inference, we consider structured variants of this problem with additional convex polyhedral constraints. We propose a new cubic regularized Newton method for this problem and present novel worst-case and local computational guarantees for our algorithm. We extend earlier work by Nesterov and Polyak to the case of a self-concordant objective with polyhedral constraints, such as the ones considered herein. We propose a Frank-Wolfe method to solve the cubic regularized Newton subproblem; and derive efficient solutions for the linear optimization oracles that may be of independent interest. In the particular case of Gaussian mixtures without shape constraints, we derive bounds on how well the finite mixture problem approximates the infinite-dimensional Kiefer-Wolfowitz maximum likelihood estimator. Experiments on synthetic and real datasets suggest that our proposed algorithms exhibit improved runtimes and scalability features over existing benchmarks.

1 Introduction

In this paper, we study a problem in nonparametric density estimation—in particular, learning the components of a mixture model, which is a key problem in statistics and related disciplines. Consider a one-dimensional mixture density of the form: \( g(x) = \sum_{i=1}^{M} w_i \psi_i(x) \) where, the \( M \) components (probability densities) \( \{ \psi_i(x) \}_{i=1}^{M} \) are known, but the proportions \( \{ w_i \}_{i=1}^{n} \) are unknown, and need to be estimated from the data at hand.

1.1 Learning nonparametric mixture proportions

Suppose we are given \( N \) samples \( \{ X_j \}_{j=1}^{N} \), independently drawn from \( g(x) \), we can obtain a maximum likelihood estimate (MLE) of the mixture proportions or weights via the following convex optimization problem:

\[
\min_w \quad -\frac{1}{N} \sum_{j \in [N]} \log \left( \sum_{i \in [M]} w_i B_{ij} \right) \\
\text{s.t.} \quad w \in \Delta_M := \{ w : \sum_{i \in [M]} w_i = 1, w_i \geq 0, i \in [M] \}
\]

where, \( B_{ij} = \psi_i(X_j) \geq 0 \) is the evaluation of the density \( \psi_i \) at point \( X_j \) for all \( i,j \). One of our goals in this paper is to present new algorithms for (1.1) with associated computational guarantees, that scale to instances with \( N \approx 10^6 \) and \( M \approx 10^3 \). Problem (1.1) has a rich history in statistics: this arises, for example, in the context of empirical Bayes estimation \([22, 17, 20, 8]\). Several choices of the bases functions

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\{\psi_i\} are possible—see for example [20], and references therein. A notable example arising in Gaussian sequence models [18], is to consider \(\psi_i(x) := \varphi(x - \mu_i)\) where, \(\varphi\) is the standard Gaussian density and the location parameter \(\mu_i\) is pre-specified for all \(i \in [M]\). In this case, problem (1.1) can be interpreted as a finite-dimensional approximation of the original formulation of the Kiefer-Wolfowitz nonparametric MLE [19]. Given an infinite mixture \(g_Q(x) = \int_\mathbb{R} \varphi(x - \mu) dQ(\mu)\) where, \(Q\) is a probability distribution on \(\mathbb{R}\), the Kiefer-Wolfowitz nonparametric MLE estimates \(Q\) given \(N\) independent samples from \(g_Q\). This infinite dimensional problem admits a finite dimensional solution with \(Q\) supported on \(N\) unknown atoms [19,22]. Since these atoms can be hard to locate, it is common to resort to discrete approximations like (1.1) for a suitable pre-specified grid of \(\{\mu_i\}\)-values. In this paper, we present bounds that quantify how well an optimal solution to a discretized problem (1.1) (with a-priori specified atoms), approximates a solution to the infinite dimensional Kiefer-Wolfowitz MLE problem.

As noted by [20], while versions of problem (1.1) originated in the 1890s, the utility of this estimator and the abundance of large-scale datasets have necessitated solving problem (1.1) at scale (e.g., with \(N \approx 10^5\) - \(10^6\) and \(M \approx 10^3\)). A popular algorithm for (1.1) is based on the Expectation Maximization (EM) algorithm [17] see for example, which is known to have slow convergence behavior in practice [22,20]. [22] observed that solving a dual of (1.1) via Mosek’s interior point solver, led to improvements over EM-based methods. Recently, [20] propose an interesting approach based on sequential quadratic programming for (1.1) that offers notable improvements over [22,21]. [20] also use low-rank approximations of \(B\), active set updates, among other clever tricks to obtain computational improvements. Global complexity guarantees of these methods appear to be unknown. In this paper, we present a novel computational framework (with global complexity guarantees) that applies to Problem (1.1); and a constrained variant of this problem, arising in the context of shape constrained density estimation [12], as we discuss next.

1.2 Learning nonparametric mixtures with shape constraints

In many applications, practitioners have prior knowledge about the shape of the underlying density. In these cases, it is desirable to incorporate such qualitative shape constraints into the density estimation procedure—this falls under the purview of shape constrained inference [12] which dates back to at least 1960s with the seminal work of [10]. Due to their usefulness and applicability in a wide variety of domains, the last 10 years or so has witnessed a significant interest in shape constrained inference in terms of methodology development—see [32] for a recent overview.

We consider a structured variant of (1.1) which allows for density estimation under shape constraints. That is, we assume the density \(x \mapsto \sum_{i \in [M]} w_i \psi_i(x)\) obeys a pre-specified shape constraint such as monotonicity (e.g., decreasing), convexity, unimodality, among others [12]. To this end, we consider a special family of basis functions, the Bernstein polynomial bases [5,31 Ch 7], which are well-known for their (a) appealing shape-preserving properties, and (b) ability to approximate any smooth function over a compact support to high accuracy. Density estimation with Bernstein polynomials have been studied in the statistics community [37,2,9,36], though the exact framework and algorithms we explore herein appear to be novel, to our knowledge. Given an interval \([0,1]\) (say \(1\)) the Bernstein polynomials of degree \(M\) are given by a linear combination of the following Bernstein basis elements

\[
\tilde{b}_m(x) = \begin{cases} 
\frac{\Gamma(M+1)}{\Gamma(m+1) \Gamma(M-m+1)} x^{m-1} (1-x)^{M-m} & \text{if } x \in [0,1] \\
0 & \text{otherwise}
\end{cases}
\]

for \(m \in [M]\); and \(\Gamma(\cdot)\) is the standard Gamma function. This leads to a family of 1D smooth densities on the unit interval, of the form \(g_B(x) = \sum_{m=1}^M w_m \tilde{b}_m(x)\) where the mixture proportions (given by \(w\)) lie on the \(M\)-dimensional simplex (i.e., \(\Delta_M\)). Note that \(\tilde{b}_m(x)\) is a Beta-density with shape parameters \(m\) and \(M - m + 1\); and \(g_B(x)\) can be interpreted as a finite mixture of Beta-densities.

\footnote{For a general compact interval \([a,b] \subset \mathbb{R}\), one can obtain a suitable bases representation via a standard affine transformation mapping \([a,b]\) to \([0,1]\).}
Estimation under polyhedral shape constraints. An appealing property of the Bernstein bases representation is their shape preserving nature \[5, 31\]: a shape constraint on \( m \mapsto w_m \) translates to a shape constraint on \( x \mapsto g_B(x) \), restricted to its support \([0, 1] \). In particular, consider the following examples:

- If \( w_m \leq w_{m+1}, m \in [M - 1] \), i.e., \( m \mapsto w_m \) is an increasing sequence, then \( x \mapsto g_B(x) \) is increasing.
  Similarly, if \( m \mapsto w_m \) is decreasing, then \( x \mapsto g_B(x) \) is a decreasing density.

- If \( 2w_m \geq w_{m-1} + w_{m+1} \) for all \( 2 \leq m \leq M - 1 \), i.e., \( m \mapsto w_m \) is concave, then \( x \mapsto g_B(x) \) is concave.
  Similarly, if \( m \mapsto w_m \) is convex, then \( x \mapsto g_B(x) \) is convex.

The shape preserving property also extends to combinations of constraints mentioned above: for example, when the sequence \( m \mapsto w_m \) is decreasing and convex, then so is the density \( x \mapsto g_B(x) \). For all these shape constraints, \( w \) lies in a convex polyhedral set.

In order to estimate the mixture density \( g_B(x) \), we estimate the weights \( \{ w_m \}^M \) such that they lie in the \( M \)-dimensional unit simplex and in addition, obey suitable shape constraints. The MLE for this setup is given by a constrained version of (1.1):

\[
\min_w f(w) := -\frac{1}{N} \sum_{j=1}^N \log(\sum_{i\in[M]} w_i B_{ij}) \quad \text{s.t.} \quad w \in C := \Delta_M \cap S.
\] (1.3)

where, \( B_{ij} = \psi_i(X_j) = \tilde{b}_i(X_j) \); and \( S \) is a convex polyhedron corresponding to the shape constraint.\(^2\)

In addition to the shape constraints mentioned earlier, another useful shape restricted family arises when \( m \mapsto w_m \) is a unimodal sequence \([5, 36]\) i.e., a sequence with one mode or maximum \(\tilde{m} \). A unimodal sequence \( \{ w_m \} \) leads to a unimodal density \( g_B(x) \) \([5]\). In order to obtain the maximum likelihood estimate of \( g_B(x) \) under the assumption that it is unimodal (but the mode location is unknown), we will need to minimize \( f(w) \) over all unimodal sequences \( w \), lying on the unit simplex. If we know that the unimodal sequence \( m \mapsto w_m \) has a mode at \( m_0 \in [M] \), then \( w \) lies in a convex polyhedral set \( C_{m_0} \) (say)—this falls into the framework of (1.3). To find the best modal location, we will need to find the location \( m_0 \in [M] \) that leads to the largest log-likelihood—this can be done by a one-dimensional search over \( m_0 \) (for further details, see Section 4.1.7). A detailed discussion of the different polyhedral shape constraints we consider in this paper can be found in Section 4.1.

The presence of additional (shape) constraints in (1.3) poses further algorithmic/scalability challenges, compared to the special case (1.1), discussed earlier. Our main goal in this paper is to present a new scalable computational framework for (1.3) with computational guarantees.

For motivation, Figure 1 illustrates density estimates available from solutions of (1.3). We consider a synthetic dataset where the underlying density is decreasing; and estimate the density by solving (1.3) for two choices of \( S \): (a) Here we consider \( S = \mathbb{R}^M \) (with no shape constraint), and (b) \( S \) corresponds to all decreasing sequences \( m \mapsto w_m \). Figure 1 shows that without shape constraints, the estimated density can have spurious wiggly artifacts, which disappear under shape constraints. The estimated weights \( w \), are shown in the right panel.

Earlier work in statistics has studied density estimation under various shape constraints: examples include, convex \([13]\), monotone \([11]\), convex and decreasing \([13]\) shape constraints.\(^3\) As an example of a concave density, we can consider the triangular distribution on \([0, 1] \). —Section 6 presents our numerical experience with shape-constrained densities arising in real-world datasets. The approach we pursue here,

\(^2\)For example, \( S = \{ w \in \mathbb{R}^M : w_1 \leq \cdots \leq w_M \} \) implies that \( x \mapsto g_B(x) \) is decreasing. See Section 4 for details.

\(^3\)In this paper, for a unimodal sequence \( \{ w_m \}^M \), we use the convention that the sequence is first increasing and then decreasing, with a maximum located somewhere in \( \{ 1, \ldots, M \} \).

\(^4\)Another important family of shape constrained densities are log-concave densities \([33]\). While a log-concavity constraint on the weights \( \{ w_i \} \) leads to a log-concave density \( x \mapsto g_B(x) \) [22], see for example], a log-concavity constraint on \( w_i \)'s is not convex; and hence does not fall into our framework. This being said, log-concave densities are unimodal, and our framework can address unimodal densities on a compact support.
Figure 1: [Left panel] Nonparametric density estimates obtained from (1.3) under two different settings: (a) no shape restriction; (b) a decreasing constraint. We draw $N = 5000$ independent samples, each $X_i$ was taken to be the absolute value of a standard Gaussian (values $\geq 3$ were discarded)—all $X_i$-values were then re-scaled to $[0, 1]$. We consider $M = 100$ Bernstein bases elements for both estimators. [Right panel] shows the estimated weight vector $w$ as available from (1.3).

based on learning the proportions of a nonparametric mixture of Bernstein polynomials, differs from these earlier approaches—the density estimate available from (1.3), satisfies the imposed shape constraint and is also smooth. On the other hand, nonparametric density estimation under shape constraints such as monotonicity, convexity (for example) do not lead to smooth estimators.

### 1.3 Contributions

In this paper we study a new algorithmic framework for nonparametric density estimation with possible shape constraints. Our approach is based on a maximum likelihood framework to learn the proportions of a finite mixture model subject to polyhedral constraints; and is given by Problem (1.3). To our knowledge, the general form of estimator (1.3) that we consider here, has not been studied earlier—though, special instances of this framework has been studied before [20, 22, 36, 17, see for example]. In the special case of Problem (1.1) when the bases elements correspond to a Gaussian location mixture family, we present guarantees on how well a solution to the finite mixture problem approximates the infinite version of Kiefer-Wolfowitz nonparametric MLE [19].

Our algorithm for (1.3) is based on a Newton method with cubic regularization, a related method was first proposed by [30] for a different family of optimization problems. Specifically, the setup of [30] does not apply to our setting as we have a self-concordant objective function $f$ with (possibly) unbounded gradients, and polyhedral constraints. Our proposed algorithm at every iteration solves a modified Newton step: this is a second order local model for $f$ with an additional cubic regularization that depends upon the local geometry of $f$ (see Section 3 for details). We establish a worst case $O(1/k^2)$ convergence rate of our algorithm (where, $k$ denotes the number of cubic regularized Newton steps); and also derive a local quadratic convergence guarantee. For every cubic Newton step, we need to solve a structured convex problem for which we use Frank-Wolfe methods [7, 23]. We present nearly closed-form solutions for the linear optimization oracles arising in the context of the Frank-Wolfe algorithms. To our knowledge, these linear optimization oracles have not been studied before, and may be of independent interest.

We numerically compare our algorithms for (1.3) with different choices of $C$, versus various existing benchmarks for both synthetic and real datasets. For the special case of (1.1), our approach leads up to a 3X-5X improvement in runtime over the recent solver [20]; and a 10X-improvement over the commercial solver Mosek (both in terms of obtaining a moderate-accuracy solution). Furthermore, in the presence of shape constraints, our approach can lead to a 20X-improvement in runtimes over Mosek, and is more memory-friendly (especially, for larger problem instances).
1.4 Related Work

Damped Newton methods [29] are commonly used for unconstrained problems with a self-concordant objective. [28, 29] present computational guarantees of damped Newton for unconstrained minimization of self-concordant functions. [35] generalize such damped Newton methods for optimization over additional (simple) constraints; and establish computational guarantees—these methods have been further generalized by [34], motivated by applications in statistics and machine learning.

In a different line of work, [30] introduced a cubic regularized Newton algorithm in the context of a convex optimization problem of the form $\min_{x \in \mathbb{R}^d} H(x)$ where, the convex function $H$ has a Lipschitz continuous Hessian: $\|\nabla^2 H(x) - \nabla^2 H(y)\| \leq L \|x - y\|$ for all $x, y$ (here, $\| \cdot \|$ is the Euclidean norm), for some constant $L > 0$. As noted by [30], a unique aspect of the cubic Newton method is that it leads to a global worst case convergence guarantee of $O(1/k^2)$, similar guarantees are not generally available for Newton-type methods with few exceptions. [30] also show local quadratic convergence guarantees for the cubic Newton method. However, as mentioned earlier, these results do not directly carry over to the setting of (1.3) as our objective function $f(\cdot)$ does not have a Lipschitz continuous Hessian; additionally, Problem (1.3) is a constrained optimization problem. A main technical contribution of our work is to address these challenges.

In other work pertaining to first order methods, [6] presents an analysis of the Frank Wolfe method for self-concordant objective functions with a possible constraint (e.g., a simplex or the $\ell_1$-ball constraint). Proximal gradient methods [35] have also been proposed for a similar family of problems. During the preparation of this manuscript, we became aware of a recent work [26] who also consider the minimization of a family of self-concordant functions with possible constraints. They propose a proximal damped Newton-method where the resulting sub-problem is solved via Frank Wolfe methods, leading to a double-loop algorithm. [26] study problems in portfolio optimization, the D-optimal design and logistic regression.

As mentioned earlier, recently [20] presents a specialized algorithm for (1.1) leading to improvements over Mosek’s interior point algorithms [22, 21] and the EM algorithm [17]. The method of [20] however does not apply to the shape constrained problem (1.3). [20] do not discuss complexity guarantees for their proposed approach.

Organization. The rest of the paper is organized as follows. Section 3 presents our main algorithm, along with its global and local computational guarantees. In Section 4 we discuss how to solve the cubic-regularized Newton step via Frank Wolfe along with the linear optimization oracles. In Section 5 we derive bounds on how well a solution to the finite mixture problem approximates the infinite dimensional Kiefer-Wolfowitz problem. Section 6 presents numerical results for our proposed method and comparisons with several benchmarks. Proofs of all results and additional technical details can be found in the Supplement.

2 Notation and Preliminaries

For an integer $n \geq 1$, let $[n] := \{1, 2, ..., n\}$. We let $\mathbb{R}^n := \{x \in \mathbb{R}^n : x_i \geq 0 \forall i \in [n]\}$ denote the nonnegative orthant; $\mathbb{R}^n_+ := \{x \in \mathbb{R}^n : x_i > 0 \forall i \in [n]\}$ denote the interior of $\mathbb{R}^n_+$; and $1_n$ denote the vector in $\mathbb{R}^n$ with all coordinates being 1. For any $M \times M$ positive semidefinite matrix $A$, we define $\|w\|_A := \sqrt{w^T A w}$ for any vector $w \in \mathbb{R}^M$; $A[w, u] := u^T A w$ for any vectors $w, u$; and write $A[u]^2 := A[u, u]$. Moreover, for any symmetric tensor $T \in \mathbb{R}^{M \times M \times M}$ and vectors $u, v, w \in \mathbb{R}^M$, we define $T[u, v, w] := \sum_{i,j,k} T[i,j,k] u_i v_j w_k$ and use the shorthand $T[u]^3 := T[u, u, u]$. For any function $g$ that is thrice continuously differentiable on
an open set \( U \subseteq R^M \), and \( w \in U \), let \( \nabla^3 f(w) \in R^{M \times M \times M} \) be the tensor of third-order derivatives:

\[
[\nabla^3 f(w)]_{i,j,k} = \frac{\partial^3}{\partial w_i \partial w_j \partial w_k} f(w), \quad i,j,k \in \{1, \ldots, M\}.
\]

For any two symmetric matrices \( A, \tilde{A} \subseteq R^{n \times n} \), we use the notation \( A \preceq \tilde{A} \) if \( \tilde{A} - A \) is positive semidefinite, and \( A \succeq \tilde{A} \) if \( A - \tilde{A} \) is positive semidefinite. For matrix \( B = ((B_{ij})_{i,j} \subseteq R^{M \times N} \) in (1.3) let the \( j \)-th column be denoted by \( B_j := [B_{1j}, B_{2j}, \ldots, B_{Mj}]^\top \subseteq R^M \) for \( j \in \{1, \ldots, N\} \).

### 2.1 Preliminaries on self-concordant functions

We present some basic properties of self-concordant functions following [29] that we use. For further details, see [29].

Let \( Q \) be an open nonempty convex subset of \( R^n \). A thrice continuously differentiable function \( F : Q \to R \) is called \( \alpha \)-self-concordant if it is convex and for any \( x \in Q, u \subseteq R^n \), it holds

\[
|\nabla^3 F(x)|u, u, u| \leq 2\alpha^{-1/2}(\nabla^2 F(x)|u, u|)^{3/2}.
\]

For the same function \( F \) and \( x \in Q \), let us define:

\[
\|u\|_{F,x} := ((1/\alpha)\nabla^2 F(x)|u, u|)^{1/2}.
\]

For any \( y \in Q \) such that \( \bar{r} := \|x - y\|_{F,x} < 1 \), we have the following ordering:

\[
(1 - \bar{r})^2 \nabla^2 F(x) \preceq \nabla^2 F(y) \preceq \frac{1}{(1 - \bar{r})^2} \nabla^2 F(x).
\]

If a function \( F \) is \( 1 \)-self-concordant on \( Q \), then it holds

\[
F(y) \geq F(x) + \nabla F(x)^\top (y - x) + \rho (\|y - x\|_{\nabla^2 F(x)})
\]

where the function \( \rho : R_+ \to R_+ \) is given by \( \rho(t) = t - \log(1 + t) \).

The following result [28, Section 4.1.3] follows from the definition of self-concordance.

**Lemma 2.1** The function \( w \mapsto f(w) \) defined in (1.3) is \((1/N)\)-self-concordant.

### 3 A cubic-regularized Newton method for Problem (1.3)

In this section, we develop our proposed algorithmic framework for problem (1.3). For \( f, y \in \mathcal{C} \), define

\[
\Phi_f(y, w) := f(w) + \nabla f(w)^\top (y - w) + \frac{1}{2} \nabla^2 f(w)[y - w]^2
\]

as a local second order model for \( y \mapsto f(y) \) around the point \( w \).

Our proposed method is presented in Algorithm 1 which is a modification of the original cubic regularized Newton method by [30] proposed for a different family of problems.

Note that Step 2 in Algorithm 1 differs from that proposed in [30]—the cubic regularization term we use \((L_k/6)\|\nabla^2 f(w_k)[y - w_k]\|^3/2\), depends upon the local curvature of the objective function; and a local \( L_k \). In contrast, [30] uses a cubic regularization term \( L/6\|y - w_k\|^2 \) (note the use of the Euclidean norm) and a fixed value of the Lipschitz constant (of the Hessian), \( L \). Intuitively speaking, the regularization term in (3.2) restricts the distance of the update \( y^k \) from \( w_k \), by adapting to the local geometry of the self-concordant function \( f(\cdot) \). If the regularization term is too small, and the condition (3.3) in step 3 does not hold, then we increase \( L_k \). In Section 3.1, we prove that \( \sup_{k \geq 1} \{L_k\} \) will be bounded by a constant multiple of \( N \) (this does not depend upon the data \( B \) or the constraints), implying that \( L_k \) can be increased for at most a finite number of times.
Algorithm 1 A cubic regularized Newton method for Problem (1.3)

Input: initial point \( w^0 \in C \); initial regularization parameter \( L_0 > 0 \); two non-negative sequences \( \{\gamma_i\}_{i=1}^\infty \) and \( \{\rho_i\}_{i=1}^\infty \); enlarging parameter \( \beta > 1 \).

For \( k = 1, 2, \ldots \)
1. Set \( L_k = L_{k-1} \).
2. Find an approximate solution \( y^k \) of
\[
\min_{y \in C} \left\{ h_f(y, w^k) := \Phi_f(y, w^k) + \frac{L_k}{6}\|y - w^k\|^3_{\nabla^2 f(w^k)} \right\}.
\]

3. If
\[
f(y^k) \leq \Phi_f(y^k, w^k) + \frac{L_k}{6}\|y^k - w^k\|^3_{\nabla^2 f(w^k)} + \gamma_k,
\]
let \( w^{k+1} \) be a point satisfying
\[
f(w^{k+1}) \leq f(w^k) \quad \text{and} \quad f(w^{k+1}) \leq f(y^k) + \rho_k.
\]

Else, let \( L_k = \beta L_k \) and go back to step 2.

Note that Algorithm 1 allows for an inexact solution of sub-problem (3.2). As we discuss in Section 4, this sub-problem cannot be solved in closed form—we use a Frank Wolfe method to approximately solve the sub-problems efficiently. As long as the accuracy of solving (3.2) suitably decreases as the algorithm proceeds, the global convergence still holds (See Section 3.1).

Finally, Algorithm 1 allows for a flexible choice of \( w^{k+1} \) as long as it satisfies condition (3.4) with a sequence of tolerances \( \{\rho_i\}_{i=1}^\infty \). A natural special case is \( w^{k+1} = y^k \) with \( \rho_k = 0 \)—In our numerical experiments, we observe that this flexibility can be helpful in the initial stages of the algorithm and can lead to improved computational performance and an overall reduction of running times.

Finally, we note that Algorithm 1 is different from both the damped Newton method in [29] and the cubic-regularized Newton method in [30].

3.1 Computational guarantees

Here we establish the convergence properties of Algorithm 1. In Section 3.1.1, we establish a global (worst case) sublinear \( O(1/k^2) \) rate of convergence for Algorithm 1 (See Theorem 3.3). An ingredient in this proof is that the adaptive parameter \( L_k \) is bounded above by a constant that does not depend upon the problem data \( B \) or the constraints (cf Lemma 3.2). In Section 3.1.2, we establish a local quadratic convergence of Algorithm 1 in terms of \( \|w^k - w^*\|_{H_*} \) where, \( w^* \) is an optimal solution of Problem (1.3) and \( H_* = \nabla^2 f(w^*) \) is the Hessian of the objective at an optimal solution. Proofs of results in this section appear in Section B.1.

3.1.1 A global sublinear convergence rate

We make a mild assumption pertaining to the updates (3.2) in Algorithm 1.

Assumption 3.1 Suppose \( y^k \) (computed in Step 2 of Algorithm 1) satisfies
\[
\Phi_f(y^k, w^k) + \frac{L_k}{6}\|y^k - w^k\|^3_{\nabla^2 f(w^k)} \leq f(w^k).
\]

Note that condition (3.5) is satisfied if we set \( y^k = w^k \), hence Assumption 3.1 should be satisfied by any reasonable solution of sub-problem (3.2). The following lemma makes use of Assumption 3.1 to establish that the sequence \( \{L_k\} \) is bounded.
Lemma 3.2 (Boundedness of $L_k$) Let $f(\cdot)$ be defined in (1.3) and $\{L_k\}_{k=0}^\infty$ be the parameters generated in Algorithm 1. Suppose Assumption 3.1 is satisfied. If we take $\beta \in (1, 2)$ in Algorithm 2, then

$$L_k \leq \max\{48N, L_0\} \quad \forall k \geq 1. \quad (3.6)$$

Lemma 3.2 shows that $L_k$ is bounded by a constant that depends on $N$, but not the data $B$. This is a consequence of the self-concordance property of $f(\cdot)$. Based on our numerical experience however, it appears that the worst-case bound in (3.6) is conservative.

Before stating the global convergence result, we introduce some new notations. Let us define the sub-level set

$$X^0 := \{w \in C : f(w) \leq f(w^0)\},$$

where $w^0$ is an initialization for Algorithm 1. Let $w^*$ be an optimal solution of (1.3) and define

$$C_1 := \sup_{w \in X^0} \frac{1}{N} \sum_{i=1}^N \max \left\{ \left| \frac{\langle B_i, w - w^* \rangle}{\langle B_i, w \rangle} \right|^3, \left| \frac{\langle B_i, w - w^* \rangle}{\langle B_i, w^* \rangle} \right|^3 \right\}, \quad \text{and}$$

$$C := (1/3) \max \left\{ 1 + \sup_{k \geq 0} L_k/2 \right\} C_1, \quad f(w^0) - f^*.$$  \hspace{1cm} (3.7)

Note that $C_1$ defined above, is finite.\footnote{In addition, by Lemma 3.2, $C$ is also finite. Let $f^*$ be the optimal objective value of (1.3). With these notations, we can state the following global convergence result:}

Theorem 3.3 (Global sublinear convergence) Let $\{w^k\}_{k=1}^\infty$ be the sequence from Algorithm 1. Let $\delta_k$ be a measure of how close $y^k$ is to minimizing Problem (3.2), that is,

$$\delta_k := h_f(y^k, w^k) - \min_{y \in C} h_f(y, w^k). \quad (3.8)$$

For $i \geq 1$ let $E_i := \gamma_i + \rho_i + \delta_i$. Then for all $k \geq 2$ it holds

$$f(w^{k+1}) - f^* \leq \frac{30C}{(k + 2)^2} + \frac{1}{(k + 1)^3} \sum_{i=1}^k (i + 3)^3 E_i.$$  \hspace{1cm} (3.9)

The following corollary states that under mild assumptions on the sequence $\{\delta_k, \gamma_k, \rho_k\}_{k \geq 1}$, Algorithm 1 converges to the minimum of (1.3) at a sublinear rate.

Corollary 3.4 Under the statements of Theorem 3.3 if the sequences $\{\gamma_k\}_{k=1}^\infty$, $\{\rho_k\}_{k=1}^\infty$ are set such that $\sum_{k=1}^\infty (\gamma_k + \rho_k)k^3 < \infty$, and the errors $\delta_k$ of solving sub-problems also satisfy $\sum_{k=1}^\infty \delta_k k^3 < \infty$, then Algorithm 1 has a global convergence rate $O(1/k^2)$.

Particular choices of the parameters $\delta_k, \gamma_k$, and $\rho_k$ are discussed in Section 6.

3.1.2 A local quadratic convergence rate

Theorem 3.5 below presents the local convergence properties of Algorithm 1 when $E_k = 0$ for all $k$. The proof is based on the analysis of the cubic regularized Newton method in [30] combined with basic properties of self-concordant functions. For this result we assume the matrix $B$ has full row rank – this implies the Hessian $\nabla^2 f(w)$ is positive definite for all $w \in C$ with $f(w) < \infty$. Our local convergence rate is stated using the norm $\| \cdot \|$ of $\nabla^2 f(w^*)$, similar to the local convergence rates in [35] for the damped Newton method.

\footnote{To see this, note that if $C_1 = \infty$, then we can find a sequence $\tilde{w}^k \in X^0$ such that $f(\tilde{w}^k) \to \infty$ as $k \to \infty$, which is a contradiction to the fact $\tilde{w}^k \in X^0$.}
Theorem 3.5 (Local quadratic convergence) Consider a special case of Algorithm 1 with \( \delta_k = \gamma_k = \rho_k = 0 \) and let \( w^{k+1} = y^k \) in Step 3. Let \( \{w^k\}_{k=0}^\infty \) be the iterates from Algorithm 1 and let \( L := \sup_{k \geq 0} \{L_k\} \) and \( H_* := \nabla^2 f(w^*) \). If for some \( K > 0 \), the following holds:

\[
(6\sqrt{N} + 2L)\|w^K - w^*\|_{H_*} \leq 1.
\]

Then for all \( k \geq K \), we have

\[
\|w^{k+1} - w^*\|_{H_*} \leq (6\sqrt{N} + 2L)\|w^k - w^*\|_{H_*}^2.
\]

4 Solving the cubic regularized Newton step with Frank-Wolfe

To implement Algorithm 1 we need an efficient method for (approximately) solving the cubic regularized Newton step (3.2). We use the Frank-Wolfe method with away steps \([15, 24]\) for this purpose. Frank-Wolfe method \([7, 16]\) is a classical algorithm for constrained convex optimization with a compact constraint set. It is called a “projection-free” method since at every iteration, we need access to a linear programming (LP) oracle (over the constraint set). The Away-step Frank-Wolfe (AFW) is a variant of the classical Frank-Wolfe method which usually leads to improved sparsity properties and enjoys a global linear convergence rate when the objective function is strongly convex and the constraint set is a polytope.\(^6\) Owing to space constraints, a formal description of our AFW algorithm is presented in Section A. For improved practical performance, AFW requires efficient solutions to the LP oracles and efficient methods to store a subset of vertices of the polyhedral constraint set, as we discuss next.

4.1 Solving the LP oracle

We discuss how to efficiently solve the LP oracle

\[
\min_{w \in C} \langle g, w \rangle \tag{4.1}
\]

for the different choices of the polyhedral set \( C \) that we consider here. In particular, we provide a description of the set of vertices \( V(C) \), which leads to a solution of (4.1). This can also be used to compute the away step, which requires solving a linear oracle over a subset of vertices.

Proofs of all technical results in this section can be found in Section B.2.

4.1.1 No shape restriction

The constraint \( C = \Delta_M \), the \( M \)-dimensional unit simplex, has \( M \) vertices, corresponding to the standard orthogonal bases elements \( \{e_i\}_{i=1}^M \). Here, solving the LP (4.1) is equivalent to finding the minimum value of \( g \).

4.1.2 Monotonicity constraint

For monotone density estimation via formulation \([1, 3]\) with Bernstein polynomial bases, we consider the following choices for the polyhedral set \( C \):

\[
C^- = \{ w \in \mathbb{R}^M : 1^T_M w = 1, \ w \geq 0, \ w_1 \geq \cdots \geq w_M \},
\]

\[
C^+ = \{ w \in \mathbb{R}^M : 1^T_M w = 1, \ w \geq 0, \ w_1 \leq \cdots \leq w_M \} \tag{4.2}
\]

which correspond to monotonically decreasing and increasing sequences (densities), respectively. We show below that after a linear transformation, the constraint sets in (4.2) can be transformed to the standard simplex, for which the LP oracle can be solved in closed form.

\(^6\)We note that there are several variants of Frank-Wolfe \([8]\) see for example that result in improvements over the basic version of the Frank-Wolfe method. We use the away-step variant for convenience, though other choices are also possible.
Proposition 4.1 (Decreasing) Let \( U \in \mathbb{R}^{M \times M} \) be an upper triangular matrix with \( U_{i,j} = 1/j \) for \( j \geq i \) and \( i \in [M] \). Then, we can equivalently write \( C^- \) as

\[
C^- = U(\Delta_M) := \left\{ y \in \mathbb{R}^M : 1_M^\top y = 1, \ y \geq 0 \right\}.
\]

For any given \( g \in \mathbb{R}^M \), the LP (4.1) (with \( C = C^- \)), is equivalent to solving

\[
\min_y \langle U^\top g, y \rangle \ \text{s.t.} \ 1_M^\top y = 1, \ y \geq 0
\]

which is equivalent to finding the minimum value in the vector \( U^\top g \). By exploiting the structure of matrix \( U \), computing \( U^\top g \) only needs \( O(M) \) operations.

Similarly, when \( C = C^+ \) (increasing sequence), we arrive at the following proposition.

Proposition 4.2 (Increasing) Let \( U \in \mathbb{R}^{M \times M} \) be a lower triangular matrix with \( U_{i,j} = 1 / (M - j + 1) \) for \( i \geq j \) and \( j \in [M] \). Then we have

\[
C^+ = U(\Delta_M) := \left\{ y \in \mathbb{R}^M : 1_M^\top y = 1, \ y \geq 0 \right\}.
\]

The LP oracle (4.1) (for \( C = C^+ \)) can be solved in a manner similar to the case of \( C^- \) — we omit the details for brevity.

4.1.3 Concavity constraint

For concave density estimation with a Bernstein polynomial bases (see Section 1.2), in Problem (1.3), we consider \( C = C^\wedge \), where

\[
C^\wedge = \left\{ w \in \mathbb{R}^M : 1_M^\top w = 1, \ w \geq 0, \ w \text{ is concave} \right\}.
\]

The following proposition provides a description of the extreme points of the set \( C^\wedge \).

Proposition 4.3 (Concave) \( C^\wedge \) has \( M \) vertices, which are given by

\[
v_1 = \frac{2}{M(M-1)} (0, 1, ..., M-1)^\top, \ v_M = \frac{2}{M(M-1)} (M-1, M-2, ..., 1, 0)^\top,
\]

\[
v_j = (0, p_j, ..., (j-1)p_j, (M-j-1)q_j, (M-j-2)q_j, ..., q_j, 0)^\top \quad 2 \leq j \leq M-1,
\]

where \( p_j = 2 / ((M - 1)(j - 1)) \) and \( q_j = 2 / ((M - 1)(M - j)) \) for all \( 2 \leq j \leq M-1 \).

Let \( V \) be the matrix whose columns are \( v_1, \ldots, v_M \). For any given \( g \in \mathbb{R}^M \), the LP oracle \( \min_{w \in C^\wedge} \langle g, w \rangle \) amounts to solving the following problem

\[
\min_y \langle V^\top g, y \rangle \ \text{s.t.} \ 1_M^\top y = 1, \ y \geq 0
\]

which is equivalent to finding the minimum entry in the vector \( V^\top g \). A careful analysis shows that computing \( V^\top g \) only requires \( O(M) \) operations.

4.1.4 Convexity constraint

Similar to Section 4.1.3 (concavity constraint), we consider the case when \( C \) in (1.3) corresponds to a convex sequence, resulting in a convex density estimate. Here, in Problem (1.3), we take \( C = C^\vee \) where,

\[
C^\vee = \left\{ w \in \mathbb{R}^M : 1_M^\top w = 1, \ w \geq 0, \ w \text{ is convex} \right\}.
\]

For any \( k \geq 0 \), let \( 0_k \) denote a vector in \( \mathbb{R}^k \) with all coordinates being 0. The following proposition describes the vertices of \( C^\vee \).
Proposition 4.4 (Convex) $\mathcal{C}^\vee$ has $2M$ vertices, which are given by

$$\bigcup_{k=1}^{M} \left\{ a_k^{-1}(0_{M-k}^T, 1, 2, \ldots, k), a_k^{-1}(k, k-1, \ldots, 2, 1_{M-k}^T) \right\}$$

where $a_k = (k + 1)/2$ for all $k \in [M]$.

By Proposition 4.4 solving the LP oracle (4.1) with $\mathcal{C} = \mathcal{C}^\vee$ amounts to computing

$$\min \left\{ \min_{1 \leq k \leq M} \left\{ a_k^{-1} \sum_{i=1}^{k} ig_{i+k-M} \right\}, \min_{1 \leq k \leq M} \left\{ a_k^{-1} \sum_{i=1}^{k} ig_{k+1-i} \right\} \right\}.$$  

With a careful cost accounting, the above can be computed within $O(M)$ operations.

4.1.5 Concavity and monotonicity restriction

We consider the cases when $\mathcal{C}$ corresponds to a combination of concavity and monotonity constraints:

$$\mathcal{C}^{\land+} = \left\{ w \in \mathbb{R}^M : 1_M^T w = 1, w \geq 0, w \text{ is increasing and concave} \right\},$$

$$\mathcal{C}^{\land-} = \left\{ w \in \mathbb{R}^M : 1_M^T w = 1, w \geq 0, w \text{ is decreasing and concave} \right\}.$$  

Following our discussion in Section 4.1.2, if we set $\mathcal{C} = \mathcal{C}^{\land+}$ in (1.3) and use Bernstein polynomial bases, we obtain a maximum likelihood density estimate that is concave and increasing. Similarly, $\mathcal{C}^{\land-}$ leads to a density that is concave and decreasing. Propositions 4.5 and 4.6 below describe the set of vertices of $\mathcal{C}^{\land+}$ and $\mathcal{C}^{\land-}$, respectively.

Proposition 4.5 (Concave and increasing) $\mathcal{C}^{\land+}$ has $M$ vertices, which are given by

$$v_1 = M^{-1} 1_M, \quad v_M = r_M(0, 1, 2, \ldots, M-1)^T,$$

$$v_i = r_i(0, 1, \ldots, i-2, i-1, (i-1)1_{M-i}^T)^T, \quad 2 \leq i \leq M-1,$$

where $r_i = 2/((2M-i)(i-1))$ for $2 \leq i \leq M$.

Similar to Proposition 4.5, we present the corresponding proposition for $\mathcal{C}^{\land-}$, whose proof is omitted due to brevity.

Proposition 4.6 (Concave and decreasing) $\mathcal{C}^{\land-}$ has $M$ vertices, which are given by

$$v_1 = M^{-1} 1_M, \quad v_M = r_M(M-1, M-2, \ldots, 1, 0)^T,$$

$$v_i = r_i((i-1)1_{M-i}^T, i-1, i-2, \ldots, 1, 0)^T, \quad 2 \leq i \leq M-1,$$

where $r_i = 2/((2M-i)(i-1))$ for $2 \leq i \leq M$.

In light of Propositions 4.5 and 4.6, we can efficiently compute the corresponding LP oracles (4.1) with $\mathcal{C} = \mathcal{C}^{\land+}$ and $\mathcal{C} = \mathcal{C}^{\land-}$.

4.1.6 Convexity and monotonicity restriction

We consider the cases when $\mathcal{C}$ corresponds to a combination of convexity and monotonity constraints. Here, the constraint set $\mathcal{C}$ is one of the following:

$$\mathcal{C}^{\lor+} = \left\{ w \in \mathbb{R}^M : 1_M^T w = 1, w \geq 0, w \text{ is convex and increasing} \right\},$$

$$\mathcal{C}^{\lor-} = \left\{ w \in \mathbb{R}^M : 1_M^T w = 1, w \geq 0, w \text{ is convex and decreasing} \right\}.$$  

The following proposition describes the set of vertices of $\mathcal{C}^{\lor+}$.
Proposition 4.7 (Convex and increasing) $C^{v+}$ has $M$ vertices, which are given by:
\[
v_i = \frac{2}{i(i+1)} (0_{M-i}^\top, 1, 2, ..., i) = 1, 1 \leq i \leq M-1; \text{ and } v_M = \frac{1}{M} 1_M.
\]

Similarly, we have the following proposition for $C^{v-}$, whose proof is omitted.

Proposition 4.8 (Convex and decreasing) $C^{v-}$ has $M$ vertices, which are given by:
\[
v_i = \frac{2}{i(i+1)} (i, i-1, ..., 2, 1, 0_{M-i}) = 1, 1 \leq i \leq M-1; \text{ and } v_M = \frac{1}{M} 1_M.
\]

Using Propositions 4.7 and 4.8, one can maintain the active vertices and solve the LP oracles, in a manner similar to our earlier discussions.

### 4.1.7 Unimodality constraint

We consider a special case of (1.1) when the $i$-th mixture component is a Gaussian density with unit variance and mean $\mu_i$ for $i \in [M]$. In this case, Problem (1.3) with $C$ vertices of $\mathcal{C}$ can be interpreted as a finite dimensional version of the original Keifer-Wolfowitz nonparametric MLE problem [19, 22].

\[
C_{k}^{um} = \{w \in \mathbb{R}^M : 1_m^\top w = 1, \ w_1 \leq \cdots \leq w_k, \ w_k \geq \cdots \geq w_M\}.
\]

(4.5)

To estimate $g_B(x)$ under a unimodality constraint on $w$ where the mode location is unknown, we solve Problem (1.3) with $C = C_{k}^{um}$ for each $k \in [M]$. Then we choose the value of $k$ which minimizes the negative log-likelihood or equivalently, the objective $f(w)$ in (1.3). This leads to the MLE for the mixture density $g_B(x)$ under the assumption of unimodality.

We now discuss how to solve the LP oracle when $w \in C_{k}^{um}$ for a fixed $k$. The following result lists all vertices of $C_{k}^{um}$.

Proposition 4.9 $C_{k}^{um}$ has $k(M-k+1)$ vertices, which are given by: $v_{k_1,k_2}$ for $1 \leq k_1 \leq k \leq k_2 \leq M$, where the $i$-th element in $v_{k_1,k_2} \in \mathbb{R}^M$ is:
\[
v_i^{k_1,k_2} = \begin{cases} 0 & \text{for } i < k_1 \text{ or } i > k_2 \\ \frac{1}{(k_2 - k_1 + 1)} & \text{for } k_1 \leq i \leq k_2. \end{cases}
\]

Let $U$ be the matrix with columns being the vertices of $C_{k}^{um}$. For a given $g \in \mathbb{R}^M$, solving the linear oracle $\min_{w \in C_{k}^{um}} \langle g, w \rangle$ amounts to finding the minimum entry in the vector $U^\top g$. This requires $O(k(M-k))$ operations with a careful manipulation.

### 5 Approximation guarantees for the Kiefer-Wolfowitz MLE

We consider a special case of (1.1) when the $i$-th mixture component is a Gaussian density with unit variance and mean $\mu_i$ for $i \in [M]$. In this case, Problem (1.1) can be interpreted as a finite dimensional version of the original Keifer-Wolfowitz nonparametric MLE problem [19, 22].

\[
p^* := \min_{g} - \sum_{i=1}^{N} \log \left( \int \varphi(X_i - \mu)dQ(\mu) \right)
\]

(5.1)

That is, $m \mapsto w_m$ is increasing at the beginning and then decreasing, with a maximum located somewhere in $\{1, \ldots, M\}$.
where $Q$ runs over all mixing distributions (of the location parameter, $\mu$) on $\mathbb{R}$. Note that a solution to (5.1) admits a finite dimensional solution [22], which can be described via a dual formulation of (5.1), as presented below.

**Theorem 5.1** (Theorem 2 of [22]) (Duality of (5.1)) Problem (5.1) has a minimizer $Q^*$, which is an atomic probability measure with at most $N$ atoms. The locations, $\{\mu_j^*\}$, and the masses, $\{\nu_j^*\}$, at these $N$ locations can be found via the following dual characterization:

$$\max_{\nu \in \mathbb{R}^N_+} \sum_{i=1}^N \log \nu_i \quad \text{s.t.} \quad \sum_{i=1}^N \nu_i \varphi(X_i - \mu) \leq N \quad \forall \mu \in \mathbb{R}. \tag{5.2}$$

The solution $\nu^*$ of (5.2) satisfies the extremal equations $\sum_j \varphi(X_i - \mu_j^*) \nu_j^* = 1/\nu_i^*, \ i \in [N]$, and $\mu_j^*$’s are exactly those values of $\mu$ at which the dual constraint is active.

The dual objective in (5.2) contains $N$ decision variables, but the constraints are infinite dimensional. While an optimal solution to (5.1) contains $N$ atoms, these locations are not known; and it is not clear how to efficiently identify these locations without solving the infinite-dimensional problem. [23,14] present algorithms to approximate this infinite dimensional problem (5.1). In particular, [25] proposes a vertex-directional method and provides bounds for the computed solution. We explore some properties of the commonly-used discretized version of (5.1) where $Q$ is supported on a pre-specified discrete set of atoms between $\min X_i$ and $\max X_i$—this version can be written in the form (1.1) and solved by Algorithm 1.

Note that if $G = \{\hat{\mu}_1, \cdots, \hat{\mu}_M\}$ ($\hat{\mu}_1 < \cdots < \hat{\mu}_M$) denotes a pre-specified set of $M$ atoms, then the discrete version of (5.1) is

$$\hat{\rho}_G := \min_{w \in \mathbb{R}^M} - \sum_{i=1}^N \log \left( \sum_{j=1}^M w_j \varphi(X_i - \hat{\mu}_j) \right) \quad \text{s.t.} \quad w \geq 0, \ \sum_{i \in [M]} w_i = 1. \tag{5.3}$$

The following proposition presents a dual of (5.3).

**Proposition 5.2** (Duality for finite dimensional approximation) The optimal objective of (5.3) equals the optimal objective of the following dual problem:

$$\max_{\nu \in \mathbb{R}^N} \sum_{i=1}^N \log \nu_i \quad \text{s.t.} \quad \sum_{i=1}^N \nu_i \varphi(X_i - \hat{\mu}_j) \leq N \quad \forall j \in [M], \ \nu \geq 0. \tag{5.4}$$

Furthermore, an optimal solution $\hat{\nu}$ of (5.3) and the optimal solution $\hat{\nu}$ of (5.4) are linked by $\sum_{j=1}^M \hat{\nu}_j \varphi(X_i - \hat{\mu}_j) = 1/\hat{\nu}_i$ for all $i \in [N]$. If for some $j \in [M]$ we have a strict inequality $\sum_{i=1}^N \nu_i \varphi(X_i - \hat{\mu}_j) < N$, then by complementary slackness, we have $\hat{\nu}_j = 0$.

The optimal objective value $\hat{\rho}_G$ of (5.3) is larger than the optimal objective value $p^*$ of (5.1). In the following, we present an upper bound on $\hat{\rho}_G - p^*$, which depends upon the discrete set of atoms $G$. To derive our result, we make use of the observation that $\varphi$ is Lipschitz continuous over $\mathbb{R}$, that is, for all $t_1, t_2 \in \mathbb{R}, |\varphi(t_1) - \varphi(t_2)| \leq 1/(\sqrt{2\pi})|t_1 - t_2|$.

**Proposition 5.3** (Primal optimality gap) Let $G = \{\hat{\mu}_1, \cdots, \hat{\mu}_M\}$ (with $\hat{\mu}_1 < \cdots < \hat{\mu}_M$) be a pre-specified set of discretized locations satisfying $\mu_1 \leq \min_{i \in [N]} X_i \leq \max_{i \in [N]} X_i \leq \hat{\mu}_M$. Let $\hat{\rho}_G$ be the optimal value of (5.3), and let $p^*$ denote the optimal value of the infinite dimensional problem (5.1). Let $\nu$ be the optimal solution of (5.4). Suppose $\Gamma > 0$ satisfies $\Gamma \geq \max_{\nu \in \mathbb{R}} \sum_{i=1}^N \nu_i \varphi(X_i - \mu)$. Then it holds

$$p^* \leq \hat{\rho}_G \leq p^* + N \log(\Gamma/N). \tag{5.5}$$
Let $\Delta G$ be the largest spacing among ordered atoms in $\mathcal{G}$, that is, $\Delta G := \max_i (\hat{\mu}_{i+1} - \hat{\mu}_i)$. Then we have

$$p^* \leq \hat{p}_G \leq p^* + N \log \left( 1 + \frac{\Delta G}{\sqrt{8 \pi e}} \frac{1}{N} \sum_{i=1}^N \hat{\nu}_i \right). \quad (5.6)$$

As a consequence of Proposition 5.3 if $\nabla G \approx 0$, then $p^* \approx \hat{p}_G$. Using Proposition 5.3 we present the following bound on the proximity of the dual solutions corresponding to the finite and infinite-dimensional problems.

**Proposition 5.4** (Error bound on dual optimal solutions) Let $\mathcal{G}$, $\hat{p}_G$ and $p^*$ be the same as in Proposition 5.3. Let $\hat{\nu}$ and $\nu^*$ be the optimal solutions of (5.4) and (5.2) respectively. Then it holds

$$\left( \sum_{i=1}^N (\nu^*_i - \hat{\nu}_i)^2 / \nu^2_i \right)^{1/2} \leq \rho^{-1}(\hat{p}_G - p^*), \quad (5.7)$$

where, $\rho^{-1}(t)$ denotes the inverse of the (strictly increasing) function $\rho(t) = t - \log(1 + t)$, defined on $[0, \infty)$.

### 6 Experiments

In this section we compare the numerical performance of our proposed Algorithm 1 versus other benchmarks for Problem (1.3) for different choices of $C$ on both synthetic and real datasets. Our algorithms are written in Python 3.7.4 and can be found at

[https://github.com/wanghaoyue123/Nonparametric-density-estimation-with-shape-constraints](https://github.com/wanghaoyue123/Nonparametric-density-estimation-with-shape-constraints)

All computations are performed on MIT Sloan’s engaging cluster with 1 CPU and 32GB RAM.

#### 6.1 Synthetic data experiments

**6.1.1 Solving Problem (1.1)**

We first consider the problem of estimating mixture proportions with no shape constraint; and compare our algorithm with several benchmarks on synthetic datasets in terms of optimizing (1.1).

**Setup.** We generate iid samples $X_1, \ldots, X_N$ from a Gaussian mixture density with 5 components: $g^1_B(x) = \sum_{i=1}^5 w_i^1 N(\mu_i^1, (\sigma_i^1)^2)$ with mixture proportions $(w_1^1, \ldots, w_5^1) = (0.6, 0.05, 0.15, 0.1, 0.1)$, location parameters $(\mu_1^1, \ldots, \mu_5^1) = (0.4, 5.5, -3.5, 4.5)$, and standard deviations $(\sigma_1^1, \ldots, \sigma_5^1) = (1, 0.5, 1, 0.25, 0.25)$. To approximate the underlying density $g^1_B(x)$, we consider a mixture of $M$ Gaussian densities: The basis elements are given by $\psi_i(x) = \varphi((x - \mu_i)/\sigma)$ for $i \in [M]$, and $\{\mu_i\}_{i=1}^M$ form an equi-spaced grid between the smallest and largest values in $X_1, \ldots, X_N$. Note that the true underlying density $g^1_B(x)$ is not a member of $g_B(x) = \sum_{i=1}^M w_i \psi_i(x)$, as each basis element $\psi_i$ has variance $\sigma^2$.

**Benchmarks and metrics.** We compare Algorithm 1 with (i) the commercial solver Mosek 11 using CVXPY interface; (ii) the sequential quadratic programming based method (MIXSQP) introduced in 20, (iii) the Frank-Wolfe method (FW) in 8, and (iv) proximal gradient descent (PGD) in 35.

In Table I, we present the runtimes of these five methods for different values of $M \in \{200, 500, 1000\}$ and $N \in \{10^5, 2 \times 10^5, 5 \times 10^5\}$. We set the standard deviation of the mixture components to $\sigma = 0.2$ (this value is chosen so that the resulting density leads to a good visual fit). For each method, Table I presents the following metrics: (a) Time: the time (s) needed for an algorithm to output a solution. (b) Relative Error: For an output solution $\hat{w}$ (computed by an algorithm), we define the relative error as

$$\text{Relative Error} = (f(\hat{w}) - f^*) / \max \{1, |f^*|\}$$

---

Footnotes:

1. Some implementation details of Algorithm 1 can be found in Section D.
2. For FW and PGD we use the public code available at [https://github.com/kamil-safin/SCFW](https://github.com/kamil-safin/SCFW).
where, $f^*$ is the (estimated) optimal objective value as obtained by Mosek\textsuperscript{19} In Table 1, the time and relative error for each method is reported as time/error; and for Mosek, we only report the runtime as the relative error is zero. In our experiment, we use Mosek with its default setting. For MIXSQP we also use the default setting, but set a loose convergence tolerance of 0.03. The FW and PGD algorithms are terminated as soon as they reach a solution with a relative error smaller than $10^{-4}$. In Algorithm 1, we solve every cubic Newton step with AFW; we terminate our method as soon as its relative error falls below $10^{-4}$. See Section D for additional implementation details of Algorithm 1.

Table 1 suggests that our proposed approach can be faster than other methods—we obtain approximately a 3X-5X improvement over the next best method (MIXSQP), to reach a solution with relative error $\sim 10^{-4}$–$10^{-5}$. We note that [20] use a low-rank approximation of $B$ for improved computational performance. We do not use low-rank approximations in our implementations, but note that they may lead to further improvements. The interior point solver of Mosek also works quite well; and we obtain up to a 10X improvement over Mosek on some instances. Compared to Mosek, our method appears to be more memory efficient—see for example, the instance with $M = 1000$ and $N = 5 \times 10^5$.

| $N$ | $M$ | Mosek | MIXSQP | FW | PGD | Algorithm 1 |
|-----|-----|-------|--------|----|-----|-------------|
|     |     | time (s) | time(s)/error | time(s)/error | time(s)/error | time(s)/error |
| 1e5 | 200 | 63.2 | 23.8/1.1e-04 | 189.9/1.0e-04 | 101.8/9.6e-05 | 8.6/8.4e-05 |
|     | 500 | 102.9 | 76.6/1.3e-04 | 188.5/1.0e-04 | 270.0/9.9e-05 | 23.9/8.7e-05 |
|     | 1000 | 186.7 | 186.4/8.2e-05 | 414.4/9.7e-05 | 575.0/9.8e-05 | 60.7/9.8e-05 |
| 2e5 | 200 | 114.1 | 47.5/9.1e-05 | 477.5/1.0e-04 | 323.9/9.9e-05 | 13.5/5.9e-05 |
|     | 500 | 207.4 | 165.4/9.2e-05 | 1075.5/1.0e-04 | 856.4/9.8e-05 | 36.7/6.5e-05 |
|     | 1000 | 372.2 | 329.2/9.2e-05 | 1851.9/9.9e-05 | 1729.0/9.9e-05 | 98.7/6.4e-05 |
| 5e5 | 200 | 361.5 | 110.2/1.2e-04 | 1183.6/1.0e-04 | 1094.8/1.0e-04 | 27.1/5.6e-05 |
|     | 500 | 608.6 | 329.1/1.2e-04 | 2609.5/1.0e-04 | 3186.1/1.0e-04 | 88.9/5.5e-05 |
|     | 1000 | O.M. | 738.0/1.2e-04 | 2781.9/9.8e-05 | 6747.7/1.0e-04 | 236.5/5.9e-05 |

Table 1: Comparison of timings for density estimation with no shape constraints i.e., Problem (1.1). For each method, we present time(s) and (relative) error as defined in the text. Here “O.M.” refers to the instance where Mosek runs out of memory (32G).

6.1.2 Solving Problem (1.3): with shape constraints

For density estimation with shape constraints, we present results for two settings: one with a concave density, and the other involving a density that is convex and increasing.

We generate $N$ iid samples from the true density $g^\dagger_B(x) = \sum_{m=1}^{5} w_m^\dagger h_m(x)$, which is a finite mixture of 5 Beta-densities. The concave density $g^\dagger_B(x)$ is obtained by choosing $(w_1^\dagger, ..., w_5^\dagger) = (0.05, 0.3, 0.3, 0.3, 0.05)$. To obtain a density $g^\dagger_B(x)$ which is increasing and convex, we use $(w_1^\dagger, ..., w_5^\dagger) = (0.05, 0.05, 0.1, 0.25, 0.55)$. For each case, we learn the density $g^\dagger_B$ using a mixture of $M$ Bernstein densities with knots located uniformly in the interval $[0, 1]$—we obtain the mixture weights by solving Problem (1.3) (with the corresponding shape constraint). See Table 2 for results.

Unlike (1.1), there are no specialized benchmarks for the shape constrained problem (1.3). We only compare our method with Mosek. When Mosek does not run into memory issues, our method outperforms Mosek in runtime by a factor of 3X–20X, with a reasonably good accuracy $10^{-4}$ $\sim 10^{-5}$. For larger problems, our approach works well but Mosek would not run due to memory issues.

\textsuperscript{19}For the examples where Mosek fails to output a solution due to insufficient memory (we limit memory to 32GB), we run Mosek with 128GB memory to obtain the value of $f^\dagger$. 


Table 2: Comparison of timings for density estimation with shape constraints—we consider Problem \(1.3\) with two shape constraints: [left] concave, [right] convex and increasing. Mosek runs into memory issues (O.M.) for some larger instances.

### 6.2 Real data example

We illustrate our approach on real-world data from the US Census Bureau to demonstrate examples of shape-constrained density estimation for some covariates. The data is publicly available in US Census Planning Database 2020 that provides a range of demographic, socioeconomic, housing and census operational data [4]. It includes covariates from Census 2010 and 2014-2018 American Community Survey (ACS), aggregated at both Census tract level as well as block level in the country. We consider tract level data, which has approximately 74,000 samples and 500 covariates. We consider the marginal density estimation for 4 different features (denoted as feature-1,..,feature-4) to illustrate our density estimation procedure with different shape constraints, such as decreasing, increasing, convex and concave—all of which can be handled by Problem \(1.3\).

Figure 2 shows a visualization of the estimated densities for 4 different covariates. Figure 2 (a) compares our density estimate with Grenander’s monotone density estimator [10]. We see that Grenander’s estimator is not smooth whilst our estimator is smooth (due to the choice of the Bernstein polynomials as bases elements). Our estimator appears to be more expressive near \(x = 0\). Figure 2 (c) shows two of our estimators: one convex, and the other decreasing. The inset shows a zoomed-in version of the right tail showing the contrasting behavior between the convex and decreasing density estimates. Figure 2 (d) shows two estimators: one with no shape constraint \(1.1\) and the other with a concave shape constraint. The shape constrained density estimator appears to be less ‘wiggly’ than the unconstrained variant—consistent with our observation in Figure 1.

For the same dataset, Table 3 presents running times of our method versus Mosek for Problem \(1.3\) using Bernstein bases elements and different shape constraints as shown in the table. We observe that our algorithm reaches a reasonable accuracy in runtimes that are smaller than Mosek. We see up to a 15X improvement in runtimes over Mosek.

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11 The features correspond to: feature-1: number of children under age 18 living in households below poverty line. feature-2: percentage of population who are citizens of the United States at birth. feature-3: percentage of population that identify as “Mexican”, “Puerto Rican”, “Cuban”, or “another Hispanic, Latino, or Spanish origin”. feature-4: Percentage of children of age 3 and 4 that are enrolled in school. All these numbers pertain to the ACS database. All features have been normalized within the interval \([0, 1]\) before performing density estimation.
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![Estimated Density (ours) vs Estimated Density (Grenander) for different shape restrictions](image)

**Figure 2:** Marginal probability density estimates of 4 covariates (all normalized between [0, 1]) from the ACS dataset under different shape restrictions: decreasing, increasing, convex and concave as shown in the headings for each sub-figure. Estimators are obtained by solving (1.3) with Bernstein bases with $M = 500$ components. For (a), (b) the x-axis ranges have been truncated to aid visualization.
| Census Feature | Shape Constraint \((S \text{ in } (1.3))\) | \(M\) | Mosek time (s) | Algorithm 1 time (s)/ error |
|----------------|----------------------------------|------|----------------|---------------------------|
| feature-1      | Decreasing                       | 100  | 18.7           | 7.0/9.9e-5               |
|                |                                  | 500  | 51.5           | 11.1/1e-4                |
|                |                                  | 1000 | 79.2           | 27.5/8.9e-5              |
| feature-2      | Increasing                       | 100  | 31.8           | 6.4/2.0e-5               |
|                |                                  | 500  | 74.7           | 6.7/7.9e-5               |
|                |                                  | 1000 | 116.9          | 17.2/8.46e-5             |
| feature-3      | Convex                           | 100  | 28.5           | 2.1/6.3e-5               |
|                |                                  | 500  | 65.3           | 7.7/8.8e-5               |
|                |                                  | 1000 | 102.7          | 20.9/9.4e-5              |
| feature-4      | Concave                          | 100  | 23.2           | 1.15/6.7e-5              |
|                |                                  | 500  | 76.9           | 4.8/7.1e-5               |
|                |                                  | 1000 | 158.7          | 10.7/8.2e-5              |

Table 3: Density estimation with shape constraints for Problem \((1.3)\) on four ACS features from the Census Bureau (see Figure 2 for corresponding visualizations). Here, \(N \approx 74,000\) and we take different values of \(M\). We compare Mosek vs our method (Algorithm 1). We report running time (s) and solution accuracy i.e., relative error—reported as time/error.
References

[1] Erling D Andersen and Knud D Andersen. The mosek interior point optimizer for linear programming: an implementation of the homogeneous algorithm. In *High performance optimization*, pages 197–232. Springer, 2000.

[2] G Jogesh Babu, Angelo J Canty, and Yogendra P Chaubey. Application of bernstein polynomials for smooth estimation of a distribution and density function. *Journal of Statistical Planning and Inference*, 105(2):377–392, 2002.

[3] Lawrence D Brown and Eitan Greenshtein. Nonparametric empirical bayes and compound decision approaches to estimation of a high-dimensional vector of normal means. *The Annals of Statistics*, pages 1685–1704, 2009.

[4] US Census Bureau. Planning database, Jun 2020.

[5] Jesús M Carnicer and Juan Manuel Pena. Shape preserving representations and optimality of the bernstein basis. *Advances in Computational Mathematics*, 1(2):173–196, 1993.

[6] Pavel Dvurechensky, Petr Ostroukhov, Kamil Safin, Shimrit Shtern, and Mathias Staudigl. Self-concordant analysis of frank-wolfe algorithms. In *International Conference on Machine Learning*, pages 2814–2824. PMLR, 2020.

[7] M. Frank and P. Wolfe. An algorithm for quadratic programming. *Naval Research Logistics Quarterly*, 1956.

[8] Robert M Freund, Paul Grigas, and Rahul Mazumder. An extended frank-wolfe method with “in-face” directions, and its application to low-rank matrix completion. *SIAM Journal on optimization*, 27(1):319–346, 2017.

[9] Subhashis Ghosal. Convergence rates for density estimation with bernstein polynomials. *The Annals of Statistics*, 29(5):1264–1280, 2001.

[10] Ulf Grenander. On the theory of mortality measurement: part ii. *Scandinavian Actuarial Journal*, 1956(2):125–153, 1956.

[11] P Groeneboom. Estimating a monotone density. inproceedings of the berkeley conference in honor of jerzy neyman and jack kiefer, 1985.

[12] Piet Groeneboom and Geurt Jongbloed. *Nonparametric estimation under shape constraints*, volume 38. Cambridge University Press, 2014.

[13] Piet Groeneboom, Geurt Jongbloed, and Jon A Wellner. Estimation of a convex function: characterizations and asymptotic theory. *Annals of Statistics*, 29(6):1653–1698, 2001.

[14] Piet Groeneboom, Geurt Jongbloed, and Jon A Wellner. The support reduction algorithm for computing non-parametric function estimates in mixture models. *Scandinavian Journal of Statistics*, 35(3):385–399, 2008.

[15] Jacques Guélat and Patrice Marcotte. Some comments on wolfe’s ‘away step’. *Mathematical Programming*, 35(1):110–119, 1986.

[16] Martin Jaggi. Revisiting Frank-Wolfe: Projection-free sparse convex optimization. In *Proceedings of the 30th International Conference on Machine Learning*, pages 427–435, 2013.

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

[18] Iain M Johnstone and Bernard W Silverman. Needles and straw in haystacks: Empirical bayes estimates of possibly sparse sequences. *Annals of Statistics*, 32(4):1594–1649, 2004.

[19] 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.

[20] 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.

[21] Roger Koenker and Jiaying Gu. Rebayes: an r package for empirical bayes mixture methods. *Journal of Statistical Software*, 82(1):1–26, 2017.

[22] 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, April 2014.

[23] Simon Lacoste-Julien and Martin Jaggi. On the global linear convergence of frank-wolfe optimization variants. In *Proceedings of the 28th International Conference on Neural Information Processing Systems - Volume 1*, NIPS’15, page 496–504, Cambridge, MA, USA, 2015. MIT Press.

[24] Simon Lacoste-Julien and Martin Jaggi. On the global linear convergence of frank-wolfe optimization variants. *arXiv preprint arXiv:1511.05932*, 2015.
[25] Bruce G Lindsay. The geometry of mixture likelihoods: a general theory. *The annals of statistics*, pages 86–94, 1983.

[26] Deyi Liu, Volkan Cevher, and Quoc Tran-Dinh. A newton frank-wolfe method for constrained self-concordant minimization. *arXiv preprint arXiv:2002.07003*, 2020.

[27] Xiaosheng Mu. Log-concavity of a mixture of beta distributions. *Statistics & Probability Letters*, 99:125–130, 2015.

[28] Yurii Nesterov. *Introductory lectures on convex optimization: A basic course*, volume 87. Springer Science & Business Media, 2013.

[29] Yurii Nesterov and Arkadii Nemirovskii. *Interior-point polynomial algorithms in convex programming*. SIAM, 1994.

[30] Yurii Nesterov and Boris T Polyak. Cubic regularization of newton method and its global performance. *Mathematical Programming*, 108(1):177–205, 2006.

[31] George M Phillips. *Interpolation and approximation by polynomials*, volume 14. Springer Science & Business Media, 2003.

[32] Richard Samworth and Bodhisattva Sen. Special issue on” nonparametric inference under shape constraints”*. 2018.

[33] Richard J Samworth. Recent progress in log-concave density estimation. *Statistical Science*, 33(4):493–509, 2018.

[34] Tianxiao Sun and Quoc Tran-Dinh. Generalized self-concordant functions: a recipe for newton-type methods. *Mathematical Programming*, 178(1):145–213, 2019.

[35] Quoc Tran Dinh, Anastasios Kyrillidis, and Volkan Cevher. Composite self-concordant minimization. *Journal of Machine Learning Research*, 16(ARTICLE):371–416, 2015.

[36] Bradley C Turnbull and Sujit K Ghosh. Unimodal density estimation using bernstein polynomials. *Computational Statistics & Data Analysis*, 72:13–29, 2014.

[37] Richard A Vitale. A bernstein polynomial approach to density function estimation. In *Statistical inference and related topics*, pages 87–99. Elsevier, 1975.
A Frank-Wolfe algorithm with away steps

Below we present the details for Frank-Wolfe algorithm with away steps [15, 24]. For notational convenience, we denote the objective $h_f(y, w^k)$ in (3.2) by

$$G(z) := \Phi_f(z, w^k) + \frac{L_k}{6} \|z - w^k\|^2_{\nabla^2 f(w^k)}.$$

In addition, let $V(C)$ denote the set of vertices of the constraint set $C$ (which is a bounded convex polyhedron in our problem). In the AFW algorithm (see Algorithm 2), we start from some $z^0$ which is a vertex of $C$. In iteration $t$, $z^t$ can always be represented as a convex combination of at most $t$ vertices $V(z^t) \subset V(C)$, which we write as $z^t = \sum_{v \in V(z^t)} \lambda_v(z^t)v$, where $\lambda_v(z^t) > 0$ for $v \in V(z^t)$, and $\sum_{v \in V(z^t)} \lambda_v(z^t) = 1$. We keep track of the set of vertices $V(z^t)$ and the weight vector $\lambda(z^t)$, and choose between the Frank-Wolfe step and away step (See Algorithm 2 Step 1). After a step is taken and we move to $z^{t+1}$, we update the set of vertices and weights to $V(z^{t+1})$ and $\lambda(z^{t+1})$, respectively. More precisely, we update $V(z^{t+1})$ and $\lambda(z^{t+1})$ in the following way: For a Frank-Wolfe step, let $V(z^{t+1}) = \{s^t\}$ if $\alpha_t = 1$; otherwise $V(z^{t+1}) = V(z^t) \cup \{s^t\}$. Also, we have $\lambda_v(z^{t+1}) := (1 - \alpha_t)\lambda_v(z^t) + \alpha_t$ and $\lambda_v(z^{t+1}) = (1 - \alpha_t)\lambda_v(z^t)$ for $v \in V(z^t) \setminus \{s^t\}$. For an away step, let $V(z^{t+1}) = V(z^t) \setminus \{v^t\}$ if $\alpha_t = \alpha_{\text{max}}$; otherwise $V(z^{t+1}) = V(z^t)$. Also, we have $\lambda_v(z^{t+1}) := (1 + \alpha_t)\lambda_v(z^t) - \alpha_t$ and $\lambda_v(z^{t+1}) := (1 + \alpha_t)\lambda_v$ for $v \in V(z^t) \setminus \{v^t\}$.

**Algorithm 2** Away-step Frank-Wolfe method (AFW) [15, 24]

Starting from $z^0 \in V(C)$. Set $V(z^0) = \{z^0\}$ and $\lambda_v(z^0) = 1$.

For $t = 0, 1, 2, \ldots$

1. $s^t := \arg\min_{z \in C} \langle \nabla G(z^t), z \rangle$, $v^t := \arg\max_{z \in V(z^t)} \langle \nabla G(z^t), z \rangle$.
   - if $\langle \nabla G(z^t), s^t - z^t \rangle < \langle \nabla G(z^t), z^t - v^t \rangle$: (Frank-Wolfe step)
     $$d^t := s^t - z^t; \quad \alpha_{\text{max}} = 1.$$
   - else: (away step)
     $$d^t := z^t - v^t; \quad \alpha_{\text{max}} = \lambda_v(z^t)/(1 - \lambda_v(z^t))$$
2. $z^{t+1} = z^t + \alpha_t d^t$; where $\alpha_t \in \arg\min_{\alpha \in [0, \alpha_{\text{max}}]} G(z^t + \alpha d^t)$.
3. Update $V(z^{t+1})$ and $\lambda(z^{t+1})$ (see text for details).

B Postponed Proofs

B.1 Proofs on Computational Guarantees

B.1.1 Proof of Lemma 3.2

It suffices to show that if $L_k \geq 24N$, condition (3.3) must be satisfied. (If this is true, then noting that $\beta \in (1, 2)$, we know $L_k \leq \max\{48N, L_0\}$.) For $i \in [N]$, recall that $B_i := [B_{1i}, B_{2i}, \ldots, B_{Mi}]^T \in \mathbb{R}^M$. Define

$$\mu_i(y, w) := \langle B_i, w - y \rangle / \langle B_i, w \rangle.$$

Then it holds that

$$\langle \nabla f(w), y - w \rangle = \frac{1}{N} \sum_{i=1}^N \mu_i(y, w)$$

and

$$\nabla^2 f(w)[y - w]^2 = \frac{1}{N} \sum_{i=1}^N (y - w)^T (\langle B_i, w \rangle)^{-2} B_i B_i^T (y - w) = \frac{1}{N} \sum_{i=1}^N \mu_i(y, w)^2.$$
As a result, recalling the definition of $\Phi_f$ in (3.1), we have
\[
\Phi_f(y, w) + (L/6)\|y - w\|^2_{\nabla^2 f(w)} - f(w) = \frac{1}{N} \sum_{i=1}^{N} \left\{ \mu_i(y, w) + \frac{1}{2} \mu_i(y, w)^2 \right\} + \frac{L}{6} \left( \frac{1}{N} \sum_{i=1}^{N} \mu_i(y, w)^2 \right)^{3/2}
\]
for all $w, y$ and $L$. From Assumption 3.1, we have
\[
\frac{1}{N} \sum_{i=1}^{N} \left\{ \mu_i(y^k, w^k) + \frac{1}{2} \mu_i(y^k, w^k)^2 \right\} + \frac{L_k}{6} \left( \frac{1}{N} \sum_{i=1}^{N} \mu_i(y^k, w^k)^2 \right)^{3/2} \leq 0 \quad (2.2)
\]
Let $p := \frac{1}{N} \sum_{i=1}^{N} \mu_i(y^k, w^k)$ and $q := (\frac{1}{N} \sum_{i=1}^{N} \mu_i(y^k, w^k)^2)^{1/2}$, then (2.2) is equivalent to $p + (1/2)q^2 + (L_k/6)q^3 \leq 0$. By Jensen’s inequality, it holds $p^2 \leq q^2$, so we have
\[
(L_k/6)q^3 \leq (1/2)q^2 + (L_k/6)q^3 \leq -p \leq q,
\]
and thus $q \leq (6/L_k)^{1/2}$. Recall that $q^2 = \nabla^2 f(w_k)[y^k - w^k]^2$, and making use of the definition of $\| \cdot \|_{F,x}$ (see (2.1)) along with Lemma 2.1, we have:
\[
\sqrt{N}q = \sqrt{N\nabla^2 f(w_k)[y^k - w^k]^2} = \|y^k - w^k\|_{f,w_k}.
\]
By using the observation $q \leq (6/L_k)^{1/2}$ and the assumption $L_k \geq 24N$, we have $\sigma_k := \|y^k - w^k\|_{f,w_k} = \sqrt{N}q \leq 1/2$. We have the following chain of inequalities
\[
\left| f(y^k) - f(w_k) - \langle \nabla f(w_k), y^k - w_k \rangle - \frac{1}{2} \nabla^2 f(w_k)[y^k - w^k]^2 \right| \leq 2\sqrt{N} \int_{[0,1]^3} t^2 s |\nabla^2 f(w_k)(y^k - w^k)| ds dt dr
\]
\[
\leq 3 \sqrt{N} |\nabla^2 f(w_k)(y^k - w^k)|^{3/2} \int_{[0,1]^3} t^2 s \ ds \ dt \ dr
\]
where (i) is from Taylor formula (see Lemma C.1), (ii) uses the fact that $f$ is a $1/N$-self concordant function, (iii) is from (2.2), and (iv) is from $\sigma_k \leq 1/2$. As a result, using $L_k \geq 24N$, we have:
\[
f(y^k) \leq \Phi_f(y^k, w_k) + 3\sqrt{N} |\nabla^2 f(w_k)(y^k - w^k)|^{3/2}
\]
\[
\leq \Phi_f(y^k, w_k) + (L_k/6) |\nabla^2 f(w_k)(y^k - w^k)|^{3/2}
\]
and hence Condition (3.3) is satisfied for any non-negative $\gamma_k$.

**B.1.2 Proof of Theorem 3.3**

From Step 3 of Algorithm 1 and Assumption 3.1, we have
\[
f(w^{k+1}) \leq f(y^k) + \rho_k
\]
\[
\leq \Phi_f(y^k, w^k) + \frac{L_k}{6} \|y^k - w^k\|_{\nabla^2 f(w_k)}^3 + \rho_k + \gamma_k
\]
\[
\leq \min_{y \in C} \left\{ \Phi_f(y, w^k) + \frac{L_k}{6} \|y - w^k\|_{\nabla^2 f(w_k)}^3 \right\} + E_k \quad (2.3)
\]
where the first inequality is by \([3.4]\), the second inequality is by \([3.3]\), and the third inequality follows from \([3.2]\) and the definitions of \(\delta_k\) and \(E_k\). Recall that \(w^*\) is an optimal solution of \((1.3)\). For \(\tau \in [0, 1]\), let \(w^*(\tau) := \tau w^* + (1 - \tau)w_k\). Restricting the minimization in \((2.3)\) to this line segment joining \(w_k\) and \(w^*\), we have

\[
f(w^{k+1}) \leq \min_{\tau \in [0, 1]} \left\{ \Phi_f(w^k(\tau), w^k) + \frac{L_k \tau^3}{6} \| w^* - w^k \|^3_{\nabla^2 f(w^k)} \right\} + E_k. \tag{2.4}
\]

By Taylor’s expansion in Lemma \([C.1]\), we have

\[
\Phi_f(w^k(\tau), w^k) = f(w^k(\tau)) + \int_{[0, 1]^3} \frac{2}{N} \sum_{i=1}^{N} t^2 s \left( \frac{\langle B_i, w^k(\tau) - w^k \rangle}{\langle B_i, w^k + \text{str}(w^k(\tau) - w^k) \rangle} \right)^3 \, ds \, dt \, dr. \tag{2.5}
\]

Note that

\[
\frac{2}{N} \sum_{i=1}^{N} \left( \frac{\langle B_i, w^k(\tau) - w^k \rangle}{\langle B_i, w^k + \text{str}(w^k(\tau) - w^k) \rangle} \right)^3 = \frac{2}{N} \sum_{i=1}^{N} \tau^3 \left( \frac{\langle B_i, w^* - w^k \rangle}{(1 - \text{str}\tau)(\langle B_i, w^* \rangle) + \text{str}\tau(\langle B_i, w^* \rangle)} \right)^3 \tag{2.6}
\]

\[
\leq \frac{2}{N} \sum_{i=1}^{N} \tau^3 \max \left\{ \left| \frac{\langle B_i, w^* - w^k \rangle}{\langle B_i, w^* \rangle} \right|^3, \left| \frac{\langle B_i, w^* - w^k \rangle}{\langle B_i, w^k \rangle} \right|^3 \right\} \leq 2C_1 \tau^3
\]

where, the first inequality is because \(a/((1 - \alpha)b + ac) \leq \max\{a/b, a/c\}\) for all \(a, b, c \geq 0\) and \(\alpha \in [0, 1]\), and the last inequality is from the definition of \(C_1\) in \([3.7]\) and the fact that \(w^k \in X^0\) for all \(k \geq 1\). By \((2.5)\) and \((2.6)\) we have

\[
\Phi_f(w^k(\tau), w^k) \leq f(w^k(\tau)) + 2C_1 \tau^3 \int_{[0, 1]^3} t^2 s \, ds \, dt \, dr = f(w^k(\tau)) + \frac{C_1 \tau^3}{3}. \tag{2.7}
\]

On the other hand, note that \(\| w^* - w^k \|^2_{\nabla^2 f(w^k)} = \frac{1}{N} \sum_{i=1}^{N} \langle B_i, w^* - w^k \rangle^2 / \langle B_i, w^k \rangle^2\), so

\[
\| w^* - w^k \|^3_{\nabla^2 f(w^k)} \leq \frac{1}{N} \sum_{i=1}^{N} \left| \frac{\langle B_i, w^* - w^k \rangle}{\langle B_i, w^k \rangle} \right|^3 \leq C_1, \tag{2.8}
\]

where we use Jensen’s inequality for the first inequality; and \([3.7]\) for the second inequality. Combining inequalities \((2.4), (2.7)\) and \((2.8)\), we obtain

\[
f(w^{k+1}) \leq f(w^k(\tau)) + \frac{C_1 \tau^3}{3} + \frac{1}{6} \sup_{k \geq 0} \{L_k\} C_1 \tau^3 + E_k \leq f(w^k(\tau)) + C \tau^3 + E_k \tag{2.9}
\]

where, the second inequality uses the definition of \(C\) in \([3.7]\). Using the convexity of \(\tau \mapsto f(w^k(\tau))\) in line \((2.9)\), we obtain

\[
f(w^{k+1}) \leq (1 - \tau) f(w^k) + \tau f^* + C \tau^3 + E_k \tag{2.10}
\]

which holds for all \(\tau \in [0, 1]\). Taking \(\tau_k = 3/(k + 3)\) above, we get

\[
f(w^{k+1}) - f^* \leq (1 - \tau_k)(f(w^k) - f^*) + \frac{27C}{(k + 3)^2} + E_k. \tag{2.11}
\]
Let \( T_0 = 1 \) and \( T_k = \prod_{i=1}^{k}(1 - \tau_i) \), then we have
\[
T_k = \frac{6}{(k+1)(k+2)(k+3)} \quad \text{for } k \geq 1.
\]

It follows from (2.11) and the definition of \( T_k \) that
\[
\frac{1}{T_k}(f(w^{k+1}) - f^*) \leq \frac{1}{T_{k-1}}(f(w^k) - f^*) + \frac{27C}{(k+3)^3T_k} + \frac{E_k}{T_k}.
\]

Summing the above over \( k \) yields
\[
\frac{1}{T_k}(f(w^{k+1}) - f^*) \leq \frac{1}{T_0}(f(w^1) - f^*) + \sum_{i=1}^{k} \frac{27C}{(i+3)^3T_i} + \sum_{i=1}^{k} \frac{E_i}{T_i}.
\] (2.12)

Note that
\[
(f(w^1) - f^*) \leq f(w^0) - f^* \leq C, \quad T_0 = 1 \quad \text{and} \quad 27/(T_i(i+3)^3) \leq 9/2,
\]
which when used in (2.12), leads to
\[
\frac{1}{T_k}(f(w^{k+1}) - f^*) \leq C + \frac{9}{2}kC + \sum_{i=1}^{k} \frac{E_i}{T_i} \leq 5kC + \sum_{i=1}^{k} \frac{E_i}{T_i}
\]
where the second inequality uses the assumption \( k \geq 2 \). As a result,
\[
f(w^{k+1}) - f^* \leq \frac{30C}{(k+2)(k+3)} + \frac{1}{(k+1)(k+2)(k+3)} \sum_{i=1}^{k} (i+1)(i+2)(i+3)E_i
\]
\[
\leq \frac{30C}{(k+2)^2} + \frac{1}{(k+1)^3} \sum_{i=1}^{k} (i+3)^3E_i
\]
which completes the proof.

**B.1.3 Proof of Theorem 3.5**

In this proof, for notational convenience, we use the shorthand notations:
\[
H_k := \nabla^2 f(w^k), \quad \eta_k := \|w^k - w^*\|_{H_k} \quad \text{and} \quad \eta'_k := \|w^{k+1} - w^*\|_{H_k}.
\]

Suppose for some \( k \geq K \), we have:
\[
(6\sqrt{N} + 2\bar{L})\|w^k - w^*\|_{H_*} \leq 1.
\] (2.13)

It suffices to prove that
\[
\|w^{k+1} - w^*\|_{H_*} \leq (6\sqrt{N} + 2\bar{L})\|w^k - w^*\|_{H_*}^2.
\] (2.14)

This is because, by (2.13) and (2.14) it follows that \((6\sqrt{N} + 2\bar{L})\|w^{k+1} - w^*\|_{H_*} \leq 1\)---we can then apply the same arguments for \( k + 1 \) in place of \( k \) and prove Theorem 3.5 by induction.

Below we prove (2.14) assuming that (2.13) holds true. First, note that by condition (2.13), we have
\[
\|w^k - w^*\|_{f,w^*} = \sqrt{N}\|w^k - w^*\|_{H_*} \leq 1/6.
\] (2.15)

Hence by (2.2) we have
\[
(25/36)H_* \leq H_k \leq (36/25)H_*.
\] (2.16)
Let $h$ be the indicator function of the set $C$, that is, $h(w) = 0$ for $w \in C$ and $h(w) = \infty$ for $w \notin C$. Since by our assumption, $y^k = w^{k+1}$ is a minimizer for (3.2), we have
\[
\nabla f(w^k) + \mu_k \nabla^2 f(w^k)(w^{k+1} - w^k) + v^{k+1} = 0,
\]
where $v^{k+1} \in \partial h(w^{k+1})$ and $\mu_k := 1 + \frac{L_k}{2} \|w^{k+1} - w^k\|_{H_k}$. On the other hand, since $w^*$ is the optimal solution to (1.3), there exists $v^* \in \partial h(w^*)$ such that $\nabla f(w^*) + v^* = 0$—this leads to
\[
\nabla f(w^k) - \nabla f(w^*) + \mu_k \nabla^2 f(w^k)(w^{k+1} - w^k) + v^{k+1} - v^* = 0. \tag{2.17}
\]
Multiplying both sides of (2.17) by $w^{k+1} - w^*$, and in view of $(w^{k+1} - w^*)^T (v^{k+1} - v^*) \geq 0$ (since $h$ is a convex function), we have
\[
0 \geq (w^{k+1} - w^*)^T \left( \nabla f(w^k) - \nabla f(w^*) + \mu_k \nabla^2 f(w^k)(w^{k+1} - w^k) \right)
= (w^{k+1} - w^*)^T \left( \nabla f(w^k) - \nabla f(w^*) - \mu_k \nabla^2 f(w^k)(w^* - w^k) \right) + \mu_k \|w^{k+1} - w^*\|_{H_k}^2.
\]
Recall that $\eta'_k = \|w^{k+1} - w^*\|_{H_k}$. Hence from the above, we get:
\[
\mu_k (\eta'_k)^2 \leq (w^{k+1} - w^*)^T \left( \nabla f(w^k) - \nabla f(w^*) - \mu_k \nabla^2 f(w^k)(w^* - w^k) \right)
\leq \eta'_k \|H_k^{-1/2} \left( \nabla f(w^*) - \nabla f(w^k) - \mu_k \nabla^2 f(w^k)(w^* - w^k) \right)\|_2,
\]
and hence
\[
\mu_k \eta'_k \leq \|H_k^{-1/2} \left( \nabla f(w^*) - \nabla f(w^k) - \mu_k \nabla^2 f(w^k)(w^* - w^k) \right)\|_2
\leq \|H_k^{-1/2} \left( \nabla f(w^*) - \nabla f(w^k) - \nabla^2 f(w^k)(w^* - w^k) \right)\|_2
\leq (L_k/2) \|w^{k+1} - w^k\|_{H_k} \|w^k - w^*\|_{H_k}. \tag{2.18}
\]
where the second inequality in (2.18) makes use of the definition of $\mu_k = 1 + \frac{L_k}{2} \|w^{k+1} - w^k\|_{H_k}$. Let us denote
\[
J_1 := \|H_k^{-1/2} \left( \nabla f(w^*) - \nabla f(w^k) - \nabla^2 f(w^k)(w^* - w^k) \right)\|_2 \quad \text{and} \quad J_2 := (L_k/2) \|w^{k+1} - w^k\|_{H_k} \|w^k - w^*\|_{H_k}.
\]
Then (2.18) reduces to
\[
\mu_k \eta'_k \leq J_1 + J_2. \tag{2.19}
\]
By the definition of $J_1$ one has
\[
J_1 = \left\| \int_0^1 H_k^{-1/2} \left( \nabla^2 f(w^k(t)) - \nabla^2 f(w^k) \right)(w^* - w^k) dt \right\|_2, \tag{2.20}
\]
where $w^k(t) = w^k + t(w^* - w^k)$.
Let
\[
r := \|w^k - w^*\|_{f,w^k} = \sqrt{N} \|w^k - w^*\|_{H_k}.
\]
By (2.16) we have
\[
r \leq (6/5) \sqrt{N} \|w^k - w^*\|_{H_k} = (6/5) \|w^k - w^*\|_{f,w^k} \leq 1/5, \tag{2.21}
\]
where, the second inequality is by (2.15).
For any $t \in [0,1]$, by the definition of $r$ and (2.21), we have
\[
\|w^k(t) - w^k\|_{f,w^k} = t \|w^* - w^k\|_{f,w^k} = tr \leq 1/5 < 1.
\]
where, the inequality in (2.27) follows by noting that
\[
\nabla^2 f(w^k(t)) - \nabla^2 f(w^k) \preceq (1 - tr)^{-2} - 1 \nabla^2 f(w^k) \preceq 3tr\nabla^2 f(w^k) ,
\]
where the last inequality is by \( tr \in [0, 1/5] \) and Lemma C.3. Similarly, we can obtain:
\[
\nabla^2 f(w^k(t)) - \nabla^2 f(w^k) \succeq (1 - tr)^2 - 1 \nabla^2 f(w^k) \succeq -3tr\nabla^2 f(w^k) .
\]
Combining (2.22) and (2.23), and using Lemma C.2 with \( \bar{A} = \nabla^2 f(w^k(t)) - \nabla^2 f(w^k) \) and \( \bar{B} = 3tr\nabla^2 f(w^k) = 3trH_k \), we have \( \bar{A}B^{-1}A \leq \bar{B} \), which implies:
\[
\|H_k^{-1/2}(\nabla^2 f(w^k(t)) - \nabla^2 f(w^k))(w^* - w^k)\|_2 \leq 3tr\|w^* - w^k\|_{H_k}.
\]
(2.24)
Note that \( r = \|w^k - w^*\|_{f, w^k} = \sqrt{N}\|w^k - w^*\|_{H_k} = \sqrt{N}\eta_k \) and \( \|w^k - w^*\|_{H_k} = \eta_k \), so (2.24) is equivalent to
\[
\|H_k^{-1/2}(\nabla^2 f(w^k(t)) - \nabla^2 f(w^k))(w^* - w^k)\|_2 \leq 3t\sqrt{N}\eta_k^2.
\]
(2.25)
By (2.20) and the convexity of the norm \( \| \cdot \|_2 \), one has
\[
J_1 \leq \int_0^1 \|H_k^{-1/2}(\nabla^2 f(w^k(t)) - \nabla^2 f(w^k))(w^* - w^k)\|_2 dt \leq (3/2)\sqrt{N}\eta_k^2
\]
(2.26)
where, the second inequality is by (2.25) and \( \int_0^1 t dt = 1/2 \). On the other hand,
\[
J_2 = (L_k/2)\|w^{k+1} - w^k\|_{H_k}\|w^k - w^*\|_{H_k} \leq (L/2)(\eta_k + \eta_k')\eta_k
\]
(2.27)
where, the inequality in (2.27) follows by noting that \( L_k \leq \bar{L} \) and
\[
\|w^{k+1} - w^k\|_{H_k} \leq \|w^{k+1} - w^*\|_{H_k} + \|w^k - w^*\|_{H_k} = \eta_k + \eta_k'.
\]
Combining (2.19), (2.26) and (2.27), we have
\[
\mu_k\eta_k' \leq (3/2)\sqrt{N}\eta_k^2 + (\bar{L}/2)(\eta_k + \eta_k')\eta_k .
\]
(2.28)
By (2.16) and assumption (2.13) we have
\[
\bar{L}\eta_k = \bar{L}\|w^k - w^*\|_{H_k} \leq (6/5)\bar{L}\|w^k - w^*\|_{H_*} \leq 1,
\]
which implies \( 1/2 - \bar{L}\eta_k/2 \geq 0 \). Hence we have
\[
\eta_k'/2 \leq \eta_k' = \eta_k' \leq \eta_k + \eta_k'/2
\]
(2.29)
where the second inequality is because \( \mu_k \geq 1 \), and the third inequality is by (2.28). From (2.29) and the definitions of \( \eta_k \) and \( \eta_k' \), we have
\[
\|w^{k+1} - w^*\|_{H_k} \leq (3\sqrt{N} + \bar{L})\|w^k - w^*\|^2_{H_k}.
\]
(2.30)
From (2.30) and using (2.16), we have
\[
\|w^{k+1} - w^*\|_{H_*} \leq (6/5)^3(3\sqrt{N} + \bar{L})\|w^k - w^*\|^2_{H_*} \leq (6\sqrt{N} + 2\bar{L})\|w^k - w^*\|^2_{H_*},
\]
which completes the proof.
B.2 Proofs: computing the LP oracles

B.2.1 Proof of Proposition 4.1

If \( w \in C^- \), define \( y \in \mathbb{R}^M \) by \( y_M = Mw_M \) and \( y_i = i(w_i - w_{i+1}) \) for \( i \in [M-1] \). Then equivalently we have \( w = Uy \). Moreover, by the definition of \( C^- \), we have \( y \geq 0 \) and \( 1_M^T y = Mw_M + \sum_{i=1}^{M-1} i(w_i - w_{i+1}) = \sum_{j=1}^M w_j = 1 \). Hence \( y \in \Delta_M \), so we have proved \( C^- \subseteq U(\Delta_M) \).

On the other hand, suppose \( y \in \Delta_M \), and let \( w = Uy \). Then \( 1_M^T w = 1_M^T Uy = 1_M^T y = 1 \); additionally, we have \( w \geq 0 \) and \( w_1 \geq w_2 \geq \cdots \geq w_M \). Hence \( w = Uy \in C^- \), and \( C^- = U(\Delta_M) \).

B.2.2 Proof of Proposition 4.3

We divide all the inequality constraints in the set \( C^\wedge \), defined in (4.3), into two groups:

\[
(g1): \quad w_i \geq 0, \quad i \in [M]; \quad (g2): \quad 2w_i \geq w_{i-1} + w_{i+1}, \quad 2 \leq i \leq M - 1.
\]

Suppose \( \bar{w} \) is a vertex of \( C^\wedge \). By the definition of a vertex, \( \bar{w} \) is given by a solution to a system of \( M \) independent equations. Since there is one equality constraint \( 1_M^T \bar{w} = 1 \), there must exist \( M - 1 \) independent inequality constraints from (g1) and (g2), for which equality holds. Since (g2) contains \( M - 2 \) constraints, there must exist some \( i \in [M] \) such that \( \bar{w}_i = 0 \). By the concavity constraints, it is easy to see that \( \#\{i : \bar{w}_i = 0\} \leq 2 \), since otherwise, all coordinates will be zero.

If \( \#\{i : \bar{w}_i = 0\} = 1 \), then either \( \bar{w}_1 = 0 \) or \( \bar{w}_M = 0 \), and all constraints in (g2) will be active—this implies \( \bar{w} \) is linear. Combined with the fact that \( 1_M^T \bar{w} = 1 \), it follows that \( \bar{w} \) must be either \( v_1 \) or \( v_M \).

If \( \#\{i : \bar{w}_i = 0\} = 2 \), then we must have \( \bar{w}_1 = 0 \) and \( \bar{w}_M = 0 \), and the \( M - 3 \) constraints in (g2) will be active at \( \bar{w} \). As a result, \( \bar{w} \) is piecewise linear with two pieces. Combined with the constraint that \( 1_M^T \bar{w} = 1 \), we know that \( \bar{w} \) must be one of the points \( v_2, \ldots, v_{M-1} \).

Finally, it is easy to check that any point among \( v_1, \ldots, v_M \) satisfies \( M - 1 \) active inequality constraints, hence it is a vertex. This completes the proof of this proposition.

B.2.3 Proof of Proposition 4.4

We divide all the inequality constraints in the set \( C^\vee \), defined in (4.4), into two groups:

\[
(g1): \quad w_i \geq 0, \quad i \in [M]; \quad (g2): \quad 2w_i \leq w_{i-1} + w_{i+1}, \quad 2 \leq i \leq M - 1.
\]

Suppose \( \bar{w} \) is a vertex of \( C^\vee \). Since there is one equality constraint \( 1_M^T \bar{w} = 1 \), a vertex must have \( M - 1 \) independent active inequality constraints that are also independent to the equality constraint. Since (g2) has \( M - 2 \) constraints, there must exist some \( i \in [M] \) such that \( \bar{w}_i = 0 \). By the convexity constraints in (g2), it can be seen that there exists a pair \((i_1, i_2)\) with \( 1 \leq i_1 \leq i_2 \leq M \) such that

\[
\bar{w}_i = 0 \quad \text{for} \quad i_1 \leq i \leq i_2; \quad \text{and} \quad \bar{w}_i > 0 \quad \text{for} \quad 1 \leq i < i_1, \quad \text{or} \quad M \geq i > i_2.
\]

We claim that either \( i_1 = 1 \) or \( i_2 = M \). Otherwise, suppose \( 1 < i_1 \leq i_2 < M \), then by the definition of \( i_1 \) and \( i_2 \), there are \( i_2 - i_1 + 1 \) active constraints in (g1), and there are at most \( (i_1 - 2) + (M - i_2 - 1) \) active constraints in (g2) that are independent to those active constraints in (g1)—in total, there are at most \( M - 2 \) independent inequality constraints that are active, which is not possible for a vertex \( \bar{w} \).

If \( i_1 = 1 \), then there are \( i_2 \) active constraints in (g1). For \( \bar{w} \) to be a vertex, we need at least \( M - 1 - i_2 \) active constraints in (g2) that are independent to the active constraints in (g1). By the definition of \( i_2 \), we must have \( 2w_{i_2} < w_{i_2-1} + w_{i_2+1} \), so we should have \( 2w_i = w_{i-1} + w_{i+1} \) for all \( i_2 + 1 \leq i \leq M - 1 \) (in order that there are \( M - 1 - i_2 \) active constraints in (g2)). In this case, using the equality constraint \( 1_M^T w = 1 \), we can see that \( \bar{w} \) is of the form

\[
a_k^{-1}(0_{M-k}, 1, 2, \ldots, k)
\]

27
for some $1 \leq k \leq M$. On the other hand, we can verify that any point of the above form satisfies $M - 1$ active inequality constraints, and is hence a vertex.

Similarly, if $i_2 = M$, we can show that a vertex $\bar{w}$ must be of the form

$$a_k^{-1}(k, k-1, \ldots, 2, 1, 0^\top_{M-k})$$

for some $1 \leq k \leq M$.

**B.2.4 Proof of Proposition 4.5**

Note that under the constraints $2w_i \geq w_{i-1} + w_{i+1}$ for $2 \leq i \leq M - 1$, the single inequality $w_{M-1} \leq w_M$ will imply $w_1 \leq \cdots \leq w_M$. As a result, we can rewrite $C^{\lor+}$ as follows:

$$C^{\lor+} = \{ w \in \mathbb{R}^M : 1_M^\top w = 1, w \geq 0, w \text{ is concave}, w_{M-1} \leq w_M \}.$$  

In the following, we separate all the inequality constraints above into 3 groups:

$$(g1) : w_i \geq 0, \; i \in [M]; \quad (g2) : 2w_i \geq w_{i-1} + w_{i+1}, \; 2 \leq i \leq M - 1; \quad (g3) : w_{M-1} \leq w_M.$$  

Let $\bar{w}$ be a vertex of $C^{\lor+}$. We first claim that for all $2 \leq i \leq M$, we must have $\bar{w}_i > 0$. Suppose (for the sake of contradiction), for some $2 \leq i \leq M$ it holds that $\bar{w}_i = 0$, then by the increasing constraints and $\bar{w} \geq 0$, we have $\bar{w}_j = 0$ for all $1 \leq j \leq i$. Moreover, by the concavity constraints, we have $\bar{w}_k = 0$ for all $i \leq k \leq M$. As a result, $\bar{w} = 0$, which is a contradiction to $1_M^\top \bar{w} = 1$.

When $\bar{w}_1$ is also positive, in order that there are $M$ independent active constraints in total, all constraints in (g2) and (g3) should be active, and hence $\bar{w}_i = \bar{w}_j$ for all $1 \leq i, j \leq M$. Combining with $1_M^\top \bar{w} = 1$, we have $\bar{w} = v_1$. When $\bar{w}_1 = 0$ and the constraint in (g3) is not active, in order that there are $M$ independent active constraints in total, all constraints in (g2) should be active. Combining with $1_M^\top \bar{w} = 1$, we obtain $\bar{w} = w_M$. When $\bar{w}_1 = 0$ and the constraint in (g3) is active, in order that there are $M$ independent active constraints in total, there are at least $M - 3$ constraints in (g2) being active, which means $\bar{w}$ is piecewise linear with two pieces, and is a constant on the second piece (since $w_{M-1} = w_M$). Combining with $1_M^\top \bar{w} = 1$, we know that $\bar{w}$ must be among $\{v_2, \ldots, v_{M-1}\}$.

On the other hand, it is easy to check that $v_1, \ldots, v_M$ indeed satisfy $M$ independent active constraints, hence they are indeed vertices of $C^{\lor+}$.

**B.2.5 Proof of Proposition 4.7**

Note that under the convexity constraints $2w_i \leq w_{i-1} + w_{i+1}$ for $2 \leq i \leq M - 1$, the single inequality $w_1 \leq w_2$ will imply $w_1 \leq \cdots \leq w_M$. As a result, we can rewrite $C^{\land+}$ as follows:

$$C^{\land+} = \{ w \in \mathbb{R}^M : 1_M^\top w = 1, w \geq 0, w \text{ is convex}, w_1 \leq w_2 \}.$$  

In the following, we separate all the inequality constraints above into 3 groups:

$$(g1) : w_i \geq 0, \; i \in [M]; \quad (g2) : 2w_i \leq w_{i-1} + w_{i+1}, \; 2 \leq i \leq M - 1; \quad (g3) : w_1 \leq w_2.$$  

Now let $\bar{w}$ be a vertex of $C^{\land+}$. If $\bar{w}_1 > 0$, then by the increasing constraints, $\bar{w}_i > 0$ for all $i \in [M]$, and all constraints in (g1) are inactive. In order that there are $M$ independent active constraints at $\bar{w}$, all constraints in (g2) and (g3) should be active, and hence $\bar{w}_i = \bar{w}_j$ for all $1 \leq i, j \leq M$. Since also $1_M^\top \bar{w} = 1$, we have $\bar{w} = v_1$.

If $\bar{w}_1 = 0$ and $\bar{w}_2 > \bar{w}_1$, in order that there are $M$ independent active constraints at $\bar{w}$, all constraints in (g2) should be active, hence $\bar{w}$ is linear. Combined with $1_M^\top \bar{w} = 1$, we have $\bar{w} = v_{M-1}$. If $\bar{w}_1 = 0$ and $\bar{w}_1 = \bar{w}_2$, in order that there are $M$ independent active constraints at $\bar{w}$, there are at least $M - 3$ active constraints in (g2), which means $\bar{w}$ is piecewise linear, and is a constant on the first piece (since $\bar{w}_1 = \bar{w}_2$). Combined with $1_M^\top \bar{w} = 1$, we know that $\bar{w}$ must be one of $v_1, \ldots, v_{M-2}$.

On the other hand, it is easy to check that $v_1, \ldots, v_M$ indeed satisfy $M$ independent active constraints, and are vertices of $C^{\land+}$.
B.2.6 Proof of Proposition 4.9

In the proof, we use the notation \( C_k^{um}(M) \) for \( C^{um} \) to highlight the dependence on \( M \).

We first show that for all \( k \in [M] \), if \( \bar{w} \) is a vertex of \( C_k^{um}(M) \) satisfying \( \bar{w}_i > 0 \) for all \( i \in [M] \), then \( \bar{w} = (1/M)1_M \). Indeed, since \( \bar{w} \) is a vertex of \( C_k^{um}(M) \), there are \( M \) independent active constraints at \( \bar{w} \). Since there is only one equality constraint in the definition of \( C_k^{um}(M) \), there are at least \( M - 1 \) independent inequality constraints for which equality holds at \( \bar{w} \). We separate all the inequality constraints in \( C_k^{um}(M) \) into 3 groups:

\[
(g1) : w_i \geq 0, \ i \in [M]; \quad (g2) : w_{i-1} \leq w_i, \ 2 \leq i \leq k; \quad (g3) : w_i \geq w_{i+1}, \ k \leq i \leq M-1.
\]

Since \( \bar{w}_i > 0 \) for all \( i \in [M] \), no constraints in \( g1 \) are active. Since there are \( (k - 1) + (M - k) = M - 1 \) constraints in \( g2 \) and \( g3 \), all the constraints in \( g2 \) and \( g3 \) are active at \( \bar{w} \). This implies \( \bar{w} = (1/M)1_M \).

Below we prove the main conclusion. Let \( \bar{w} \) be a vertex of \( C_k^{um}(M) \). By the constraints in \( C_k^{um}(M) \), \( \bar{w} \) is a unimodal vector with all coordinates being non-negative, so there exist \( k_1, k_2 \) satisfying \( 1 \leq k_1 \leq k \leq k_2 \leq M \) such that \( \bar{w}_i > 0 \) for all \( k_1 \leq i \leq k_2 \) and \( \bar{w}_i = 0 \) for all \( i < k_1 \) or \( i > k_2 \). Let \( \bar{u} \in \mathbb{R}^{k_2-k_1+1} \) be the subvector of \( \bar{w} \) restricted to the positive entries — that is, \( \bar{u}_i = \bar{w}_{i+k_1-1} \) for \( i \in [k_2-k_1+1] \). Then \( \bar{u} \) is a vertex of \( C_{k_2-k_1+1}(k_2 - k_1 + 1) \). Since otherwise this is a contradiction to our assumption that \( \bar{w} \) is a vertex of \( C_k^{um}(M) \).

From the discussion in the earlier paragraph, we have \( \bar{u}_i = 1/(k_2 - k_1 + 1) \) for all \( i \in [k_2 - k_1 + 1] \). This implies \( \bar{w} = \nu^{k_1,k_2} \).

On the other hand, it is easy to check that for all \( 1 \leq k_1 \leq k \leq k_2 \leq M \), the vector \( \nu^{k_1,k_2} \) satisfies \( M \) independent active constraints, so it is indeed a vertex of \( C_k^{um}(M) \). This completes the proof.

B.3 Proofs from Section 5

B.3.1 Proof of Proposition 5.3

It is immediate from the definition that \( p^* \leq \hat{p}_G \). On the other hand, define \( \bar{v}_i := N\hat{v}_i/\Gamma \) for \( i \in [N] \). Then by our assumption on \( \Gamma \), it holds

\[
\max_{\mu \in \mathbb{R}} \sum_{i=1}^{N} \bar{v}_i \varphi(X_i - \mu) = \frac{N}{\Gamma} \max_{\mu \in \mathbb{R}} \sum_{i=1}^{N} \hat{v}_i \varphi(X_i - \mu) \leq N,
\]

hence \( \bar{v} \) is a feasible solution of the (infinite) dual problem \((5.2)\). As a result,

\[
p^* \geq \sum_{i=1}^{N} \log \bar{v}_i = \sum_{i=1}^{N} \log \hat{v}_i + N \log(N/\Gamma) = \hat{p}_G - N \log(\Gamma/N)
\]

where the last equality is because \( \hat{p} \) is the optimal solution of \((5.4)\). This completes the proof of \((5.5)\).

Finally, since \( \bar{v} \) is a solution of \((5.4)\), it holds \( \sum_{i=1}^{N} \hat{v}_i \varphi(X_i - \bar{\mu}_j) \leq N \) for all \( j \in [M] \). Denote \( X_{\min} = \min_{i \in [N]} X_i \) and \( X_{\max} = \max_{i \in [N]} X_i \). Since \( \varphi \) is Lipschitz continuous, for any \( \mu \in [X_{\min}, X_{\max}] \), there exists \( j \in [M] \) such that \( |\mu - \bar{\mu}_j| \leq \Delta G/2 \), hence it holds

\[
\left| \sum_{i=1}^{N} \hat{v}_i \varphi(X_i - \mu) - \sum_{i=1}^{N} \hat{v}_i \varphi(X_i - \bar{\mu}_j) \right| \leq \sum_{i=1}^{N} \left| \hat{v}_i \right| \frac{1}{\sqrt{2\pi} e} \Delta G \leq \sum_{i=1}^{N} \hat{v}_i \leq N + \frac{\Delta G}{\sqrt{8\pi} e} \sum_{i=1}^{N} \hat{v}_i.
\]

On the other hand, it is easy to check that the function \( \mu \mapsto \sum_{i=1}^{N} \hat{v}_i \varphi(X_i - \mu) \) is increasing on \((-\infty, X_{\min}]\) and decreasing on \([X_{\max}, \infty)\), hence

\[
\max_{\mu \in \mathbb{R}} \sum_{i=1}^{N} \hat{v}_i \varphi(X_i - \mu) \leq N + \frac{\Delta G}{\sqrt{8\pi} e} \sum_{i=1}^{N} \hat{v}_i.
\]

The above when combined with \((5.5)\) leads to \((5.6)\).
B.3.2 Proof of Proposition 5.4
Recall that the function $F(\nu) := -\sum_{i=1}^{N} \log \nu_i$ is 1-self-concordant on $\mathbb{R}^{N}_{++}$. By (2.3) we have
\[
\sum_{i=1}^{N} (\log(\hat{\nu}_i) - \log(\nu_i^*)) \geq \langle \nabla F(\hat{\nu}), \nu^* - \hat{\nu} \rangle + \rho \left( \frac{(\sum_{i=1}^{N} (\nu_i^* - \hat{\nu}_i)^2)^{1/2}}{} \right).
\] (2.32)

Let $S$ be the feasible region of (5.4). Since $\hat{\nu}$ is the optimal solution of (5.4), and $\nu^*$ is in $S$, it holds $\langle \nabla F(\hat{\nu}), \nu^* - \hat{\nu} \rangle \geq 0$. As a result, (2.32) implies
\[
\hat{\rho} - p^* = \sum_{i=1}^{N} (\log(\hat{\nu}_i) - \log(\nu_i^*)) \geq \rho \left( \frac{(\sum_{i=1}^{N} (\nu_i^* - \hat{\nu}_i)^2)^{1/2}}{} \right).
\]

The proof is complete by taking the inverse of $\rho(\cdot)$.

C Auxiliary results

Lemma C.1 For any third-order continuous differentiable function $f(\cdot)$ on a open set $Q \subseteq \mathbb{R}^M$ and any $w, y \in Q$, it holds
\[
f(y) - f(w) - \langle \nabla f(w), y - w \rangle - \frac{1}{2} \nabla^2 f(w)[y - w]^2
= \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} t^2 s \nabla^3 f(w + rst(y - w))[y - w]^3 dt ds dr.
\]

Proof. Note that
\[
f(y) - f(w) - \langle \nabla f(w), y - w \rangle = \int_{0}^{1} [\nabla f(w + t(y - w)) - \nabla f(w)]^T (y - w) dt
= \int_{0}^{1} \int_{0}^{1} t \nabla^2 f(w + ts(y - w))[y - w]^2 ds dt.
\]

Hence it holds that
\[
f(y) - f(w) - \langle \nabla f(w), y - w \rangle - \frac{1}{2} \nabla^2 f(w)[y - w]^2
= \int_{0}^{1} \int_{0}^{1} t (\nabla^2 f(w + st(y - w)) - \nabla^2 f(w))[y - w]^2 ds dt
= \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} t^2 s \nabla^3 f(w + str(y - w))[y - w]^3 dr ds dt.
\]

\[
\square
\]

Lemma C.2 Let $\bar{A} \in \mathbb{R}^{n \times n}$ be a symmetric matrix and $\bar{B} \in \mathbb{R}^{n \times n}$ be a positive definite matrix (and hence invertible). Suppose $\bar{A} \preceq \bar{B}$ and $\bar{A} \succeq - \bar{B}$, then it holds $\bar{A} \bar{B}^{-1} \bar{A} \preceq \bar{B}$.

Proof. Let $P$ be a nonsingular matrix such that $P^\top \bar{B} P = I_n$. By assumption, we have
\[-I_n \preceq P^\top \bar{A} P \preceq I_n \Rightarrow (P^\top \bar{A} P)^2 \preceq I_n \]

Therefore,
\[
P^\top \bar{A} B^{-1} \bar{A} P = P^\top \bar{A} P \cdot (P^\top \bar{B} P)^{-1} \cdot P^\top \bar{A} P = (P^\top \bar{A} P)^2 \preceq I_n
\]
which is equivalent to
\[
\bar{A} \bar{B}^{-1} \bar{A} \preceq P^{-T} P^{-1} = \bar{B}.
\]

\[
\square
\]
Lemma C.3 For any \( x \in [0, 1/5] \), it holds

\[
(1 - x)^{-2} - 1 \leq 3x \quad \text{and} \quad (1 - x)^2 - 1 \geq -3x.
\] (3.1)

Proof. Note that the function \( g(x) = (1 - x)^{-2} - 1 - 3x \) is convex on \([0, 1/5]\), with \( g(0) = 0 \) and \( g(1/5) = 25/16 - 1 - 3/5 = 9/16 - 9/15 < 0 \), so \( g(x) \leq 0 \) for all \( x \in [0, 1/5] \). For the second inequality, note that \( (1 - x)^2 - 1 = x^2 - 2x \geq -2x \geq -3x \) for all \( x \geq 0 \). □

D Experimental Details

For experiments in Section 6.1.1, for Algorithm 1, we use \( \gamma_k = \rho_k = 0.8^k \), and initialize with \( w^0 = (1/M)1_M \). We set initially \( L_0 = 3/\sqrt{2} \), and the enlargement parameter \( \beta = 1.5 \). For the first 10 iterations of Algorithm 1, we try a shorter step-size \( w_{k+1} = w_k + 0.5(y_k - w_k) \). If this shorter step is accepted by (3.5), then we use this shorter step. Otherwise, we use a full step \( w_{k+1} = y_k \). After 10 iterations, we use the default full step \( w_{k+1} = y_k \) for \( k > 10 \). We terminate the Away-step Frank-Wolfe (AFW) method for subproblem (3.2) as follows: in the \( k \)-th outer iteration, let \( h^{k,t} \) be the objective value of the subproblem (3.2) in the \( t \)-th iteration of Algorithm 2. We terminate Algorithm 2 at iteration \( t \) if \( |h^{k,t} - h^{k,t-1}| / \max\{|h^{k,t-1}|, 1\} < \text{tol}_k \) for some given \( \text{tol}_k > 0 \). In particular, we set \( \text{tol}_k = 10^{-8} \) for \( k \leq 3 \), \( \text{tol}_k = 10^{-9} \) for \( 4 \leq k \leq 9 \), and \( \text{tol}_k = 10^{-10} \) for \( k \geq 10 \).

For experiments in Section 6.1.2, we adopt the same parameter specifications mentioned above, except that we don’t try the shorter steps (\( w_{k+1} = w_k + 0.5(y_k - w_k) \)).

For experiments in Section 6.2, we adopt the same parameter specifications as in Section 6.1.1 except that we try 5 iterations of shorter steps instead of 10.