

Maximum Likelihood Estimation for Learning Populations of Parameters

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Abstract

Consider a setting with N independent individuals, each with an unknown parameter, $p_i \in [0, 1]$ drawn from some unknown distribution P^* . After observing the outcomes of t independent Bernoulli trials, i.e., $X_i \sim \text{Binomial}(t, p_i)$ per individual, our objective is to accurately estimate P^* . This problem arises in numerous domains, including the social sciences, psychology, health-care, and biology, where the size of the population under study is usually large while the number of observations per individual is often limited.

Our main result shows that, in the regime where $t \ll N$, the maximum likelihood estimator (MLE) is both statistically minimax optimal and efficiently computable. Precisely, for sufficiently large N , the MLE achieves the information theoretic optimal error bound of $\mathcal{O}(\frac{1}{t})$ for $t < c \log N$, with regards to the earth mover's distance (between the estimated and true distributions). More generally, in an exponentially large interval of t beyond $c \log N$, the MLE achieves the minimax error bound of $\mathcal{O}(\frac{1}{\sqrt{t \log N}})$. In contrast, regardless of how large N is, the naive "plug-in" estimator for this problem only achieves the sub-optimal error of $\Theta(\frac{1}{\sqrt{t}})$.

1 Introduction

The problem of learning a distribution of parameters over a population arises in several domains such as social sciences, psychology, medicine, and biology [Lor65, LC75, Mil86, PD90, CC94, BLW00]. While the number of individuals in the population can be very large, the number of observations available per individual is often very limited, which prohibits accurate estimation of the parameter of interest per individual. In such sparse observation scenarios, *how accurately can we estimate the distribution of parameters over the population?*

In the 1960's F. M. Lord studied the problem of estimating the distribution of parameters over a population in the context of psychological testing [Lor65, Lor69]. Consider a study involving a large number of independent individuals. Each individual has an unknown probability p_i of answering a question correctly. Given the scores of these individuals on a test with a small set of questions, the goal is to estimate the underlying distribution of the p_i 's. Such an estimated distribution can be used in downstream tasks, like testing if the distribution of scores is uniform or multimodal, or comparing two tests of the same psychological trait.

We use the lens of sparse regime analysis for this problem of learning a population of parameters. Our analysis is inspired by the recent advances in a related problem of estimating discrete distributions and their properties such as, entropy and support size, when the number of observations is much smaller than the support size of the distribution [VV11a, VV11b, JVHW15, WY15, VV16, WY16, OSW16, ADOS17, JHW18, HJW18]. However, we note that our setting is not the same as estimating a discrete distribution. For instance, the probabilities

sum to 1 for a discrete distribution, where as, the true parameters in our setting need not sum to 1.

There have been several classical works on non-parametric mixture models in general [Tur76, Sim76, Lai78, Lin83a, Lin83b, Böh89, LK92] and binomial mixture models in particular [Cre79, Woo99] which have studied the geometry of the maximum likelihood estimator (MLE), the optimality conditions, identifiability, and uniqueness of the MLE solution, and algorithms for computing the optimal solution to the MLE. However, the statistical analysis of how accurately the MLE recovers the underlying distribution has not been addressed. In this paper, we fill this gap, and show that the MLE achieves the optimal error bound with regards to the earth mover's distance (or Wasserstein-1 distance, Definition 3.1) between the estimated and true distributions (equivalently, the l_1 -distance between the CDF's).

1.1 Problem set-up and summary of results

The setting considered in [Lor69] can be modeled as follows. Consider a set of N independent coins, each with its own unknown bias $p_i \in [0, 1]$ drawn independently from some unknown distribution P^* over $[0, 1]$. That is, the probability of seeing a head when coin i is tossed is p_i . For each coin i , we get to observe the outcome of t independent tosses, denoted by, $X_i \sim \text{Binomial}(t, p_i)$. Our goal is to estimate the unknown distribution P^* from $\{X_i\}_{i=1}^N$.

The MLE for this problem is formulated as follows:

$$\hat{P}_{\text{mle}} \in \arg \max_{Q \in \mathcal{D}} \sum_{i=1}^N \log \int_0^1 \binom{t}{X_i} y^{X_i} (1-y)^{t-X_i} dQ(y),$$

where \mathcal{D} is the set of all distributions on $[0, 1]$.

Our Contribution: We bound the earth mover's distance (or the Wasserstein-1 distance) between the true distribution P^* and the MLE solution \hat{P}_{mle} , and show that:

Theorem 1.1. (Informal statement)

- The MLE achieves an error bound of

$$W_1(P^*, \hat{P}_{\text{mle}}) = \mathcal{O}_\delta \left(\frac{1}{t} \right),^1$$

when $t = \mathcal{O}(\log N)$. The bound of $\Theta\left(\frac{1}{t}\right)$ is information theoretically optimal up to a constant factor.

- The MLE achieves an error bound of

$$W_1(P^*, \hat{P}_{\text{mle}}) = \mathcal{O}_\delta \left(\frac{1}{\sqrt{t \log N}} \right),$$

when $t \in [\Omega(\log N), \mathcal{O}(N^{2/9-\epsilon})]$, and this bound is information theoretically optimal in this regime.

Table 1 summarizes our results in comparison to other estimators. While the moment matching estimator [TKV17] achieves the same minimax optimal error bound as the MLE when $t = \mathcal{O}(\log N)$, it fails when $t = \Omega(\log N)$ due to high variance in the larger moments. While the local moment matching approach [HJW18] could theoretically avoid this weakness, it involves hyperparameter tuning which makes it difficult to work with in practice (Remark 3.3 in Section 3). In contrast, the MLE naturally adapts itself and achieves the optimal rates in different regimes without the need for any parameter tuning. Furthermore, our analysis involves bounding the coefficients of Bernstein polynomials approximating Lipschitz-1 functions (Proposition 4.2). This question is of independent interest with implications to general polynomial approximation theory as well as applications in computer graphics.

¹ $\mathcal{O}_\delta(\cdot)$ hides $\log(1/\delta)$ in the bound for it to hold with probability at least $1 - 2\delta$.

Table 1: Comparison of results

Estimators	Bound on EMD
Empirical Estimator	$\Theta\left(\frac{1}{\sqrt{t}}\right) + \Theta\left(\frac{1}{\sqrt{N}}\right)$ in all regimes
Moment Matching [TKV17]	<ul style="list-style-type: none"> • $\Theta\left(\frac{1}{t}\right)$, when $t = \mathcal{O}(\log N)$ • Fails when $t = \Omega(\log N)$
MLE (this paper)	<ul style="list-style-type: none"> • $\Theta\left(\frac{1}{t}\right)$, when $t = \mathcal{O}(\log N)$ • $\Theta\left(\frac{1}{\sqrt{t \log N}}\right)$, when $t \in [\Omega(\log N), \mathcal{O}(N^{2/9-\epsilon})]$

1.2 Outline

The rest of the paper is organized as follows. In Section 2, we discuss the related works. In Section 3, we describe the maximum likelihood estimator for the problem and formally state our main results. We provide the outline of the proofs of our main results in Section 4. The details of the proofs are available in the appendix. Finally, we conclude in Section 5 by discussing some open questions for future research directions.

2 Related Works

Starting from [Lor69], there has been a great deal of interest in the problem of estimating the distribution of true scores of a population of independent entities. Maximum likelihood estimation for non-parametric mixture models has been studied extensively [LC75, Cre79, Lai78, Tur76, LK92]. [Lin83a] and [Lin83b] delineate the geometry of the MLE landscape for non-parametric mixture models in general, and specifically for exponential family respectively. [Woo99] further discusses the issue of uniqueness of the solution for mixture of binomials and the relationship with the moment space. As mentioned in the introduction, the accuracy of the MLE solution for this formulation has not been studied in the literature. Our work fills in this gap by showing that the MLE solution is minimax optimal when $t \ll N$.

In a recent work [TKV17], the authors proposed a *moment matching estimator* to estimate the unknown distribution of the biases in the regime where the number of tosses per coin $t = \mathcal{O}(\log N)$. This estimator finds a distribution on $[0, 1]$ that closely matches the first t empirical moments of the unknown distribution that can be estimated using the observations. This moment matching estimator has an error bound of $\mathcal{O}\left(\frac{1}{t}\right) + \mathcal{O}_\delta\left(2^t t \sqrt{\frac{\log t}{N}}\right)$ in Wasserstein-1 distance. Furthermore, [TKV17] also showed that $\Omega\left(\frac{1}{t}\right)$ is a lower bound in this setting. The main weakness of this method of moments approach is that it fails to obtain the optimal rate when $t > c \log N$.

A tangentially related problem is that of estimating a discrete distribution and its sym-

metric properties² such as, entropy and support size, when the number of observations is much smaller than the support size of the distribution. This is a well-studied classical problem in statistics [FCW43, GT56, ET76]. It has received a lot of interest in the past decade and continues to be a very active area of research [Pan03, OSVZ04, AOP09, ADM⁺10, VV11a, VV13, JVHW15, WY15, VV16, WY16, OSW16, ADOS17, JHW18, HJW18]. Recent work [HJW18] used local moment matching to provide bounds on estimating symmetric properties of discrete distributions under the Wasserstein-1 distance. This technique of local moment matching can be used in our setting to improve the bounds obtained in [TKV17] in the regime where $t > c \log N$. We discuss this more in Section 3.2.

In a similar spirit to our work, a series of works [AOP09, ADM⁺10, ADOS17] examined the *profile* or *pattern* maximum likelihood as a unifying framework for estimating symmetric properties of a discrete distribution. Unlike in our setting, it is computationally challenging to compute the exact maximum likelihood estimator, and the question becomes how to efficiently approximate it (see e.g. [Von12]).

3 Main Results

Before formally stating our results, we introduce some notation, discuss the MLE objective and define the Wasserstein-1 metric used to measure the accuracy of estimation.

Notation: Recall that N is the number of independent coins and t is the number of tosses per coin. The biases of the coins are denoted by $\{p_i\}_{i=1}^N$, where each $p_i \in [0, 1]$ is drawn from some unknown distribution P^* on $[0, 1]$. The set of observations is $\{X_i\}_{i=1}^N$, where $X_i \sim \text{Binomial}(t, p_i)$. For $s \in \{0, 1, \dots, t\}$, let n_s denote the number of coins that show s heads out of t tosses. Let h_s^{obs} denote the fraction of coins that show s heads.

$$n_s := \sum_{i=1}^N \mathbf{1}_{\{X_i=s\}}, \quad h_s^{\text{obs}} := \frac{n_s}{N}, \quad (1)$$

where $\mathbf{1}_{\mathcal{A}}$ is indicator function for set \mathcal{A} . $\mathbf{h}^{\text{obs}} := \{h_0^{\text{obs}}, h_1^{\text{obs}}, \dots, h_t^{\text{obs}}\}$ is the observed *fingerprint*. Since the identity of the coins is not important to estimate the distribution of the biases, the observed fingerprint is a sufficient statistics for the estimation problem.

MLE Objective: The MLE estimate of the distribution of biases given the observations $\{X_i\}_{i=1}^N$ is,

$$\begin{aligned} \hat{P}_{\text{mle}} &\in \arg \max_{Q \in \mathcal{D}} \sum_{i=1}^N \log \int_0^1 \binom{t}{X_i} y^{X_i} (1-y)^{t-X_i} dQ(y), \\ &= \arg \max_{Q \in \mathcal{D}} \sum_{s=0}^t n_s \log \underbrace{\int_0^1 \binom{t}{s} y^s (1-y)^{t-s} q(y) dy}_{=: E_Q[h_s]}, \end{aligned}$$

where \mathcal{D} is the set of all distributions on $[0, 1]$, n_s is the number of coins that see s heads out of t tosses, and $E_Q[h_s]$ is the expected fraction of the population that sees s heads out of t tosses under the distribution Q . Equivalently, the MLE can be written in terms of the

²A function over a discrete distribution is said to be a *symmetric function* if it remains invariant to the relabeling of the domain symbols.

fingerprint as follows,

$$\hat{P}_{\text{mle}} \in \arg \max_{Q \in \mathcal{D}} \sum_{s=0}^t h_s^{\text{obs}} \log E_Q[h_s], \quad (2)$$

$$= \arg \min_{Q \in \mathcal{D}} \text{KL}(\mathbf{h}^{\text{obs}}, E_Q[\mathbf{h}]), \quad (3)$$

where $\text{KL}(A, B)$ is the Kullback-Leibler divergence³ between distributions A and B , \mathbf{h}^{obs} is the observed fingerprint vector and $E_Q[\mathbf{h}]$ denotes the expected fingerprint vector when the biases are drawn from distribution Q .

Remark 3.1. The set \mathcal{D} of all distributions over $[0, 1]$ is convex. Furthermore, the objective function of the MLE (Equation 3) is convex in Q and strictly convex in the valid fingerprints, $\{E_Q[h_s]\}_{s=0}^t$. While there is a unique $E_{\hat{P}_{\text{mle}}}[\mathbf{h}]$ that minimizes the objective (3), there can be many distributions $Q^* \in \mathcal{D}$ that can give rise to the optimal expected fingerprint. Moreover, while the fingerprint vector \mathbf{h} lives in Δ^t , the t -dimensional simplex in \mathbb{R}^{t+1} , not all vectors in Δ^t can be valid fingerprints. The set of all valid fingerprints is a small convex subset of Δ^t . Very often \mathbf{h}^{obs} falls outside the set of valid fingerprints and the solution to the MLE is the closest projection under the KL divergence onto the valid fingerprint set. Furthermore, the fingerprints are related to moments via a linear transform. The geometry of the set of valid fingerprints therefore can also be described using moments. For more details on this geometric description we refer the reader to [Woo99].

Wasserstein-1 Distance: We measure the accuracy of our estimator using the Wasserstein-1 distance or the earth mover's distance (EMD) between two probability distributions over the interval $[0, 1]$ which is defined as:

Definition 3.1 (Wasserstein-1 or earth mover's distance).

$$W_1(P, Q) := \inf_{\gamma \in \Gamma(P, Q)} \int_{x=0}^1 \int_{y=0}^1 |x - y| d\gamma(x, y), \quad (4)$$

where $\Gamma(P, Q)$ is a collection of all the joint distributions on $[0, 1]^2$ with marginals P and Q . A dual definition due to Kantorovich and Rubinstein [KR58] of this metric is as follows:

$$W_1(P, Q) := \sup_{f \in \text{Lip}(1)} \int_0^1 f(x)(p(x) - q(x))dx, \quad (5)$$

$$= \sup_{f \in \text{Lip}(1)} (E_P[f] - E_Q[f]), \quad (6)$$

where p and q are the probability density functions of the distributions P and Q respectively, and $\text{Lip}(1)$ denotes the set of Lipschitz-1 functions.

Wassertein-1 distance is a natural choice to measure the accuracy of an estimator in our setting. E.g., suppose the true distribution P^* is $\delta(0.5) = 1$. Let P_1 with $\delta(0.45) = 1$ and P_2 with $\delta(0) = \delta(1) = \frac{1}{2}$ be the output of two estimators. The Wassertein-1 distance, $W_1(P^*, P_1) = 0.05$ and $W_1(P^*, P_2) = 0.5$, clearly distinguishes the first estimate to be much better than the second. In contrast, the total variation distance between both P_1 and P_2 to the truth is 1 and the KL divergence to the truth in both cases is infinite.

³KL divergence between two discrete distributions A and B supported on \mathcal{X} is defined as $\text{KL}(A, B) = \sum_{x \in \mathcal{X}} A(x) \log \frac{A(x)}{B(x)}$.

3.1 Small sample regime

We first focus on the regime where the number of observations per coin, $t = \mathcal{O}(\log N)$. Consider the problem setup in Section 1.1. The following theorem gives a bound on the Wasserstein-1 distance between the MLE (Equation 3) and the true underlying distribution.

Theorem 3.1 (Small Sample Regime). When $t = \mathcal{O}(\log N)$, the Wasserstein-1 distance between an optimal solution to the MLE, denoted by \hat{P}_{mle} and the true underlying distribution P^* can be bounded with probability at least $1 - 2\delta$ as follows,

$$W_1(P^*, \hat{P}_{\text{mle}}) \leq \mathcal{O}_\delta \left(\frac{1}{t} \right). \quad (7)$$

For constant δ , this $\mathcal{O}(\frac{1}{t})$ rate is information theoretically optimal due to the following result (Proposition 1 in [TKV17]):

Proposition 3.1 (Lower Bound [TKV17]). Let P denote a distribution over $[0, 1]$. Let $\mathbf{X} := \{X_i\}_{i=1}^N$ be random variables with $X_i \sim \text{Binomial}(t, p_i)$ where p_i is drawn independently from P . Let f be an estimator that maps \mathbf{X} to a distribution $f(\mathbf{X})$. For every fixed t , the following lower bound holds for all N :

$$\inf_f \sup_P \mathbb{E} [W_1(P, f(\mathbf{X}))] > \frac{1}{4t}. \quad (8)$$

3.2 Medium sample regime

In this section we consider the regime where the number of observations per coin t is greater than $\Omega(\log N)$. For the same setting as before (Section 1.1), the following theorem provides a bound on the Wasserstein-1 distance between the MLE solution and the true distribution.

Theorem 3.2 (Medium Sample Regime). There exists $\epsilon > 0$, such that, for $t \in [\Omega(\log N), \mathcal{O}(N^{2/9-\epsilon})]$, with probability at least $1 - 2\delta$,

$$W_1(P^*, \hat{P}_{\text{mle}}) \leq \mathcal{O}_\delta \left(\frac{1}{\sqrt{t \log N}} \right). \quad (9)$$

We prove a matching $\Omega(\frac{1}{\sqrt{t \log N}})$ lower bound on the minimax rate for estimating the population of parameters under Wasserstein-1 distance. The lower bound is formalized in the following theorem.

Theorem 3.3. Let P be a distribution over $[0, 1]$. Let $\mathbf{X} := \{X_i\}_{i=1}^N$ be random variables with $X_i \sim \text{Binomial}(t, p_i)$ where p_i is drawn independently from P . Let f be an estimator that maps \mathbf{X} to a distribution $f(\mathbf{X})$. For every t, N s.t. $t \leq \frac{N^{2(\epsilon^4-1)}}{36}$, the following lower bound holds:

$$\inf_f \sup_P \mathbb{E} [W_1(P, f(\mathbf{X}))] > \frac{1}{3e^4 \sqrt{t \log N}}. \quad (10)$$

This lower bound, combined with the $\Theta(\frac{1}{t})$ lower bound shown in [TKV17], implies that the MLE is minimax optimal up to a constant factor in both the regimes.

Remark 3.2 (Conjecture). We believe that the range of t for which the bound in Equation 9 holds is larger than that guaranteed in Theorem 3.2. With the current proof framework, it seems likely that the interval of t in which Theorem 3.2 holds can be improved to

$$t \in \left[\Omega(\log N), \mathcal{O}(N^{2/3-\epsilon}) \right].$$

Details on why we believe that this interval should hold are described in Section 5.1.

Remark 3.3 (Local Moment Matching). The moment matching estimator in [TKV17] fails when t is larger than $\Omega(\log N)$ because the t -th order moments cannot be estimated accurately in that regime. This causes the second term in the error bound $\mathcal{O}\left(\frac{1}{t}\right) + \mathcal{O}_\delta\left(2^t t \sqrt{\frac{\log t}{N}}\right)$ to become large. Naturally, one might consider matching only the first $\log N$ moments which can be reliably estimated. In addition, the parameter interval $[0, 1]$ can be split into blocks, and the moment matching can be done in each block locally by utilizing the fact that for large t , X_i/t tightly concentrates around p_i . The local moment matching was first introduced in a recent work by [HJW18] in the setting of learning discrete distributions. Potentially, one may apply the local moment matching approach to our setting of learning populations of parameters which will likely yield an algorithm that achieves the same Wasserstein-1 distance error as the MLE, $\mathcal{O}(\max(\frac{1}{\sqrt{t \log N}}, \frac{1}{t}))$ in the $t \ll N$ regime. The algorithm will degenerate to the one developed in [TKV17] in the $t = \mathcal{O}(\log N)$ regime. However, from a practical perspective, the local moment matching algorithm is quite unwieldy. It involves significant parameter tuning and special treatment for the edge cases. Some techniques used in local moment matching, e.g. using a fixed blocks partition of $[0, 1]$ and matching the first $\log N$ moments for all the blocks, are quite crude and likely lose large constant factors both in theory and in practice. Therefore, we expect the local moment matching to have inferior performance than the MLE approach in practice. We include a brief sketch of how one may apply the local moment matching approach to our setting in Appendix C.

Remark 3.4 (Empirical Estimator). The naive “plug-in” estimator for the underlying distribution is the sorted estimates of the biases of the coins. This incurs an error of $\mathcal{O}\left(\frac{1}{\sqrt{t}}\right) + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$ in the earth movers distance (or l_1 –distance between the estimated and the true CDFs), where the first term is due to the error in estimating the biases of the coins from t outcomes, and the second term is due to estimating the error in the estimated CDF using N coins. If the number of tosses per coin is very large, that is, $t \gg N$, then we can estimate individual biases pretty well, and obtain an empirical CDF that can estimate P^* incurring an overall error rate of $\mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$. However, in the regime of interest, the number of observations per coin is small, i.e., $t \ll N$ (*sparse regime*). The empirical estimates of the biases in this regime are very crude. Thus, when t is small, even with a very large population (large N), the empirical estimator does not perform better on the task of estimating the underlying distribution than on estimating the biases itself which incurs a $\Theta\left(\frac{1}{\sqrt{t}}\right)$ error.

4 Proof Sketches

In this section we provide proof sketches for the main results stated in Section 3. The details are provided in the appendix.

4.1 Bound on Wasserstein-1 distance

Proofs of Theorems 3.1 and 3.2 involve bounding the Wasserstein-1 distance between the true distribution P^* and the MLE estimate \hat{P}_{MLE} . Recall the dual definition of Wasserstein-1 distance or the earth movers distance between two distributions P and Q supported on $[0, 1]$,

$$W_1(P, Q) = \sup_{f \in \text{Lip}(1)} \int_0^1 f(x)(p(x) - q(x))dx,$$

where p and q are the probability density functions of the distributions P and Q respectively, and $\text{Lip}(1)$ denotes the set of Lipschitz-1 functions. Any Lipschitz-1 function f on $[0, 1]$ can

be approximated using Bernstein polynomials as, $\hat{f}(x) := \sum_{j=0}^t b_j \binom{t}{j} x^j (1-x)^{t-j}$. Using this approximation for any Lipschitz-1 function f , we obtain the following bound,

$$\begin{aligned} \int_0^1 f(x)(p(x) - q(x))dx &= \int_0^1 (f(x) - \hat{f}(x))(p(x) - q(x))dx + \int_0^1 \hat{f}(x)(p(x) - q(x))dx, \\ &\leq 2\|f - \hat{f}\|_\infty + \int_0^1 \sum_{j=0}^t b_j \binom{t}{j} x^j (1-x)^{t-j} (p(x) - q(x))dx, \\ &= 2\|f - \hat{f}\|_\infty + \sum_{j=0}^t b_j (\mathbb{E}_P[h_j] - \mathbb{E}_Q[h_j]), \end{aligned} \quad (11)$$

where $\|f - \hat{f}\|_\infty := \max_{x \in [0,1]} |f(x) - \hat{f}(x)|$ is the polynomial approximation error. Therefore, the Wasserstein-1 distance (Definition 5) between the true distribution P^* and MLE estimate \hat{P}_{mle} can be bounded as follows,

$$\begin{aligned} &W_1(P^*, \hat{P}_{\text{mle}}) \\ &\leq \sup_{f \in \text{Lip}(1)} \left\{ \underbrace{2\|f - \hat{f}\|_\infty}_{(a)} + \underbrace{\sum_{j=0}^t b_j (\mathbb{E}_{P^*}[h_j] - h_j^{\text{obs}})}_{(b)} + \underbrace{\sum_{j=0}^t b_j (h_j^{\text{obs}} - \mathbb{E}_{\hat{P}_{\text{mle}}}[h_j])}_{(c)} \right\} \end{aligned} \quad (12)$$

The first term (a) in the above bound (Equation 12) is the approximation error for using Bernstein polynomials to approximate Lipschitz-1 functions. The second term (b) is the error due to sampling. The third term (c) is the estimation error in matching the fingerprints.

4.2 Concentration of fingerprints

We bound the second term in Equation 12 using the following lemma.

Lemma 4.1. With probability at least $1 - \delta$,

$$\left| \sum_{j=0}^t b_j (h_j^{\text{obs}} - \mathbb{E}_{P^*}[h_j]) \right| \leq \mathcal{O} \left(\max_j |b_j| \sqrt{\frac{\log 1/\delta}{N}} \right). \quad (13)$$

Proof. Recall that h_s^{obs} is the fraction of the population that sees s heads out of t tosses and $\mathbb{E}_{P^*}[h_s]$ is the expected fingerprint under the true distribution which is exactly $\mathbb{E}[h_s^{\text{obs}}]$, and we will use $\mathbb{E}[h_s^{\text{obs}}]$ and $\mathbb{E}_{P^*}[h_s]$ interchangeably. Define, $\phi(X) := \sum_{s=0}^t b_s (h_s^{\text{obs}} - \mathbb{E}[h_s^{\text{obs}}])$, that is,

$$\phi(X) = \frac{1}{N} \sum_{i=1}^N \sum_{s=0}^t b_s (\mathbb{1}_{\{X_i=s\}} - \mathbb{E}[h_s^{\text{obs}}]).$$

Note that $\mathbb{E}[\phi(X)] = 0$. Note that X_i is a sum of t independent Bernoulli random variables,

$$X_i := \sum_{s=0}^t Y_s^{(i)},$$

where $Y_s^{(i)} \sim \text{Bernoulli}(p_i)$. Let $\phi_{i'}(X)$ be ϕ with one of the t tosses of coin i being re-drawn, say $Y_s^{(i)'} \sim \text{Bernoulli}(p_i)$. Let X_i' denote the number of heads seen by coin i with the replaced

coin toss. Note that X'_i can differ from X_i by at most ± 1 . Therefore, we can bound the difference in $\phi(X)$ and $\phi_{i'}(X)$ as follows,

$$|\phi(X) - \phi_{i'}(X)| \leq \max_{0 \leq s \leq t} |b_s| \frac{2}{N}.$$

By McDiarmid's Inequality, for some absolute constants $C, c > 0$,

$$\Pr(|\phi(X)| \geq \epsilon) \leq C \exp\left(-\frac{cN\epsilon^2}{4(\max_s |b_s|)^2}\right).$$

Hence, with probability at least $1 - \delta$,

$$\left| \sum_{j=0}^t b_j (h_j^{\text{obs}} - \mathbb{E}_{P^*}[h_j]) \right| \leq \mathcal{O}\left(\max_j |b_j| \sqrt{\frac{\log 1/\delta}{N}}\right). \quad (14)$$

□

4.3 Bound on error term due to MLE

We bound the third term in Equation 12 using the following lemma.

Lemma 4.2. For $3 \leq t \leq \sqrt{C_0 N} + 2$, where $C_0 > 0$ is a constant, w. p. $1 - \delta$,

$$\begin{aligned} \left| \sum_{j=0}^t b_j (h_j^{\text{obs}} - \mathbb{E}_{P_{\text{mle}}}[h_j]) \right| &\leq \max_j |b_j| \sum_{j=0}^t |h_j^{\text{obs}} - \mathbb{E}_{P_{\text{mle}}}[h_j]|, \\ &\leq \max_j |b_j| \sqrt{2 \ln 2} \sqrt{\frac{t}{2N} \log \frac{4N}{t} + \frac{1}{N} \log \frac{3e}{\delta}}. \end{aligned} \quad (15)$$

Proof. Let P_{mle} be an optimal solution to the MLE and P^* be the true distribution. By optimality of the MLE solution, we have the following inequality,

$$\text{KL}(\mathbf{h}^{\text{obs}}, \mathbb{E}_{P_{\text{mle}}}[\mathbf{h}]) \leq \text{KL}(\mathbf{h}^{\text{obs}}, \mathbb{E}_{P^*}[\mathbf{h}]). \quad (16)$$

Proposition 4.1 (Pinsker's Inequality [CT12]). For discrete distributions P and Q :

$$\text{KL}(P, Q) \geq \frac{1}{2 \ln 2} \|P - Q\|_1^2. \quad (17)$$

Using Pinsker's inequality and the optimality of the MLE solution, we can bound term (c) in Equation (12) as follows:

$$\begin{aligned} \left| \sum_{j=0}^t b_j (h_j^{\text{obs}} - \mathbb{E}_{P_{\text{mle}}}[h_j]) \right| &\leq \sum_{j=0}^t |b_j| |h_j^{\text{obs}} - \mathbb{E}_{P_{\text{mle}}}[h_j]|, \\ &\leq \max_j |b_j| \sum_{j=0}^t |h_j^{\text{obs}} - \mathbb{E}_{P_{\text{mle}}}[h_j]|, \\ &\leq \max_j |b_j| \sqrt{2 \ln 2 \text{KL}(\mathbf{h}^{\text{obs}}, \mathbb{E}_{P_{\text{mle}}}[\mathbf{h}])}, \end{aligned} \quad (18)$$

$$\leq \max_j |b_j| \sqrt{2 \ln 2 \text{KL}(\mathbf{h}^{\text{obs}}, \mathbb{E}_{P^*}[\mathbf{h}])}. \quad (19)$$

Using the recent results on bounds on KL divergence between empirical observations and the true distribution for discrete distributions [MJT⁺18], for $3 \leq t \leq \sqrt{C_0 N} + 2$, w. p. $1 - \delta$,

$$\left| \sum_{j=0}^t b_j (h_j^{\text{obs}} - \mathbb{E}_{P_{\text{mle}}}[h_j]) \right| \leq \max_j |b_j| \sqrt{2 \ln 2} \sqrt{\frac{t}{2N} \log \frac{4N}{t} + \frac{1}{N} \log \frac{3e}{\delta}}.$$

□

4.4 Bounding the polynomial approximation error

In this section we bound $\max_j |b_j|$ as well as term (a) in Equation 12, both of which are related to polynomial approximation of Lipschitz-1 functions using Bernstein polynomials. Let f be any Lipschitz-1 function on $[0, 1]$. Let \hat{f} be a polynomial approximation of f using Bernstein polynomials of degree t :

$$\hat{f}(x) = \sum_{j=0}^t b_j \binom{t}{j} x^j (1-x)^{t-j} := \sum_{j=0}^t b_j B_j^t(x), \quad (20)$$

where,

$$B_j^t(x) := \binom{t}{j} x^j (1-x)^{t-j},$$

is j -th Bernstein polynomial of degree t , for $j = 0, 1, \dots, t$. Our goal is to bound the uniform approximation error,

$$\|f - \hat{f}\|_\infty := \max_{x \in [0,1]} |f(x) - \hat{f}(x)|,$$

while controlling the magnitude $|b_j|$, of the coefficients. We note that $\max_j |b_j|$ appears in the bounds of the error terms (b) and (c) in Equation (11). Therefore, it is important to control it while bounding the polynomial approximation error to obtain tight bounds on the Wasserstein-1 metric in different regimes of t and N .

Bernstein [Ber12, Lor53] used $t+1$ uniform samples of the function f on $[0, 1]$, $f(\frac{j}{t})$, $j = 0, 1, \dots, t$, as the coefficients in Equation 20 to prove Weierstrass Approximation Theorem and showed that the uniform approximation error of such an approximation is $\|f - \hat{f}\|_\infty \leq \frac{C}{\sqrt{t}}$, where C is a constant. Since we are interested in approximating Lipschitz-1 functions on $[0, 1]$, the co-efficients used, $|f(\frac{j}{t})|$ are constants, as w.l.o.g, $|f| \leq \frac{1}{2}$. However, this approximation is not sufficient to show the bounds in Theorems 3.1 and 3.2. Therefore, the question of interest is: *Can we obtain better uniform approximation error using Bernstein polynomials with other bounded coefficients?* The following proposition answers this question.

Proposition 4.2. Any Lipschitz-1 function on $[0, 1]$ can be approximated using Bernstein polynomials (Equation 20) of degree t , with an uniform approximation error of

1. $\mathcal{O}(\frac{1}{t})$ with $\max_j |b_j| \leq \sqrt{t} 2^t$.
2. $\mathcal{O}(\frac{1}{k})$ with $\max_j |b_j| \leq \sqrt{k}(t+1)e^{\frac{k^2}{t}}$, for $k < t$.

We are now ready to prove our main results in Theorem 3.1 and Theorem 3.2. We postpone the proof of Proposition 4.2 to the end of this section.

Proof of Theorem 3.1. The first approximation result in Proposition 4.2 with Lemma 4.1 and Lemma 4.2 gives the following bound on the Wasserstein-1 distance between the MLE estimate and the true distribution,

$$W_1(P^*, \hat{P}_{\text{mle}}) \leq \mathcal{O}\left(\frac{1}{t}\right) + \mathcal{O}\left(2^t t \sqrt{\frac{1}{N} \log \frac{1}{\delta}}\right),$$

with probability at least $1 - 2\delta$. Therefore, for $t = \mathcal{O}(\log N)$, we obtain the bound in Theorem 3.1. \square

Proof of Theorem 3.2. With $k = \sqrt{t \log N^c}$, for appropriate choice of $c > 0$, we obtain a bound of

$$\max_j |b_j| \leq t^{1/4}(t+1) (\log N^c)^{1/4} N^c,$$

on the coefficients with a uniform approximation error $\mathcal{O}\left(\frac{1}{\sqrt{t \log N}}\right)$. Combining this bound with Lemma 4.1 and Lemma 4.2 gives the following bound,

$$W_1(P^*, \hat{P}_{\text{mle}}) \leq \mathcal{O}\left(\frac{1}{\sqrt{t \log N}}\right) + \mathcal{O}\left((t \log N^c)^{1/4}(t+1)N^c \sqrt{\frac{t}{N} \log \frac{1}{\delta}}\right),$$

with probability at least $1 - 2\delta$. Therefore, for t above $\Omega(\log N)$, and $t = \mathcal{O}(N^{2/9-\epsilon})$ for $\epsilon > 0$ such that $N^\epsilon = \mathcal{O}(N^{4c/9} c^{1/9} (\log N)^{1/3})$, we obtain the result in Theorem 3.2. \square

Proof sketch of Proposition 4.2: The key idea of our proof is to approximate f using Chebyshev polynomials of degree $k \leq t$, which are then expressed as linear combinations of Bernstein polynomials of degree t to obtain appropriate bounds on the coefficients $|b_j|$. Let \tilde{T}_m denote Chebyshev polynomial of degree m shifted to $[0, 1]$ which satisfy the following recursive relation:

$$\tilde{T}_m(x) = (4x - 2)\tilde{T}_{m-1} - \tilde{T}_{m-2}(x), \quad m = 2, 3, \dots,$$

and $\tilde{T}_0(x) = 1$, $\tilde{T}_1(x) = 2x - 1$. We use the following lemma regarding Chebyshev polynomial approximation. The proof is available in Appendix A.1.

Lemma 4.3. Given any Lipschitz-1 function $f(x)$ on $[0, 1]$, there exists a degree k polynomial in the form of $\hat{f}_k(x) = \sum_{m=0}^k a_m \tilde{T}_m(x)$ that approximates $f(x)$ with error $\|f - \hat{f}_k\|_\infty = \mathcal{O}(\frac{1}{k})$, where $\tilde{T}_m(x)$ denotes Chebyshev polynomial of degree m shifted to $[0, 1]$. Further, the coefficients $(a_0, a_1, a_2, \dots, a_k)$ satisfies $\|a\|_2 \leq 1$.

Chebyshev polynomial \tilde{T}_m , can be written in terms of Bernstein-Bezier polynomials of degree m as follows [Rab03]:

$$\tilde{T}_m(x) = \sum_{i=0}^m (-1)^{m-i} \frac{\binom{2m}{2i}}{\binom{m}{i}} B_i^m(x). \quad (21)$$

Note that the coefficients of B_i^m can be at most 2^m . To prove the first part of the proposition, we approximate the Lipschitz-1 function $f(x)$ using degree $k = t$ Chebyshev polynomial approximation provided by Lemma 4.3 with error $\mathcal{O}(\frac{1}{t})$. This gives an upper bound of 2^t on the coefficients of Bernstein polynomial. To show the second part of the proposition, we need to bound the coefficients of the Bernstein polynomials when the degree of Chebyshev approximation satisfies $k < t$.

Degree raising: Bernstein polynomials of degree $m < t$ can be raised to degree t as:

$$B_i^m(x) = \sum_{j=i}^{i+t-m} \frac{\binom{m}{i} \binom{t-m}{j-i}}{\binom{t}{j}} B_j^t(x). \quad (22)$$

Using degree raising of Bernstein polynomials, we can write shifted Chebyshev polynomials of degree $m < t$ in terms of Bernstein polynomials of degree t as,

$$\begin{aligned} \tilde{T}_m(x) &= \sum_{i=0}^m (-1)^{m-i} \frac{\binom{2m}{2i}}{\binom{m}{i}} \sum_{j=i}^{i+t-m} \frac{\binom{m}{i} \binom{t-m}{j-i}}{\binom{t}{j}} B_j^t(x), \\ &=: \sum_{j=0}^t C(t, m, j) B_j^t(x), \end{aligned} \quad (23)$$

where the coefficient of j -th Bernstein polynomial of degree t is given by⁴,

$$C(t, m, j) := \sum_{l=0}^j (-1)^{m-l} \frac{\binom{2m}{2l} \binom{t-m}{j-l}}{\binom{t}{j}}. \quad (24)$$

With the closed form expressions of the coefficients of the Bernstein polynomials, what remains is to establish upper bounds of these coefficients. The following is a generating function for $C(t, m, j) \binom{t}{j}$,

$$(1+z)^{t-m} \frac{(1+i\sqrt{z})^{2m} + (1-i\sqrt{z})^{2m}}{2} = \sum_{j=0}^t C(t, m, j) \binom{t}{j} z^{t-j}. \quad (25)$$

Using Beta function, the binomial terms in the denominator can be written as,

$$\binom{t}{j}^{-1} = (t+1) \int_0^1 (1-u)^j u^{t-j} du.$$

Combining, we obtain the following generating function for the coefficients,

$$\frac{\sum_{j=0}^t C(t, m, j) z^{t-j}}{t+1} = \int_0^1 (1-u) + uz)^{t-m} \frac{(\sqrt{1-u} + i\sqrt{uz})^{2m} + (\sqrt{1-u} - i\sqrt{uz})^{2m}}{2} du$$

We bound the generating function of the coefficients on the unit circle and use Parseval's theorem to prove the following lemma (details are available in Appendix A.2).

Lemma 4.4. The l_2 -norm of the coefficients of B_j^t can be bounded as follows,

$$\sqrt{\sum_{j=0}^t |C(t, m, j)|^2} \leq (t+1) e^{\frac{m^2}{t}}. \quad (26)$$

And, hence the coefficients of B_j^t can be bounded as follows,

$$|C(t, m, j)| \leq (t+1) e^{\frac{m^2}{t}}. \quad (27)$$

Let f be a Lipschitz-1 function on $[0, 1]$. Let f_k be the polynomial approximation using Chebyshev polynomials upto degree k obtained from Lemma 4.3. We re-write each \tilde{T}_m using Bernstein polynomials of degree k followed by degree raising to t .

$$\begin{aligned} f_k(x) &= \sum_{m=0}^k a_m \tilde{T}_m(x) = \sum_{m=0}^k a_m \left(\sum_{j=0}^t C(t, m, j) B_j^t(x) \right), \\ &= \sum_{j=0}^t \left(\sum_{m=0}^k a_m C(t, m, j) \right) B_j^t(x), \\ &=: \sum_{j=0}^t b_j B_j^t(x). \end{aligned} \quad (28)$$

Since $\|a\|_2 \leq 1$, and from Equation 27, we obtain the following bound on the coefficients, for $j = 0, 1, 2, \dots, t$,

$$\begin{aligned} |b_j| &= \left| \sum_{m=0}^k a_m C(t, m, j) \right| \leq \sum_{m=0}^k |a_m| |C(t, m, j)|, \\ &\leq \sqrt{k} \max_m |C(t, m, j)| \leq \sqrt{k} (t+1) e^{\frac{k^2}{t}}, \end{aligned} \quad (29)$$

where we have applied Lemma 4.3 and Lemma 4.4. This conclude the proof of Proposition 4.2.

⁴For positive integers $a, b > 0$, $\binom{a}{b} = 0$ when $a < b$.

4.5 Lower bound for medium t regime

The basic idea of the proof of Theorem 3.3 is to construct a pair of distributions P, Q whose first $\Theta(\log N)$ moments match and $W_1(P, Q) = \Theta(\frac{1}{\sqrt{t \log N}})$. With N coins sampled from these distributions, each with t flips, we argue that it is information theoretically hard to distinguish the two distributions. We need the following two propositions for the proof, where Proposition 4.3 gives the existence of such a pair of distributions and Proposition 4.4 shows they are hard to distinguish. The proofs of these propositions are provided in Appendix B.

Proposition 4.3. For any positive integer s , there exists a pair of distributions P and Q supported on $[a, b]$ where $0 < a < b$ such that P and Q have identical first s moments, and $W_1(P, Q) \geq \frac{(b-a)}{2s}$.

Proposition 4.4. Let P and Q be two distributions, supported on $\left[\frac{1}{2} - \sqrt{\frac{\log N}{t}}, \frac{1}{2} + \sqrt{\frac{\log N}{t}}\right]$, whose first $L := e^4 \log N$ moments match. Let $p \sim P$ and $q \sim Q$. Let $X \sim \text{Binomial}(t, p)$ and $Y \sim \text{Binomial}(t, q)$. Then the total variation distance between X and Y satisfies,

$$\text{TV}(X, Y) \leq \frac{2\sqrt{t}}{Ne^4}.$$

The proof of Theorem 3.3 follows from these two propositions.

Proof of Theorem 3.3. We first apply Proposition 4.3 to construct a pair of distributions P and Q supported on $\left[\frac{1}{2} - \sqrt{\frac{\log N}{t}}, \frac{1}{2} + \sqrt{\frac{\log N}{t}}\right]$ such that their first $L := e^4 \log N$ moments match, and $W_1(P, Q) \geq \frac{1}{e^4} \frac{1}{\sqrt{t \log N}}$. Let $\mathbf{X} := \{X_i\}_{i=1}^N$ be random variables with $X_i \sim \text{Binomial}(t, p_i)$ where p_i is drawn independently from P . Let $\mathbf{Y} := \{Y_i\}_{i=1}^N$ be random variables with $Y_i \sim \text{Binomial}(t, q_i)$ where q_i is drawn independently from Q . Denote P_N as the joint distribution of \mathbf{X} and Q_N as the joint distribution of \mathbf{Y} . It follows from Proposition 4.4 that $\text{TV}(X_i, Y_i) \leq \frac{2\sqrt{t}}{Ne^4}$. By the property of the product distribution, for $t \leq \frac{N^{2(e^4-1)}}{36}$, $\text{TV}(P_N, Q_N) \leq \frac{2\sqrt{t}}{Ne^4-1} \leq \frac{1}{3}$, which implies that the minimax error is at least $\frac{1}{3e^4\sqrt{t \log N}}$. \square

5 Discussion and Future Directions

We consider the problem of learning the distribution of parameters over a heterogeneous population and show that the MLE achieves optimal error bounds with respect to Wasserstein-1 distance in the sparse observation setting. A future direction of work is to incorporate prior knowledge about the properties of the underlying distribution, such as, smoothness, as additional constraints to the MLE optimization problem. Another direction of interest is to extend the analysis to provide guarantees in general Wasserstein- p norms. In a different direction, a natural question of interest is estimating the properties of the underlying distribution. While the MLE can be used as a plug-in solution to estimate properties of the underlying distribution, it is possible that certain properties could be directly estimated more accurately. Still, one could imagine an analog of the results of [ADOS17], who showed that in the related setting of drawing samples from a single discrete distribution over a large alphabet, for a large class of properties, applying the plug-in estimator to the results of the “profile” maximum likelihood distribution yields a nearly optimal estimator.

5.1 Discussion

We conjecture that the right bound on the coefficients of B_j^t for every $m \leq t$ to be,

$$|C(t, m, j)| \leq e^{\frac{m^2}{t}}, \quad j = 0, 1, 2, \dots, t. \quad (30)$$

In fact, for a fixed m , the coefficients $C(t, m, j)$ should converge to points sampled uniformly from $T_m(x)$ as $t \rightarrow \infty$ by Bernstein's approximation. So, the bound on the coefficients should converge to 1 as $t \rightarrow \infty$.

Furthermore, we believe that the bound on the error due to the MLE could be improved to mirror that for the observed fingerprints, that is, $\left| \sum_{j=0}^t b_j (h_j - \mathbb{E}_{P_{\text{mle}}}(h_j)) \right| \leq \mathcal{O} \left(\max_j |b_j| \sqrt{\frac{\log 1/\delta}{N}} \right)$. Therefore, our conjecture for the upper bound on the range of t in Theorem 3.2 is $\mathcal{O}(N^{2/3-\epsilon})$.

The question of polynomial approximation of Lipschitz-1 functions using Bernstein polynomials with bounded coefficients is an interesting problem on its own, with implications to general polynomial approximation theory and applications in computer graphics.

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A Proofs of Lemma 4.3 and Lemma 4.4

In this section we provide proofs for Lemma 4.3 and Lemma 4.4 used to prove Theorem 3.1 and Theorem 3.2.

A.1 Chebyshev polynomial approximation: Proof of Lemma 4.3

In this section, we focus on proving Lemma 4.3. The existence of the Chebyshev polynomial approximation with error $\mathcal{O}(1/k)$ is shown using the following result,

Lemma A.1. [Jac21, BD69] Given any Lipschitz-1 function $f(x)$ on $[0, 1]$, there exists a degree k polynomial in the form of $f_k(x) = \sum_{m=0}^k a_m \tilde{T}_m(x)$ that approximates $f(x)$ with error $\max_{x \in [0,1]} |f(x) - f_k(x)| = \mathcal{O}(\frac{1}{k})$, where $\tilde{T}_m(x)$ denotes Chebyshev polynomial of degree m shifted to $[0, 1]$.

We now show that the coefficients satisfy $\|a\|_2^2 \leq 1$. Let \tilde{T}_m denote Chebyshev polynomial of degree m shifted to $[0, 1]$ which satisfy the following recursive relation:

$$\tilde{T}_m(x) = (4x - 2)\tilde{T}_{m-1} - \tilde{T}_{m-2}(x), \quad m = 2, 3, \dots,$$

and $\tilde{T}_0(x) = 1$, $\tilde{T}_1(x) = 2x - 1$. Shifted Chebyshev polynomials form a sequence of orthogonal polynomials with respect to the weight $\frac{1}{\sqrt{4x-4x^2}}$:

$$\int_0^1 \tilde{T}_m(x) \tilde{T}_n(x) \frac{dx}{\sqrt{4x-4x^2}} = \begin{cases} 0 & \text{if } m \neq n \\ \frac{\pi}{2} & \text{if } m = n = 0 \\ \frac{\pi}{4} & \text{if } m = n \neq 0. \end{cases} \quad (31)$$

Let f be a Lipschitz-1 function on $[0, 1]$. Let f_k be degree k polynomial approximation of f using Chebyshev polynomials up to degree k ,

$$f_k(x) = \sum_{m=0}^k a_m \tilde{T}_m(x). \quad (32)$$

Since f is Lipschitz-1 on $[0, 1]$, w.l.o.g. $|f_k(x)| \leq 1/2$ for all $x \in [0, 1]$. So, $|a_m| \leq 1$. Furthermore, the norm of the coefficient vector can be bounded as follows:

$$\begin{aligned} \int_0^1 |f_k(x)|^2 \frac{dy}{\sqrt{4x-4x^2}} &= \sum_{m,n=0}^k a_m a_n \int_0^1 \tilde{T}_m(x) \tilde{T}_n(x) \frac{dy}{\sqrt{4x-4x^2}} \\ &= a_0^2 \frac{\pi}{2} + \sum_{m=1}^k a_m^2 \frac{\pi}{4} = a_0^2 \frac{\pi}{4} + \sum_{m=0}^k a_m^2 \frac{\pi}{4}. \end{aligned} \quad (33)$$

Since $|f_k(x)| \leq 1/2$ for all $x \in [0, 1]$ and $\int_0^1 \frac{dy}{\sqrt{4x-4x^2}} = \frac{\pi}{2}$, we obtain the following bound,

$$a_0^2 \frac{\pi}{4} + \|a\|_2^2 \frac{\pi}{4} \leq \frac{\pi}{8}. \quad (34)$$

Hence, $\|a\|_2^2 \leq 1$. Along with Lemma A.1, this completes the proof of Lemma 4.3.

A.2 Bound on generating function: Proof of Lemma 4.4

Using degree raising of Bernstein polynomials, we can write the shifted Chebyshev polynomials of degree $m < t$ in terms of Bernstein polynomials of degree t as follows,

$$\begin{aligned} \tilde{T}_m(x) &= \sum_{i=0}^m (-1)^{m-i} \frac{\binom{2m}{2i}}{\binom{m}{i}} \sum_{j=i}^{i+t-m} \frac{\binom{m}{i} \binom{t-m}{j-i}}{\binom{t}{j}} B_j^t(x), \\ &=: \sum_{j=0}^t C(t, m, j) B_j^t(x), \end{aligned} \quad (35)$$

where the coefficient of j -th Bernstein polynomial of degree t is given by⁵,

$$C(t, m, j) := \sum_{l=0}^j (-1)^{m-l} \frac{\binom{2m}{2l} \binom{t-m}{j-l}}{\binom{t}{j}}. \quad (36)$$

Following is a generating function for the coefficients multiplied by the Binomial terms,

$$\begin{aligned} (1+z)^{t-m} \frac{(1+i\sqrt{z})^{2m} + (1-i\sqrt{z})^{2m}}{2} \\ = \sum_{j=0}^t C(t, m, j) \binom{t}{j} z^{t-j}. \end{aligned} \quad (37)$$

Using the Beta function the binomial terms in the denominator can be written as,

$$\binom{t}{j}^{-1} = (t+1) \int_0^1 (1-u)^j u^{t-j} du.$$

Combing with Equation 37, we obtain the following generating function for the coefficients,

$$(t+1) \int_0^1 ((1-u) + uz)^{t-m} \frac{(\sqrt{1-u} + i\sqrt{uz})^{2m} + (\sqrt{1-u} - i\sqrt{uz})^{2m}}{2} du \quad (38)$$

$$= \sum_{j=0}^t \left(\frac{\sum_{l=0}^j (-1)^{m-l} \binom{2m}{2l} \binom{t-m}{j-l}}{\binom{t}{j}} \right) z^{t-j} \quad (39)$$

⁵For positive integers $a, b > 0$, $\binom{a}{b} = 0$ when $a < b$.

Our goal is to bound the generating function Equation 38 on the unit circle. Let $i\sqrt{z} = \cos \theta + i \sin \theta$, then $z = \cos(\pi + 2\theta) + i \sin(\pi + 2\theta) = -\cos(2\theta) - i \sin(2\theta)$. We bound the norm of $((1-u) + uz)^{t-m} \frac{(\sqrt{1-u} + i\sqrt{uz})^{2m} + (\sqrt{1-u} - i\sqrt{uz})^{2m}}{2}$ by bounding the norm of $(1-u) + uz$ and $(\sqrt{1-u} + i\sqrt{uz})$ which can be expressed as follows,

$$\begin{aligned} |(1-u) + uz|^2 &= (1 - u(1 + \cos(2\theta)))^2 + u^2 \sin^2(2\theta) \\ &= 1 + (2u^2 - 2u)(1 + \cos 2\theta); \end{aligned}$$

$$|\sqrt{1-u} + i\sqrt{uz}|^2 = (\sqrt{1-u} + \sqrt{u} \cos \theta)^2 + u \sin^2 \theta = 1 + 2\sqrt{u-u^2} \cos \theta.$$

Thus, we can bound the logarithm of the magnitude of the integrand as follows,

$$\begin{aligned} &\log \left| ((1-u) + uz)^{t-m} \left(\frac{(\sqrt{1-u} + i\sqrt{uz})^{2m} + (\sqrt{1-u} - i\sqrt{uz})^{2m}}{2} \right) \right| \\ &\leq \frac{t-m}{2} \log((1 - u(1 + \cos(2\theta)))^2 + u^2 \sin^2(2\theta)) + m \log((\sqrt{1-u} + \sqrt{u} \cos \theta)^2 + u \sin^2 \theta) \\ &=: B(\theta, v). \end{aligned} \quad (40)$$

Let $v = \frac{1}{2} - u$. Taking the derivative of $B(\theta, v)$ with respect to θ and v , we get the following two expressions:

$$\begin{aligned} \frac{dB(\theta, v)}{d\theta} &= -4v \cos(\theta) \left(\frac{2(m-t) \cos(\theta)}{(4v^2 - 1) \cos(2\theta) + 4v^2 + 1} + \frac{m}{-4v^2 \cos(\theta) + \cos(\theta) + \sqrt{1-4v^2}} \right) \\ \frac{dB(\theta, v)}{dv} &= \frac{(4v^2 - 1)(m-t) \sin(2\theta)}{(4v^2 - 1) \cos(2\theta) + 4v^2 + 1} - \frac{m\sqrt{1-4v^2} \sin(\theta)}{\sqrt{1-4v^2} \cos(\theta) + 1} \end{aligned}$$

In order to find the maximum of the function, we solve for θ, v such that the above two expressions equal 0. Ignoring the solutions where $\theta = 0$ which are clearly not the maximum, we have $\theta = \arccos[m/t]$ and $v = 0$. Plugging in the solution to the upper bound in Equation 40, we obtain the following upper bound on the logarithm of the magnitude of the integrand of the generating function,

$$B(\theta, v) \leq \underbrace{\frac{t-m}{2} \log \left(1 - \frac{m^2}{t^2} \right)}_{<0} + m \log \left(1 + \frac{m}{t} \right) \leq m \log \left(1 + \frac{m}{t} \right) \leq \frac{m^2}{t}.$$

Therefore, Equation 38 can be bounded by $e^{m^2/t}(t+1)$. Hence, for all z on the unit circle, Equation 39 is bounded by $(t+1)e^{m^2/t}$.

Proposition A.1. Given a degree $d-1$ real polynomial $p(x) = \sum_{i=0}^{d-1} a_i x^i$ that satisfies $|p(x)| \leq c$ for all complex numbers $|x| = 1$, the sum of the squares of the coefficients satisfies $\sum_{i=0}^{d-1} a_i^2 \leq c^2$.

Proof. Let $g_k = p(x_k)$ where $x_k = e^{-\frac{2\pi i k}{d}}$ for $k = 0, 1, \dots, d-1$. By the assumption, we have $|g_k| \leq c$ for all k . Notice that $(g_0, g_1, \dots, g_{d-1})$ is the discrete Fourier transform of the coefficient vector $(a_0, a_1, \dots, a_{d-1})$. Hence, by Parseval's theorem, we have $\sum_{i=0}^{d-1} a_i^2 = \frac{1}{d} \sum_{k=0}^{d-1} g_k^2 \leq c^2$. \square

From Proposition A.1, we obtain the following bound the l_2 -norm of the coefficients,

$$\sqrt{\sum_{j=0}^t |C(t, m, j)|^2} \leq (t+1)e^{\frac{m^2}{t}}. \quad (41)$$

Using the above bound, each of the coefficient can be bounded as follows:

$$|C(t, m, j)| \leq (t+1)e^{\frac{m^2}{t}}.$$

This completes the proof of Lemma 4.4.

B Proof of Theorem 3.3

In this section, we provide the detailed proofs of Proposition 4.3 and Proposition 4.4 that are used to prove Theorem 3.3.

B.1 Proof of Proposition 4.3

Proposition 4.3 states the following: For any positive integer s , there exists a pair of distributions P, Q supported on $[a, b]$ where $0 < a < b$ such that P and Q have identical first s moments, and $W_1(P, Q) \geq \frac{(b-a)}{2s}$.

Proof. Our proof leverages the following result from [TKV17],

Lemma B.1 ([TKV17], Lemma 3). For any positive integer s , there exists a pair of distributions P', Q' supported on $[0, 1]$ such that P' and Q' have identical first s moments, and $W_1(P', Q') \geq \frac{1}{2s}$.

The pair of distributions P' and Q' supported on $[0, 1]$ can be transformed to a pair of distributions P and Q supported on $[a, b]$, where $0 < a < b$, via transformation $P(x) = \frac{1}{b-a} P' \left(\frac{x-a}{b-a} \right)$. We show that P and Q have identical first s moments as follows. For $k \leq s$,

$$\begin{aligned} \int_a^b P(x) x^k dx &= \int_a^b \frac{1}{b-a} P' \left(\frac{x-a}{b-a} \right) x^k dx \\ &= \int_0^1 P'(y) (y(b-a) + a)^k dy \\ &= \int_0^1 Q'(y) (y(b-a) + a)^k dy \\ &= \int_a^b Q(x) x^k dx. \end{aligned}$$

□

B.2 Proof of Proposition 4.4

Proposition 4.4 states the following: Let P and Q be two distributions supported on the interval $\left[\frac{1}{2} - \sqrt{\frac{\log N}{t}}, \frac{1}{2} + \sqrt{\frac{\log N}{t}} \right]$, whose first $L := e^4 \log N$ moments match. Let $p \sim P$, $X \sim \text{Binomial}(t, p)$, $q \sim Q$ and $Y \sim \text{Binomial}(t, q)$. The total variation distance between X and Y satisfies

$$\text{TV}(X, Y) \leq \frac{2\sqrt{t}}{Ne^4}.$$

Proof. The total variation distance between X and Y is

$$\begin{aligned} \text{TV}(X, Y) &= \sum_{j=0}^t \left| \mathbb{E}_{p \sim P} \left[\binom{t}{j} p^j (1-p)^{t-j} \right] - \mathbb{E}_{q \sim Q} \left[\binom{t}{j} q^j (1-q)^{t-j} \right] \right| \\ &= \sum_{j=0}^t \left| \mathbb{E}_{p \sim P} [B_j(p)] - \mathbb{E}_{q \sim Q} [B_j(q)] \right|, \end{aligned}$$

where $B_j(p) = \binom{t}{j} p^j (1-p)^{t-j}$ is the j -th Bernstein polynomial of degree t . Expanding the Bernstein polynomial at $p = \frac{1}{2}$ we get,

$$B_j(p) = \sum_{k=0}^{\infty} \frac{B_j^{(k)} \left(\frac{1}{2} \right)}{k!} \left(p - \frac{1}{2} \right)^k,$$

where $B_j^{(k)}(a) := \frac{d^k B_j(x)}{dx^k} \Big|_{x=a}$. Therefore, we can bound the total variation distance between X and Y as follows,

$$\begin{aligned} \text{TV}(X, Y) &= \sum_{j=0}^t \left| \sum_{k=0}^{\infty} \frac{B_j^{(k)}\left(\frac{1}{2}\right)}{k!} \mathbb{E} \left[\left(p - \frac{1}{2}\right)^k \right] - \sum_{k=0}^{\infty} \frac{B_j^{(k)}\left(\frac{1}{2}\right)}{k!} \mathbb{E} \left[\left(q - \frac{1}{2}\right)^k \right] \right| \\ &\leq \sum_{k=0}^{\infty} \sum_{j=0}^t \left| \frac{B_j^{(k)}\left(\frac{1}{2}\right)}{k!} \right| \left| \mathbb{E} \left[\left(p - \frac{1}{2}\right)^k \right] - \mathbb{E} \left[\left(q - \frac{1}{2}\right)^k \right] \right| \\ &\leq 2 \sum_{k=L+1}^{\infty} \sum_{j=0}^t \left| \frac{B_j^{(k)}\left(\frac{1}{2}\right)}{k!} \right| \left(\frac{\log N}{t} \right)^{\frac{k}{2}}. \end{aligned}$$

The last inequality follows from the fact that $\mathbb{E} \left[\left(p - \frac{1}{2}\right)^k \right] \leq \left(\frac{\log N}{t} \right)^{\frac{k}{2}}$, since P and Q are supported on $\left[\frac{1}{2} - \sqrt{\frac{\log N}{t}}, \frac{1}{2} + \sqrt{\frac{\log N}{t}} \right]$ and their first L moments match. Further, applying Proposition B.1, we obtain the following bound,

$$\begin{aligned} \text{TV}(X, Y) &\leq 2 \sum_{k=L+1}^{\infty} \frac{\sqrt{t} e^k t^{k/2}}{k^{k/2}} \left(\frac{\log N}{t} \right)^{\frac{k}{2}} = 2 \sum_{k=L+1}^{\infty} \frac{\sqrt{t} e^k (\log N)^{k/2}}{k^{k/2}}, \\ &\leq 2\sqrt{t} \sum_{k=L+1}^{\infty} \left(\frac{e^2 \log N}{L} \right)^{k/2}, \\ &= 2\sqrt{t} \sum_{k=L+1}^{\infty} \left(\frac{1}{e} \right)^k, \quad (\text{since } L = e^4 \log N), \\ &\leq 2\sqrt{t} e^{-e^4 \log N} \leq \frac{2\sqrt{t}}{N^{e^4}}. \end{aligned}$$

□

Proposition B.1.

$$\sum_{j=0}^t \left| \frac{B_j^{(k)}\left(\frac{1}{2}\right)}{k!} \right| \leq \frac{\sqrt{t} e^k t^{k/2}}{k^{k/2}}.$$

Proof. Each term involving the k -th order derivative of Bernstein polynomial $B_j(x)$ evaluated at $\frac{1}{2}$ can be written as:

$$\begin{aligned} \frac{B_j^{(k)}\left(\frac{1}{2}\right)}{k!} &= \frac{1}{2^t} \binom{t}{k} \sum_{i=0}^k \binom{k}{i} \binom{t-k}{j-i} (-1)^{(k-i)}, \\ &= (-1)^k \frac{1}{2^t} \binom{t}{k} K_j(k; t), \end{aligned}$$

where $K_j(k; t)$ is the Kravchuk polynomial.

We then apply Proposition A.1 to obtain an upper bound for $\sqrt{\sum_{j=0}^t K_j^2(k; t)}$ by bounding the generating function of Kravchuk Polynomial. The generating function of the Kravchuk polynomials is

$$\sum_{j=0}^t K_j(k; t) z^j = (1+z)^{t-k} (1-z)^k.$$

Our aim is to bound the absolute value of the generating function evaluated on the unit circle. Define $z = \cos \theta + i \sin \theta$. The absolute value of the generating function is $|(1+z)^{t-k}(1-z)^k| = 2^t \cos^{t-k}(\frac{\theta}{2}) \sin^k(\frac{\theta}{2})$ which achieves maximum at $\theta = 2 \arcsin(\sqrt{k/t})$ with value $2^t (\frac{t-k}{t})^{(t-k)/2} (\frac{k}{t})^{k/2}$. Hence, it follows from Proposition A.1 that

$$\begin{aligned} \sum_{j=0}^t \left| \frac{B_j^{(k)}(\frac{1}{2})}{k!} \right| &\leq \frac{1}{2^t} \binom{t}{k} \sqrt{t} \sqrt{\sum_{j=0}^t K_j^2(k; t)} \\ &\leq \binom{t}{k} \sqrt{t} \left(\frac{t-k}{t} \right)^{(t-k)/2} \left(\frac{k}{t} \right)^{k/2}. \end{aligned}$$

Finally, it follows from $\binom{t}{k} \leq (\frac{et}{k})^k$ and $(1 - \frac{k}{t})^{(t-k)/2} \leq e^{(k^2/t-k)/2}$ that

$$\sum_{j=0}^t \left| \frac{B_j^{(k)}(\frac{1}{2})}{k!} \right| \leq \frac{\sqrt{t} e^{(k^2/(t-k))/2} t^{k/2}}{k^{k/2}} \leq \frac{\sqrt{t} e^k t^{k/2}}{k^{k/2}}.$$

□

C Local moment matching

In this section, we provide a high-level idea of how the local moment matching [JHW18] can be extended to obtain an algorithm to estimate the distribution of the parameters. The algorithm consists of three steps:

1. **Binning:** We divide the coin flips into two batches. The first batch of the data consists of the result of the first $t/2$ coin flips of each coin, and we call the first batch of samples X'_1, X'_2, \dots, X'_N and the second batch of samples X_1, X_2, \dots, X_N . We define disjoint intervals

$$I_j := \left[\frac{(j-1)^2 c_1 \log N}{t}, \frac{j^2 c_1 \log N}{t} \right], \quad (42)$$

for $j = 1, 2, \dots, M := \sqrt{\frac{t}{c_2 \log N}}$ (assuming $\sqrt{\frac{t}{c_2 \log N}}$ be an integer). We define $l_j = \frac{(j-1)^2 c_1 \log N}{t}$, $r_j = \frac{j^2 c_1 \log N}{t}$ to be the left and right end of the j -th interval. The i -th coin is assigned to interval (bin) j if $X'_i/t \in I_j$.

2. **Moment estimation:** In the second step, we estimate the first $c_2 \log N$ 'th moments of the coins in each interval (bin). Here the k -th moment of the coins in the j -th bin is defined to be $m_k^{(j)} := \sum_{X'_i/t \in I_j} (p_i - l_j)^k$. It follows from Lemma 1 of [TKV17] that $\frac{\binom{X_i}{l}}{\binom{t}{l}}$ is an unbiased estimator for p_i^l . Hence, $\sum_{l=0}^k \binom{k}{l} (-l_j)^{k-l} \frac{\binom{X_i}{l}}{\binom{t}{l}}$ is an unbiased estimator of $(p_i - l_j)^k$. We compute $\sum_{X'_i/t \in I_j} \sum_{l=0}^k \binom{k}{l} (-l_j)^{k-l} \frac{\binom{X_i}{l}}{\binom{t}{l}}$ as an estimate of the k -th moment of the j -th bin for all $k = 0, 1, \dots, c_2 \log N$, and denote it as $\hat{m}_k^{(j)}$.
3. **Distribution recovery:** In the third step, for each bin j , we solve a linear programming (see e.g. Algorithm 1 of [TKV17]) to recover a distribution μ_j supported on $\tilde{I}_j := [\frac{(j-\frac{3}{2})^2 c_1 \log N}{t}, \frac{(j+1)^2 c_1 \log N}{t}]$ whose first $c_2 \log N$ moments closely match our estimation $\hat{m}_1^{(j)}, \hat{m}_2^{(j)}, \dots, \hat{m}_{c_2 \log N}^{(j)}$. Finally, we output $\hat{P}_{lmm} = \sum_j \mu_j$ as the estimate.