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# Learning discrete distributions with infinite support

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## Abstract

We present a novel approach to estimating discrete distributions with (potentially) infinite support in the total variation metric. In a departure from the established paradigm, we make no structural assumptions whatsoever on the sampling distribution. In such a setting, distribution-free risk bounds are impossible, and the best one could hope for is a fully empirical data-dependent bound. We derive precisely such bounds, and demonstrate that these are, in a well-defined sense, the best possible. Our main discovery is that the half-norm of the empirical distribution provides tight upper and lower estimates on the empirical risk. Furthermore, this quantity decays at a nearly optimal rate as a function of the true distribution. The optimality follows from a minimax result, of possible independent interest. Additional structural results are provided, including an exact Rademacher complexity calculation and apparently a first connection between the total variation risk and the missing mass.

## 1 Introduction

Estimating a discrete distribution in the total variation (TV) metric is a central problem in computer science and statistics (see, e.g., Han et al. [2015], Kamath et al. [2015], Orlitsky and Suresh [2015] and the references therein). The TV metric, which we use throughout the paper, is a natural and abundantly motivated choice [Devroye and Lugosi, 2001]. For support size  $d$ , a sample of size  $\mathcal{O}(d/\varepsilon^2)$  suffices for the maximum-likelihood estimator (MLE) to be  $\varepsilon$ -close (with constant probability) to the unknown target distribution. A matching lower bound is known [Anthony and Bartlett, 1999], and has been computed down to the exact constants [Kamath et al., 2015].

Classic VC theory — and, in particular, the aforementioned results — imply that for infinite support, no distribution-free sample complexity bound is possible. If  $\mu$  is the target distribution and  $\hat{\mu}_m$  is its empirical (i.e., MLE) estimate based on  $m$  iid samples, then Berend and Kontorovich [2013] showed that

$$\frac{1}{4}\Lambda_m(\mu) - \frac{1}{4\sqrt{m}} \leq \mathbb{E}[\|\mu - \hat{\mu}_m\|_{\text{TV}}] \leq \Lambda_m(\mu), \quad m \geq 2, \quad (1)$$

where

$$\Lambda_m(\mu) = \sum_{j \in \mathbb{N}: \mu(j) < 1/m} \mu(j) + \frac{1}{2\sqrt{m}} \sum_{j \in \mathbb{N}: \mu(j) \geq 1/m} \sqrt{\mu(j)}. \quad (2)$$

The quantity  $\Lambda_m(\boldsymbol{\mu})$  has the advantage of always being finite and of decaying to 0 as  $m \rightarrow \infty$ . The bound in (1) suggests that  $\Lambda_m(\boldsymbol{\mu})$ , or a closely related measure, controls the sample complexity for learning discrete distributions in TV. Further supporting the foregoing intuition is the observation that for finite support size  $d$  and  $m \gg 1$ , we have  $\Lambda_m \lesssim \sqrt{d/m}$ , recovering the known minimax rate. Additionally, a closely related measure turns out to control a minimax risk rate in a sense made precise in Theorem 2.5.

One shortcoming of (1) is that the lower bound only holds for the MLE, leaving the possibility that a different estimator could achieve significantly improved bounds. Another shortcoming of (1) and related estimates is that they are not *empirical*, in that they depend on the unknown quantity we are trying to estimate. A fully empirical bound, on the other hand, would give a high-probability estimate on  $\|\boldsymbol{\mu} - \hat{\boldsymbol{\mu}}_m\|_{\text{TV}}$  solely in terms of observable quantities such as  $\hat{\boldsymbol{\mu}}_m$ . Of course, such a bound should also be non-trivial, in the sense of improving with growing sample size and approaching 0 as  $m \rightarrow \infty$ . A further desideratum might be something akin to *instance optimality*: We would like the rate at which the empirical bound decays to be “the best” possible for the given  $\boldsymbol{\mu}$ , in an appropriate sense. Our analogue of instance optimality is inspired by, but distinct from, that of Valiant and Valiant [2016], as discussed in detail in Related work below.

**Our contributions.** We address the shortcomings of existing estimators detailed above by providing a fully empirical bound on  $\|\boldsymbol{\mu} - \hat{\boldsymbol{\mu}}_m\|_{\text{TV}}$ . Our main discovery is that the quantity  $\Phi_m(\hat{\boldsymbol{\mu}}_m) := \frac{1}{\sqrt{m}} \sum_{j \in \mathbb{N}} \sqrt{\hat{\boldsymbol{\mu}}_m(j)}$  satisfies all of the desiderata posed above for an empirical bound. As we show in Theorems 2.1 and 2.2,  $\Phi_m(\hat{\boldsymbol{\mu}}_m)$  provides tight, high-probability upper and lower bounds on  $\|\boldsymbol{\mu} - \hat{\boldsymbol{\mu}}_m\|_{\text{TV}}$ . Further, Theorem 2.3 shows that  $\mathbb{E}[\Phi_m(\hat{\boldsymbol{\mu}}_m)]$  behaves as  $\Lambda_m(\boldsymbol{\mu})$  defined in (2). Finally, a result in the spirit of instance optimality, Theorem 2.4, shows that no other estimator-bound pair can improve upon  $(\hat{\boldsymbol{\mu}}_m, \Phi_m)$ , other than by small constants. The latter follows from a minimax bound of independent interest, Theorem 2.5. Additional structural results are provided, including an exact Rademacher complexity calculation and a connection (apparently the first) between the total variation risk and the missing mass.

**Definitions, notation and setting.** As we are dealing with discrete distributions, there is no loss of generality in taking our sample space to be the natural numbers  $\mathbb{N} = \{1, 2, 3, \dots\}$ . For  $k \in \mathbb{N}$ , we write  $[k] := \{i \in \mathbb{N} : i \leq k\}$ . The set of all distributions on  $\mathbb{N}$  will be denoted by  $\Delta_{\mathbb{N}}$ , which we enlarge to include the “deficient” distributions:  $\Delta_{\mathbb{N}} \subset \Delta_{\mathbb{N}}^{\circ} := \{\boldsymbol{\mu} \in [0, 1]^{\mathbb{N}} : \sum_{i \in \mathbb{N}} \boldsymbol{\mu}(i) \leq 1\}$ . For  $d \in \mathbb{N}$ , we write  $\Delta_d \subset \Delta_{\mathbb{N}}$  to denote those  $\boldsymbol{\mu}$  whose support is contained in  $[d]$ .

For  $\boldsymbol{\mu} \in \Delta_{\mathbb{N}}^{\circ}$  and  $I \subseteq \mathbb{N}$ , we write  $\boldsymbol{\mu}(I) = \sum_{i \in I} \boldsymbol{\mu}(i)$ . We define the *decreasing permutation* of  $\boldsymbol{\mu} \in \Delta_{\mathbb{N}}^{\circ}$ , denoted by  $\boldsymbol{\mu}^{\downarrow}$ , to be the sequence  $(\boldsymbol{\mu}(i))_{i \in \mathbb{N}}$  sorted in non-increasing order, achieved by a<sup>1</sup> permutation  $\Pi_{\boldsymbol{\mu}}^{\downarrow} : \mathbb{N} \rightarrow \mathbb{N}$ ; thus,  $\boldsymbol{\mu}^{\downarrow}(i) = \boldsymbol{\mu}(\Pi_{\boldsymbol{\mu}}^{\downarrow}(i))$ . For  $0 < \eta < 1$ , define  $T_{\boldsymbol{\mu}}(\eta) \in \mathbb{N}$  as the least  $t$  for which  $\sum_{i > t} \boldsymbol{\mu}^{\downarrow}(i) < \eta$ . This induces a truncation of  $\boldsymbol{\mu}$ , denoted by  $\boldsymbol{\mu}[\eta] \in \Delta_{\mathbb{N}}^{\circ}$  and defined by  $\boldsymbol{\mu}[\eta](i) = \mathbf{1}[\Pi_{\boldsymbol{\mu}}^{\downarrow}(i) \leq T_{\boldsymbol{\mu}}(\eta)]\boldsymbol{\mu}(i)$ .

For  $\boldsymbol{\mu}, \boldsymbol{\nu} \in \Delta_{\mathbb{N}}^{\circ}$ , we define the *total variation distance* in terms of the  $\ell_1$  norm:

$$\|\boldsymbol{\mu} - \boldsymbol{\nu}\|_{\text{TV}} := \frac{1}{2} \|\boldsymbol{\mu} - \boldsymbol{\nu}\|_1 = \frac{1}{2} \sum_{i \in \mathbb{N}} |\boldsymbol{\mu}(i) - \boldsymbol{\nu}(i)|. \quad (3)$$

For  $\boldsymbol{\mu} \in \Delta_{\mathbb{N}}^{\circ}$ , we also define the *half-norm*<sup>2</sup> as

$$\|\boldsymbol{\mu}\|_{1/2} := \left( \sum_{i \in \Omega} \sqrt{\boldsymbol{\mu}(i)} \right)^2; \quad (4)$$

note that while  $\|\boldsymbol{\mu}\|_{1/2}$  may be infinite, we have  $\|\boldsymbol{\mu}\|_{1/2} \leq \|\boldsymbol{\mu}\|_0$ , where the latter denotes the support size.

For  $m \in \mathbb{N}$  and  $\boldsymbol{\mu} \in \Delta_{\mathbb{N}}$ , we write  $\mathbf{X} = (X_1, \dots, X_m) \sim \boldsymbol{\mu}^m$  to mean that the components of the vector  $\mathbf{X}$  are drawn iid from from  $\boldsymbol{\mu}$ . We reserve  $\hat{\boldsymbol{\mu}}_m \in \Delta_{\mathbb{N}}$  for the empirical measure induced by the sample  $\mathbf{X}$ , i.e.  $\hat{\boldsymbol{\mu}}_m(i) := \frac{1}{m} \sum_{t \in [m]} \mathbf{1}[X_t = i]$ ; the term MLE will be used interchangeably.

<sup>1</sup>While  $\boldsymbol{\mu}^{\downarrow}$  is uniquely defined,  $\Pi_{\boldsymbol{\mu}}^{\downarrow}$  is not. Uniqueness could be ensured by taking the lexicographically first permutation, but will not be needed for our results.

<sup>2</sup>The half-norm is not a proper vector-space norm, as it lacks sub-additivity.

For the class of boolean functions over the integers  $\{f: \mathbb{N} \rightarrow \{0, 1\}\}$ , which we denote by  $\{0, 1\}^{\mathbb{N}}$ , recall the definition of the *empirical Rademacher complexity* [Mohri et al., 2012, Definition 3.1] conditional on the sample  $\mathbf{X}$ :

$$\hat{\mathfrak{R}}_m(\mathbf{X}) := \mathbb{E}_{\boldsymbol{\sigma}} \left[ \sup_{f \in \{0, 1\}^{\mathbb{N}}} \frac{1}{m} \sum_{t=1}^m \sigma_t f(X_t) \right], \quad (5)$$

where  $\boldsymbol{\sigma} = (\sigma_1, \dots, \sigma_m) \sim \text{Uniform}(\{-1, 1\}^m)$ . The expectation of the above random quantity is the *Rademacher complexity* [Mohri et al., 2012, Definition 3.2]:

$$\mathfrak{R}_m := \mathbb{E}_{\mathbf{X} \sim \mu^m} [\hat{\mathfrak{R}}(\mathbf{X})]. \quad (6)$$

**Related work.** Given the classical nature of the problem, a comprehensive literature survey is beyond our scope; the standard texts Devroye and Györfi [1985], Devroye and Lugosi [2001] provide much of the requisite background. Chapter 6.5 of the latter makes a compelling case for the TV metric used in this paper, but see Waggoner [2015] and the works cited therein for results on other  $\ell_p$  norms. Though surveying all of the relevant literature is a formidable task, a relatively streamlined narrative may be distilled. Conceptually, the simplest case is that of  $\|\mu\|_0 < \infty$  (i.e., finite support). Since learning a distribution over  $[d]$  in TV is equivalent to agnostically learning the function class  $\{0, 1\}^d$ , standard VC theory [Anthony and Bartlett, 1999, Kontorovich and Pinelis, 2019] entails that the MLE achieves the minimax risk rate of  $\sqrt{d/m}$  over all  $\mu \in \Delta_{\mathbb{N}}$  with  $\|\mu\|_0 \leq d$ . An immediate consequence is that in order to obtain quantitative risk rates for the case of infinite support, one must assume some sort of structure [Diakonikolas, 2016]. One can, for example, obtain minimax rates for  $\mu$  with bounded entropy [Han et al., 2015], or, say, bounded half-norm (as we do here). Alternatively, one can restrict one’s attention to a finite class  $\mathcal{Q} \subset \Delta_{\mathbb{N}}$ ; here too, optimal results are known [Bousquet et al., 2019]. Berend and Kontorovich [2013] was one of the few works that made no assumptions on  $\mu \in \Delta_{\mathbb{N}}$ , but only gave non-empirical bounds.

Our work departs from the paradigm of a-priori constraints on the unknown sampling distribution. Instead, our estimates hold for all  $\mu \in \Delta_{\mathbb{N}}$ . Of course, this must come at a price: no a-priori sample complexity bounds are possible in this setting. Absent any prior knowledge regarding  $\mu$ , one can only hope for sample-dependent *empirical* bounds, and we indeed obtain these. Further, our empirical bounds are essentially the best possible, as formalized in Theorem 2.4. The latter result may be thought of as a learning-theoretic analogue of being *instance-optimal*, as introduced by Valiant and Valiant [2017] in the testing framework. Instance optimality is a very natural notion in the context of testing whether an unknown sampling distribution  $\mu$  is identical to or  $\varepsilon$ -far from a given reference one,  $\mu_0$ . For example, Valiant and Valiant discovered that a truncated  $2/3$ -norm of  $\mu_0$  — i.e., a quantity closely related to  $\|\mu_0\|_{2/3}$  — controls the complexity of the testing problem in TV distance. Instance optimality is more difficult to formalize for distribution learning, since for any given  $\mu \in \Delta_{\mathbb{N}}$ , there is a trivial “learner” with  $\mu$  hard-coded inside. Valiant and Valiant [2016] defined this notion in terms of competing against an oracle who knows the distribution up to a permutation of the atoms, and did not provide empirical confidence intervals. We do derive fully empirical bounds, and further show that they are impossible to improve upon — by *any estimator* — other than by constants. Our results suggest that the half-norm  $\|\mu\|_{1/2}$  plays a role in learning analogous to that of  $\|\mu\|_{2/3}$  in testing. As an intriguing aside, we note that the half-norm corresponds to the Tsallis  $q$ -entropy with  $q = 1/2$ , which was shown to be an optimal regularizer in some stochastic and adversarial bandit settings [Zimmert and Seldin, 2019]. We leave the question of investigating a deeper connection between the two results for future work.

## 2 Main results

In this section, we formally state our main results. Recall from the Definitions that the sample  $\mathbf{X} = (X_1, \dots, X_m) \sim \mu^m$  induces the empirical measure (MLE)  $\hat{\mu}_m$ , and that a key quantity in our bounds is

$$\Phi_m(\hat{\mu}_m) = \frac{1}{\sqrt{m}} \|\hat{\mu}_m\|_{1/2}^{1/2} = \frac{1}{\sqrt{m}} \sum_{j \in \mathbb{N}} \sqrt{\hat{\mu}_m(j)}. \quad (7)$$

Our first result is a fully empirical, high-probability upper bound on  $\|\hat{\mu}_m - \mu\|_{\text{TV}}$  in terms of  $\Phi_m(\hat{\mu}_m)$ :

**Theorem 2.1.** For all  $m \in \mathbb{N}$ ,  $\delta \in (0, 1)$ , and  $\boldsymbol{\mu} \in \Delta_{\mathbb{N}}$ , we have that

$$\|\hat{\boldsymbol{\mu}}_m - \boldsymbol{\mu}\|_{\text{TV}} \leq \Phi_m(\hat{\boldsymbol{\mu}}_m) + 3\sqrt{\frac{\log \frac{2}{\delta}}{2m}}$$

holds with probability at least  $1 - \delta$ . We also have

$$\mathbb{E}[\|\hat{\boldsymbol{\mu}}_m - \boldsymbol{\mu}\|_{\text{TV}}] \leq \mathbb{E}[\Phi_m(\hat{\boldsymbol{\mu}}_m)].$$

Since  $\|\hat{\boldsymbol{\mu}}_m\|_{1/2} \leq \|\hat{\boldsymbol{\mu}}_m\|_0 \leq \|\boldsymbol{\mu}\|_0$ , this recovers the minimax rate of  $\sqrt{d/m}$  for  $\boldsymbol{\mu} \in \Delta_{\mathbb{N}}$  with  $\|\boldsymbol{\mu}\|_0 \leq d$ . We also provide a matching lower bound:

**Theorem 2.2.** For all  $m \in \mathbb{N}$ ,  $\delta \in (0, 1)$ , and  $\boldsymbol{\mu} \in \Delta_{\mathbb{N}}$ , we have that

$$\|\hat{\boldsymbol{\mu}}_m - \boldsymbol{\mu}\|_{\text{TV}} \geq \frac{1}{4\sqrt{2}}\Phi_m(\hat{\boldsymbol{\mu}}_m) - 3\sqrt{\frac{\log \frac{2}{\delta}}{m}}$$

holds with probability at least  $1 - \delta$ .

Our empirical measure  $\Phi_m(\hat{\boldsymbol{\mu}}_m)$  is never much worse than the non-empirical  $\Lambda_m(\boldsymbol{\mu})$ , defined in (2):

**Theorem 2.3.** For all  $m \in \mathbb{N}$  and  $\boldsymbol{\mu} \in \Delta_{\mathbb{N}}$  we have

$$\mathbb{E}[\Phi_m(\hat{\boldsymbol{\mu}}_m)] \leq 2\Lambda_m(\boldsymbol{\mu})$$

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

$$\Phi_m(\hat{\boldsymbol{\mu}}_m) \leq 2\Lambda_m(\boldsymbol{\mu}) + \sqrt{\log(1/\delta)/m}.$$

Furthermore, no other estimator-bound pair  $(\tilde{\boldsymbol{\mu}}_m, \Psi_m)$  can improve upon  $(\hat{\boldsymbol{\mu}}_m, \Phi_m)$ , other than by a constant. This is the ‘‘instance optimality’’ result alluded to above:

**Theorem 2.4.** There exist universal constants  $a, b > 0$  such that the following holds. For any estimator-bound pair  $(\tilde{\boldsymbol{\mu}}_m, \Psi_m)$  and any continuous function  $\theta: \mathbb{R}_+ \rightarrow \mathbb{R}_+$  such that

$$\mathbb{E}[\|\tilde{\boldsymbol{\mu}}_m - \boldsymbol{\mu}\|_{\text{TV}}] \leq \mathbb{E}[\Psi_m(\tilde{\boldsymbol{\mu}}_m)] \leq \theta\left(\mathbb{E}[\Phi_m(\hat{\boldsymbol{\mu}}_m)]\right)$$

holds for all  $\boldsymbol{\mu} \in \Delta_{\mathbb{N}}$ ,  $\theta$  necessarily verifies

$$\inf_{0 < x < b} \frac{\theta(x)}{x} \geq \frac{1}{a}.$$

The next result, framed in the high-probability setting, draws a direct parallel between our characterization of the learning sample complexity via the half-norm and Valiant and Valiant [2017]’s characterization of the testing sample complexity via the 2/3-norm. The truncation is needed to ensure finiteness, since the  $\|\boldsymbol{\mu}\|_{1/2} = \infty$  for heavy-tailed distributions (e.g.  $\boldsymbol{\mu}(i) \propto 1/i^2$ ).

**Theorem 2.5.** There is a universal constant  $C > 0$  such that for all  $\Lambda \geq 2$  and  $0 < \varepsilon, \delta < 1$ , the MLE  $\hat{\boldsymbol{\mu}}_m$  verifies the following optimality property: For all  $\boldsymbol{\mu} \in \Delta_{\mathbb{N}}$  with  $\|\boldsymbol{\mu}[2\varepsilon\delta/9]\|_{1/2} \leq \Lambda$ , we have

$$m \geq C\varepsilon^{-2} \max\{\Lambda, \log(1/\delta)\} \implies \mathbb{P}(\|\hat{\boldsymbol{\mu}}_m - \boldsymbol{\mu}\|_{\text{TV}} < \varepsilon) \geq 1 - \delta.$$

On the other hand, for any estimator  $\tilde{\boldsymbol{\mu}}_m: \mathbb{N}^m \rightarrow \Delta_{\mathbb{N}}$  there is a  $\boldsymbol{\mu} \in \Delta_{\mathbb{N}}$  with  $\max\{\|\boldsymbol{\mu}[\varepsilon/18]\|_{1/2}, \|\boldsymbol{\mu}[2\varepsilon\delta/9]\|_{1/2}\} \leq \Lambda$  such that:

$$m < C\varepsilon^{-2} \min\{\Lambda, \log(1/\delta)\} \implies \mathbb{P}(\|\tilde{\boldsymbol{\mu}}_m - \boldsymbol{\mu}\|_{\text{TV}} \geq \varepsilon) \geq \min\{3/4, 1 - \delta\}.$$

The above is a simplified statement chosen for brevity; a considerably refined version is stated and proved in Theorem 3.1.

### 3 Proofs

#### 3.1 Proof of Theorem 2.1

The proof consists of two parts. The first is contained in Lemma 3.1, which provides a high-probability empirical upper bound, and an expectation bound, similar to Theorem 2.1, but in terms of  $\hat{\mathfrak{R}}_m(\mathbf{X})$  instead of  $\Phi_m(\hat{\boldsymbol{\mu}}_m)$ . The second part, contained in Lemma 3.2, provides an estimate of  $\hat{\mathfrak{R}}_m(\mathbf{X})$  in terms of  $\Phi_m(\hat{\boldsymbol{\mu}}_m)$ .

**Lemma 3.1.** *For all  $m \in \mathbb{N}$ ,  $\delta \in (0, 1)$ , and  $\boldsymbol{\mu} \in \Delta_{\mathbb{N}}$ , we have that*

$$\|\hat{\boldsymbol{\mu}}_m - \boldsymbol{\mu}\|_{\text{TV}} \leq 2\hat{\mathfrak{R}}_m(\mathbf{X}) + 3\sqrt{\frac{\log \frac{2}{\delta}}{2m}}$$

holds with probability at least  $1 - \delta$ . We also have,

$$\mathbb{E} [\|\hat{\boldsymbol{\mu}}_m - \boldsymbol{\mu}\|_{\text{TV}}] \leq 2\mathfrak{R}_m. \quad (8)$$

*Proof.* The high-probability bound from the observation,

$$\|\hat{\boldsymbol{\mu}}_m - \boldsymbol{\mu}\|_{\text{TV}} := \sup_{A \subseteq \mathbb{N}} (\boldsymbol{\mu}(A) - \hat{\boldsymbol{\mu}}_m(A)) = \sup_{f \in \mathcal{F}} \left( \mathbb{E}_{X \sim \boldsymbol{\mu}} [f(X)] - \frac{1}{m} \sum_{i=1}^m f(X_i) \right) \quad (9)$$

where  $\mathcal{F} := \{\mathbb{I}_A | A \subseteq \mathbb{N}\} = \{0, 1\}^{\mathbb{N}}$ , combined with [Mohri et al., 2012, Theorem 3.3], which states: Let  $\mathcal{G}$  be a family of functions from  $\mathcal{Z}$  to  $[0, 1]$  and let  $\nu$  be a distribution supported on a subset of  $\mathcal{Z}$ . Then, for any  $\delta > 0$ , with probability at least  $1 - \delta$  over  $\mathbf{Z} = (Z_1, \dots, Z_m) \sim \nu^m$ , the following holds:

$$\sup_{g \in \mathcal{G}} \left( \mathbb{E}_{Z \sim \nu} [g(Z)] - \frac{1}{m} \sum_{i=1}^m g(Z_i) \right) \leq 2\hat{\mathfrak{R}}_m(\mathbf{Z}) + 3\sqrt{\frac{\log \frac{2}{\delta}}{2m}}.$$

Plugging in  $\mathcal{F}$  for  $\mathcal{G}$  and  $\boldsymbol{\mu}$  for  $\nu$  in the above theorem completes the proof of the high-probability bound. The expectation bound (eq. (8)) follows from the observation at eq. (9) and a symmetrization argument [Mohri et al., 2012, eq. (3.8) to (3.13)].  $\square$

In order to complete the proof, we apply

**Lemma 3.2** (Empirical Rademacher estimates). *Let  $\mathbf{X} = (X_1, \dots, X_m)$  and let  $\hat{\boldsymbol{\mu}}_m$  be the empirical measure constructed from the sample  $\mathbf{X}$ . Then,*

$$\frac{1}{2\sqrt{2}} \Phi_m(\hat{\boldsymbol{\mu}}_m) \leq \hat{\mathfrak{R}}_m(\mathbf{X}) \leq \frac{1}{2} \Phi_m(\hat{\boldsymbol{\mu}}_m).$$

*Proof.* The proof is based on an argument that was also developed in [Scott and Nowak, 2006, Section 7.1, Appendix E.] in the context of histograms and dyadic decision trees, and that was credited to Gilles Blanchard.

Let  $\hat{S} = \{X_i | i \in [m]\}$  be the empirical support according to the sample  $\mathbf{X} = (X_1, X_2, \dots, X_m)$ . Then,

$$\begin{aligned} m\hat{\mathfrak{R}}_m(\mathbf{X}) &= \mathbb{E}_{\boldsymbol{\sigma}} \left[ \sup_{f \in \{0,1\}^{\mathbb{N}}} \sum_{i=1}^m \sigma_i f(X_i) \right] = \mathbb{E}_{\boldsymbol{\sigma}} \left[ \sup_{A \subseteq \hat{S}} \sum_{i=1}^m \sigma_i \mathbb{I}_A(X_i) \right] \\ &= \sum_{x \in \hat{S}} \mathbb{E}_{\boldsymbol{\sigma}} \left[ \sup_{A \subseteq \{x\}} \sum_{i: X_i=x} \sigma_i \mathbb{I}_A(X_i) \right] = \sum_{x \in \hat{S}} \mathbb{E}_{\boldsymbol{\sigma}} \left[ \left( \sum_{i: X_i=x} \sigma_i \right)_+ \right] = \sum_{x \in \hat{S}} \frac{1}{2} \mathbb{E}_{\boldsymbol{\sigma}} \left[ \left| \sum_{i=1}^m \sigma_i \right| \right], \end{aligned}$$

where the last equality follows from counting  $\{i : X_i = x\}$  and the symmetry of the random variable  $\sum_{i=1}^m \sigma_i$  for all  $n \in \mathbb{N}$ . Now, by Khintchine's inequality, for  $0 < p < \infty$  and  $x_1, x_2, \dots, x_m \in \mathbb{C}$  we have

$$A_p \left( \sum_{i=1}^m |x_i|^2 \right)^{1/2} \leq \left( \mathbb{E}_{\boldsymbol{\sigma}} \left[ \left| \sum_{i=1}^m x_i \sigma_i \right|^p \right] \right)^{1/p} \leq B_p \left( \sum_{i=1}^m |x_i|^2 \right)^{1/2},$$

where  $A_p, B_p > 0$  are constants depending on  $p$ . Sharp values for  $A_p, B_p$  were found by Haagerup [1981]. In particular, for  $p = 1$  he found that  $A_1 = \frac{1}{\sqrt{2}}$  and  $B_1 = 1$ . By using Khintchine's inequality for each  $\mathbb{E}_\sigma \left[ \left| \sum_{i=1}^m \hat{\mu}_m(x) \sigma_i \right| \right]$  with these constants, we get

$$\frac{1}{\sqrt{2}} \sqrt{m \hat{\mu}_m(x)} \leq \mathbb{E}_\sigma \left[ \left| \sum_{i=1}^m \sigma_i \right| \right] \leq \sqrt{m \hat{\mu}_m(x)},$$

and hence

$$\frac{1}{2\sqrt{2}} \sum_{x \in \hat{S}} \sqrt{m \hat{\mu}_m(x)} \leq m \hat{\mathfrak{R}}_m(\mathbf{X}) \leq \frac{1}{2} \sum_{x \in \hat{S}} \sqrt{m \hat{\mu}_m(x)}.$$

Dividing by  $m$  completes the proof.  $\square$

Remark: We also give an exact expression for  $\hat{\mathfrak{R}}_m(\mathbf{X})$  in Lemma A.1, and show in Corollary A.1 with a more delicate analysis that

$$\frac{\|\hat{\mu}_m\|_{1/2}^{1/2}}{\sqrt{2\pi m}} - \frac{3}{2} \sqrt{\frac{1}{2\pi}} \frac{1}{m^{3/2}} \|\hat{\mu}_m^+\|_{-1/2}^{-1/2} \leq \hat{\mathfrak{R}}_m(\mathbf{X}) \leq \frac{\|\hat{\mu}_m\|_{1/2}^{1/2}}{\sqrt{2\pi m}} + \sqrt{\frac{1}{2\pi}} \frac{1}{m^{3/2}} \|\hat{\mu}_m^+\|_{-1/2}^{-1/2}.$$

### 3.2 Proof of Theorem 2.2

The proof follows from applying the lower bound of Lemma 3.2 to the following lemma:

**Lemma 3.3** (lower bound by empirical Rademacher). *For all  $m \in \mathbb{N}$ ,  $\delta \in (0, 1)$ , and  $\mu \in \Delta_{\mathbb{N}}$ , we have that*

$$\|\hat{\mu}_m - \mu\|_{\text{TV}} \geq \frac{1}{2} \hat{\mathfrak{R}}_m(\mathbf{X}) - 3 \sqrt{\frac{\log \frac{2}{\delta}}{m}}$$

holds with probability at least  $1 - \delta$ .

*Proof.* The proof is closely based on [Wainwright, 2019, Proposition 4.12], which states: Let  $\mathbf{Y} = (Y_1, \dots, Y_m) \sim \nu^m$  for some distribution  $\nu$  on  $\mathcal{Z}$ , let  $\mathcal{G} \subseteq [-b, b]^{\mathcal{Z}}$  be a function class, and let  $\sigma = (\sigma_1, \dots, \sigma_m) \sim \text{Uniform}(\{-1, 1\}^m)$ . Then

$$\sup_{g \in \mathcal{G}} \left| \mathbb{E}_{Y \sim \nu} [g(Y)] - \frac{1}{m} \sum_{i=1}^m g(Y_i) \right| \geq \frac{1}{2} \mathbb{E}_{\sigma, \mathbf{Y}} \left[ \sup_{g \in \mathcal{G}} \left| \frac{1}{m} \sum_{i=1}^m \sigma_i g(Y_i) \right| \right] - \frac{\sup_{g \in \mathcal{G}} |\mathbb{E}_{Y \sim \nu} [g(Y)]|}{2\sqrt{m}} - \delta \quad (10)$$

holds with probability at least  $1 - e^{-\frac{n\delta^2}{2b^2}}$ . Plugging in  $\mathbf{X}$  for  $\mathbf{Y}$ ,  $\mu$  for  $\nu$ ,  $\mathbb{N}$  for  $\mathcal{Z}$ , 1 for  $b$ , and  $\mathcal{F} := \{\mathbb{I}_A | A \subseteq \mathbb{N}\} = \{0, 1\}^{\mathbb{N}}$  for  $\mathcal{G}$  in (10) together with observing that

$$\begin{aligned} \|\hat{\mu}_m - \mu\|_{\text{TV}} &:= \sup_{A \subseteq \mathbb{N}} (\mu(A) - \hat{\mu}_m(A)) = \sup_{f \in \mathcal{F}} \left| \mathbb{E}_{X \sim \mu} [f(X)] - \frac{1}{m} \sum_{i=1}^m f(X_i) \right|, \\ \mathbb{E}_{\sigma, \mathbf{X}} \left[ \sup_{f \in \mathcal{F}} \left| \frac{1}{m} \sum_{i=1}^m \sigma_i f(X_i) \right| \right] &\geq \mathfrak{R}_m, \quad \text{and} \quad \sup_{f \in \mathcal{F}} \left| \mathbb{E}_{X \sim \mu} [f(X)] \right| = 1, \end{aligned}$$

followed by some algebraic manipulation we get

$$\|\hat{\mu}_m - \mu\|_{\text{TV}} \geq \frac{1}{2} \mathfrak{R}_m - \frac{1}{2\sqrt{m}} - \sqrt{\frac{2 \log \frac{2}{\delta}}{m}} \quad (11)$$

with probability at least  $1 - \delta/2$ . Applying McDiarmid's inequality to the  $1/m$ -bounded-differences function  $\hat{\mathfrak{R}}_m(\mathbf{X})$  (similar to [Mohri et al., 2012, Eq. (3.14)]) we get:

$$\frac{1}{2} \mathfrak{R}_m \geq \frac{1}{2} \hat{\mathfrak{R}}_m(\mathbf{X}) - \frac{1}{2} \sqrt{\frac{\log \frac{2}{\delta}}{2m}} \quad (12)$$

with probability at least  $1 - \delta/2$ . To conclude the proof, combine (11) and (12) with the union bound to get:

$$\|\widehat{\boldsymbol{\mu}}_m - \boldsymbol{\mu}\|_{\text{TV}} \geq \frac{1}{2} \widehat{\mathfrak{R}}_m(\mathbf{X}) - \frac{1}{2\sqrt{m}} - \frac{1}{2} \sqrt{\frac{\log \frac{2}{\delta}}{2m}} - \sqrt{\frac{2 \log \frac{2}{\delta}}{m}}$$

with probability at least  $1 - \delta$ , and use the fact  $-\frac{1}{2\sqrt{m}} - \frac{1}{2} \sqrt{\frac{\log \frac{2}{\delta}}{2m}} - \sqrt{\frac{2 \log \frac{2}{\delta}}{m}} \geq -3\sqrt{\frac{\log \frac{2}{\delta}}{m}}$  for all  $m \in \mathbb{N}, \delta \in (0, 1)$ .  $\square$

**Remark 3.1.** We note that by using a more careful analysis, the constants of Theorem 2.2 can be improved to yield, under the same assumptions,  $\|\widehat{\boldsymbol{\mu}}_m - \boldsymbol{\mu}\|_{\text{TV}} \geq \frac{1}{2} \widehat{\mathfrak{R}}_m(\mathbf{X}) - \frac{1}{4\sqrt{m}} - \frac{3}{2} \sqrt{\frac{\log \frac{2}{\delta}}{2m}}$  with probability at least  $1 - \delta$ .

### 3.3 Proof of Theorem 2.3

Invoking Fubini's theorem, we write

$$\frac{1}{\sqrt{m}} \mathbb{E} \left[ \|\widehat{\boldsymbol{\mu}}_m\|_{1/2}^{1/2} \right] = \frac{1}{m} \sum_{i=1}^{\infty} \mathbb{E}_{X \sim \text{Bin}(m, \boldsymbol{\mu}(i))} \left[ \sqrt{X} \right].$$

Since  $X \in \{0, 1, 2, \dots\}$ , we have  $\sqrt{X} \leq X$  and hence  $\mathbb{E} \left[ \sqrt{X} \right] \leq \mathbb{E} [X]$ . On the other hand, Jensen's inequality implies  $\mathbb{E} \left[ \sqrt{X} \right] \leq \sqrt{\mathbb{E} [X]}$ , whence

$$\frac{1}{\sqrt{m}} \mathbb{E} \left[ \|\widehat{\boldsymbol{\mu}}_m\|_{1/2}^{1/2} \right] \leq \frac{1}{m} \sum_{i=1}^{\infty} \min\{\sqrt{m\boldsymbol{\mu}(i)}, m\boldsymbol{\mu}(i)\} \quad (13)$$

$$= \sum_{i: \boldsymbol{\mu}(i) \leq 1/m} \boldsymbol{\mu}(i) + \frac{1}{\sqrt{m}} \sum_{i: \boldsymbol{\mu}(i) > 1/m} \sqrt{\boldsymbol{\mu}(i)} \leq 2\Lambda_m(\boldsymbol{\mu}). \quad (14)$$

The high-probability bound follows from applying McDiarmid's inequality to the  $2/m$ -bounded-differences function: for all  $\delta \in (0, 1)$ , we have

$$\Phi_m(\widehat{\boldsymbol{\mu}}_m) \leq \mathbb{E} [\Phi_m(\widehat{\boldsymbol{\mu}}_m)] + \sqrt{\log(1/\delta)/m}.$$

$\square$

### 3.4 Statement and proof of the refined version of Theorem 2.5

**Theorem 3.1.** *There is a universal constant  $C > 0$  such that for all  $\Lambda \geq 2$  and  $0 < \varepsilon, \delta < 1$ , the MLE verifies the following optimality property: For all  $\boldsymbol{\mu} \in \Delta_{\mathbb{N}}$  with  $\|\boldsymbol{\mu}[2\varepsilon\delta/9]\|_{1/2} \leq \Lambda$ , if  $(X_1, \dots, X_m) \sim \boldsymbol{\mu}^m$  and  $m \geq \frac{C}{\varepsilon^2} \max\{\Lambda, \ln \delta^{-1}\}$ , then  $\|\widehat{\boldsymbol{\mu}}_m - \boldsymbol{\mu}\|_{\text{TV}} < \varepsilon$  holds with probability at least  $1 - \delta$ .*

*On the other hand, for all  $\Lambda \geq 2$  and  $0 < \varepsilon < 1/16, 0 < \delta < 1$ , for any estimator  $\bar{\boldsymbol{\mu}}: \mathbb{N}^m \rightarrow \Delta_{\mathbb{N}}$  there is a  $\boldsymbol{\mu} \in \Delta_{\mathbb{N}}$  with  $\|\boldsymbol{\mu}[\varepsilon/18]\|_{1/2} \leq \Lambda$  such that  $\bar{\boldsymbol{\mu}}$  must require at least  $m \geq \frac{C}{\varepsilon^2} \Lambda$  samples in order for  $\|\bar{\boldsymbol{\mu}} - \boldsymbol{\mu}\|_{\text{TV}} < \varepsilon$  to hold with probability at least  $3/4$ , and for any estimator  $\bar{\boldsymbol{\nu}}: \mathbb{N}^m \rightarrow \Delta_{\mathbb{N}}$  there is a  $\boldsymbol{\nu} \in \Delta_{\mathbb{N}}$  with  $\|\boldsymbol{\nu}[2\varepsilon\delta/9]\|_{1/2} \leq \Lambda$ , such that  $\bar{\boldsymbol{\nu}}$  must require at least  $m \geq \frac{C}{\varepsilon^2} \ln \frac{1}{\delta}$  samples in order for  $\|\bar{\boldsymbol{\nu}} - \boldsymbol{\nu}\|_{\text{TV}} < \varepsilon$  to hold with probability at least  $1 - \delta$ .*

**Minimax risk.** For any  $\Lambda \in [2, \infty), 0 < \varepsilon, \delta < 1$ , we define the minimax risk

$$\mathcal{R}_m(\Lambda, \varepsilon, \delta) := \inf_{\bar{\boldsymbol{\mu}}} \sup_{\boldsymbol{\mu}: \|\boldsymbol{\mu}[2\varepsilon\delta/9]\|_{1/2} < \Lambda} \mathbb{P}_{\mathbf{X} \sim \boldsymbol{\mu}^m} (\|\bar{\boldsymbol{\mu}} - \boldsymbol{\mu}\|_{\text{TV}} > \varepsilon),$$

where the infimum is taken over all functions  $\bar{\boldsymbol{\mu}}: \mathbb{N}^m \rightarrow \Delta_{\mathbb{N}}$ , and the supremum is taken over the subset of distributions such that  $\|\boldsymbol{\mu}[2\varepsilon\delta/9]\|_{1/2} < \Lambda$ .

**Upper bound.** Let  $\Lambda \in [2, \infty)$ ,  $0 < \varepsilon, \delta < 1$ ,  $\boldsymbol{\mu} \in \Delta_{\mathbb{N}}$ , such that  $\|\boldsymbol{\mu}[2\varepsilon\delta/9]\|_{1/2} \leq \Lambda$ ,  $m \in \mathbb{N}$ ,  $(X_1, \dots, X_m) \sim \boldsymbol{\mu}$  and let  $\hat{\boldsymbol{\mu}}_m$  be the MLE. For  $\eta > 0$ , consider the two truncated distributions  $\boldsymbol{\mu}[\eta]$  and  $\hat{\boldsymbol{\mu}}'_m$ , where we define the latter as

$$\hat{\boldsymbol{\mu}}'_m(i) := \hat{\boldsymbol{\mu}}_m(i) \mathbf{1}[\boldsymbol{\mu}[\eta](i) > 0], \quad i \in \mathbb{N}.$$

By the triangle inequality,  $\mathbb{P}(\|\hat{\boldsymbol{\mu}}_m - \boldsymbol{\mu}\|_{\text{TV}} > \varepsilon) \leq \mathbb{P}(\mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3 > \varepsilon)$ , where

$$\mathcal{E}_1 := \|\hat{\boldsymbol{\mu}}_m - \hat{\boldsymbol{\mu}}'_m\|_{\text{TV}}, \quad \mathcal{E}_2 := \|\hat{\boldsymbol{\mu}}'_m - \boldsymbol{\mu}[2\varepsilon\delta/9]\|_{\text{TV}}, \quad \mathcal{E}_3 := \|\boldsymbol{\mu}[2\varepsilon\delta/9] - \boldsymbol{\mu}\|_{\text{TV}}.$$

By Markov's inequality,

$$\begin{aligned} \mathbb{P}\left(\mathcal{E}_1 > \frac{\varepsilon}{3}\right) &\leq \frac{3}{\varepsilon} \mathbb{E}[\|\hat{\boldsymbol{\mu}}_m - \hat{\boldsymbol{\mu}}'_m\|_{\text{TV}}] = \frac{3}{2\varepsilon} \mathbb{E}\left[\sum_{i=1}^{\infty} |\hat{\boldsymbol{\mu}}_m(i) - \hat{\boldsymbol{\mu}}'_m(i)|\right] \\ &= \frac{3}{2\varepsilon} \mathbb{E}\left[\frac{1}{m} \sum_{i \in \mathbb{N}: \Pi_{\boldsymbol{\mu}}(i) > T_{\boldsymbol{\mu}}(\eta)} \sum_{t=1}^m \mathbf{1}[X_t = i]\right] = \frac{3}{2\varepsilon} \mathbb{P}(\Pi_{\boldsymbol{\mu}}(X_t) > T_{\boldsymbol{\mu}}(\eta)) \leq \frac{\delta}{3}. \end{aligned}$$

Moreover,  $\mathcal{E}_3 = \frac{1}{2} \sum_{i > T_{\boldsymbol{\mu}}(\eta)}^{\infty} \boldsymbol{\mu}^{\downarrow}(i) \leq \frac{\varepsilon\delta}{9} \leq \frac{\varepsilon}{3}$ . In order to apply the union bound, it remains to handle  $\mathbb{P}(\mathcal{E}_2 > \varepsilon/3)$ . This is achieved in two standard steps. The first follows an argument similar to that of [Berend and Kontorovich, 2013, Lemma 5], that bounds from above the quantity in expectation using Jensen's inequality,  $\mathbb{E}[\mathcal{E}_2] \leq \frac{\|\boldsymbol{\mu}[2\varepsilon\delta/9]\|_{1/2}^{1/2}}{\sqrt{m}} \leq \sqrt{\frac{\Lambda}{m}}$ . An application of McDiarmid's inequality controls the fluctuations around the expectation [Berend and Kontorovich, 2013, (7.5)] and concludes the proof.  $\square$

**Sample complexity lower bound**  $m = \Omega\left(\frac{\log \delta^{-1}}{\varepsilon^2}\right)$ . See Lemma B.1.

**Sample complexity lower bound**  $m = \Omega\left(\frac{\Lambda}{\varepsilon^2}\right)$ . Let  $\varepsilon \in (0, 1/16)$  and  $\Lambda > 2$ . First observe that  $\Lambda/2 \leq 2\lfloor \Lambda/2 \rfloor \leq \Lambda$ , and  $2\lfloor \Lambda/2 \rfloor \in 2\mathbb{N}$ . As a result,

$$\begin{aligned} \mathcal{R}_m(\Lambda, \varepsilon, \delta) &\stackrel{(i)}{\geq} \inf_{\bar{\boldsymbol{\mu}}} \sup_{\boldsymbol{\mu}: \|\boldsymbol{\mu}[2\varepsilon\delta/9]\|_{1/2} \leq 2\lfloor \Lambda/2 \rfloor} \mathbb{P}_{\mathbf{X} \sim \boldsymbol{\mu}^m}(\|\bar{\boldsymbol{\mu}} - \boldsymbol{\mu}\|_{\text{TV}} > \varepsilon) \\ &\stackrel{(ii)}{\geq} \inf_{\bar{\boldsymbol{\mu}}} \sup_{\boldsymbol{\mu} \in \Delta_{2\lfloor \Lambda/2 \rfloor}} \mathbb{P}_{\mathbf{X} \sim \boldsymbol{\mu}^m}(\|\bar{\boldsymbol{\mu}} - \boldsymbol{\mu}\|_{\text{TV}} > \varepsilon) \stackrel{(iii)}{\geq} \frac{1}{2} \left(1 - \frac{mC\varepsilon^2}{2\lfloor \Lambda/2 \rfloor}\right) \geq \frac{1}{2} \left(1 - \frac{2mC\varepsilon^2}{\Lambda}\right) \end{aligned}$$

where (i) and (ii) follow from taking the supremum over increasingly smaller sets, (iii) is Lemma B.2 invoked for  $2\lfloor \Lambda/2 \rfloor \in \mathbb{N}$ , and  $C > 0$  is a universal constant. To conclude,  $m \leq \frac{\Lambda}{4C\varepsilon^2} \implies \mathcal{R}_m(\Lambda, \varepsilon, \delta) \geq 1/4$ , which yields the second lower bound.  $\square$

Remark: The universal constant in the lower bound obtained by Tsybakov's method at Lemma B.2 is suboptimal, and we give a short proof in the appendix for completeness. We refer the reader to the more involved methods of Kamath et al. [2015] for obtaining tighter bounds.

### 3.5 Proof of Theorem 2.4

Let  $d \in 2\mathbb{N}$  and  $m \in \mathbb{N}$ , and restrict the problem to  $\boldsymbol{\mu} \in \Delta_d$ . Let  $\varepsilon \in (0, 1/16)$ . By Lemma B.2,  $\bar{\mathcal{R}}_m(d, \varepsilon) := \inf_{\bar{\boldsymbol{\mu}}} \sup_{\boldsymbol{\mu} \in \Delta_d} \mathbb{P}(\|\bar{\boldsymbol{\mu}} - \boldsymbol{\mu}\|_{\text{TV}} > \varepsilon) \geq \frac{1}{2} \left(1 - \frac{Cm\varepsilon^2}{d}\right)$  for some  $C > 0$ , whence Markov's inequality yields

$$\frac{1}{2} \left(1 - \frac{Cm\varepsilon^2}{d}\right) \leq \frac{1}{\varepsilon} \inf_{\bar{\boldsymbol{\mu}}} \sup_{\boldsymbol{\mu} \in \Delta_d} \mathbb{E}[\|\bar{\boldsymbol{\mu}} - \boldsymbol{\mu}\|_{\text{TV}}].$$

Restrict  $m \geq \frac{d}{b^2}$ , with  $b := \sqrt{3C/16}$  and set  $\varepsilon = \sqrt{\frac{d}{3Cm}}$ , so that

$$\inf_{\bar{\boldsymbol{\mu}}} \sup_{\boldsymbol{\mu} \in \Delta_d} \mathbb{E}[\|\bar{\boldsymbol{\mu}} - \boldsymbol{\mu}\|_{\text{TV}}] \geq \frac{1}{a} \sqrt{\frac{d}{m}}, \quad \text{where } a := \sqrt{27C} \quad (15)$$



Suppose that  $\theta(\sqrt{d/m}) < \frac{1}{a}\sqrt{\frac{d}{m}}$ , then by hypothesis,

$$\inf_{\tilde{\mu}} \sup_{\mu \in \Delta_d} \mathbb{E} [\|\tilde{\mu} - \mu\|_{\text{TV}}] \leq \sup_{\mu \in \Delta_d} \mathbb{E} [\Psi_m(\tilde{\mu}_m)] \leq \sup_{\mu \in \Delta_d} \theta \left( \mathbb{E} [\Phi_m] \right).$$

For  $\mu \in \Delta_d$ ,  $\mathbb{E} \left[ \sqrt{\frac{\|\tilde{\mu}_m\|_{1/2}}{m}} \right] \leq \sqrt{\frac{d}{m}}$ . It follows that

$$\sup_{\mu \in \Delta_d} \theta \left( \mathbb{E} [\Phi_m] \right) \leq \theta \left( \sqrt{\frac{d}{m}} \right) < \frac{1}{a} \sqrt{\frac{d}{m}},$$

which contradicts (15). We have therefore established, for

$$r \in R := \left\{ \sqrt{d/m} : (m, d) \in \mathbb{N} \times 2\mathbb{N}, m \geq \frac{d}{b^2} \right\},$$

the lower bound  $\theta(r) \geq r/a$ . We extend the lower bound to the open interval  $(0, b)$ , by observing that  $R$  is dense in  $(0, b)$  followed by a continuity argument.  $\square$

## Broader Impact

This work is of purely theoretical nature and does not present any foreseeable societal consequence.

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