Dualizing Le Cam’s method, with applications to estimating the unseens

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Abstract

One of the most commonly used techniques for proving statistical lower bounds, Le Cam’s method, has been the method of choice for functional estimation. This paper aims at explaining the effectiveness of Le Cam’s method from an optimization perspective. Under a variety of settings it is shown that the maximization problem that searches for the best lower bound provided by Le Cam’s method, upon dualizing, becomes a minimization problem that optimizes the bias-variance tradeoff among a family of estimators. While Le Cam’s method can be used with arbitrary distance, our duality result applies specifically to the $\chi^2$-divergence, thus singling it out as a natural choice for quadratic risk. For estimating linear functionals of a distribution our work strengthens prior results of Dohono-Liu [DL91] (for quadratic loss) by dropping the Hölderian assumption on the modulus of continuity. For exponential families our results improve those of Juditsky-Nemirovski [JN09] by characterizing the minimax risk for the quadratic loss under weaker assumptions on the exponential family.

We also provide an extension to the high-dimensional setting for estimating separable functionals. Notably, coupled with tools from complex analysis, this method is particularly effective for characterizing the “elbow effect” — the phase transition from parametric to nonparametric rates. As the main application of our methodology, we consider three problems in the area of “estimating the unseens”, recovering the prior result of [PSW17] on population recovery and, in addition, obtaining two new ones:

- **Distinct elements problem**: Randomly sampling a fraction $p$ of colored balls from an urn containing $d$ balls in total, the optimal normalized estimation error of the number of distinct colors in the urn is within logarithmic factors of $d^{-\frac{1}{2}} \min\{\frac{1}{4}, \frac{1}{2}\}$, exhibiting an elbow at $p = \frac{1}{2}$;
- **Fisher’s species problem**: Given $n$ independent samples drawn from an unknown distribution, the optimal normalized prediction error of the number of unseen symbols in the next (unobserved) $r \cdot n$ samples is within logarithmic factors of $n^{-\min\{\frac{1}{4}, \frac{1}{2}\}}$, exhibiting an elbow at $r = 1$.

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1 Introduction

One of the most commonly used tools for statistical lower bound is Le Cam’s method (or the two-point method) [LC86]. To explain its rationale, consider the following general setup of functional estimation: Let $X_1, \ldots, X_n$ be iid samples drawn from some distribution $P_\theta$ parameterized by $\theta \in \Theta$. Given these samples, the goal is to estimate some real-valued functional $T(\theta)$. The minimax quadratic risk (mean-squared error) is defined as follows

$$R^*_n = \inf_{\hat{T}} \sup_{\theta \in \Theta} \mathbb{E}_\theta[(\hat{T} - T(\theta))^2]$$

where the infimum is taken over all estimators $\hat{T}$ that are measurable with respect to $X_1, \ldots, X_n$. Then Le Cam’s method yields the following lower bound (cf., e.g., [Tsy09, Sec 2.3]):

$$R^*_n \geq c(\epsilon) \sup_{\theta, \theta' \in \Theta} \left\{ |T(\theta) - T(\theta')|^2 : \text{TV}(P_\theta \otimes P_{\theta'}^n, P_{\theta'} \otimes P_{\theta}^n) \leq 1 - \epsilon \right\}.$$

where $\epsilon$ is typically chosen to be a small constant and $c(\epsilon)$ is some constant that only depends on $\epsilon$; the rationale is that testing is easier (statistically) than estimation. Indeed, the constraint in (2) ensures that the two hypotheses cannot be reliably tested and hence the worst-case statistical risk is lower bounded by the separation of the functional values. A more convenient form that avoids product distributions is the following in terms of the $\chi^2$-divergence:

$$R^*_n \geq c \sup_{\theta, \theta' \in \Theta} \left\{ |T(\theta) - T(\theta')|^2 : \chi^2(P_\theta \parallel P_{\theta'}^n) \leq \frac{1}{n} \right\},$$

where $\chi^2$ is the Kullback-Leibler divergence.

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for some absolute constant $c$, thanks to the inequality $\chi^2(P\|Q) \geq \log \frac{1}{2(1-\text{TV}(P,Q))}$ [Tsy09, Sec. 2.4] and the tensorization property $\chi^2(P^\otimes n\|Q^\otimes n) = (1 + \chi^2(P\|Q))^n - 1$. Similar lower bounds can be obtained by replacing $\chi^2$ in (2) with the squared Hellinger distance $H^2(P_\theta, P_{\theta'})$ or the Kullback-Leibler (KL) divergence $D(P_\theta\|P_{\theta'})$; nevertheless, the $\chi^2$-version is perhaps the most popular since the second moment nature of the $\chi^2$-divergence renders it frequently easy to compute. In virtually all problems of functional estimation, the lower bound follows from applying (3) or the variants thereof (such as the version with two priors), which often turn out to be rate-optimal.

This papers aims at explaining the effectiveness of Le Cam’s method, specifically the version (3) based on the $\chi^2$-divergence, from an optimization perspective. The main observation is the following: For certain problems such as estimating linear functionals in the density model (with possibly indirect observations), under suitable conditions, the maximization in (3) can be viewed as a convex optimization problem, whose dual problem corresponds to (within constant factors) a minimization problem that optimizes the bias-variance tradeoff. This perspective yields the following characterization of the minimax rate in terms of the $\chi^2$-modulus of continuity:¹

$$R^*_n \asymp \sup_{\theta,\theta'\in\Theta} \left\{ \left[ T(\theta) - T(\theta') \right]^2 : \chi^2(P_\theta\|P_{\theta'}) \leq \frac{1}{n} \right\},$$

which strengthens the prior result of Donoho-Liu [DL91] for linear functionals. In addition, we show the result holds for exponential families for estimating functionals linear in the mean parameters, which strengthens the prior result of Donoho-Liu [DL91] for linear functionals. In addition, we show the follow characterizing the of the minimax rate in terms of the $\chi^2$-modulus of continuity:¹

$$\sup_{\pi,\pi'\in\Pi} \left\{ \left[ \int T(\theta)\pi(d\theta) - \int T(\theta)\pi'(d\theta) \right]^2 : \chi^2(P_\pi\|P_{\pi'}) \leq \frac{1}{d} \right\}.$$

where the supremum is taken over all pairs of priors in the constraint set $\Pi = \{ \pi : \int c(\theta)\pi(d\theta) \leq 1 \}$ and $P_\pi = \int P_\theta\pi(d\theta)$ denotes the mixture distribution. This result gives conditions under which the generalized version of Le Cam’s method using two priors (also known as fuzzy hypotheses testing [Tsy09, Sec. 2.7.4]) is tight.

The duality view in this paper is in fact natural. Indeed, the classical minimax theorem in decision theory states that, under regularity assumptions,

$$\inf_{T} \sup_{\theta\in\Theta} \mathbb{E}_\theta[(\hat{T} - T(\theta))^2] = \sup_{\pi\in\Pi(\Theta)} \inf_{\pi\rightarrow\pi} [(\hat{T} - T(\theta))^2]$$

This can also be interpreted from the duality perspective,² where the primal variables corresponds to (randomized) estimators and the dual variables correspond to priors. However, the duality

¹Throughout the paper, for any sequences $\{a_n\}$ and $\{b_n\}$ of positive numbers, we write $a_n \gtrless b_n$ if $a_n \geq cb_n$ holds for all $n$ and some absolute constant $c > 0$, $a_n \precsim b_n$ if $a_n \gtrsim b_n$, and $a_n \asymp b_n$ if both $a_n \gtrsim b_n$ and $a_n \precsim b_n$ hold.

²This follows from standard arguments in optimization by rewriting the left-hand side as $\inf_{t} \{ t : \mathbb{E}_\theta[(\hat{T} - T(\theta))^2] \leq t, \forall \theta \in \Theta \}$ and the Lagrange multipliers correspond to priors. When both $X$ and $\theta$ are finitely-valued, (6) is simply the duality of linear programming (LP).
view of (6) is unwieldy except in special cases or simple univariate problems, because finding the least favorable prior that maximizes the Bayes risk is a difficult infinite-dimensional optimization problem. In this vein, results such as (4) and (5) can be viewed as approximate version of the general minimax theorem that applies to functional estimation.

To produce concrete results of rate of convergence, one needs to evaluate the value of the maximization program such as (5). Using tools from complex analysis, we do so for a number of problems and obtain new results on the sharp rate of convergence, characterizing, in particular, the “elbow effect”, that is, the phase transition from parametric to nonparametric rates. As the main application of our methodology, we consider three problems in the area of “estimating the unseens”, namely, population recovery, distinct elements problem, and Fisher’s species problem. In addition to recovering the prior result of [PSW17] on the sharp rate of population recovery, we establish the following new results:

- Distinct elements problem: Randomly sampling a fraction $p$ of colored balls from an urn containing $d$ balls in total, the goal is to estimate the number of distinct colors in the urn [RRSS09, Val11, WY18]. We show that, as $d \to \infty$, the optimal normalized estimation error is within logarithmic factors of $d^{-\frac{1}{2}} \min\{\frac{d}{p}, 1\}$, exhibiting an elbow at $p = \frac{1}{2}$;

- Fisher’s species problem: Given $n$ independent samples drawn from an unknown distribution, the goal is to predict the number of unseen symbols in the next (unobserved) $r \cdot n$ samples [FCW43, ET76, OSW16]. We show that, as $n \to \infty$, the optimal normalized prediction error is within logarithmic factors of $n^{-\min\{\frac{1}{r}, \frac{1}{2}\}}$, exhibiting an elbow at $r = 1$.

We emphasize that in obtaining the above results, we do not demonstrate an explicit choice of the optimal estimator; instead, capitalizing on the duality between the minimization problem over the linear estimators and the maximization that produces the best Le Cam lower bound, we bound the value of the dual problem from above, thereby showing the achievability of the optimal rates. This is conceptually distinct from previous explicit construction of linear estimators such as kernel-based methods for density estimation [Tsy09] or smoothed estimators in the context of species problems [OSW16] (which do not attain the optimal rate). Nevertheless, the estimators can be constructed in polynomial time as solutions to certain linear programs.

Before proceeding to the discussion of the related literature, let us mention that the duality view in this paper need not be limited to functional estimation. In a companion paper [JPW19] we extend the methods to estimating the distribution itself (with respect to the total variation loss) in the context of the distinct elements problem. The connection to functional estimation is that estimating the distribution in total variation is equivalent to simultaneously estimating all bounded linear functionals; this view enables us to analyze minimum-distance estimators in the duality framework.

1.1 Related work

A celebrated result of Donoho-Liu [DL91] relates the minimax rate of estimating linear functionals to the Hellinger modulus of continuity. For the density estimation models, under certain assumptions, it is shown that the minimax rate coincides with the right-hand side of (3) with $H^2$ in place of the $\chi^2$-divergence. However, the constant factors may not be universal and depend on the problem or its hyper-parameters, thus precluding the application to high-dimensional problems. More importantly, the proof (of the upper bound) in [DL91] is based on constructing an estimator
via pairwise hypotheses tests, by means of a binary search on the functional value. While this method can deal with general loss function, the limitation is that it assumes the Hölderianity of the modulus of continuity in order to show tightness. We refer the readers to Section 2.5 for a detailed comparison of the results.

The prior work that is closest to ours in spirit is that of Juditsky-Nemirovski [JN09], where the main technology was also convex optimization and the minimax theorem. As opposed to the squared loss, they considered the $\epsilon$-quantile loss and the corresponding minimax risk:

$$R^*_{n,\epsilon} = \inf_{\hat{T}} \inf_{r} \{ r : \sup_{\theta \in \Theta} P_\theta[|\hat{T} - T(\theta)| > r] \leq \epsilon \}.$$  

For exponential families, under certain convexity assumptions, it is shown (cf. [JN09, Theorem 3.1 and Proposition 3.1]) that $R^*_{n,\epsilon}$ is within absolute constant factors of the Hellinger modulus of continuity, provided that $\exp(-o(n)) \leq \epsilon \leq \frac{1}{4}$. We extend this result to quadratic risk under more relaxed assumptions (see Section 4.3 for details). Note that the quadratic risk result cannot be obtained through the usual route of integrating the high-probability risk bound, since the estimator for $\epsilon$-quantile loss potentially depends on $\epsilon$. On the other hand, one can deduce the result on $\epsilon$-quantile loss for constant $\epsilon$ from that for quadratic risk by applying the Markov inequality.4 Notwithstanding these improvements, the main advantage of our approach is its versatility, as witnessed, e.g., by the treatment of the high-dimensional case.

Other examples that operationalized the duality perspective for statistical estimation include the following:

- The linear programming (LP) duality between the risk of the optimal linear estimator and the best Le Cam lower bound based on the total variation was recognized in [PSW17, Theorem 4] for linear functional estimation in discrete problems; this is the precursor to the present paper. However, this result in general has a $\sqrt{n}$-gap in the convergence rate, which was mended in an ad hoc manner in [PSW17] for specific problems. In fact, similar proof technique was previously employed by Moitra-Saks in [MS13] to upper bound the value of the dual LP in order to establish statistical upper bounds, although the connection that the dual program in fact corresponds to the minimax lower bound was missing.

- The duality between the best polynomial approximation and the moment matching problem was leveraged in [WY16, WY19, JVHW15] for estimating symmetric functionals, such as the Shannon entropy and support size, of distributions supported on large domains. As opposed to optimizing over general linear estimators, the construction is by using approximating polynomials whose uniform approximation error bound the bias. Matching minimax lower bound is obtained by using the solution of the dual problem (moment matching) to construct priors. In similar context of estimating distribution functionals, general sample complexity bounds are obtained [VV11] based on linear programming duality.

### 1.2 Organization

The rest of the paper is organized as follows. Section 2 presents the main result for estimating linear functionals of a distribution (with possibly indirect observations) under a general setup. We provide two examples: population recovery (Section 2.3) and density estimation (Section 2.4), which are finite-dimensional and infinite-dimensional application of the main theorem respectively. Section 3 extend the result to estimating separable functions in high-dimensional models. The methods are

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4However, for small $\epsilon$ the results of [JN09] are not implied by the quadratic risk result in this paper.
then applied to the distinct elements problem (Section 3.1) and Fisher’s species extrapolation problem (Section 3.2) to yield sharp minimax rates of convergence. Finally, in Section 4 we extend the result for exponential families under weaker assumptions than those in [JN09]. To present a simple motivating example and to exhibit the duality perspective in a familiar problem, in Section 4.1 we revisit the classical Gaussian white noise model and re-derive the classical result of Ibragimov and Has’minskii [HI84]. For readers unfamiliar with this type of argument, it might be helpful to start with Section 4.1.

Section 5 contains the proofs of Theorems 8–10; further technical results and proofs are collected in Appendices A and B.

2 Linear functionals

Let \( \Theta \) and \( \mathcal{X} \) be measurable spaces and \( P : \Theta \to \mathcal{X} \) a transition probability kernel between them. Denote by \( \mathcal{P}(\Theta) \) the set of all probability distributions on \( \Theta \) and let \( \Pi \) be a (given) subset of \( \mathcal{P}(\Theta) \). Let \( T(\pi) \) be a functional of \( \pi \in \Pi \). We define the minimax rate of estimating \( T \) using samples \( X_1, \ldots, X_n \sim \pi P \) as:

\[
R^*(n) \triangleq \inf_{T} \sup_{\pi \in \Pi} \mathbb{E}[|\hat{T}(X_1, \ldots, X_n) - T(\pi)|^2].
\]

When \( P \) is the identity kernel, the samples are simply drawn from \( \pi \); otherwise, the samples are indirect observations.

We also define the modulus of continuity of functional \( T \) with respect to various distances (and quasi-distances) between distributions \( \pi P \):

\[
\delta_{\chi^2}(t) = \sup \{ T(\pi') - T(\pi) : \chi^2(\pi' P \| \pi P) \leq t^2, \pi, \pi' \in \Pi \} \tag{7}
\]
\[
\delta_{H^2}(t) = \sup \{ T(\pi') - T(\pi) : H^2(\pi' P, \pi P) \leq t^2, \pi, \pi' \in \Pi \} \tag{8}
\]
\[
\delta_{TV}(t) = \sup \{ T(\pi') - T(\pi) : TV(\pi' P, \pi P) \leq t, \pi, \pi' \in \Pi \} \tag{9}
\]

where \( TV(F, G) = \sup_E |F(E) - G(E)| \) is the total variation, \( H^2(F, G) = \int d\nu \left( \sqrt{\frac{dF}{d\nu}} - \sqrt{\frac{dG}{d\nu}} \right)^2 \)

is the squared Hellinger distance. Finally, the \( \chi^2 \)-divergence is defined as \( \chi^2(F \| G) = \infty \) if \( F \not\ll G \) and otherwise \( \chi^2(F \| G) = \int dG \left( \frac{dF}{dG} \right)^2 - 1 \). We note that \( TV(F, G) \) and \( H(F, G) \) are distances on \( \mathcal{P} \). For a signed measure \( \mu \) its total variation norm is denoted \( \|\mu\|_{TV} \), so that \( TV(F, G) = \|F - G\|_{TV} \).

2.1 General properties of \( \delta(t) \)

Proposition 1. Let \( T(\pi) \) be affine in \( \pi \). Then

1. (Concavity) \( \delta_{H^2}(\cdot) \) and \( \delta_{TV}(\cdot) \) are concave.
2. (Subadditivity) For any \( c \in [0, 1] \) and \( t \geq 0 \) we have:

\[
\delta_{TV}(ct) \geq c\delta_{TV}(t) \tag{10}
\]
\[
\delta_{H^2}(ct) \geq c\delta_{H^2}(t) \tag{11}
\]
\[
\delta_{\chi^2}(ct) \geq c^2\delta_{\chi^2}(t) \tag{12}
\]

3. (Comparison of various \( \delta \)’s) For all \( t \geq 0 \) we have

\[
\frac{1}{2} \delta_{H^2}(t) \leq \delta_{\chi^2}(t) \leq \delta_{H^2}(t) \leq \delta_{TV}(t) \leq \delta_{H^2}(\sqrt{2}t). \tag{13}
\]
4. (Superlinearity) Let $\Delta_{\text{max}} \triangleq \sup\{T(\pi') - T(\pi) : \pi, \pi' \in \Pi\}$, then

$$\delta_{H^2}(t) \geq \Delta_{\text{max}} \frac{t}{2}. \quad (14)$$

Proof. The first property follows from the fact that $\text{TV}(P,Q)$ and $H(P,Q)$ are both convex in the pair $(P,Q)$ (in fact they are distances). The second one for TV and $H^2$ follows from the first and the fact that $\delta(0) = 0$, while for $\chi^2$ it follows from the convexity of $(P,Q) \mapsto \chi^2(P\|Q)$ and hence the concavity of $s \mapsto \delta_{\chi^2}(\sqrt{s})$. For the third, we recall standard bounds (cf. e.g. [Tsy09, Sec. 2.4.1]): For any pair of distributions $P,Q$ we have

$$H^2(P,Q)/2 \leq \text{TV}(P,Q) \leq H(P,Q), \quad (15)$$

and

$$H^2(P,Q) \leq 2 - \frac{2}{\sqrt{1 + \chi^2(P\|Q)}} \leq \chi^2(P\|Q). \quad (16)$$

Together (15) and (16) establish all inequalities in (13) except the left-most one. For the latter we recall from [LC86, p. 48]:

$$\frac{1}{2}H^2(P,Q) \leq \chi^2 \left( P \left\| \frac{P + Q}{2} \right\| \right) \leq H^2(P,Q). \quad (17)$$

Thus, for any $(\pi, \pi')$ that are feasible for the $\delta_{H^2}(t)$ problem, then $\pi_0 \triangleq \frac{\pi + \pi'}{2}$ and $\pi'_0 \triangleq \pi'$ are feasible for the $\delta_{\chi^2}(t)$ problem, since $\chi^2(\pi'_0 P\|\pi_0 P) \leq t^2$ according to (17), and satisfy $|T(\pi_0) - T(\pi'_0)| = \frac{1}{2}|T(\pi) - T(\pi')|.$

Finally, (14) follows from (12) and the observation that $\delta_{H^2}(2) = \Delta_{\text{max}}$ since $H^2 \leq 2$ by definition. \qed

2.2 Main result: Minimax rate for linear functionals

Our main result is the following:

**Theorem 2.** Suppose that $(\Theta, \mathcal{X}, P, T, \Pi)$ satisfy the following assumptions:

A1 The functional $\pi \mapsto T(\pi)$ is affine;

A2 The set $\Pi$ is convex;

A3 There exists a vector space of functions $\mathcal{F}$ on $\mathcal{X}$ such that $\mathcal{F}$ contains constants and is dense in $L_2(\mathcal{X}, \pi P)$ for every $\pi \in \Pi$;

A4 There exists a topology on $\Pi$ such that:

A4a It is coarse enough that $\Pi$ is compact;

A4b It is fine enough that $T(\pi), \pi P f$ and $\pi P(\mathcal{F})$ are continuous in $\pi \in \Pi$ for all $f \in \mathcal{F}$.

Then

$$\frac{1}{l} \delta_{\chi^2}(\frac{1}{\sqrt{n}})^2 \leq R^*(n) \leq \delta_{\chi^2}(\frac{1}{\sqrt{n}})^2. \quad (18)$$

Some remarks are in order:

1. If $\Theta$ and $\mathcal{X}$ are finite, then $\mathcal{F}$ can be taken to be all functions on $\mathcal{X}$ and assumptions A3 and A4 are automatic.
2. If $\mathcal{X}$ is a normal topological space, then every probability measure $\nu$ is regular [DS58, IV.6.2] and the set $\mathcal{F}$ of all bounded continuous functions is dense in $L_2(\mathcal{X}, \nu)$, cf. [DS58, IV.8.19]. Other convenient choices of $\mathcal{F}$ are all Lipschitz functions (and Wasserstein $W_1$-convergence), all polynomials, trigonometric polynomials or sums of exponentials.

3. The continuity of $\pi Pf$ under the weak topology on $\Pi$ can be assured by demanding a (strong Feller) property for kernel $P$: For any bounded measurable $f$, $Pf$ is bounded continuous.

Proof. The lower bound simply follows from the $\chi^2$-version of Le Cam’s method. Consider a pair of distributions $\pi, \pi'$ such that $\chi^2(\pi'\|\pi P) \leq \frac{a}{n}$ for some $a > 0$ to be optimized. From the tensorization property of $\chi^2$-divergence we have

$$\chi^2((\pi' P)\otimes n \| (\pi P)\otimes n) = (1 + \chi^2(\pi' P)((\pi P)))^n \leq e^a - 1. \quad (19)$$

Using Brown-Low’s two-point lower bound [BL96] and optimizing over the pair $\pi, \pi'$, we have

$$R^*(n) \geq \sup_{\pi, \pi': \chi^2(\pi' P)\| P \leq \frac{a}{n}} \left( \frac{(T(\pi) - T(\pi'))^2}{1 + \sqrt{1 + \chi^2((\pi' P)\otimes n \| (\pi P)\otimes n)}} \right)^2 = \frac{\delta^2}{a^2} \left( \frac{\sqrt{n}}{a} \right)^2. \quad (20)$$

Using (12) and optimizing over $a > 0$, we obtain

$$R^*(n) \geq \delta^2 \left( \frac{1}{\sqrt{n}} \right)^2 \sup_{a > 0} \frac{a}{\left( 1 + e^{a/2} \right)^2} \geq 1/6.5. \quad (21)$$

To prove an upper bound we consider estimators of the form

$$\hat{T}_g(X_1, \ldots, X_n) = \frac{1}{n} \sum_{i=1}^n g(X_i), \quad (22)$$

where $g \in \mathcal{F}$. For convenience we denote $X^n = (X_1, \ldots, X_n)$. We analyze the quadratic risk of this estimator by decomposing it into bias and variance part:

$$\mathbb{E}_{X^n \sim \pi Pf}[(\hat{T}_g(X^n) - T(\pi))^2] \leq \frac{1}{n} \text{Var}_{\pi P}[g] + |T(\pi) - \pi Pg|^2 \quad (23)$$

Taking worst-case $\pi$ and optimizing over $g$ we get

$$\sqrt{R^*(n)} \leq \inf_g \sup_{\pi \in \Pi} \left\{ \frac{1}{\sqrt{n}} \sqrt{\text{Var}_{\pi P}[g] + |T(\pi) - \pi Pg|} \right\} = \delta_t \left( \frac{1}{\sqrt{n}} \right),$$

where

$$\delta_t(t) \triangleq \inf_g \sup_{\pi} \left\{ t \sqrt{\text{Var}_{\pi P}[g] + |T(\pi) - \pi Pg|} \right\} \quad (24)$$

The proof is completed by applying the next proposition.

**Proposition 3.** Under the conditions of Theorem 2, we have

$$\delta_a(t) \leq \delta_{\chi^2}(t) \quad \forall t \geq 0. \quad (25)$$

Furthermore, the supremum over $\pi, \pi'$ in the definition of $\delta_{\chi^2}$ is achieved: There exist $\pi^*, \pi'^* \in \Pi$ s.t. $\delta_{\chi^2}(t) = T(\pi'^*) - T(\pi^*)$ and $\chi^2(\pi'^* P \| \pi^* P) \leq t^2$. 

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Before proving the proposition, we recall the minimax theorem due to Ky Fan \cite[Theorem 2]{Fan53}.

**Theorem 4** (Ky Fan). Let \( X \) be a compact space and \( Y \) an arbitrary set (not topologized). Let \( f : X \times Y \to \mathbb{R} \) be such that for every \( y \in Y \), \( x \mapsto f(x, y) \) is upper semicontinuous on \( X \). If \( f \) is concave-convex-like on \( X \times Y \), then

\[
\max_{x \in X} \inf_{y \in Y} f(x, y) = \inf_{y \in Y} \max_{x \in X} f(x, y).
\]

We remind that the function \( f \) is concave-convex-like on \( X \times Y \) if a) for any two \( x_1, x_2 \in X \) and \( \lambda \in [0, 1] \) there exists \( x_3 \in X \) such that for all \( y \in Y \):

\[
\lambda f(x_1, y) + (1 - \lambda) f(x_2, y) \leq f(x_3, y)
\]

and b) for any two \( y_1, y_2 \in Y \) and \( \lambda \in [0, 1] \) there exists \( y_3 \in Y \) such that for all \( x \in X \):

\[
\lambda f(x, y_1) + (1 - \lambda) f(x, y_2) \geq f(x, y_3).
\]

**Proof of Proposition 3.** We aim to apply the minimax theorem in order to get a more convenient expression for \( \delta(t) \). The function

\[
(\pi, g) \mapsto \sqrt{\text{Var}_{\pi P}[g]} + |T(\pi) - \pi Pg|
\]

satisfies all the conditions except for the concavity in \( \pi \) due to the last term (it is convex instead of concave). To mend this consider the following upper bound

\[
|T(\pi) - \pi Pg| \leq \sup_{\xi \in [0, 2], \pi' \in \Pi} T(\pi) - \pi Pg - \xi(T(\pi') - \pi' Pg).
\]

Indeed, if \( T(\pi) - \pi Pg > 0 \), take \( \xi = 0 \); otherwise, take \( \pi' = \pi, \xi = 2 \).

So letting \( u = (\pi, \pi', \xi) \in U \triangleq \Pi \times \Pi \times [0, 2] \) we consider the following function on \( U \times F \):

\[
F_t(u, g) \triangleq T(\pi) - \pi Pg - \xi(T(\pi') - \pi' Pg) + t\sqrt{\text{Var}_{\pi P}[g]}
\]

We claim it is concave-convex-like. Convexity in \( g \) is easy: the term \( |T(\pi) - \pi Pg| \) is clearly convex, whereas the convexity of \( g \mapsto \sqrt{\text{Var}_{\mu}[g]} \) follows from observation that without loss of generality we may assume \( \mathbb{E}_\mu[g] = 0 \) and then \( \sqrt{\text{Var}_{\mu}[g]} = \|g\|_{L^2(\mu)} \) is a norm (hence convex).

We proceed to checking the concave-like property of \( F_t(u, g) \) in \( u \). Define for convenience,

\[
a(\pi) \triangleq T(\pi) - \pi Pg, \quad b(\pi) = t\sqrt{\text{Var}_{\pi P}[g]}
\]

It is clear that \( a(\pi) \) is affine, whereas \( b(\pi) \) is concave. Indeed, \( \sqrt{\cdot} \) is a concave and increasing scalar function, whereas \( \text{Var}_\mu[g] = \mu(g^2) - (\mu g)^2 \) is concave in \( g \). So for \( u = (\pi, \pi', \xi) \) we have

\[
F_t(u, g) = a(\pi) - \xi a(\pi') + b(\pi).
\]

(27)

Consider \( u_1 = (\pi_1, \pi'_1, \xi_1) \) and \( u_2 = (\pi_2, \pi'_2, \xi_2) \) and \( \lambda \in [0, 1] \). First, suppose that \( \xi_1 = \xi_2 = 0 \). We see that in this case

\[
\lambda F_t(u_1, g) + (1 - \lambda) F_t(u_2, g) \leq F_t(\lambda u_1 + (1 - \lambda)u_2, g)
\]

\footnote{There it is stated for Hausdorff \( X \), but this condition is not necessary, e.g., \cite{BZ86}. Note that in defining convex-concave-like property we mandate it hold for all \( 0 \leq t \leq 1 \) in (26), but it is also known that minimax theorem holds for functions that only satisfy, e.g., \( t = 1/2 \), see \cite{Kon68}.}
since from (27) we see that \( F_t \) is concave in \( \pi \). Then, taking \( u_3 = \lambda u_1 + (1 - \lambda)u_2 \) satisfies (26). Next, assume that either \( \xi_1 > 0 \) or \( \xi_2 > 0 \). Then define

\[
\pi_3 \triangleq \lambda \pi_1 + (1 - \lambda)\pi_2, \quad \pi'_3 \triangleq \frac{\lambda \xi_1}{\xi_3} \pi'_1 + \frac{(1 - \lambda)\xi_2}{\xi_3} \pi'_2, \quad \xi_3 \triangleq \lambda \xi_1 + (1 - \lambda)\xi_2.
\]

And set \( u_3 = (\pi_3, \pi'_3, \xi_3) \). We claim that

\[
\lambda F_t(u_1, g) + (1 - \lambda)F_t(u_2, g) \leq F_t(u_3, g).
\]

Indeed, we have from affinity of \( a(\cdot) \):

\[
a \left( \frac{\lambda \xi_1}{\xi_3} \pi'_1 + \frac{(1 - \lambda)\xi_2}{\xi_3} \pi'_2 \right) = \frac{\lambda \xi_1}{\xi_3} a(\pi'_1) + \frac{(1 - \lambda)\xi_2}{\xi_3} a(\pi'_2).
\]

Therefore, we have

\[
\lambda a(\pi_1) + (1 - \lambda) a(\pi_2) = a(\pi_3)
\]

\[
\lambda \xi_1 a(\pi'_1) + (1 - \lambda) \xi_2 a(\pi'_2) = \xi_3 a(\pi'_3)
\]

\[
\lambda b(\pi_1) + (1 - \lambda) b(\pi_2) \leq b(\pi_3).
\]

These three statements together with (27) prove (28).

Knowing that \( F_t \) is concave-convex-like, for applying the minimax theorem we only need to check that \( u \mapsto F_t(u, g) \) is continuous for all \( g \) and that \( U \) is compact. This is satisfied by the assumption \( A4 \) of Theorem 2. Applying Theorem 4, we have

\[
\delta_u(t) \leq \inf_{g \in \mathcal{F}} \sup_{u \in U} F_t(u, g) = \inf_{g \in \mathcal{F}} \max_{u \in U} F_t(u, g) = \max_{u \in U} \inf_{g \in \mathcal{F}} F_t(u, g).
\]

Next, to evaluate the rightmost term, fix \( u = (\pi, \pi', \xi) \in U \) and consider the optimization

\[
\psi_t(u) = \inf_{g \in \mathcal{F}} \{(\xi, \pi' - \pi) P g + t \sqrt{\text{Var}_\pi P[g]}\}.
\]

We claim that

\[
\psi_t(u) = \begin{cases} 
-\infty, & \xi \neq 1 \\
-\infty, & \xi = 1, \chi^2(\pi' P | \pi P) > t^2 \\
0, & \text{otherwise}
\end{cases}
\]

which implies the desired (25) by continuing (29):

\[
\max_{u \in U} \inf_{g \in \mathcal{F}} F_t(u, g) = \max\{T(\pi') - T(\pi) : \chi^2(\pi' P | \pi P) \leq t^2, \pi \in \Pi, \pi' \in \Pi\}.
\]

To prove (31), we first recall that \( \mathcal{F} \) contains constants. Thus if \( \xi \neq 1 \), we have that the first term in (30) can be driven to \( -\infty \), while keeping the second term zero, by taking \( g = c1 \) and \( c \to \pm \infty \). So fix \( \xi = 1 \). Recall a variational characterization of the \( \chi^2 \)-divergence:

\[
\chi^2(\mu || \nu) = \sup_{g \in \mathcal{G}} \{ (\mathbb{E}_\mu [g] - \mathbb{E}_\nu [g])^2 : \text{Var}_\nu [g] \leq 1 \},
\]

\[
\text{For completeness, here is short proof of (32). First, assume } \chi^2(\mu || \nu) < \infty. \text{ Denoting } f = \frac{d\mu}{d\nu} \text{ and assuming without loss of generality that } \mathbb{E}_\nu [g] = 0 \text{ we have } |\mathbb{E}_\nu [g] - \mathbb{E}_\mu [g]|^2 \leq \text{Var}_\nu [g] \text{Var}_\nu f, \text{ which completes the proof since } \text{Var}_\nu f = \chi^2(\mu || \nu). \text{ For the other direction, simply approximate } f \text{ by elements of } \mathcal{G}. \text{ If } \chi^2(\mu || \nu) = \infty, \text{ set } f_n = \min(f, n) \text{ and let } n \to \infty.
\]
where $\mathcal{G}$ is any subset that is dense in $L_2(\nu)$. Thus, if $\chi^2(\pi'P\|\pi P) > t^2$ (in particular, if $\pi'P \ll \pi P$) there must exist $g_0 \in \mathcal{F}$ such that

$$
\pi'Pg_0 - \pi Pg_0 < -t \quad \text{Var}_{\pi P}[g_0] \leq 1
$$

Thus taking $g = cg_0$ and $c \to \infty$ in (30) we again obtain that $\psi_t(u) = -\infty$. In the remaining case, $\chi^2(\pi'P\|\pi P) \leq t^2$ and again from (32) we have that for any $g \in \mathcal{F}$

$$(\pi' - \pi)Pg \geq -t \sqrt{\text{Var}_{\pi P}[g]} ,$$

and thus $\psi_t(u) \geq 0$, while 0 is achievable by taking $g = 0$. $\square$

2.3 Application: Population recovery

For a positive integer $d$, consider the following three specializations of Theorem 2, namely the following tuples $(\Theta, \mathcal{X}, P, T, \Pi)$:

1. $\Theta = \{0, 1\}^d$, $T(\pi) = \pi(0)$, where 0 is the all-zero string, $\Pi = \mathcal{P}(\Theta)$, $\mathcal{X} = \{0, 1, ?\}^d$, and the kernel $P$ is given by

$$
P^{(1)}_{\theta} = \prod_{t=1}^d Q(\cdot|\theta_t), \quad Q(b|a) = \begin{cases} 
\epsilon, & b = ? \\
1 - \epsilon, & b = a
\end{cases}
$$

(i.e. each coordinate of $\theta$ is erased independently with probability $\epsilon$).

2. $\Theta = \{0, \ldots, d\}$, $T(\pi) = \pi(0)$, $\Pi = \mathcal{P}(\Theta)$, $\mathcal{X} = \mathbb{Z}_+ \times \mathbb{Z}_+$ and $P$ equals

$$
P^{(2)}_{\theta} = \text{Binom}(\theta, 1 - \epsilon) \otimes \text{Binom}(d - \theta, 1 - \epsilon),
$$

where $\text{Binom}(n, p)$ stands for the binomial distribution with $n$ independent trials and success probability $p$.

3. $\Theta = \{0, \ldots, d\}$, $T(\pi) = \pi(0)$, $\Pi = \mathcal{P}(\Theta)$, $\mathcal{X} = \mathbb{Z}_+$ and $P$ equals

$$
P^{(3)}_{\theta} = \text{Binom}(\theta, 1 - \epsilon).
$$

We will denote the minimax quadratic risk for estimating $T(\pi)$ based on $n$ iid samples by $R^*_i(n, d)$ and the modulus of continuity function by $\delta^{(i)}_{\chi^2}(t, d)$, for $i = 1, 2, 3$, respectively.

The first model $P^{(1)}$ corresponds to the so-called “lossy population recovery” – a problem initially considered in [DRWY12, WY12] in the context of learning DNFs with partial observations, and further investigated in [BIMP13, MS13, LZ15, DST16, PSW17]. This problem can also be viewed as a special instance of learning mixtures of discrete distributions in the framework of [KMR+94]. Here the parameter $\pi$ is an arbitrary distribution on the $d$-dimensional Hamming space $\{0, 1\}^d$. For $n$ iid random binary strings drawn from $\pi$, we observe their erased version, where each bit is erased with probability $\epsilon$. The goal is to estimate the weight of the all-zero string $\pi(0)$. It has been shown in [DRWY12] (cf. [PSW17, Appendix A]) estimating the entire distribution $\pi$ in the sup norm can be reduced to estimating $\pi(0)$ in terms of both sample and time complexity.

It is easy to see that from permutation invariance, in the context of $P^{(1)}$, to estimate $\pi(0)$ it is sufficient to summarize each sample $X_i$ into its number of 1’s and 0’s. Correspondingly, the set of distributions in the definition of the minimax risk can be safely restricted to permutation
invariant distributions on \( \{0, 1\}^d \). With these reductions we arrive at the second model \( P^{(2)} \) which is statistically equivalent. Thus,

\[
R_{(1)}^*(n, d) = R_{(2)}^*(n, d), \quad \delta_{\chi^2}^{(1)}(t, d) = \delta_{\chi^2}^{(2)}(t, d).
\]

The third setting corresponds to ignoring the number of 0’s in the second setting (i.e. restricting to estimators that only depend on the number of 1’s in each sample). Since we reduce the observation space, it is clear that

\[
R_{(3)}^*(n, d) \geq R_{(2)}^*(n, d), \quad \delta_{\chi^2}^{(3)}(t, d) \geq \delta_{\chi^2}^{(2)}(t, d)
\]

In fact, the reverse direction is almost true, since the number of 0’s provides negligible information for estimating \( \pi(0) \) [PSW17].

The minimax risk of population recovery has been characterized within logarithmic factors in [PSW17]. Next we deduce this result from the general Theorem 2, which boils down to characterizing the \( \delta_{\chi^2} \) function. The following result can be distilled from [PSW17] (a proof is given in Appendix B for completeness):

**Lemma 5.** For any \( t \geq 0, d \geq 1 \) we have

\[
\delta_{\chi^2}^{(3)}(t, d) \leq t^{\min(1, \frac{1-\epsilon}{\epsilon})}. \tag{36}
\]

Conversely, for \( \epsilon > 1/2 \) there exists \( t_0 = t_0(\epsilon) \) and \( C = C(\epsilon) \) such that

\[
\delta_{\chi^2}^{(3)}(t, d) \geq C \left( \frac{t}{\ln \frac{1}{t}} \right)^{\frac{1-\epsilon}{\epsilon}}, \tag{37}
\]

provided that \( t \leq t_0 \) and \( d \geq C \ln^2 \frac{1}{t} \). Furthermore, if \( d \geq Ct^{-2} \ln^4 \frac{1}{t} \) then also

\[
\delta_{\chi^2}^{(2)}(t, d) \geq C \left( \frac{t}{\ln \frac{1}{t}} \right)^{\frac{1-\epsilon}{\epsilon}}. \tag{38}
\]

Applying the general Theorem 2 together with Lemma 5, we obtain the following characterization of the minimax risks, where the rate of convergence exhibits an elbow effect at erasure probability \( \epsilon = \frac{1}{2} \):

**Corollary 6 (PSW17).** For all three minimax risks \( i = 1, 2, 3 \), the following holds:

- If \( \epsilon \in (0, \frac{1}{2}) \), then for any \( d \),
  \[
  \frac{1}{28n} \leq R_{(i)}^*(n, d) \leq \frac{1}{n};
  \]

- If \( \epsilon \in (\frac{1}{2}, 1) \), then there exists a constant \( C = C(\epsilon) > 0 \) such that we have
  \[
  \frac{1}{C} (n \log^2 n)^{-\frac{1-\epsilon}{\epsilon}} \leq R_{(i)}^*(n, d) \leq n^{-\frac{1+\epsilon}{\epsilon}}
  \]

  where the lower bound holds provided that \( d \geq C n \log^4 n \).
2.4 Application: Density estimation

As another application of Theorem 2, we consider the classical setting of density estimation under smoothness conditions. For simplicity, we focus on the one-dimensional setting where \( \rho \) is a probability density function on \([-1,1]\) and belongs to the Hölder class \( \mathcal{P}(\beta, L) \), namely, \(|\rho(x) - \rho(y)| \leq L|x - y|^{\beta}\) for any \( x, y \in [-1,1] \). Given \( n \) iid samples drawn from \( \rho \), the goal is to estimate the value of the density at point zero \( \rho(0) \). So the minimax risk is given by

\[
R^*(n) = \inf_{\hat{\rho}} \sup_{\rho} \mathbb{E}_{X_i \sim \rho} \left| \hat{\rho}(X_1, \ldots, X_n) - \rho(0) \right|^2.
\]

We now verify that this setting fulfills the assumptions of Theorem 2. First, we have \( \Theta = \mathcal{X} = [-1,1] \), the identity kernel \( P(x, E) = 1\{x \in E\} \). We take \( \mathcal{F} = C[-1,1] \) to be all continuous functions on \([-1,1]\). Note that by identifying a measure \( \pi \) on \([-1,1]\) with its density \( \rho \), we can set \( T(\pi) = \rho(0) \) and view \( \Pi \) as a subset of \( C[-1,1] \):

\[
\Pi = \{ \rho \in C[-1,1] : |\rho(x) - \rho(y)| \leq L|x - y|^{\beta} \}.
\]

If we endow \( \Pi \) and \( C[-1,1] \) with the topology of uniform convergence, then \( \Pi \) becomes a closed convex subset of \( C[-1,1] \) and the Arzela-Ascoli theorem [DS58, IV.6.7] implies that \( \Pi \) is in fact compact. Finally, it is clear that \( \rho \mapsto \rho(0) \), \( \rho \mapsto \int_{[-1,1]} \rho(x)f(x)dx \) and \( \rho \mapsto \int_{[-1,1]} \rho(x)f^2(x)dx \) are all continuous on \( \Pi \) for any \( f \in C[-1,1] \).

So all assumptions A1-A4 of the theorem are satisfied and the minimax quadratic risk is determined within absolute constant factors by \( \delta_{\chi^2}(\frac{1}{\sqrt{n}})^2 \). It is well-known that the modulus continuity here satisfies the following (a proof is given in Appendix B for completeness):

**Lemma 7.** There exist constants \( c_0, c_1 \) depending on \( \beta \) and \( L \), such that for all \( t > 0 \),

\[
c_0 t^{\frac{2\beta}{\beta+\tau}} \leq \delta_{\chi^2}(t) \leq c_1 t^{\frac{2\beta}{\beta+\tau}}.
\]

Applying Theorem 2, we recover the classical result:

\[
\inf_{T} \sup_{f \in \mathcal{P}(\beta, L)} \mathbb{E}_{X_1, \ldots, X_n \sim f} \left| T(X_1, \ldots, X_n) - f(0) \right|^2 \asymp_{\beta, L} \frac{1}{n^{\frac{2\beta}{\beta+\tau}}}.
\]

Further, Theorem 2 ensures that empirical-mean estimators of the form \( \hat{T} = \frac{1}{n} \sum_{i=1}^{n} g(X_i) \) are rate optimal for some appropriately chosen function \( g \). Indeed, kernel density estimates are of this form, which achieve the minimax rate for suitably chosen kernel and bandwidth (cf. e.g. [Tsy09, Section 1.2]).

2.5 Comparison to Donoho-Liu [DL91]

Theorem 2 is very similar to a celebrated result of Donoho-Liu [DL91], who showed that in the same setting, as \( n \to \infty \), one has

\[
C_0 \delta_{H^2}(\frac{1}{\sqrt{n}})^2 \leq R^*(n) \leq C_1 \delta_{H^2}(\frac{1}{\sqrt{n}})^2;
\]

for some constants \( C_0, C_1 \), i.e. that the minimax rate for estimating the linear functionals \( T \) coincides with *modulus of continuity* of \( T \) with respect to Hellinger distance. In view of (13), \( \delta_{H^2} \asymp \delta_{\chi^2} \) and thus (40) seems like exactly what Theorem 2 claims.
What is different are two things. Firstly, the technical assumptions required in [DL91] are: A1, A2 (from Theorem 2), boundedness sup π∈Π |T(π)| < ∞ and Hölderianity of δ_{H2}:

\[ \delta_{H2}(t) = Ct^r + o(t^r) \]

for some \( C, r > 0 \) as \( t \to 0 \). Barring the latter, the assumptions are weaker than in Theorem 2.

The second, and crucial, difference is the fact that (40) only holds for a fixed statistical problem \((\Theta, X, P, T, \Pi)\) and as \( n \to \infty \), i.e. the proportionality constants in (40) are not uniform and can be problem dependent. This precludes one to analyze questions where the problem size (e.g. dimension) varies with the sample size \( n \), etc. For example, in the population recovery problem considered in Section 2.3 for any fixed \( d \) and \( n \to \infty \) we get parametric rate \( R^*(n) \asymp \frac{1}{n} \). To get interesting phase-transitions one needs to let \( d \) slowly grow – and this cannot be handled in the setup of [DL91] where the problem is first fixed and then analyzed in the large-sample asymptotics of \( n \to \infty \).

The third difference is the method of proof. While we (indirectly, via duality) show the existence of a good linear estimator, Donoho and Liu construct an estimator via binary search, which entails decomposing the problem into a dyadic sequence of hypothesis testing problems between two composite hypotheses of the form \( \{ \pi : T(\pi) < a \} \) vs \( \{ \pi : T(\pi) > b \} \). The advantage of their method is that it can handle loss functions other than the quadratic loss. The advantage of our method is that our estimator is simply an empirical average of a certain function, that, in discrete cases, can be efficiently pre-computed by convex or linear programming. Furthermore, even for continuous models, the infinite-dimensional LP can be effectively “finite-dimensionalized” leading to computational efficient construction of optimal estimators (see Theorems 9 and 10 for examples).

Overall, the advantage of our method is getting explicit universal constants comparing \( R^*(n) \) and \( \delta_{\chi^2}(\frac{1}{\sqrt{n}}) \). Another advantage is that our method also extends (as we show next) to problems of estimating symmetric functionals of high-dimensional parameters.

### 3 Extension 1: High-dimensional functional estimation

In this section we consider the following setting: A \( d \)-dimensional parameter \( \theta = (\theta_1, \ldots, \theta_d) \in \Theta_c \) is given. The constraint set \( \Theta_c \) is defined as

\[ \Theta_c = \left\{ \theta \in \Theta^\otimes d : \frac{1}{d} \sum_{i=1}^{d} c(\theta_i) \leq 1 \right\}, \]

for some cost function \( c : \Theta \to \mathbb{R} \). Let \( P : \Theta \to \mathcal{X} \) be a transition kernel. Given the data \( X = (X_1, \ldots, X_d) \), where \( X_i \sim P_{\theta_i} \) independently, the goal is to estimate a separable functional \( T_d(\theta) \):

\[ T_d(\theta) = \frac{1}{d} \sum_{i=1}^{d} T(\theta_i), \]

where \( T : \Theta \to \mathbb{R} \). The minimax quadratic risk is defined as

\[ R^*(d) = \inf_{\hat{T}} \sup_{\theta \in \Theta_c} \mathbb{E}[|\hat{T}(X) - T_d(\theta)|^2] \]

where the infimum is taken over all measurable function \( \hat{T} : \mathcal{X}^d \to \mathbb{R} \).

Many problems studied in the high-dimensional functional estimation literature are of the above type. For example, in the Gaussian model where \( X_i \sim N(\theta_i, 1) \), estimation of linear \((T(\theta) = \theta)\) and quadratic functional \((T(\theta) = \theta^2)\) has been well-studied and more recently under sparsity
assumptions which correspond to adding further constraints with \( c(\theta) = 1_{\{|\theta|>0\}} \) or \( c(\theta) = |\theta|^q \) [CCTV16,CCT17]. Estimation of non-smooth functional such as the \( \ell_1 \)-norm \( (T(\theta) = |\theta|) \) has been studied by Cai-Low [CL11].

We define the following convex set of probability distributions

\[
\Pi = \{ \pi \in \mathcal{P}(\Theta) : \mathbb{E}_\pi[c(\theta)] \leq 1 \}.
\]

We will slightly abuse notation and extend \( T(\theta) \) to \( T(\pi) \) for \( \pi \in \Pi \) by linearity:

\[
T(\pi) = \int_\Theta T(\theta) \pi(d\theta).
\]

Our technical assumptions below will imply this integral indeed exists. Finally, with \( \Pi \) and \( T : \Pi \to \mathbb{R} \) defined, we also define \( \delta_{\chi^2}(\cdot) \) via (7).

The main idea of this section is that the stated minimax problem is very similar to a problem where, instead of adversarially selected vector \( \theta \), one generates each coordinate \( \theta_i \) independently from for some prior \( \pi \in \Pi \), and instead of \( T_\theta(\theta) \) one estimates \( \mathbb{E}[T_\theta(\theta)] = T(\pi) \), which is a linear functional of \( \pi \). The latter problem falls into the purview of Section 2 and hence its minimax rate is given by \( \delta_{\chi^2}(\frac{1}{\sqrt{d}}) \). Thus, it seems natural to expect that

\[
R^*(d) \asymp \delta_{\chi^2}(\frac{1}{\sqrt{d}}) \tag{42}
\]

up to universal constants. Alas, such statement is not true without conditions, as the next example demonstrates. However, the good news is that such counterexamples only occur in the “uninteresting” case of \( R^*(d) = 0 \) or \( R^*(d) \asymp \frac{1}{\sqrt{d}} \) (parametric rate).

**Example 1.** Let \( \Theta = \mathcal{X} = \{0,1\} \), \( c(\theta) = 0 \), \( T(\theta) = \theta \) and consider the observation model \( \mathbb{P}[X = \theta] = 1 - \mathbb{P}[X = 1 - \theta] = \tau \) (the binary symmetric channel). From (13) and (14) we obtain that for any \( \tau \geq 0 \) (including \( \tau = 0 \)): \( \delta_{\chi^2}(t) \geq \frac{\tau}{4} \). At the same time, a simple unbiased estimator \( \hat{T}(X_1, \ldots, X_d) = \frac{1}{d(1-2\tau)} \sum_{i=1}^d 1\{X_i = 1\} - \tau \) achieves

\[
R^*(d) \leq \frac{\sqrt{\tau(1-\tau)}}{|1-2\tau|} \frac{1}{\sqrt{d}}.
\]

One immediate conclusion is that at \( \tau = 0 \) we have \( R^*(d) = 0 \) while \( \delta_{\chi^2}(t) > 0 \) for all \( t > 0 \). Furthermore, even when \( \tau > 0 \) and \( R^*(d) \asymp \delta_{\chi^2}(1/\sqrt{d}) \asymp \frac{1}{\sqrt{d}} \), the proportionality constant in the first relation blows up. In other words, \( \lim_{\tau \to 0} \frac{R^*(d)}{\delta_{\chi^2}(1/\sqrt{d})} = 0 \) and we cannot expect the relation (42) to hold universally.

**Remark 1** (Parametric lower bound). Consider the high-dimensional setting where the constraint function \( c \) and the functional \( T \) are both fixed and the dimension \( d \) grows. There is a general dichotomy: either risk \( R^*(d) = 0 \) or \( R^*(d) = \Omega(\frac{1}{\sqrt{d}}) \). Indeed, either there exists a pair \( \theta_a, \theta_b \in \Theta \) s.t. \( T(\theta_a) \neq T(\theta_b) \) and \( \text{TV}(P_{\theta_a}, P_{\theta_b}) < 1 \), or there is no such pair. In the latter case, we have \( T(\theta) = g(X_1) \) (i.e. \( T(\theta) \) is a deterministic function of a single sample), and thus \( R^*(d) = 0 \) for any \( d \geq 1 \). In the former case, we can lower bound \( R^*(d) \) by the Bayes risk when \( \theta \) has iid components with \( \mathbb{P}[\theta_i = \theta_a] = \mathbb{P}[\theta_i = \theta_b] = \frac{1}{2} \). Clearly, the corresponding Bayesian risk is \( \Omega(1/\sqrt{d}) \).

---

7 This prior needs to be modified if \( c(\theta_a) > 1 \) or \( c(\theta_b) > 1 \). Specifically, choose an arbitrary \( \theta_0 \) such that \( c(\theta_0) < 1 \). Then we can choose \( \theta \) iid from \( \pi = (1-\epsilon)\delta_{\theta_0} + \frac{\epsilon}{2}(\delta_{\theta_a} + \delta_{\theta_b}) \) for sufficiently small constant \( \epsilon \).
The main result of this section is (see Section 5.1 for a proof):

**Theorem 8.** Suppose that \((\Theta, \mathcal{X}, P, T = T(\pi), \Pi)\) satisfy conditions A1-A4 of Theorem 2. Then

\[
R^*(d) \leq \delta_{\chi^2} \left( \frac{1}{\sqrt{d}} \right).
\]

Furthermore, if the following extra conditions are satisfied

A5 \(K_V = \sup_{\pi \in \Pi} \text{Var}_{\theta \sim \pi}[T(\theta)] \leq \infty\)

A6 Cost function \(c \geq 0\) and there exists \(\theta_0 \in \Theta\) with \(c(\theta_0) = 0\)

Then

\[
R^*(d) \geq \frac{1}{62} \delta_{\chi^2} \left( \frac{1}{\sqrt{d}} \right) - \sqrt{\frac{K_V}{4d}}.
\]

**Remark 2.** Before considering new applications in discrete high-dimensional problems, as a quick application, consider the problem of estimating the \(\ell_1\)-norm of a vector in the Gaussian location model \([CL11]\), where \(X_i \sim N(\theta_i, 1)\), \(T(\theta) = |\theta|\) and \(T(\theta) = \|\theta\|_1\), and \(\theta \in \Theta = [-1, 1]^d\). Using the method of polynomial approximation and moment matching, it was shown in \([CL11]\) that \(R^*(d) = \Theta((\log \log \frac{1}{\delta}))^2\) (in fact, the sharp constant as \(d \to \infty\) was also found). To see how this result follows from Theorem 8, note that \(K_V = 1\), we have

\[
\delta_{\chi^2}(t) = \sup \left\{ \int |\theta| \pi'(d\theta) - \int |\theta| \pi''(d\theta) : \chi^2(\pi' * N(0, 1)) \leq t^2 \right\}.
\]

Here \(*\) denotes convolution, and the supremum is take over \(\pi, \pi' \in \mathcal{P}([-1, 1])\). The speed of convergence of \(\delta_{\chi^2}(t)\) when \(t \to 0\) is extremely slow and thus its behavior governs the minimax rate. Indeed, one can show that (see Appendix B)

\[
\delta_{\chi^2}(t) = \Theta \left( \frac{\log \log \frac{1}{t}}{\log \frac{1}{t}} \right),
\]

recovering the result of \([CL11]\).

However, if the parameter space is unbounded with \(\Theta = \mathbb{R}^d\) we have \(K_V = \infty\) and lower bound in Theorem 8 is not applicable. Nevertheless, applying a truncation argument, it was shown in \([CL11]\) that \(R^*(d) \asymp \frac{1}{\log d}\).

### 3.1 Application: Distinct Elements problem

The distinct element problem refers to the following question: Given \(n\) balls randomly drawn from an urn containing \(d\) colored balls, how to estimate the total number \(N\) of distinct colors in the urn? This problem has been investigated in a sequence of work \([CCMN00, RRSS09, Val11, Val12, WY18]\) in both the theoretical computer science and the statistics community; see \([WY18, Table 1]\) for a summary of the state of the art. These results typically aim at the sublinear regime, where the number of samples satisfies \(n = o(d)\). In particular, it is known that the optimal sample complexity for (normalized) consistent estimate is \(\Theta(\frac{d}{\log d})\). For the linear regime, say, 1% of the balls are observed, existing results do not yield tight characterization of the optimal estimation accuracy. In this section, we will apply the general Theorem 8 to determine the minimax risk up to logarithmic.
factors in the linear regime, and reveal an elbow effect in the optimal rate of convergence that precisely occurs at sampling ratio $\frac{1}{2}$.

Specifically, let us consider the following version of the distinct elements problem, where the number of balls in the urn is at most $d$ and unknown a priori. Without loss of generality, assume that the number of colors in the universe (not necessarily in the urn) is $d$, and indexed then by $\{d\} = \{1, \ldots, d\}$. Let $\theta_i \in \mathbb{Z}_+$ be the number of balls of the $i$th color, $i = 1, \ldots, d$. Thus, the parameter $\theta = (\theta_1, \ldots, \theta_d)$ is constrained to belong to the set

$$\Theta_c = \left\{ \theta \in \mathbb{Z}^d_+ : \frac{1}{d} \sum_{i=1}^d \theta_i \leq 1 \right\}.$$  

We shall work with the Bernoulli sampling model with sampling ratio $p$, where the color of each ball is observed independently with probability $p$. To conform to the notations in the previous section, instead of estimating the number of distinct colors $N \triangleq \sum_{i=1}^d 1\{\theta_i \geq 1\}$, we estimate a normalized quantity

$$T_d(\theta) \triangleq \frac{1}{d} \sum_{i=1}^d 1\{\theta_i \geq 1\}.$$  

The minimax quadratic risk $R^*(d)$ is defined as in (41).

The following theorem (proved in Section 5.2) determines the sharp minimax risk up to logarithmic factors in the linear sampling regime ($p$ being a constant). Note that the upper bound is explicit and non-asymptotic, which allows us to recover the prior result on the optimal sampling complexity $\Omega(d \log d)$, i.e. $p = \Omega\left(\frac{1}{\log d}\right)$, for consistent estimation.

**Theorem 9.** Fix $p \in (0, 1)$. There exists a constant $c = c(p) > 0$ such that

- if $p \geq \frac{1}{2}$, then

$$R^*(d) \leq \frac{1}{d} \quad \text{(47)}$$

- if $p < \frac{1}{2}$, then

$$c(d \log d)^{-\frac{p}{1-p}} \leq R^*(d) \leq d^{-\frac{p}{1-p}}, \quad \text{(48)}$$

where the upper bound holds for all $d$ and the the lower bound holds for all $d \geq d_0 = d_0(p)$. Furthermore, an estimator achieving the upper bound can be constructed in time $O(d^a)$ for some absolute constant $a$.

**Remark 3** (Linear estimator). One particular consequence of Theorem 8 is that it shows the optimality of the following empirical-mean estimator:

$$\hat{T} = \sum_{i \in [d]} g(N_i),$$

where $N_i$ is the observed number of balls of the $i$th color. Such estimators are commonly known as linear estimators, since it can be equivalently expressed as linear combinations of profiles (also known as fingerprints) [OSW16, VV11]:

$$\hat{T} = \sum_{j \geq 0} g(j) \Phi_j,$$
called the \( j \)th profile, denotes the number of colors that occurred exactly \( j \) times in the sample.

In practice, it is desirable to have \( g(0) = 0 \), in which case the estimator is fully data-driven and adaptive to the total number of possible colors. Next we show that this additional constraint can be fulfilled without sacrificing the minimax rate. Recall the definition of \( \delta_a \) in (24), which gives the best bias-variance tradeoff among linear estimators. In view of Proposition 3, we have the universal relation (thanks to duality) \( \delta_a(t) \leq \delta_X(t) \). In view of (78), dropping the variance term, we conclude that there exists \( g : \mathbb{Z}_+ \rightarrow \mathbb{R} \), such that \( \sup_{\theta \in \mathbb{Z}} [E_{N \sim \text{Binom}(\theta, p)}[g(N)] - T(\theta)] \leq d^{-\frac{1}{2}} \min(1, \frac{p}{1-p}) \), where \( T(\theta) = 1_{\{\theta \geq 1\}} \). Particularizing to \( \theta = 0 \), we have \( |g(0)| \leq d^{-\frac{1}{2}} \min(1, \frac{p}{1-p}) \). This shows that the modified estimator \( \tilde{g} \) given by \( \tilde{g}(0) = 0 \) and \( \tilde{g}(j) = g(j) \) for all \( j \geq 1 \) continues to achieve the optimal rate in Theorem 9.

### 3.2 Application: Fisher’s species problem

Dating back to Fisher [FCW43], predicting the unseen species is a classical question in statistics, where we observe \( n \) iid samples \( X_1, \ldots, X_n \) drawn from an unknown probability discrete distribution \( P = (p_x) \) on some countable alphabet \( \mathcal{X} \), and the goal is to estimate the number of hitherto unobserved symbols that would be observed if \( m \) new samples \( X'_1, \ldots, X'_m \) were collected, i.e.,

\[
U = U_{n,m} \triangleq |\{X'_1, \ldots, X'_m\} \setminus \{X_1, \ldots, X_n\}|.
\]

In particular, the sequence \( m \mapsto U_{n,m} \) is called the species discovery curve, which provides a guideline on how many new species would be observed were \( m \) more samples to be collected. For this reason, extrapolating the species discovery curve is of significant interest in various fields, such as ecology [FCW43, CL92], computational linguistics [ET76], genomics [ILLL09], etc. Clearly, the more future samples we want to extrapolate, the more difficult it is to obtain a reliable prediction.

To be consistent with the existing literature as well as for the sake of technical simplicity, we consider the Poissonized version of the problem, where the number of available samples and future unobserved samples is \( N \sim \text{Poi}(n) \) and \( M \sim \text{Poi}(m) \). Denote the histogram in the observed and unobserved samples by \( N_x = \sum_{i \in [N]} 1_{\{X_i = x\}} \) and \( N'_x = \sum_{i \in [M]} 1_{\{X'_i = x\}} \), respectively. Then \( \{N_x\}_{x} \sim \text{Poi}(np_x) \) and \( \{N'_x\}_{x} \sim \text{Poi}(mp_x) \) are independent of each. In terms of histograms, the number of unseen species can be expressed as

\[
U = \sum_{x} 1_{\{N_x = 0, N'_x > 0\}}.
\]  

Let \( r \triangleq \frac{m}{n} \) denote the extrapolation ratio. Denote the normalized minimax mean squared error of estimating \( U \) by

\[
\mathcal{E}_n(r) \triangleq \inf_{\hat{U}} \sup_{P} \frac{1}{m^2} \mathbb{E}_P[(\hat{U} - U)^2],
\]

where the expectation is with respect to both the original and the future samples. We emphasize that this problem is fully non-parametric and no assumptions are imposed on the distribution \( P \).

It is known since Good and Toulmin [GT56] that an unbiased estimator for \( U \) is

\[
\hat{U}_{GT} = -\sum_{x} (-1)^{N_x} 1_{\{N_x > 0\}} = \sum_{j \geq 1} (-r)^j \Phi_j,
\]

where

\[
\Phi_j \triangleq \sum_{i} 1_{\{N_i = j\}},
\]  

(49)
where $\Phi_j$ is the $j$th profile defined in (49). If $r \leq 1$, that is, we extrapolate no more than what have been observed, this unbiased estimator achieves the (optimal) parametric rate
\[
\frac{1}{m^2} \mathbb{E}[(U - \hat{U}_{GT})^2] \lesssim \frac{1}{n}.
\] (51)

However, for $r > 1$, the variance of $\hat{U}$ is unbounded due to the exponential growth of the coefficients. Based on a technique called smoothing that modifies the unbiased estimator to obtain a good bias-variance tradeoff, Orlitsky et al [OSW16] constructed a family of estimators that encompass previous heuristics of Efron and Thisted [ET76] and provably achieve the following prediction risk:
\[
\mathcal{E}_n(r) \lesssim n^{-\log_3(1 + \frac{2}{r})}.
\] (52)

Conversely, the following lower bound is also shown in [OSW16]:
\[
\mathcal{E}_n(r) \gtrsim n^{-C/r}.
\]
for some absolute constant $C$. Thus, it is possible to extrapolate with a vanishing risk provided that $r = o(\log n)$, and this condition is the best possible. However, for fixed $r$, the optimal rate remains open. In particular, the above achievable results (51) and (52) seem to suggest an “elbow effect” in the optimal convergence rate, which transitions from parametric rate to nonparametric rate when the extrapolation ratio $r$ exceeds 1. The following result resolves this question in the positive:

**Theorem 10** (Optimal rate for predicting the unseen). Let $r > 0$ be a constant. There exist constants $c_0, c_1$ that depend only on $r$, such that the following holds.

- If $r \leq 1$, then
  \[ \frac{c_0}{n} \leq \mathcal{E}_n(r) \leq \frac{c_1}{n}; \] (53)

- If $r > 1$, then
  \[ \frac{c_0 n^{-\frac{2}{r+1}}}{\log^2 n} \leq \mathcal{E}_n(r) \leq c_1 n^{-\frac{2}{r+1}} \log^2 n. \] (54)

Furthermore, an estimator achieving the upper bound can be constructed in time $O(n^a)$ for some absolute constant $a$.

It is worth mentioning that, unlike Theorem 9, Theorem 10 does not directly follow from the general result in Theorem 8 for high-dimensional problems because of the infinite-dimensional nature of the species problem (the number of distinct species is potentially unbounded), which requires extra reduction argument. Furthermore, analyzing the behavior of the modulus of continuity (as a linear program) relies on delicate complex analysis, in particular, Hadamard’s three-lines theorem and the Paley-Wiener theorem. The proof of Theorem 10 is provided in Section 5.3.

**Remark 4** (Species versus distinct elements problem). There is an obvious connection between the species problem considered here and the distinct elements problem considered in Section 3.1: Treating the union of observed and unobserved samples $\{X_1, \ldots, X_n, X_1', \ldots, X_m'\}$ as the content of an urn, the former can be viewed as a special case of the latter with the urn size being $d = n + m$ and the fraction of observation being $p = \frac{n}{m+n} = \frac{1}{1+r}$. Thus, for the interesting case of $r > 1$, applying Theorem 9 yields the upper bound $\mathcal{E}_n(r) \leq O(n^{-\frac{1}{2}})$. Perhaps surprisingly, this strategy turns out to be suboptimal in view of Theorem 10. This suggests that the optimal estimator for the species problem is able to exploit the special structure in the color configuration arising from iid sampling.
4 Extension 2: Exponential families

4.1 Motivating example: nonparametric estimation of linear functionals in Gaussian noise

Here we show how ideas similar to that behind Theorem 2 can be used in a completely different problem. Namely, we re-derive the classical result of Ibragimov and Has’minskii [IH84] on the rate optimality (within constant factors) of affine estimators in the following problem. Consider the classical Gaussian white noise model:

$$dX_t = f(t)dt + \sigma dB_t, \quad t \in [0,1],$$

where the unknown function $f$ belong to some convex subset of density $F$. Given $X = \{X_t : t \in [0,1]\}$, the goal is to estimate some affine functional $T(f)$ (such as $T(f) = f(1/2)$). Define the minimax risk as

$$R^*(\sigma) \triangleq \sup_{f \in F} \inf_{\hat{T}} \mathbb{E}_{X \sim P_f} [(\hat{T}(X) - T(f))^2].$$

This is a special case of the $n$-sample setup in (1) with $\sigma = \frac{1}{\sqrt{n}}$. Consider a linear estimator

$$\hat{T} = \int_0^1 g(t)dX_t,$$

parameterized by some continuous compactly-supported function $g \in C^c$ to be optimized. Then the bias and variance are given respectively by

$$\mathbb{E}\hat{T} - T = \langle f, g \rangle - T(f)$$

$$\text{Var}(\hat{T}) = \sigma^2 \|g\|_2^2.$$

To bound the bias, note that, trivially,

$$\inf_{f \in F} \langle f, g \rangle - T(f) \leq \mathbb{E}\hat{T} - T \leq \sup_{f \in F} \langle f, g \rangle - T(f).$$

Without loss of generality, we can assume that $\sup_{f \in F} \langle f, g \rangle - T(f) \geq 0 \geq \inf_{f \in F} \langle f, g \rangle - T(f).$\(^8\) Therefore, we have

$$|\mathbb{E}\hat{T} - T| \leq \sup_{f \in F} \langle f, g \rangle - T(f) + \sup_{f \in F} T(f) - \langle f, g \rangle = \sup_{f,f' \in F} \langle f - f', g \rangle + T(f') - T(f).$$

Optimizing the bias-variance tradeoff over $g$ leads to the following convex optimization problem:

$$\sqrt{R^*(\sigma)} \leq \inf_{g \in C^c} \sup_{f,f' \in F} \langle f - f', g \rangle + T(f') - T(f) + \sigma \|g\|_2$$

$$= \inf_{g \in C^c} \sup_{f,f' \in F, \|z\|_2 \leq 1} \langle f - f', g \rangle + T(f') - T(f) + \sigma \langle g, z \rangle$$

$$\overset{(a)}{=} \sup_{f,f' \in F, \|z\|_2 \leq 1} \left\{ T(f') - T(f) + \inf_{g \in C^c} \langle f - f' + \sigma z, g \rangle \right\}$$

$$\overset{(b)}{=} \sup_{f,f' \in F, \|f - f'\|_2 \leq \sigma} T(f') - T(f)$$

$$\overset{(c)}{=} C \sqrt{R^*(\sigma)},$$

\(^8\)Suppose $\sup_{f \in F} \langle f, g - h \rangle = \epsilon < 0$, i.e., the estimator is always negatively biased, then replacing $g$ by $g - \epsilon$ improves the bias and retains the same variance.
where (a) follows from the minimax theorem (see, e.g., Theorem 4 in Section 2.2); (b) is simply because 
\[ \inf_{g \in C} \langle f, g \rangle = -\infty \text{ if } f \neq 0 \text{ and } 0 \text{ if } f = 0; \] 
fina lly, (c) follows from Le Cam’s two-point lower bound since the KL divergence in the white noise model is given by
\[ D(P_f || P_{f'}) = \frac{1}{2\sigma^2} \| f - f' \|_2^2, \] 
(55)
where \( P_f \) denotes the law of \( \{ X_t : t \in [0, 1] \} \) under \( f \), and \( C \) is an absolute constant. Thus we have shown that
\[ \frac{\omega(\sigma)}{C} \leq \sqrt{R^*(\sigma)} \leq \omega(\sigma). \] 
(56)
where
\[ \omega(\sigma) \triangleq \sup_{f, f' \in \mathcal{F}} \{ T(f') - T(f) : \| f - f' \|_2 \leq \sigma \}, \]
is the modulus of continuity.

The characterization (56) is the main result of [IH84] (in the refined version presented in [Don94]). Various proofs of (56) are available (although not exactly as simple as the above). First, [IH84] already used the minimax theorem to relate the performance of the best linear estimator to the modulus of continuity; however, they did not appear to make the observation that the interchanged form \( \sup_\pi \inf_{\hat{T}} \) corresponds to optimizing the two-point Le Cam lower-bound (instead they proceeded by deriving a lower bound via reduction to the worst-case one-dimensional subproblem: \( \mathcal{F}_1 = \{ \theta f_0 + (1 - \theta) f_1 : \theta \in [0, 1] \} \)). Generalizations followed in [Don94], where the minimax theorem was replaced by the fact (equivalent to minimax duality) that the worst-case risk for linear estimators is attained on the worst one-dimensional subproblem. Additionally, [Don94] showed similar results for the absolute loss and the confidence-interval (\( \epsilon \)-quantile) loss. In an attempt to generalize these results from Gaussian models to general exponential families, [JN09] returned to the use of the minimax duality and this time did connect the dual form with the Hellinger version of the two-point Le Cam method; however, [JN09] only studied the \( \epsilon \)-quantile loss.

In the next section we will provide a counterpart to results of [JN09] for square-loss and exponential families satisfying certain conditions. We note that our conditions are strictly weaker (i.e. the class of exponential families is strictly larger) than those of [JN09] – see Section 4.3 for comparison.

4.2 Estimating linear functionals of the mean parameter

Here we prove a simultaneous generalization of Theorem 2 and (56). To keep this section simple, we only consider the finite-dimensional setting.

A \( d \)-dimensional exponential family \( \{ P_\gamma \}_{\gamma \in \Gamma} \) of probability distributions on a measurable space \( \Omega \) is given by \( (\nu, X, \Gamma) \), where \( \nu \) is a measure on \( \Omega \), \( X : \Omega \to \mathbb{R}^d \) is a measurable map, \( \Gamma \subset \mathbb{R}^d \) and
\[ P_\gamma(d\omega) = \exp\{ \langle \gamma, X \rangle - C(\gamma) \} d\nu, \]
with \( \gamma \in \mathbb{R}^d \) called the natural parameter. Let \( X(\omega) = (\phi_{b,1}(\omega), \ldots, \phi_{b,d}(\omega)) \) and let \( \mathcal{F} \) be the finite-dimensional linear space spanned by basis functions \( \phi_{b,i} \), i.e., \( \langle h, X \rangle \) for \( h \in \mathbb{R}^d \). We make two standing assumptions on the exponential family:

1. The set \( \Gamma \) is open and convex; \( C(\gamma) < \infty \) for all \( \gamma \in \Gamma \).

\[ \text{Note that the second assumption is without loss of generality: if there is a linear relation between coordinates of } X, \text{ then by reducing the dimension } d \text{ we eventually will make the second assumption hold.} \]
2. For some $\gamma_0 \in \Gamma$ (and hence for all $\gamma$ by absolute continuity $P_\gamma \ll P_{\gamma_0}$), the functions $\phi_{b,1}, \ldots, \phi_{b,d}$ are linearly independent, i.e.

$$\operatorname{Var}_{P_{\gamma_0}} \langle X, h \rangle > 0 \quad \forall h \in \mathbb{R}^d \setminus \{0\}. \quad (57)$$

In addition to the natural parameter $\gamma$, we define the mean parameter $\mu$ via the forward map

$$\mu_f(\gamma) \triangleq \mathbb{E}_{P_\gamma}[X].$$

It is well known (see e.g. [Bro86]) that inside $\Gamma$ the function $\gamma \mapsto C(\gamma)$ is infinitely differentiable, whose first two derivatives give the mean and covariance of $X$:

$$\mu_f(\gamma) = \nabla C(\gamma), \quad \frac{\partial \mu_f}{\partial \gamma} = \text{Hess} C(\gamma) = \text{Cov}_{P_\gamma}[X] \triangleq \Sigma(\gamma). \quad (58)$$

The non-degeneracy assumption (57) implies

$$\Sigma(\gamma) \succ 0 \quad \forall \gamma \in \Gamma. \quad (59)$$

Since $C(\gamma)$ is, thus, strictly convex on $\Gamma$, the map $\gamma \mapsto \mu_f = \nabla C(\gamma)$ is one-to-one. Since the Jacobian of this map is non-zero everywhere on $\Gamma$, by the inverse function theorem the image $M \triangleq \mu_f(\Gamma)$ is an open set in $\mathbb{R}^d$ and, furthermore, there is an infinitely-differentiable inverse map $\gamma_r$ such that

$$\mu_f(\gamma_r(\mu)) = \mu \quad \forall \mu \in M.$$  

It is also known that Jacobian of $\gamma_r$ can be computed as

$$\frac{\partial \gamma_r(\mu)}{\partial \mu} = \Sigma^{-1}(\gamma_r(\mu)). \quad (60)$$

For convenience we denote $\tilde{P}_\mu = P_{\gamma_r(\mu)}$ and $\tilde{\Sigma}(\mu) = \Sigma(\gamma_r(\mu))$.

For a given constraint set $\Gamma_0 \subset \Gamma$ and a functional $T(\gamma)$, we define the minimax square-loss as usual

$$R^*_n(\Gamma_0) = \inf_{T} \sup_{\gamma \in \Gamma_0} \mathbb{E}_\gamma[|\hat{T}(X_1, \ldots, X_n) - T(\gamma)|^2], \quad (61)$$

where $\mathbb{E}_\gamma$ is with respect to $X_1, \ldots, X_n \overset{i.i.d.}{\sim} P_\gamma$.

The main finding in this section is that for estimating linear functionals of the mean parameter $\mu$, under certain convexity assumptions (that are strictly weaker than those in [JN09]), the minimax quadratic risk is characterized by certain moduli of continuity within universal constant factors. To this end, let $\omega_J$ and $\omega_H$ denote the modulus of continuity of $T$ on $M_0$ with respect to Jeffrey’s divergence and the Hellinger distance respectively:

$$\omega_J(t) \triangleq \sup_{\gamma, \gamma' \in \Gamma_0} \{T(\gamma) - T(\gamma') : d_J(P_\gamma, P_{\gamma'}) \leq t^2\}, \quad (62)$$

$$\omega_H(t) \triangleq \sup_{\gamma, \gamma' \in \Gamma_0} \{T(\gamma) - T(\gamma') : H(P_\gamma, P_{\gamma'}) \leq t\}, \quad (63)$$

where

$$d_J(P, Q) \triangleq D(P \parallel Q) + D(Q \parallel P) = \int dP \log \frac{dP}{dQ} + dQ \log \frac{dQ}{dP}$$

denotes Jeffrey’s divergence. We next define another divergence-like quantity:

$$d(P_{\gamma'} \parallel P_\gamma) \triangleq \sup_{\phi \in \mathcal{F}} \{\mathbb{E}_{P_\gamma}[\phi] - \mathbb{E}_{P_{\gamma'}}[\phi] : \operatorname{Var}_{P_\gamma}[\phi] \leq 1\}. \quad (64)$$
This quantity describes the dissimilarity between distributions $P_{\phi'}$ and $P_{\phi}$ in terms of the expectations of unit-variance functions in $\mathcal{F}$;\footnote{Note that without the restriction \( \phi \in \mathcal{F} \), the supremum coincides with \( \chi(P_{\phi'}\|P_{\phi}) \); see (32).} an explicit expression for $d$ is given in (133) below. The modulus of continuity of $T$ with respect to $d$ will also play a role:

\[
\delta_n(t) \triangleq \sup_{\gamma, \gamma' \in \Gamma_0} \{ T(\gamma) - T(\gamma') : d(P_{\phi'}, P_{\phi}) \leq t \}
\]

Our main result for exponential families is as follows (see Section 5.4 for a proof).

**Theorem 11.** There exist absolute constants $c_0 > 0$ and $c_1 > 0$ with the following property. Consider a subfamily of an exponential family corresponding to mean parameters $\mu \in M_0 \subset M$, where $M_0$ is a compact convex subset of $\mathbb{R}^d$. Assume that the subfamily $M_0$ satisfies the key condition

\[
\mu \mapsto \sqrt{\text{Var}_{P_{\phi}}(\phi)} \text{ is concave in } \mu \in M_0 \text{ for all } \phi \in \mathcal{F}.
\]

Let the functional $T(\gamma)$ be linear in the mean parameter, i.e.,

\[
T(\gamma) = \langle g, \mu_f(\gamma) \rangle
\]

for some $g \in \mathbb{R}^d$, and define the constraint set $\Gamma_0 = \mu_f(M_0)$. Then we have

\[
c_1 \delta_n(1/\sqrt{n}) \leq \omega_f(c_0/\sqrt{n}) \leq \sqrt{R^*_n(\Gamma_0)} \leq \delta_n(1/\sqrt{n}).
\]

A direct consequence of Theorem 11 is the following characterization of minimax rates in terms of the moduli of continuity based on Hellinger distance or Jefferey’s divergence (which turn out to be equivalent); see Appendix B for a proof.

**Corollary 12.** In the setting of Theorem 11 we have (within absolute constants):

\[
R^*_n(\Gamma_0) \asymp \omega_f^2(1/\sqrt{n}) \times \omega_H^2(1/\sqrt{n})
\]

**Remark 5.** Note that in the setting of the preceding Theorem 11, we have

\[
T(\gamma) = \mathbb{E}_{P_{\phi}}[\phi(\omega)],
\]

for some $\phi_0 \in \mathcal{F}$. Thus, it may appear that the best estimator should simply be the empirical mean of $\phi_0$, namely, $\hat{T} = \frac{1}{n} \sum_{i=1}^{n} \phi_0(\omega_i)$, which is unbiased by design. However, the catch is that $\text{Var}_{P_{\phi}}(\phi_0)$ might be too big to be optimal (such as in population recovery in Section 2.3). The main discovery here is that the concavity condition (64) guarantees the existence of some other $\phi' \in \mathcal{F}$ such that the empirical average of $\phi'$ is minimax rate-optimal.

**Example 2** (Exponential distribution). Here is an example application, which (as explained in the forthcoming Section 4.3) is outside the scope of [JN09]. For $\gamma > 0$, let $\exp(\gamma)$ denote the exponential distribution with density $\gamma e^{-\gamma x}1_{\{x > 0\}}$. Let $X$ have $d$ independent components $(X)_i \sim \exp(\gamma_i)$, $i = 1, \ldots, d$. The mean parameters are $\mu = (\gamma_1^{-1}, \ldots, \gamma_d^{-1})$. Our goal is to estimate $\sum_{i=1}^{d} \mu_i$ over the $\ell_p$-ball in $\mathbb{R}^d$: $M_0 = \{ \mu : \sum_{i=1}^{d} \mu_i^p \leq 1 \}$, where $p \geq 1$. A simple calculation shows

\[
\frac{1}{2} \left( \frac{1}{p} \right) \max(\frac{1}{2}, \frac{1}{p}) \leq \omega_f(t) \leq \frac{1}{2} \max(\frac{1}{2}, \frac{1}{p})
\]

(For $p \leq 2$ the worst pair $(\mu, \mu')$ are scaled spikes (with a single nonzero), whereas for $p > 2$ they are scaled constant vectors.) Together with Theorem 11, this establishes the minimax risk within constant factors. In this simple case the empirical mean, $\hat{T} = \frac{1}{n} \sum_{i=1}^{n} \langle X_t, 1 \rangle$, achieves optimal rate for all $p, d$. 


Remark 6. To shed some light on how assumption (64) relates to the tightness of empirical-mean estimators, we observe that the Fisher information matrix for parameter $\gamma$ is given by $I_F(\gamma) = \Sigma(\gamma)$, while for parameter $\mu$ we get $I_F(\mu) = \tilde{\Sigma}^{-1}(\mu)$. In one dimension $d = 1$, we see that (135) shows that $R_n^*(\mu_0) \leq \frac{1}{n \min I_F[\mu]}$. From the Bayesian Cramér-Rao lower bound (van Trees inequality) [GL95], we expect a similar lower bound to hold, unless $I_F(\mu)$ grows very rapidly around its minimum. The latter situation is prohibited by the assumption (64), as shown by the key inequality (140). Thus, assumption (64) enters our proof in two crucial ways: for the applicability of the minimax theorem and for taming the behavior of Fisher information. Because of the latter, it is unclear whether (64) can be extended from concavity to, say, quasi-concavity.

4.3 Comparison to Juditsky-Nemirovski [JN09]

As opposed to the squared loss (61), Juditsky-Nemirovski [JN09] considered the $\epsilon$-quantile loss and the corresponding minimax risk:

$$R_{n,\epsilon}^* = R_{n,\epsilon}^*(\Gamma_0) = \inf_{T} \inf_{\gamma \in \Gamma_0} \{ r : \sup_{\gamma \in \Gamma_0} P_\gamma[|T(X_1, \ldots, X_n) - T(\theta)| > r] \leq \epsilon \},$$

(68)

The following assumptions are made in [JN09]:

1. The ambient exponential family $(\nu, X, \Gamma)$ can be defined for $\Gamma = \mathbb{R}^d$, i.e. the natural parameters $\gamma$ can range over the entire space $\mathbb{R}^d$.

2. The functional $T(\gamma) = T(A(x))$ is affine in $x$, where $\gamma = A(x)$ is a reparametrization such that the map

$$x \mapsto C(A(x) + a) - C(A(x))$$

is concave for every $a \in \mathbb{R}^d$. (69)

Under these assumptions, it is shown that

$$\frac{1}{2} \omega_H \left( \sqrt{2 \left( 1 - e^{-\frac{1}{n} \log \frac{2}{\epsilon}} \right)} \right) \leq R_{n,\epsilon}^* \leq \frac{1}{2} \omega_H \left( \sqrt{2 \left( 1 - e^{-\frac{1}{n} \log \frac{2}{\epsilon}} \right)} \right);$$

(70)

in particular, whenever $\exp(-o(n)) \leq \epsilon < \frac{1}{5}$, we have

$$R_{n,\epsilon}^*(\Gamma_0) \approx \omega_H(1/\sqrt{n}).$$

(71)

To compare with the quadratic risk characterization in Theorem 11, first of all, in terms of results, since $R_{n,\epsilon}^* \geq \sqrt{R_n^*/\epsilon}$ by the Markov inequality, comparing (67) with (71) shows that under the assumption of [JN09], the modulus of continuity with respect to the Hellinger distance and the Jeffrey’s divergence are equivalent up to constant factors. Next we compare the assumptions of [JN09] with ours. It is not hard to see (see Appendix B for a proof) that (69) is equivalent to assuming that

$$x \mapsto \mu_f(A(x))$$

is affine and $\mu \mapsto \text{Var}_{P_\mu}[\phi]$ is concave in $\mu \in M_0$ for all $\phi \in F$. (72)

This equivalence shows that our condition (64) is strictly weaker than (72). In fact, this weakening allows applications of these results for important exponential families. For example, for the family of exponential distributions considered in Example 2 where $\Omega = \mathbb{R}$, $P_\gamma(dx) = \gamma e^{-\gamma x} dx$, $\gamma > 0$, we have that (64) holds, but (72) fails. In addition, the natural parameter ranges over a subset of $\mathbb{R}^d$, not its entirety. Another example is the normal scale model $\omega \sim \mathcal{N}(0, \sigma^2)$, $\sigma^2 > 0$ with $X = \omega^2$. For this family, again (64) holds but not (72).
5 Additional proofs

5.1 Proof of Theorem 8

Proof. To prove (43), consider estimators of the form (22) and, similarly to (23), let us analyze its risk by decomposing into bias and variance part:

\[
\sqrt{E_\theta[|\hat{T}_g(X) - T_d(\theta)|^2]} \leq \frac{1}{d} \sqrt{\sum_{i=1}^{d} \text{Var}_{P_{\theta_i}}[g]} + \frac{1}{d} \sum_{i=1}^{d} (P_{\theta_i}g - T(\theta_i)) \tag{73}
\]

Denote the empirical distribution \(\hat{\pi}\) associated with \(\theta = (\theta_1, \ldots, \theta_d)\) by \(\hat{\pi} \triangleq \frac{1}{d} \sum_{i=1}^{d} \delta_{\theta_i}\). Upper-bounding \(\sum_{i=1}^{d} \text{Var}_{P_{\theta_i}}[g] \leq d \cdot \text{Var}_{\hat{\pi}}[g]\), we continue (73) to get

\[
\sqrt{R^*(d)} \leq \inf_g \sup_{\hat{\pi}} \frac{1}{\sqrt{d}} \sqrt{\text{Var}_{\hat{\pi}}[g]} + |T(\hat{\pi}) - \hat{\pi}Pg|, \tag{74}
\]

where the supremum is taken over all empirical measures \(\hat{\pi}\) corresponding to \(\theta \in \Theta_c\). Notice that \(\hat{\pi} \in \Pi\) and so we can extend the inner supremum to \(\hat{\pi}\) ranging over all of \(\Pi\), concluding

\[
\sqrt{R^*(d)} \leq \delta_a \left(\frac{1}{\sqrt{d}}\right)
\]

with \(\delta_a(t)\) defined in (24). Applying Proposition 3 we get (43).

To prove (44), fix \(c, \gamma > 0\) (to be specified later) and consider \(\pi_0, \pi_0' \in \Pi\) such that \(\chi^2(\pi_0'P||\pi_0P) \leq \frac{c}{d}\) and \(T(\pi_0') - T(\pi_0) = \delta\). Next define distributions

\[
\pi_1 = \gamma \pi_0 + (1 - \gamma)\delta_{\theta_0}, \quad \pi_1' = \gamma \pi_0' + (1 - \gamma)\delta_{\theta_0}.
\]

From the convexity of \(\chi^2(\cdot||\cdot)\), we get

\[
\chi^2(\pi_1'P||\pi_1P) \leq \frac{\gamma c}{d}, \quad T(\pi_1') - T(\pi_1) = \gamma \delta.
\]

Denote \(\mu' = T(\pi_1'), \mu = T(\pi_1)\). Define distributions \(\nu = \pi_1^{\otimes d}, \nu' = \pi_1'^{\otimes d}\) and note that \((\pi_1P)^{\otimes d} = \nu P^{\otimes d}\). By (19) we get

\[
\text{TV}(\nu P^{\otimes d}, \nu' P^{\otimes d}) \leq \sqrt{e^{\gamma c} - 1}.
\]

Next define sets \(A, A' \subset \Theta_c\):

\[
A = \left\{ \theta \in \Theta^{\otimes d} : \sum_i c(\theta_i) \leq 1, T_d(\theta) \leq \mu - \frac{\gamma \delta}{3} \right\} \tag{75}
\]

\[
A' = \left\{ \theta \in \Theta^{\otimes d} : \sum_i c(\theta_i) \leq 1, T_d(\theta) \geq \mu' + \frac{\gamma \delta}{3} \right\}. \tag{76}
\]

From the Chebyshev and Markov inequalities we have

\[
\nu[A^c], \nu'[A'^c] \leq \gamma + \frac{9K_1}{d^2 \gamma^2 \delta^2}
\]
Next, decompose distributions \( \nu, \nu' \) as convex combinations:

\[
\nu = \nu[A] \nu_A + \nu[A^c] \nu_{A^c}, \quad \nu' = \nu'[A] \nu_A' + \nu'[A^c] \nu_{A^c}';
\]

where \( \nu_B[\cdot] \triangleq \nu[\cdot \cap E] / \nu[B] \) is the conditional version of the distribution.

By the triangle inequality and the data processing inequality of total variation, we get

\[
\text{TV}(\nu_A P^\otimes d, \nu'_A P^\otimes d) \leq \nu[A^c] + \nu'[A^c] + \text{TV}(\nu P^\otimes d, \nu' P^\otimes d).
\]

Altogether, we have a pair of distributions \( \nu_1 \triangleq \nu_A \) and \( \nu'_1 \triangleq \nu'_A \), such that \( \theta \sim \nu_1 \) satisfies a.s. \( \theta \in \Theta_c \) and \( T_d(\theta) \geq \mu - \frac{3}{2} \), and similarly for \( \nu'_1 \). Applying Le Cam’s method for quadratic risk yields the following minimax lower bound:

\[
R^* (d) \geq \frac{1}{4} \left( \frac{\gamma \delta}{3} \right)^2 (1 - t),
\]

where \( t \triangleq 2\gamma + \frac{18K_V}{\delta^2} + \sqrt{e^{7c}} - 1 \). Setting \( c = 7/4 \) and \( \gamma = \frac{1}{6} \) we get

\[
R^* (d) \geq \frac{1}{6^6} \delta^2 - \frac{K_V}{4d},
\]

and thus optimizing over the choice of \( \pi_0, \pi'_0 \):

\[
R^* (d) \geq \frac{1}{6^6} \delta^2 \left( \sqrt{\frac{7}{4d}} - \frac{K_V}{4d} \right).
\]

Applying (12) we obtain

\[
R^* (d) \geq \frac{7^2}{2^{935}} \delta^2 \left( \sqrt{\frac{1}{d}} \right) - \frac{K_V}{4d} \geq \left( \frac{1}{62} \delta^2 \left( \sqrt{\frac{1}{d}} \right) \right)^2 - \frac{K_V}{4d}.
\]

Finally, using \( \sqrt{a} - \sqrt{b} < \sqrt{a - b} \) (when the bound is non-trivial), we get (44). \( \square \)

### 5.2 Proof of Theorem 9

**Proof.** Clearly the sufficient statistic is the histogram of the observed colors, that is, \( \{N_i : i \in [d]\} \), where \( N_i \) is the number of observed balls of the \( i \)th color. Thus we have \( N_i \sim \text{Binom}(\theta_i, p) \).

Therefore, the setting of Theorem 9 is a particularization of the general Theorem 8, with \( \Theta = \mathcal{X} = \mathbb{Z}_+, P_\theta = \text{Binom}(\theta, p), c(\theta) = \theta, \Pi = \{\pi \in \mathcal{P}(\mathbb{Z}_+) : \mathbb{E}_{\theta \sim \pi} [\theta] \leq 1\} \), and \( T(\theta) = \mathbb{1}_{\{\theta \geq 1\}} \), or equivalently, \( T(\theta) = \mathbb{1}_{\{\theta = 0\}} \). Furthermore, the assumptions of Theorem 8 are fulfilled (with \( K_V \leq \frac{1}{4} \), and \( \theta_0 = 0 \)). Applying Theorem 8, it remains to characterize the behavior of \( \delta_{\chi^2}(t) \). Note that \( \delta_{\chi^2}(t) \) is closely related to \( \delta_{\chi^2}^{(3)}(t, d) \) previously studied for the population recovery problem in Section 2.3 (with \( \epsilon = 1 - p \)). Both dealing with the binomial model, the only difference is the additional moment constraint in \( \delta_{\chi^2}(t) \) and the difference in the domain (\( \mathbb{Z}_+ \) versus \( \{0, \ldots, d\} \)). Indeed, we have

\[
\delta_{\chi^2}(t) = \sup \{ \pi \theta \geq 1 \} - \pi' \pi' \theta \geq 1 \} : \chi^2 (\pi P || \pi' P) \leq t^2, \pi, \pi' \in \Pi \}
\]

\[
= \sup \{ \pi 0 \} - \pi' \{ \theta \geq 1 \} : \chi^2 (\pi P || \pi' P) \leq t^2, \pi, \pi' \in \Pi \}
\]

\[
\leq \sup \{ \pi 0 \} - \pi' \{ \theta \geq 1 \} : \chi^2 (\pi P || \pi' P) \leq t^2, \pi, \pi' \in \mathcal{P}(\mathbb{Z}_+) \} \triangleq \delta_{\chi^2}(t)
\]

\[
\leq \sup \{ \pi 0 \} - \pi' \{ \theta \geq 1 \} : \text{TV} (\pi P, \pi' P) \leq t, \pi, \pi' \in \mathcal{P}(\mathbb{Z}_+) \} \triangleq \delta_{\text{TV}}(t)
\]

(77) \hspace{1cm} (78)
where the last inequality follows from Lemma 5 (in particular (162), which shows (78) holds for $d = \infty$). This completes the proof of the upper bound in (47) and (48).

To find an estimator that achieves the above upper bound, in view of (24), it suffices to consider $\frac{1}{n} \sum_{i=1}^{n} g(X_i)$, where $g$ is the solution to the following LP (below $e_0 = (1, 0, \ldots, 0)$):

$$
\min_g \|Pg - e_0\|_\infty + \frac{1}{\sqrt{n}}\|g\|_\infty,
$$

which is equal to the dual LP

$$
\max_\Delta \{\Delta(0) : \|\Delta P\|_{TV} \leq t, \|\Delta\| \leq 1\}
$$

Since the latter is an upper bound on (77), such an estimator fulfills the desired upper bound. The above LP (with $O(d)$ variables and $O(d)$ constraints) can be solved in time that is polynomial in $d$.

Next we proceed to the lower bound. The parametric lower bound in (47) follows from Remark 1. To complete the proof of (48), it remains to show the lower bound: for any $p \leq \frac{1}{2}$,

$$
\delta_{\chi^2}(t) \geq c \left( \frac{t}{\sqrt{\log \frac{1}{t}}} \right)^{\frac{p}{1-p}}.
$$

for some constant $c = c(p)$. To this end, we demonstrate a pair of feasible $\tilde{\pi}, \tilde{\pi}' \in \Pi$ by modifying the construction in the proof of [PSW17, Lemma 12] to satisfy the additional moment constraints. Therein, it was shown that there exist probability distributions $\pi, \pi'$ on $\mathbb{Z}_+$, such that $|\pi(0) - \pi'(0)| \geq \delta$ and

$$
H^2(\pi P, \pi' P) \leq 4 \left( e\delta \log \frac{1}{\delta} \right)^{\frac{(1-p)}{p}}.
$$

More precisely, $\pi$ and $\pi'$ are obtained as follows: Let $\alpha = 1 - \frac{1}{\log \frac{1}{t}}$, $\beta = \delta \log \frac{1}{\delta}$. Define $g : \mathbb{C} \to \mathbb{C}$ by $g(z) = \beta^{1+z}$. Set

$$
f(z) = (1 - \alpha)g(\alpha z) - (1 - \alpha)g(\alpha).
$$

Define a sequence $\{\Delta_k : k \in \mathbb{Z}_+\}$ via the coefficients of the Taylor expansion of $f$, i.e., $\Delta_k \triangleq [z^k]f(z)$. Then $\Delta_k = (1 - \alpha)\alpha^k[z^k]g(z)$ for $k \geq 1$. Define the following geometric distribution $\mu$ on $\mathbb{Z}_+$ by $\mu_k \triangleq \alpha^k$. Define now $\pi$ and $\pi'$ via

$$
\pi_k \triangleq \mu_k + \Delta_k, \quad \pi'_k \triangleq \mu_k - \Delta_k.
$$

Now we estimate the mean of $\pi, \pi'$. Note that the mean of the geometric distribution $\mu$ is $\sum_{k \geq 0} k\mu_k = \frac{1}{1-\alpha} = \log \frac{1}{\Delta}$. Furthermore, since the generating function of $\Delta$ is $f$, using the facts that $f'(z) = \alpha(1 - \alpha)g'(\alpha z)$ and $g'(z) = \frac{2\log \beta}{(1-\alpha)^{2}} \beta^{\frac{1+z}{1-2}}$, we have

$$
\sum_{k \geq 0} k\Delta_k = f'(1) = \alpha(1 - \alpha)g'(\alpha) = \frac{2\alpha \log \beta}{1-\alpha} \beta^{\frac{1+z}{1-2}},
$$

Plugging in the values of $\alpha$ and $\beta$ and assuming $\delta \leq 1/e$ so that $\beta \leq 1/e$, we have $|\sum_{k \geq 0} k\Delta_k| \leq 2\delta \log^2 \frac{1}{\epsilon}$. Finally, define

$$
\tilde{\pi} = (1 - \eta)\delta_0 + \eta\pi, \quad \tilde{\pi}' = (1 - \eta)\delta_0 + \eta\pi',
$$

27
Therefore for any estimator $\hat{\theta}$ near its mean, estimating $V$ we have a parametric lower bound (cf. [GT56, OSW16]). Next we focus on proving (54) for $r > 0$ simply follows from using Good-Toulmin’s unbiased estimator and the behavior of the modulus of continuity in (83), cf. (85)-(86) below. To deal with the full species problem without restriction, some extra argument is needed, which involves the auxiliary LP (81) and introduces an extra $O(\log^2 n)$ factor in the upper bound of (54).

5.3 Proof of Theorem 10

We first present a key lemma, the proof of which requires delicate complex analysis and is postponed till the end of this subsection.

**Lemma 13.** Consider the Poisson kernel $P(\cdot | \theta) = \text{Poi}(\theta)$. For $s, t > 0$, define

$$
\delta(s, t) \triangleq \sup_{\Delta} \left\{ \int e^{-s\theta} \Delta(d\theta) : \| \Delta P \|_{TV} \leq t, \| \Delta \|_{TV} \leq 1 \right\}.
$$

where the supremum is taken over all finite signed measure $\Delta$ on $\mathbb{R}_+$. Then for any $s > 0$ and $0 \leq t \leq 1$,

$$
\delta(s, t) \leq t^{\min\{1, \frac{1}{2}\}}.
$$

Furthermore, fix $s \geq 2$ and consider $\delta_{\chi^2}(t)$ in (7) with $\Theta = \mathbb{R}_+, \mathcal{X} = \mathbb{Z}_+, P(\cdot | \theta) = \text{Poi}(\theta)$, $\Pi = \{ \pi : \int \theta \pi(d\theta) \leq 1 \}$ and $T(\theta) = e^{-s\theta}$. There exist positive constants $c = c(s), t_1 = t(s)$ such that for all $t \leq t_1$,

$$
ct^2 \log^{-2} \frac{1}{t} \leq \delta_{\chi^2}(t) \leq 2t^2.
$$

Before proving Theorem 10, we note that the species problem does not completely fall within the purview of the general high-dimensional result in Theorem 8, because the number of distinct species can be infinite. In fact, if we restrict the total number of species to $O(n)$, then the minimax rate readily follows from the general Theorem 8 coupled with the behavior of the modulus of continuity in (83), cf. (85)-(86) below. To deal with the full species problem without restriction, some extra argument is needed, which involves the auxiliary LP (81) and introduces an extra $O(\log^2 n)$ factor in the upper bound of (54).

**Proof.** The result (53) for $r \leq 1$ simply follows from using Good-Toulmin’s unbiased estimator and a parametric lower bound (cf. [GT56, OSW16]). Next we focus on proving (54) for $r > 1$.

**Lower bound.** We begin with some easy reductions. By (50), $U = \sum_x 1_{\{N_x = 0\}} - V$, where $V \triangleq \sum_x 1_{\{N_x = 0, N'_x = 0\}}$, and hence estimating $U$ and $V$ are equivalent. Next, since $V$ is concentrated near its mean, estimating $V$ and $\mathbb{E}[V]$ are essentially equivalent. Indeed, by (50) and independence, we have

$$
\text{Var}(U) = \sum_x \text{Var}(1_{\{N_x = 0, N'_x > 0\}}) \leq \mathbb{E}[U] \leq rn.
$$

Therefore for any estimator $\hat{V}$,

$$
\mathbb{E}[(\hat{V} - V)^2] \geq \frac{1}{2} \mathbb{E}[(\hat{V} - \mathbb{E}[V])^2] - \frac{1}{2} \text{Var}(V) \geq \frac{1}{2} \mathbb{E}[(\hat{V} - \mathbb{E}[V])^2] - \frac{1}{2} rn.
$$

(84)
Define \( \theta_x = np_x \) and \( T(\theta) = e^{-(r+1)\theta} \). Then \( \mathbb{E}[V] = \sum_x T(\theta_x) \).

In order to apply the general result of Theorem 8, we introduce a restricted version of the species problem, where the number of distinct species is at most \( n \). Thus any lower bound for the restricted species problem also holds for the original species problem. Denote the parameters by \( \theta = (\theta_1, \cdots, \theta_n) \in \Theta_{\text{res}} \triangleq \{ \theta \in \mathbb{R}_+^n : \sum_{i=1}^n \theta_i = n \} \). Let the optimal risk for this problem be defined as usual:

\[
\mathcal{E}_n^{(\text{res})}(r) \triangleq \inf_{\hat{V}} \sup_{\theta \in \Theta_{\text{res}}} \mathbb{E}[(\hat{V} - \mathbb{E}[V])^2].
\]  

(85)

Applying Theorem 8 with \( d = n, \ c(\theta) = \theta, \ P = \text{Poi}(\cdot), \) and \( T(\theta) = e^{-(r+1)\theta} \) (which is bounded), we obtain

\[
\delta_{\chi^2} \left( \frac{1}{\sqrt{n}} \right)^2 \geq \mathcal{E}_n^{(\text{res})}(r) \geq c \left( \delta_{\chi^2} \left( \frac{1}{\sqrt{n}} \right)^2 - \frac{1}{n} \right),
\]  

(86)

for some absolute constant \( c \). Applying (83) in Lemma 13 with \( t = \frac{1}{\sqrt{n}} \) and \( s = r + 1 \), we have a suitable lower bound on \( \delta_{\chi^2}(\frac{1}{\sqrt{n}}) \). The desired lower bound in (54) then follows from \( \mathcal{E}_n^{(\text{res})}(r) \leq \mathcal{E}_n(r) \) and (83), (84).

**Upper bound.** We start with the construction of the estimator. By Poisson splitting, at the price of replacing \( n \) by \( 2n \), we can and shall assume that we have access to two independent sets of Poisson observations \( \{N_x\} \overset{\text{ind.}}{\sim} \text{Poi}(\lambda_x) \) and \( \{N'_x\} \overset{\text{ind.}}{\sim} \text{Poi}(\lambda_x) \), where \( \lambda_x \triangleq np_x \). Fix a sequence \( h : \mathbb{Z}_+ \to \mathbb{R} \) to be optimized later. Fix a large constant \( C_0 \) and set a threshold \( b = C_0 \log n \).

Consider an estimator of the following form

\[
\hat{U} = \sum_x \hat{T}_x
\]  

(87)

where

\[
\hat{T}_x = \begin{cases} 
0 & N'_x \geq b \\
h(N_x) & N'_x < b
\end{cases}
\]  

(88)

Recall the goal is to estimate the expected number of unseen symbols that would be present in the next \( rn \) samples:

\[
T \triangleq \mathbb{E}[U] = \sum_x e^{-\lambda_x}(1 - e^{-r\lambda_x}) \triangleq T(\lambda_x).
\]

Then

\[
\mathbb{E}[(\hat{U} - U)^2] = \left( \sum_x (\mathbb{E}[\hat{T}_x] - T(\lambda_x)) \right)^2 + \text{Var}(\hat{U} - U).
\]

A simple calculation shows that (cf. [OSW16, Lemma 3])

\[
\text{Var}(\hat{U} - U) \leq n(\|h\|_\infty^2 + r).
\]  

(89)
To bound the bias, using the definition of $\hat{T}_x$ and the independence of \( \{N_x\} \) and \( \{N'_x\} \), we have:

\[
\begin{align*}
|E[\hat{T}_x - T(\lambda_x)]| &= \left|E \left[ (\hat{T}_x - T(\lambda_x)) \mathbf{1}_{\{N'_x \geq b, \lambda_x \geq \frac{b}{2}\}} + \mathbf{1}_{\{N'_x \geq b, \lambda_x \leq \frac{b}{2}\}} + \mathbf{1}_{\{N'_x \leq b, \lambda_x \leq 2b\}} + \mathbf{1}_{\{N'_x \leq b, \lambda_x \geq 2b\}} \right] \right| \\
&\leq T(\lambda_x) \mathbf{1}_{\{\lambda_x \geq \frac{b}{2}\}} + T(\lambda_x) \mathbb{P}[N'_x \geq b] \mathbf{1}_{\{\lambda_x \leq \frac{b}{2}\}} \\
&\quad + |E[h(N_x)] - T(\lambda_x)\mathbf{1}_{\{\lambda_x \leq 2b\}} + (\|h\|_\infty + 1)\mathbb{P}[N'_x \leq b] \mathbf{1}_{\{\lambda_x \geq 2b\}} | \\
&\leq \underbrace{T(\lambda_x) \mathbf{1}_{\{\lambda_x \geq \frac{b}{2}\}}} + \underbrace{T(\lambda_x) \exp(-b\kappa) \mathbf{1}_{\{\lambda_x \leq \frac{b}{2}\}}} \\
&\quad + \underbrace{|E[h(N_x)] - T(\lambda_x)\mathbf{1}_{\{\lambda_x \leq 2b\}}| + (\|h\|_\infty + 1) \exp(-b\kappa) \mathbf{1}_{\{\lambda_x \geq 2b\}}},
\end{align*}
\]

where we used the Chernoff bound for Poisson distributions [MU05, Theorem 4.4]: \( \mathbb{P}[\text{Poi}(b/2) \geq b] \leq \exp(-\kappa b) \) and \( \mathbb{P}[\text{Poi}(2b) \leq b] \leq \exp(-\kappa b) \), with \( \kappa \triangleq \log 2 - \frac{1}{2} \). Note that

\[
\sum_x \lambda_x = n. \tag{90}
\]

So

\[
\sum_x (I) \leq \sum_x e^{-\lambda_x}(1 - e^{-r\lambda_x})\mathbf{1}_{\{\lambda_x \geq \frac{b}{2}\}} \leq \sum_x e^{-\lambda_x}r\lambda_x \mathbf{1}_{\{\lambda_x \geq \frac{b}{2}\}} \leq rnn^{-\frac{C_0}{2}},
\]

and

\[
\sum_x (II) \leq \sum_x e^{-\lambda_x}(1 - e^{-r\lambda_x}) \exp(-b\kappa) \leq rnn^{-\frac{C_0\kappa}{2b}},
\]

and

\[
\sum_x (IV) \leq (\|h\|_\infty + 1)n^{-\frac{C_0\kappa}{2b}}.
\]

By choosing \( C_0 \) to be large constant, we have

\[
\sum_x (I) + (II) + (IV) \leq rnn^{-10(\|h\|_\infty + 1)}.
\]

Next we proceed to the main term (III) by solving an LP, which is directly related to the LP (81) in Lemma 13. Let \( h(k) = kg(k - 1) \) for some bounded sequence \( g : \mathbb{Z}_+ \to \mathbb{R} \) to be chosen later. Then by Stein’s identity for Poisson distributions, we have \( E[h(N_x)] = \lambda_x E[g(N_x)] \). Put

\[
S(\lambda) \triangleq \frac{T(\lambda)}{\lambda} = \frac{e^{-\lambda} - e^{-(r+1)\lambda}}{\lambda}.
\]

Then we have \( E[h(N_x)] - T(\lambda) = \lambda_x (E[g(N_x)] - S(\lambda_x)) \). Recall that the Poisson kernel \( P \) acts as follows:

- For any sequence \( g : \mathbb{Z}_+ \to \mathbb{R} \), \( Pg : \mathbb{R}_+ \to \mathbb{R} \) is a function defined via \( (Pg)(\lambda) \triangleq E[g(\text{Poi}(\lambda))] \);
- For any distribution \( \pi \) on \( \mathbb{R}_+ \), \( \pi P \) denotes the Poisson mixture whose probability mass function is given by \( (\pi P)(k) = \int e^{-\lambda}\frac{k^k}{k!} \pi(d\lambda), k \geq 0 \).
For any $t > 0$, define the following bias-variance tradeoff LP:

$$
\delta(t) \triangleq \inf_g \|S - Pg\|_{L_\infty(\mathbb{R}_+)} + t\|g\|_{\ell_\infty(\mathbb{Z}_+)},
$$

(91)

Next we bound $\delta(t)$ by the dual LP:

$$
\delta(t) \overset{(a)}{=} \inf_{g \in \ell_\infty(\mathbb{Z}_+)} \sup_{\|\Delta\|_{TV} \leq 1, \|\nu\|_{TV} \leq 1} \int (S - Pg)d\Delta + t\int gd\nu
$$

\[
\overset{(b)}{=} \sup_{\|\Delta\|_{TV} \leq 1, \|\nu\|_{TV} \leq 1} \inf_{g \in \ell_\infty(\mathbb{Z}_+)} \int (S - Pg)d\Delta + t\int gd\nu
\]

\[
\overset{(c)}{=} \sup_{\|\Delta\|_{TV} \leq 1, \|\nu\|_{TV} \leq 1} \inf_{g \in \ell_\infty(\mathbb{Z}_+)} \int Sd\Delta + \int gd(t\nu - \Delta P)
\]

\[
\overset{(d)}{=} \sup_{\Delta} \left\{ \int Sd\Delta : \|\Delta\|_{TV} \leq 1, \|\Delta P\|_{TV} \leq t \right\},
\]

(92)

where in (a) $\Delta$ and $\nu$ are finite signed measures on $\mathbb{R}_+$ and $\mathbb{Z}_+$, respectively; (b) follows from Ky Fan’s minimax theorem (Theorem 4), since $\{\Delta : \|\Delta\|_{TV} \leq 1\}$ and $\{\nu : \|\nu\|_{TV} \leq 1\}$ are compact in their respective weak topology, and for every bounded $g$, $\nu \mapsto \int gd\nu$ and $\Delta \mapsto \int (S - Pg)d\Delta$ are both weakly continuous since both $S$ and $Pg$ are bounded; (c) follows from Fubini’s theorem: $\int Pg d\Delta = \int gd(t\nu - \Delta P)$; (d) is because

$$
\inf_{g \in \ell_\infty(\mathbb{Z}_+)} \int Sd\Delta + \int gd(t\nu - \Delta P) = \begin{cases} -\infty & t\nu \neq \Delta P \\ 0 & t\nu = \Delta P \end{cases}
$$

To relate the LP (92) to the LP (81) considered in Lemma 13, the key observation is the following integral representation:

$$
S(\lambda) = \int_1^{r+1} e^{-\lambda s} ds.
$$

Interchanging the integral with the supremum in (92), we obtain the following upper bound

$$
\delta(t) \leq \int_1^{r+1} \delta(s,t) ds
$$

(93)

where $\delta(s,t)$ is defined in (81). In view of (82) and (93), we have

$$
\delta(t) \leq rt^{\frac{2}{r+1}}.
$$

(94)

Thus, for $t = \frac{1}{\sqrt{n}}$, there exists $g^* : \mathbb{Z}_+ \to \mathbb{R}$, such that

$$
\sup_{\lambda \geq 0} |E[g^*(\text{Poi}(\lambda))] - S(\lambda)| \leq rn^{-\frac{2}{r+1}}, \quad \|g^*\|_\infty \leq rn^{\frac{1}{r+1}}.
$$

(95)

Next, we truncate $g^*$. Set $\lambda_0 = 2b$ and $L = 2\lambda_0 = 4C_0 \log n$ and define $g$ by

$$
g(k) = g^*(k)1_{(k \leq L)}.
$$

(96)

Since $h(k) = kg(k - 1)$, we have $\|h\|_\infty \leq L\|g^*\|_\infty$. In view of (89) and (95), we have the variance bound

$$
\text{Var}(\bar{U} - U) \leq 4rL^2 n^{\frac{2r}{r+1}} = O(rn^{\frac{2r}{r+1}} \log^2 n).
$$
Furthermore, truncation incurs a small bias since
\[ |\mathbb{E}[g^*(N_x)1_{\{N_x > L\}}]| \leq \|g^*\|_{\infty} \mathbb{P}[N_x > L]. \]

Note that \( \mathbb{P}[\text{Poi}(\lambda) > L] \leq \lambda \sum_{i \geq L} \frac{\lambda^{i-1}}{(i-1)!} e^{-\lambda} = \lambda \mathbb{P}[\text{Poi}(\lambda) > L - 1] \). Thus
\[
\sum_x |\mathbb{E}[g^*(N_x)1_{\{N_x > L\}}]1_{\{\lambda x \leq \lambda_0\}}| \leq n\|g^*\|_{\infty} \mathbb{P}[\text{Poi}(\lambda_0) > 2\lambda_0 - 1] \]  
\[ \leq \frac{3n^2}{\frac{2}{1+\varepsilon}} \exp(-\kappa\lambda_0/2) \leq n^{-5}, \tag{97} \]

where the last step follows by \( C_0 \) being a large constant. Thus
\[
\sum_x (\text{III}) = \sum_x |\mathbb{E}[h(N_x)] - T(\lambda_x)|1_{\{\lambda x \leq \lambda_0\}} 
= \sum_x \lambda x |\mathbb{E}[g(N_x)] - S(\lambda_x)|1_{\{\lambda x \leq \lambda_0\}} \tag{98} \]
\[
\leq \sum_x \lambda x |\mathbb{E}[g^*(N_x)] - S(\lambda_x)|1_{\{\lambda x \leq \lambda_0\}} + \sum_x |\mathbb{E}[g^*(N_x)1_{\{N_x > L\}}]|1_{\{\lambda x \leq \lambda_0\}} \tag{99} \]
\[
\leq \frac{3n^2}{\frac{2}{1+\varepsilon}} + n^{-5}, \tag{100} \]

where the last step follows from (90), (95) and (97).

Putting everything together, we have
\[
\mathbb{E}[(\hat{U} - U)^2] \leq \left( \sum_x (\text{I}) + (\text{II}) + (\text{III}) + (\text{IV}) \right)^2 + \text{Var}(\hat{U} - U) = O(r^2 n^{2/1+\varepsilon} \log^2 n). \]

Dividing both sides by \( n^2 \) yields the main result (54).

Finally, we address the construction of the estimator and its computational complexity. From the above proof, combining (87), (88), (91), (96) and (97), we see that it suffices to choose an estimator of the following form
\[
\hat{U} = \sum_x g^*(N_x)1_{\{N_x < L\}}1_{\{N_x < b\}} \tag{101} \]

where \( g^* \) is the solution of the following infinite-dimensional LP:
\[
\inf_g \|S - Pg\|_{L_\infty(\{0, \lambda_0\})} + \frac{1}{\sqrt{n}} \|g\|_{\ell_\infty}, \tag{102} \]

with \((Pg)(\lambda) = \mathbb{E}_{N \sim \text{Poi}(\lambda)}[g(N)1_{\{N \leq L\}}]\). Recall that \( \lambda_0, L \) and \( b \) are all \( \Theta(\log n) \). Here the decision variable \( g : \{0, \ldots, L\} \rightarrow \mathbb{R} \) is finite-dimensional; however the objective function involves the \( L_\infty \)-norm and is equivalent to setting a continuum of constraints. It remains to show that one can find a finite-dimensional LP whose solution is as good as (102), statistically speaking. We do so by means of discretization. From the (95) we see that it suffices to consider \( \|g\|_{\infty} \leq \frac{3n^2}{\frac{2}{1+\varepsilon}} \). For some small \( \varepsilon \) to be specified, let \( m = \lceil \lambda_0/\varepsilon \rceil \) and \( M \triangleq \varepsilon \{1, \ldots, m\} \).
\[
\inf_g \|S - Pg\|_{L_\infty(M)} + \frac{1}{\sqrt{n}} \|g\|_{\ell_\infty}, \tag{103} \]

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To compare (102) and (103), note that for any \( \lambda \in [0, \lambda_0] \), there exists \( \lambda' \in M \) such that \( |\lambda - \lambda'| \leq \epsilon \). Recall that \( S(\lambda) = \frac{T(\lambda)}{\lambda} = e^{-\lambda}e^{-x(x+1)\lambda} \) is \( \lambda \)-Lipschitz in \( \lambda \) for some \( L \) depending only on \( r \). Therefore \( |S(\lambda) - S(\lambda')| \leq L\epsilon \). Furthermore, since \( D(\text{Poi}(\lambda))\|\text{Poi}(\lambda')\| = \lambda \log \frac{1}{\lambda} + \lambda' - \lambda \leq \frac{(\lambda - \lambda')^2}{\lambda} \leq \epsilon \), by Pinsker’s inequality, we have \( |(P_g(\lambda) - (P_g)(\lambda'))| \leq \|g\| \text{TV}(\text{Poi}(\lambda), \text{Poi}(\lambda')) \leq r\sqrt{\epsilon} \). Choosing \( \epsilon = \frac{1}{m^2} \), we conclude that the value of (102) and (103) only differs by \( O(n^{-1/2}) \), and solving which is an LP with \( O(\log n) \) variables and \( O(n^2) \) constraints, achieves the upper bound in (54). \( \square \)

To close this section, we prove Lemma 13. The proof relies on two key results from complex analysis: Hadamard’s three-lines theorem and the Paley-Wiener theorem.

**Proof.** We follow the same program of \( H^\infty \)-relaxation as in the proof of Theorem 5 in [PSW17]. For a complex valued function on \( U \subset \mathbb{C} \) we define \( \|f\|_{H^\infty(U)} = \sup_{z \in U} |f(z)| \). If \( f \) is holomorphic on a domain \( U \) then \( \|f\|_{H^\infty(U)} = \|f\|_{H^\infty(\partial U)} \) by the maximum principle. The open unit disk is denoted below as \( D \) and the unit circle as \( \partial D \). To each finite signed measure \( \Delta \) on \( \mathbb{R}_+ \) we associate its Laplace transform:

\[
f_\Delta(z) \triangleq \int_{\mathbb{R}_+} e^{az} \Delta(da),
\]

which is a holomorphic function on \( \{\Re \leq 0\} \) and

\[
\|f_\Delta\|_{H^\infty(\Re \leq 0)} = \|f_\Delta\|_{H^\infty(\Re = 0)} \leq \|\Delta\|_{TV} \triangleq \int_{\mathbb{R}} |\Delta|(da). \tag{104}
\]

Similarly, to each finite signed measure \( \nu \) on \( \mathbb{Z}_+ \) we associate its \( z \)-transform

\[
f_\nu(z) \triangleq \sum_{m \in \mathbb{Z}_+} \nu(m)z^m.
\]

Again, \( f_\nu \) is holomorphic on a \( D \) with

\[
\|f_\nu\|_{H^\infty(D)} = \|f_\nu\|_{H^\infty(\partial D)} \leq \|\nu\|_{TV} \triangleq \sum_{m \in \mathbb{Z}_+} |\nu(m)|. \tag{105}
\]

Furthermore, if \( f_\nu \) happens to be holomorphic on \( rD \) for \( r > 1 \), then we have from Cauchy integral formula

\[
|\nu(m)| \leq r^{-m}\|f\|_{H^\infty(rD)} \tag{106}
\]

The important observation for this proof is the following identity:

\[
f_{\Delta P}(z) = f_\Delta(z - 1), \tag{107}
\]

where \( \Delta \) and \( \Delta P \) are measures on \( \mathbb{R}_+ \) and \( \mathbb{Z}_+ \), with the latter obtained by applying the Poisson kernel \( P \) to \( \Delta \), to wit, \( \Delta P(m) = \int \frac{e^{-a}a^m}{m!} \Delta(da) \). Indeed, (107) simply follows from Fubini’s theorem:

\[
f_{\Delta P}(z) = \int \sum_{m \geq 0} \frac{e^{-a}a^m}{m!} \Delta(da) = \int e^{a(z-1)} \Delta(da) = f_\Delta(z - 1).
\]

We now proceed to proving (82):

\[
\delta(s, t) = \sup_{\Delta} \left\{ \int e^{-\delta d} \Delta(d\theta) : \|\Delta P\|_{TV} \leq t, \|\Delta\|_{TV} \leq 1 \right\}
\]

\[
= \sup_{\Delta} \{f_\Delta(-s) : \|f_\Delta\|_{H^\infty(D - 1)} \leq t, \|f_\Delta\|_{H^\infty(\Re < 0)} \leq 1 \} \tag{108}
\]

\[
\leq \sup_f \{f(-s) : \|f\|_{H^\infty(D - 1)} \leq t, \|f\|_{H^\infty(\Re < 0)} \leq 1 \} \triangleq \delta_{H^\infty}(t) \tag{109}
\]

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where (108) is by expressing the objective function in terms of Laplace transform of \( \Delta \), and relaxing the total variation constraint on \( \Delta P \) by the \( H^\infty \)-norm constraint, in view of (104), (105) and (107); (109) is by extending the optimization from Laplace transforms \( f_\Delta \) to all holomorphic functions on \( \{ \Re < 0 \} \).

To solve the optimization problem (109) we first notice that for \( s \leq 2 \), we have \(-s \in D - 1\) and thus \( \delta_{H^\infty}(t) = t \) (achieved by taking \( f(z) = t \)). Next consider \( s > 2 \). Let us reparameterize \( f(z) = g(1 + \frac{s}{z}) \). Note that (cf. Fig. 1)

\[
\| f \|_{H^\infty(\Re < 0)} = \sup_{\Re(z) < 0} |f(z)| = \sup_{\Re(z) < 0} \left| g\left(1 + \frac{s}{z}\right)\right| = \sup_{\Re(w) < 1} |g(w)| = \| g \|_{H^\infty(\Re < 1)}.
\]

Furthermore, since

\[
1 + \frac{1}{w} \in D \iff \Re(w) \leq -\frac{1}{2},
\]

we have

\[
\| f \|_{H^\infty(D - 1)} = \sup_{z \in D - 1} \left| g\left(1 + \frac{s}{z}\right)\right| = \sup_{1 + \frac{s}{w} \in D} |g(w)| = \sup_{\Re(w) < 1 - \frac{s}{2}} |g(w)| = \| g \|_{H^\infty(\Re < 1 - \frac{s}{2})}.
\]

Hence, we have

\[
\delta_{H^\infty}(t) = \sup_{g} \{ g(0) : \| g \|_{H^\infty(\Re < 1 - \frac{s}{2})} \leq t, \| g \|_{H^\infty(\Re < 1)} \leq 1 \}.
\]

By Hadamard’s three-lines theorem (see, e.g., [Sim11, Theorem 12.3]), \( x \mapsto \log \| g \|_{H^\infty(\Re < x)} \) is convex. Since \((1 - \frac{s}{2})^2 + (1 - \frac{s}{2}) = 0\), we get

\[
|g(0)| \leq \| g \|_{H^\infty(\Re < 0)} \leq \left(\| g \|_{H^\infty(\Re < 1 - \frac{s}{2})}\right)^{\frac{2}{1 - \frac{s}{2}}} \left(\| g \|_{H^\infty(\Re < 1)}\right)^{1 - \frac{2}{1 - \frac{s}{2}}} \leq t^2,
\]

for any \( g \) feasible for (111). Furthermore, this is achieved by taking \( g(z) = t^2(1 - z) \). So we have proved

\[
\delta_{H^\infty}(t) = t^2,
\]

and the optimizer in (109) is

\[
f_s(z) = t^{-\frac{s}{2}},
\]

which turns out to not depend on \( s \). This completes the proof of (82).
Next we prove (83) for $s \geq 2$. The upper bound is clear:
\[
\delta_{\chi^2}(t) \leq \delta_{TV}(t) \leq \sup_{\Delta} \left\{ \int \Delta(d\theta)e^{-s\theta} : \|\Delta P\|_{TV} \leq 2t, \|\Delta\|_{TV} \leq 2 \right\}
\]
\[
= 2\delta(s, t) \leq 2t^2
\]
where (113) is from (13), (114) is by dropping the constraint $\pi, \pi' \in \Pi$ and taking $\Delta = \pi' - \pi$, and (115) is by (82).

Finally, we prove the lower bound part of (83). To this end we need to produce a pair of distributions $\pi, \pi'$ that are feasible for $\delta_{\chi^2}(t)$. We could try to take them to be positive and negative part of the measure $\Delta$ that whose Laplace transform coincides with (112), i.e., $f_{\Delta} = f_\pi$; however, this approach does not directly work (for example, if $\Delta$ were a finite measure, its characteristic function would have been given by $e^{\frac{ic\omega}{2}}1\{\omega \neq 0\}$, which is discontinuous at $\omega = 0$ and thus not the characteristic function of any finite measure on $\mathbb{R}$). Instead, below we construct a sequence of measures approximating $\Delta$.

For each $0 < \alpha < 1$ (in the end we will take $\alpha \sim \frac{1}{\log t}$) define
\[
f_\alpha(z) = \frac{1}{(z-1)^2}e^{\frac{-2}{z-\alpha}} = \frac{1}{(z-1)^2}e^{c_\alpha/(z-\alpha)}, \quad c_\alpha \triangleq 2\log \frac{1}{t}.
\]
Let $G_\alpha$ be a real-valued function on $\mathbb{R}$ (whose existence is to be established), such that its Laplace transform is given by $f_\alpha$, i.e.
\[
\int_{\mathbb{R}} G_\alpha(a)e^{az}da = f_\alpha(z) \quad \forall z : \Re(z) \leq 0.
\]
Let $H_0$ be the following probability distribution on $\mathbb{R}_+$
\[
H_0(dx) = (1 - \lambda)\delta_0(dx) + \lambda e^{-\gamma x}1\{x \geq 0\} dx,
\]
which is a mixture of a point mass at zero and an exponential distribution. We then take
\[
\pi = H_0, \quad \pi' = (1 - \tau_0)H_0 + \xi G_\alpha,
\]
where
\[
\tau_0 = \xi \int_{\mathbb{R}} G_\alpha(x)dx = \xi f_\alpha(0) = \xi e^{-\frac{c_\alpha}{\alpha}}
\]
so that $\pi'$ is normalized. To complete the proof we have to prove that a certain choice of $(\alpha, \xi, \gamma, \lambda)$ achieves the following six goals for all sufficiently small $t$:

1. $G_\alpha$ is a real-valued density$^{11}$ supported on $\mathbb{R}_+$;
2. $\pi'$ is a probability measure (i.e. it is a positive measure);
3. $E_{\pi}[\theta] \leq 1$;
4. $E_{\pi'}[\theta] \leq 1$;

$^{11}$Although the statistical lower bound does not need it, we require $G_\alpha$ to have a density in order to apply the Paley-Wiener theorem which ensures it is supported on $\mathbb{R}_+$ and hence can be used as a valid prior.
5. The separation of means satisfies:

\[ T(\pi') - T(\pi) \geq \frac{K}{(1 + s)^2 \log^{\frac{\alpha}{4}} \frac{1}{t}} , \]

for some constant \( K \) (here and below, \( K \) denotes an absolute constant, possibly different on different lines), where recall that \( T(\pi) = \mathbb{E}_\pi[ e^{-\theta} ] \).

6. The \( \chi^2 \)-divergence satisfies:

\[ \chi^2(\pi'P \parallel \pi P) \leq t^2 . \]

We make the following choices of parameters:

\[ \gamma = \frac{\alpha}{2}, \lambda = \frac{\alpha}{4}, \xi = \frac{\alpha^2}{16}, \alpha = \frac{1}{c t} \quad (117) \]

Note that as \( t \to 0 \), all of the above vanish with \( \text{polylog}(\frac{1}{t}) \) speed.

We start with item 1. To get a formula for \( G_\alpha \) we notice that the inverse Fourier transform is well-defined. Indeed, since \( |f_\alpha(i\omega)| = \frac{1}{1 + \omega^2} \exp(-\frac{c\alpha}{\omega^2 + \alpha^2}) \), we have \( \omega \mapsto f_\alpha(i\omega) \) is in \( L^1(\mathbb{R}) \). Hence there exists a continuous bounded function \( G_\alpha \) on \( \mathbb{R} \) whose Fourier transform is given by \( f_\alpha(i\omega) \).

Moreover, \( G_\alpha \) is real-valued since \( f_\alpha(-i\omega) = (f_\alpha(i\omega))^* \), where * denotes the complex conjugation.

To ensure that \( G_\alpha \) is supported on \( \mathbb{R}^+ \), note that \( f_\alpha \) is holomorphic in \( \{ \Re \leq 0 \} \) and, furthermore,

\[ |f_\alpha(x + iy)| = \frac{1}{(1 - x)^2 + y^2} \exp \left( \frac{-c(x - \alpha)}{(x - \alpha)^2 + y^2} \right) , \]

thus

\[ \sup_{x < 0} \int_{\mathbb{R}} |f_\alpha(x + iy)|^2 dy \leq \int_{\mathbb{R}} \frac{1}{1 + y^2} dy \exp \left( \frac{c}{\alpha} \right) < \infty . \]

Then the Paley-Wiener theorem (cf. [Rud87, Theorem 19.2]) implies that \( G_\alpha \) is supported on \( \mathbb{R}^+ \).

We also get an estimate on the tail of \( G_\alpha(a) \) for \( a > 0 \) as follows: By the inverse Fourier transform,

\[
G_\alpha(a) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{\frac{\alpha t}{\omega}} \frac{1}{(i\omega - 1)^2} e^{-i\omega a} d\omega \\
= \frac{1}{2\pi i} \int_{0 - i\infty}^{0 + i\infty} e^{\frac{\alpha t}{\omega}} \frac{1}{(z - 1)^2} e^{-z a} dz \\
= \frac{1}{2\pi i} \int_{\frac{\alpha}{2} - i\infty}^{\frac{\alpha}{2} + i\infty} e^{\frac{\alpha t}{z}} \frac{1}{(z - 1)^2} e^{-z a} dz \\
= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{\frac{\alpha t}{\omega - \frac{\alpha}{2}}} \frac{1}{(i\omega + \frac{\alpha}{2} - 1)^2} e^{-(i\omega + \frac{\alpha}{2}) a} d\omega ,
\]

where in (118) we shifted the contour of integration since the integrand is holomorphic in the strip \( \{ 0 \leq \Re \leq \frac{\alpha}{2} \} \). Thus

\[
|G_\alpha(a)| \leq \frac{e^{-a^2/2}}{2\pi} \int_{-\infty}^{\infty} \frac{1}{\omega^2 + (1 - \frac{\alpha}{2})^2} d\omega \\
= \frac{1}{2(1 - \frac{\alpha}{2})} e^{-a^2/2} \leq e^{-a^2/2} ,
\]

(119)
where the last step follows from \( \int_{-\infty}^{\infty} \frac{1}{K^2 + x^2} \, dx = \frac{\pi}{K} \) and the assumption that \( \alpha \leq 1 \).

We proceed to item 2. In view of (119), to ensure the positivity of \( \pi' \) we only need to verify

\[(1 - \tau_0)\lambda \gamma e^{-a\gamma} \geq \xi e^{-\frac{a_\lambda}{s}}\]

Due to the choices in (117) this is equivalent to \( 1 - \tau_0 \geq \frac{1}{2} \) which is satisfied for sufficiently small \( t \).

For item 3, we have \( \mathbb{E}_x[\theta] = \lambda \frac{1}{2} = \frac{1}{2} \).

For item 4, we can compute the first moment of \( G_\alpha \) from its Laplace transform as follows:

\[
\int_0^\infty G_\alpha(a) da = \frac{d}{dz} \bigg|_{z=0} f_\alpha(z) = e^{-\frac{a}{\alpha}} (2 - \frac{\xi_0}{\alpha^2}) = e^{-\frac{1}{\alpha^2}(2 - \frac{1}{\alpha^2})} \to 0,
\]

since \( \alpha \to 0 \) as \( t \to 0 \). Thus, we have \( \mathbb{E}_{\pi'}[\theta] = (1 - \tau_0)\frac{1}{2} + \xi \int aG_\alpha \to \frac{1}{2} \) as \( t \to 0 \).

For item 5, note that

\[
T(G_\alpha) = \int e^{-sa}G_\alpha(a) da = f_\alpha(-s) = \frac{1}{(s+1)^2} t \frac{2}{\alpha} \geq \frac{1}{(s+1)^2} t \frac{2}{\alpha},
\]

Since \( T(H_0) = 1 - \frac{s\lambda}{s+\gamma} \in [0,1] \), by linearity, we have from (120)

\[
T(\pi') - T(\pi) = -\tau_0 \left(1 - \frac{s\lambda}{s+\gamma}\right) + \xi \int_0^\infty e^{-a}G_\alpha(a) da \geq -\tau_0 + \xi \frac{\xi_0}{(s+1)^2} t \frac{2}{\alpha}
\]

\[
(116) \xi \left(\frac{1}{s+1}\right)^2 t \frac{2}{\alpha} - e^{-4\log(\frac{1}{2})} \leq \frac{\xi}{2(s+1)^2} t \frac{2}{\alpha},
\]

where the last step holds for all sufficiently small \( t \).

Finally, for item 6, we have

\[
\chi^2((1 - \tau_0)H_0P + \xi G_\alpha P\|H_0P) = \sum_{m \geq 0} \frac{(\xi G_\alpha P(m) - \tau_0 H_0P(m))^2}{H_0P(m)} = \xi^2 \sum_{m \geq 0} \frac{G_\alpha P(m)^2}{H_0P(m)} - \tau_0^2 \leq \xi^2 \sum_{m \geq 0} \frac{G_\alpha P(m)^2}{H_0P(m)}. \quad (121)
\]

For the denominator we have

\[
H_0P(m) = (1 - \lambda)1_{\{m=0\}} + \lambda(1 - \beta)\beta^m, \quad \beta = \frac{1}{\gamma + 1}.
\]

To bound the numerator, by (107) the \( z \)-transform of \( G_\alpha \) is given by

\[
f_{G_\alpha}(z) = f_\alpha(z-1) = \frac{1}{(z-2)^2} e^{\frac{\alpha}{z} - 1 - \alpha}
\]

\[(123)\]

Our goal is to show that, for \( r = 1 + \frac{a}{\alpha} \), we have \( \|f_{G_\alpha}P\|_{H^\infty(rD)} \leq Kt \) for some constant \( K \). Indeed, the first factor in (123) is bounded by \( \|\frac{1}{(z-2)^2}\|_{H^\infty(rD)} \leq \frac{1}{(1-a/2)^2} \leq 4 \) for all sufficiently small \( t \).

For the second factor, in view of (110), for any \( \rho > 0 \) we have

\[\|e^{\rho/z}\|_{H^\infty(D-1)} = e^{-\rho/2}. \quad (124)\]

Set \( \rho = 1 + \frac{3\alpha}{4} \), we have

\[\|f_{G_\alpha}P\|_{H^\infty(rD)} \leq 4\|e^{\rho/z}\|_{H^\infty(rD-1-\alpha)} \leq 4\|e^{\rho/z}\|_{H^\infty(D-1)} = 4e^{-\frac{\rho}{2}} \leq 10t, \quad (125)\]
where (a) is by (123); (b) is because $rD - 1 - \alpha \subset \rho(D - 1)$; (c) is by (124); (d) is by the choices in (117).

From Cauchy’s integral formula (106) we obtain the estimate of the coefficients:

$$G_\alpha P(m) \leq Kr^{-m}t.$$  

(125)

Using (122) and (125) we continue (121) to get

$$\chi^2((1 - \tau_0)H_0P + \xi G_\alpha P\|H_0P) \leq Kt^2 \frac{\xi^2}{\lambda \gamma} \sum_{m \geq 0} (r^2) - m.$$  

Since $r^2 \beta = 1 + \frac{\alpha}{2\pi} + o(\alpha)$ we conclude

$$\chi^2((1 - \tau_0)H_0P + \xi G_\alpha P\|H_0P) \leq Kt^2 \frac{\xi^2}{\lambda \gamma \alpha} \leq t^2$$  

for all sufficiently small $t$ due to (117). This completes the proof of (83). 

\[\square\]

5.4 Proof of Theorem 11

Proof of Theorem 11. A routine two-point argument yields the lower bound

$$\omega_J(c_0/\sqrt{n}) \leq \sqrt{R^*_n(\Gamma_0)}.$$  

The rest of the proof consists of two main steps. First, we will show by appealing to the minimax theorem the constructive part:

$$\sqrt{R^*_n(\Gamma_0)} \leq \delta_a(1/\sqrt{n}).$$  

(126)

Next we will show that for some $c_2 > 0$ and all $t > 0$ we have

$$\omega_J(t) \geq \delta_a(ct).$$  

(127)

Since we also have $\delta_a(ct) \geq c\delta_a(t)$ (see (136) below), this will complete the proof of all inequalities in (66).

We extend the family $F$ to $F^* = \text{span}\{F, 1\}$ by adding constants. Similarly, we extend $X$ to $X^*(\omega) = (1, X(\omega)) \in \mathbb{R}^{d+1}$ by adding a constant coordinate (note that as exponential family $X^*$ no longer satisfies non-degeneracy condition (57)). We show an upper bound by considering estimators of the form

$$\hat{T} = \frac{1}{n} \sum_i \phi(\omega_i) = \frac{1}{n} \sum_i \langle \gamma^*, X_i^* \rangle,$$

where $\phi(\omega)$ is an arbitrary (to be selected) element of $F^*$, which we can represent as $\phi(\omega) = \langle \gamma^*, X(\omega) \rangle$. We have:

$$\inf_{\phi \in F^*} \sup_{\gamma \in \Gamma_0} \sqrt{E_\gamma[(T - \hat{T})^2]} \leq \inf_{\phi \in F^*} \sup_{\gamma \in \Gamma_0} \frac{1}{\sqrt{n}} \sqrt{\text{Var}_P\gamma[\phi] + |E_P\gamma[\phi] - T(\gamma)|}$$  

(128)

$$= \inf_{\phi \in F^*} \sup_{\mu \in M_0} \frac{1}{\sqrt{n}} \sqrt{\text{Var}_P\mu[\phi] + |\langle \gamma^* - g, \mu \rangle|}$$  

(129)

$$= \delta_0(1/\sqrt{n}),$$  

(130)

where $\delta_0$ is defined as

$$\delta_0(t) \overset{\Delta}{=} \inf_{\phi \in F^*} \sup_{\mu \in M_0} t \sqrt{\text{Var}_P\mu[\phi] + |\langle \gamma^* - g, \mu \rangle|}.$$  

This definition coincides with $\delta_0$ defined in Lemma 14 (Appendix A) if we set:
\[ X = \mathbb{R}^{d+1}, \Pi = \{1\} \times M_0, Y = \mathcal{F}^* \]

- Each element \( \phi \in \mathcal{F}^* \) can be written as \( \phi(\omega) = y_0 + \sum y_i \phi_{0,i}(\omega) = \langle y, X^* \rangle \), this identifies \( Y = \mathcal{F}^* \) with \( \mathbb{R}^{d+1} \).

- We establish the dual pairing between \( X \) and \( Y \) as usual \( \langle x, y \rangle = \sum_{i=0}^{d} x_i y_i \). Note that when \( x = (1, \mu) \in \Pi \) and \( y \leftrightarrow \phi \) we have \( \langle x, y \rangle = x \Phi \mu \).

- For \( x = (1, \mu) \in \Pi \) and \( y \leftrightarrow \phi \) we set \( f(x, y) = \sqrt{\text{Var}_\mu[\phi]} \)

- \( e_0 = (1,0,\ldots,0) \) corresponds to the constant function 1 in \( \mathcal{F}^* \).

Clearly \( \langle x, e_0 \rangle = \mathbb{E}_\mu[1] = 1 \) for any \( x \in \Pi \). Note also that in the definition of \( d(P_\gamma \parallel P_{\gamma'}) \) we may extend the supremum from \( \mathcal{F} \) to \( \mathcal{F}^* \) without change. With these settings, Lemma 14 shows

\[
\frac{1}{2} \delta_a(t) \leq \delta_0(t) \leq \delta_a(t).
\]

This completes the proof of (126).

We proceed to proving (127). We start with some preparatory remarks. A simple calculation reveals that

\[
d_f(P_{\gamma_1}, P_{\gamma_2}) = \langle \gamma_1 - \gamma_2, \mu_f(\gamma_1) - \mu_f(\gamma_2) \rangle .
\]

Similarly, we have the following expression for \( d \):

\[
d(\hat{P}_\mu \parallel \hat{P}_\mu) = \sup_{a \in \mathbb{R}^d} \left\{ \langle \mu - \mu', a \rangle : \langle \hat{\Sigma}(\mu)a, a \rangle \leq 1 \right\}
\]

\[
= \sqrt{\langle \hat{\Sigma}^{-1}(\mu) \Delta, \Delta \rangle}, \quad \Delta = \mu - \mu',
\]

where we used the identity

\[\sup_{y \in \mathbb{R}^d} \left\{ \langle y, b \rangle : \langle Ay, y \rangle \leq 1 \right\} = \sqrt{\langle A^{-1}b, b \rangle},\]

which follows from the Cauchy-Schwarz inequality: \( \langle y, b \rangle^2 = \langle A^{\frac{1}{2}}y, A^{-\frac{1}{2}}b \rangle^2 \leq \langle A^{-1}b, b \rangle \langle Ay, y \rangle \).

Thus, we get a more explicit formula for \( \delta_a \):

\[
\delta_a(t) = \sup_{\mu_1, \mu_2 \in M_0} \left\{ \langle \Delta, g \rangle : \langle \hat{\Sigma}^{-1}(\mu_2) \Delta, \Delta \rangle \leq t^2, \Delta = \mu_1 - \mu_2 \right\}.
\]

This expression clearly shows

\[\delta_a(ct) \geq c\delta_a(t), \quad \forall c \leq 1.\]

We next establish a key inequality connecting the behavior of \( \hat{\Sigma}^{-1}(\lambda \mu_1 + \lambda \mu_0) \) with the assumption (64). Consider the following chain of inequalities: for any \( a \in \mathbb{R}^d \),

\[
\langle \hat{\Sigma}^{-1}(\lambda \mu_1 + \lambda \mu_0)a, a \rangle = \sup_y \left\{ \langle y, a \rangle : \langle \hat{\Sigma}(\lambda \mu_1 + \lambda \mu_0)y, y \rangle \leq 1 \right\}
\]

\[
\leq \sup_y \left\{ \langle y, a \rangle : \lambda \langle \hat{\Sigma}(\mu_1)y, y \rangle + \lambda \langle \hat{\Sigma}(\mu_2)y, y \rangle \leq 1 \right\}
\]

\[
\leq \sup_y \left\{ \langle y, a \rangle : \lambda \langle \hat{\Sigma}(\mu_1)y, y \rangle \leq 1 \right\}
\]

\[= \frac{1}{\lambda} \langle \hat{\Sigma}^{-1}(\mu_1)a, a \rangle,\]

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where in (137) we used (134), in (138) we applied (64), in (139) we omitted the second term, which is non-negative by (59), and in (140) we used (134) again.

Next, we obtain an upper bound on $d_J(P_{\gamma_1}, P_{\gamma_2})$ by continuing from (131). We denote $\mu_i = \mu_f(\gamma_i), i = 1, 2$ and $\Delta = \mu_1 - \mu_2$. Notice

$$\gamma_1 - \gamma_2 = \int_0^1 \dot{\gamma}_\lambda d\lambda,$$

where with a slight abuse of notating we define $\gamma_\lambda \triangleq \gamma_r(\lambda \mu_1 + \bar{\lambda} \mu_2)$ and

$$\dot{\gamma}_\lambda = \frac{d}{d\lambda} \gamma_\lambda = \sum_{j=1}^d \frac{\partial \gamma_r}{\partial \mu_j}(\mu_{1,j} - \mu_{2,j}) = \Sigma(\gamma_\lambda)^{-1} \Delta. \quad (141)$$

Then we have

$$d_J(P_{\gamma_1}, P_{\gamma_2}) = \int_0^1 d\lambda \left\langle \hat{\Sigma}^{-1}(\lambda \mu_1 + \bar{\lambda} \mu_2) \Delta, \Delta \right\rangle \quad (142)$$

$$\leq \int_0^{1/2} d\lambda \frac{1}{\lambda} \left\langle \hat{\Sigma}^{-1}(\mu_2) \Delta, \Delta \right\rangle + \int_{1/2}^1 d\lambda \frac{1}{\lambda} \left\langle \hat{\Sigma}^{-1}(\mu_1) \Delta, \Delta \right\rangle \quad (143)$$

$$= \ln 2 \cdot \left\langle (\hat{\Sigma}^{-1}(\mu_2) + \hat{\Sigma}^{-1}(\mu_1)) \Delta, \Delta \right\rangle, \quad (144)$$

where (142) is from (141), (143) is from (140) and (144) is by computing the integrals.

Finally, consider a pair $\mu_1, \mu_2 \in M_0$ in the optimization (135), i.e. such that

$$\left\langle \hat{\Sigma}(\mu_2) \Delta, \Delta \right\rangle \leq t^2, \quad (145)$$

where as usual $\Delta = \mu_1 - \mu_2$. We set

$$\mu'_1 = \frac{2}{3} \mu_1 + \frac{1}{3} \mu_2, \quad \mu'_2 = \frac{1}{3} \mu_1 + \frac{2}{3} \mu_2. \quad (146)$$

From convexity we have $\mu'_1, \mu'_2 \in M_0$ and also

$$\left\langle \mu'_1 - \mu'_2, g \right\rangle = \frac{1}{3} \left\langle \Delta, g \right\rangle. \quad (147)$$

We claim that for some constant $c' > 0$ we have

$$d_J(\hat{P}_{\mu'_1}, \hat{P}_{\mu'_2}) \leq c't^2, \quad (148)$$

which, together with (148) would clearly establish (127). Notice that from (146) and (140) we have

$$\left\langle \hat{\Sigma}^{-1}(\mu'_1) \Delta, \Delta \right\rangle \leq 3 \left\langle \hat{\Sigma}^{-1}(\mu_2) \Delta, \Delta \right\rangle \quad (149)$$

$$\left\langle \hat{\Sigma}^{-1}(\mu'_2) \Delta, \Delta \right\rangle \leq \frac{3}{2} \left\langle \hat{\Sigma}^{-1}(\mu_2) \Delta, \Delta \right\rangle. \quad (150)$$

Hence, the left-hand side in (144) is upper-bounded by a constant multiple of $\langle \hat{\Sigma}(\mu_2) \Delta, \Delta \rangle$, which, in view of (145), shows (148).
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A Auxiliary results from convex analysis

Lemma 14 (Auxiliary convex analysis). Let $X$ and $Y$ be a dual pair of finite-dimensional vector spaces and $\Pi$ a compact convex subset of $X$. Let $f(x, y)$ be a function on $\Pi \times Y$ concave in $x$ and convex in $y$. Assume in addition:

1. There exists $e_0 \in Y$ such that $\langle x, e_0 \rangle = 1$ for any $x \in \Pi$.
2. We have $f(x, y + ce_0) = f(x, y)$ for any $c \in \mathbb{R}$.
3. For any $c \in \mathbb{R}$ we have\footnote{In particular, this implies that $f(x, y) = f(x, -y)$, $f(x, 0) = 0$ and $f \geq 0$.}

$$f(x, cy) = |c|f(x, y).$$

Fix $g \in Y$ and define the following quantities

$$d(x'\|x) \triangleq \sup \{\langle x - x', y \rangle : f(x, y) \leq 1\}, \quad (151)$$
$$d_S(x', x) \triangleq d(x', (x + x')/2), \quad (152)$$
$$\delta_0(t) \triangleq \inf_{y \in \Pi} \max_{x \in \Pi} tf(x, y) + |\langle x, g - y \rangle|, \quad (153)$$
$$\delta_1(t) \triangleq \sup_{x, x' \in \Pi} \{\langle x - x', g \rangle : d(x'\|x) \leq t\}, \quad (154)$$
$$\delta_2(t) \triangleq \sup_{x, x' \in \Pi} \{\langle x - x', g \rangle : d_S(x', x) \leq t\}. \quad (155)$$

We claim the following:

1. $d_S(x', x) = d_S(x, x')$
2. $d_S(x', x) \leq d(x\|x')$
3. $\frac{1}{2}\delta_2(t) \leq \delta_1(t) \leq \delta_2(t)$
4. And the key result:

$$\frac{1}{2}\delta_1(t) \leq \delta_0(t) \leq \delta_1(t). \quad (156)$$

Proof. 1. This is clear.

2. To prove $d(x'\|(x + x')/2) \leq d(x\|x')$ just notice that $f((x + x')/2, y) \leq 1$ implies $f(x, y) \leq 2$ by concavity and positivity.

3. Implied from above.
4. For the lower bound notice
\[
\delta_0(t) = \inf_y \sup_{x, x' \in \Pi} t \frac{f(x, y) + f(x', y)}{2} + \frac{|\langle x, g - y \rangle| + |\langle x', g - y \rangle|}{2}.
\]
In the inner supremum we set \(x, x'\) to be the ones achieving \(\delta_1(t)\). Then we have \(\langle x - x', g \rangle \geq \delta_1(t)\). Then for any \(y\) we have
\[
\langle x - x', y \rangle \leq tf(x, y).
\]
(157)

We further lower bound
\[
\delta_0(t) \geq \frac{1}{2} \inf_y t(f(x, y) + f(x', y)) + |\langle x - x', g - y \rangle|.
\]
(158)

\[
\geq \frac{1}{2} \inf_y tf(x, y) + |\langle x - x', g - y \rangle|.
\]
(159)

\[
\geq \frac{1}{2} \langle x - x', g \rangle + \frac{1}{2} \inf_y tf(x, y) - \langle x - x', y \rangle.
\]
(160)

where in the first step we used convexity of \(|\cdot|\), in the second positivity of \(f\) and in the last step \(|a| \geq a\). From (157) we conclude that \(\delta_0 \geq \frac{1}{2} \delta_1\).

To prove an upper bound we denote the convex hull \(\Pi_2 = \text{co}\{0, 2\Pi\} = \{\mu x : x \in \Pi, \mu \in [0, 2]\}\)
and notice
\[
\delta_0(t) \leq \inf_y \sup_{x, x' \in \Pi_2} tf(x, y) + \langle x - x', g - y \rangle.
\]
We now apply minimax theorem to get
\[
\delta_0(t) \leq \sup_{x \in \Pi, x' \in \Pi_2} \inf_y tf(x, y) + \langle x - x', g - y \rangle
\]
We notice that the inner infimum is \(-\infty\) unless \(\langle x - x', h \rangle = 0\), i.e. that \(x' \in \Pi\), and thus
\[
\delta_0(t) \leq \sup_{x \in \Pi, x' \in \Pi} \inf_y tf(x, y) + \langle x - x', g - y \rangle.
\]
(161)

Due to the homogeneity of \(f(x, \cdot)\) we see that further
\[
\inf_y tf(x, y) - \langle x - x', y \rangle = \begin{cases} -\infty, & d(x' || x) > t, \\ 0, & d(x' || x) \leq t \end{cases}
\]

Consequently, the right-hand side of (161) evaluates to exactly \(\delta_1(t)\).

\[\square\]

B Proof of technical results

Proof of Lemma 5. In [PSW17, Proposition 9] it is shown for any \(d \in \mathbb{N} \cup \{\infty\}\),
\[
\delta^{(3)}_{TV}(t, d) \leq t^{\min(1, \frac{1}{d})}.
\]
(162)
where \(\delta^{(3)}_{TV}(t, d)\) is defined for the same problem as \(\delta^{(3)}_{\chi^2}\) but with TV-distance in place of \(\chi^2\), cf. (9).

From the general relation \(\delta_{\chi^2} \leq \delta_{TV}\) in (13) we get (36).
Note that due to (14) and (13), for $\epsilon \leq \frac{1}{2}$ the bound (36) already establishes that

$$\frac{1}{4} t \leq \delta_{\chi^2}(t, d) \leq t, \quad i \in \{1, 2, 3\}.$$  

Next, we consider the case of $\epsilon > 1/2$. [PSW17, Lemma 12] has shown the following: For every $\delta < \frac{1}{2\sqrt{2}}$ and $d \geq \frac{2\epsilon}{\sqrt{\epsilon}} \ln \frac{1}{\delta}$ there exists a pair of probability distributions $\pi$ and $\pi'$ on $\{0, \ldots, d\}$ such that $|\pi(0) - \pi'(0)| \geq \delta$ and

$$H^2(\pi P^{(3)}, \pi' P^{(3)}) \leq 36 \left( e\delta \ln \frac{1}{\delta} \right) \frac{2\epsilon}{\sqrt{\epsilon}}.$$  

Setting the RHS to $t^2$, we conclude that there exist $t_0 = t_0(\epsilon)$ and $C = C(\epsilon)$ such that for all $t \leq t_0$ and $d \geq C \ln^2 \frac{1}{t}$, we have

$$\delta_{H^2}(t, d) \geq C \left( \frac{t}{\ln^2 1/t} \right)^{\frac{1-\epsilon}{4\epsilon}}.$$  

This implies the desired (37) in view of the general inequality $\delta_{\chi^2} \geq \frac{1}{2} \delta_{H^2}$ in (13).

Finally, to show (38) we only need to invoke [PSW17, Eqn. (61)] which shows that by adding zeros to $\pi, \pi'$ to increase the dimension from $d = \Omega(\ln^4 \frac{1}{\epsilon})$ (as before) to $d = \Omega(\frac{1}{\epsilon^2} \ln \frac{1}{\epsilon})$ we get instead of (163):

$$H^2(\pi P^{(2)}, \pi' P^{(2)}) \leq 144 \left( e\delta \ln \frac{1}{\delta} \right) \frac{2\epsilon}{\sqrt{\epsilon}}.$$  

By the same argument as above we conclude (38). □

**Proof of Lemma 7.** We first prove the upper bound. First, note that any $f \in \mathcal{P}(\beta, L)$ is everywhere bounded from above by some constant $C = C(\alpha, L)$, thanks to the fact that $f \geq 0$ and $\int f = 1$. Thus, for any $f, g \in \mathcal{P}(\beta, L)$ such that $|f(0) - g(0)| = \epsilon$ and $\chi^2(f||g) \leq t^2$, we have $\|f - g\|_2^2 \leq Ct^2$. Let $p = |f - g|$. Then $p \geq 0$ and $p$ is $(\beta, 2L)$-Hölder continuous. For sufficiently small $\epsilon$, define $h : [-1, 1] \to \mathbb{R}_+$ by $h(x) = \max\{\epsilon - 2L|x|^{\beta}, 0\}$. Then $p \geq h$ on $[-1, 1]$ pointwise and hence

$$Ct^2 \geq \|f - g\|_2^2 \geq \|h\|_2^2 = C'\epsilon^{2 + \frac{2}{\beta}}$$

for some constant $C'$ depending on $(\beta, L)$. This shows the upper bound. The lower bound follows from choosing $f$ to be the uniform distribution, and $g(x) = f(x) + c|x|^{\beta} \text{sign}(x)1_{\{|x|^{\beta} \leq \epsilon\}}$, for some small constant $c$ depending on $(\beta, L)$ and $\epsilon = t^{\frac{2\beta}{2\beta + 1}}$. □

**Proof of (46).** Let $H_k(x)$ denote the degree-$k$ Hermite polynomial and note the fact that for $X \sim N(a, 1)$, we have $\mathbb{E}[H_k(X)] = a^k$ and $\text{Var}(H_k(X)) = k! \sum_{j=0}^{k-1} \left( \frac{1}{2} \right)^j \frac{2^{2j}}{j!}$. Thus $\text{Var}(H_k(X)) \leq k! 2^k$ provided $|a| \leq 1$. Using the variational representation of the $\chi^2$-divergence (32), for any feasible solution $\pi, \pi'$ of (45), we have $|m_k(\pi) - m_k(\pi')| \leq \sqrt{k!}2^k\epsilon$, where $m_k(\pi) = \int \theta^k \pi(d\theta)$ denotes the $k$th moment of $\pi$. By existing results in approximation theory (see [CL11]), there exists a degree-$k$ polynomial $p(x) = \sum_{i=0}^{k} a_i x^i$ and a constant $C$, such that $|a_i| \leq C^k$ and sup$_{|a| \leq 1} ||a| - p(a)| \leq C$. Therefore by the triangle inequality, we have $|\int \theta^0 \pi'(d\theta) - \int \theta^0 \pi(d\theta)| \leq C + k\sqrt{k!}C^k$. Choosing $k = c\frac{\log \frac{1}{\epsilon}}{\log \log \frac{1}{\epsilon}}$ for some small constant $c$ proves the upper bound of (46).

To show the lower bound part, by the duality between best polynomial approximation and moment matching (see e.g. [WY16, Appendix E]), there exist $\pi, \pi' \in \mathcal{P}([-1, 1])$ such that $m_i(\pi) =
\[ m_i(\pi') \] for \( i = 1, \ldots, k \), and \( \int |\theta| \pi'(d\theta) - \int |\theta| \pi'(d\theta) = 2 \inf_{\deg(p)=k} \sup_{|a|\leq 1} ||a|-p(a)| \geq \frac{c}{k^2}, \] where the last inequality is well-known in the approximation theory literature \cite{CL11}. Furthermore, matching first \( k \) moments implies that the corresponding Gaussian mixture are close in \( \chi^2 \)-divergence \cite{CL11}:

\[ \chi^2(\pi' \ast \mathcal{N}(0, 1) \| \pi \ast \mathcal{N}(0, 1)) \leq \frac{c_k}{k^2}. \]

Choosing \( k = c \frac{\log \frac{1}{\delta}}{\log \log \frac{1}{\delta}} \) for some large constant \( c \) proves the desired lower bound.

**Proof of Corollary 12.** From (66) we already have that \( \sqrt{R_n^*} \asymp \omega_f(c_0/\sqrt{n}) \). Next, notice that \( \omega_f(1/\sqrt{n}) \leq \omega_f(c_0/\sqrt{c_0^2 n}) \) and then from (66) we have for all \( n \geq 2/c_0^2 \) and \( c_3 = \frac{\sqrt{2}}{c_0^2} \):

\[ \omega_f(1/\sqrt{n}) \leq \delta_a \left[ \left( c_0^2 n \right)^{-\frac{1}{2}} \right] \leq \delta_a \left( c_3/\sqrt{n} \right). \]

Dividing this inequality by \( \omega_f(c_0/\sqrt{n}) \geq \delta_a(c_2 c_0/\sqrt{n}) \) (which follows from (127)) we get

\[ 1 \leq \frac{\omega_f(1/\sqrt{n})}{\omega_f(c_0/\sqrt{n})} \leq \frac{\delta_a(c_3/\sqrt{n})}{\delta_a(c_2 c_0/\sqrt{n})} \leq \frac{c_3}{c_2 c_0}, \quad (165) \]

where in the last step we invoked (136). In all, (165) proves \( \omega_f(c_0/\sqrt{n}) \asymp \omega_f(1/\sqrt{n}) \).

To show the same claim for \( \omega_H(1/\sqrt{n}) \) we first recall that a simple application of Jensen inequality shows:

\[ -2 \log (1 - \frac{1}{2}H^2(P, Q)) = -2 \log \int \sqrt{dP dQ} \leq D(P \| Q) \]

and from symmetry we, thus have

\[ -2 \log (1 - \frac{1}{2}H^2(P, Q)) \leq \frac{1}{2}d_f(P, Q). \]

Lower bounding the left-hand side we get \( H^2(P, Q) \leq \frac{1}{2}d_f(P, Q) \leq d_f(P, Q) \) and hence \( \omega_f(t) \leq \omega_H(t) \). On the other hand, again a routine two-point argument shows for some constant \( c_4 > 0 \):

\[ \sqrt{R_n^*} \geq \omega_H(c_4/\sqrt{n}), \]

which together with (66) gives

\[ \omega_H(c_4/\sqrt{n}) \leq \sqrt{R_n^*} \leq \frac{1}{c_1} \omega_H(c_0/\sqrt{n}). \]

Arguing as before for \( \omega_H \) we conclude \( \sqrt{R_n^*} \asymp \omega_H(1/\sqrt{n}). \)

**Proof of (69) \iff (72).** To show this equivalence, first notice the representation

\[ C(\gamma + a) - C(\gamma) = \langle \mu_f(\gamma), a \rangle + \int_0^1 (1 - s) a^T \Sigma(\gamma + sa) a \, ds \]

(166)

since \( \nabla C(\gamma) = \mu_f(\gamma) \) and \( \text{Hess} C(\gamma) = \Sigma(\gamma) \) as in (58). Thus, from here (72) clearly imply (69) by virtue of

\[ a^T \Sigma(\gamma) a = \text{Var}_{P_\gamma}([X, a]). \]

(167)

Conversely, (69) implies that the function

\[ x \mapsto f_\epsilon(x) \triangleq \frac{1}{\epsilon} \left\{ C(A(x) + \epsilon a) - C(A(x)) \right\} \]

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is concave for all $\epsilon > 0$. Taking the limit $\epsilon \to 0+$, cf. (166), we conclude that $x \mapsto \langle \mu_f(A(x)), a \rangle$ is concave for any $a$ (in particular, for $-a$ as well), and hence $x \mapsto \mu_f(A(x))$ must be affine. Continuing, again from (69) we must have that

$$x \mapsto g_\epsilon(x) \triangleq \frac{1}{\epsilon} (f_\epsilon(x) - \langle \mu_f(A(x)), a \rangle)$$

is concave for any $\epsilon \neq 0$. Taking the limit as $\epsilon \to 0$, cf. (166), we conclude that $x \mapsto a^T \Sigma(A(x))a$ must be concave, which implies the second claim in (72) in view of (167). \qed

References


