Minimax Rate-Optimal Estimation of Divergences between Discrete Distributions

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Abstract

We refine the general methodology in [1] for the construction and analysis of essentially minimax estimators for a wide class of functionals of finite dimensional parameters, and elaborate on the case of discrete distributions with support size $S$ comparable with the number of observations $n$. Specifically, we determine the “smooth” and “non-smooth” regimes based on the confidence set and the smoothness of the functional. In the “non-smooth” regime, we apply an unbiased estimator for a suitable polynomial approximation of the functional. In the “smooth” regime, we construct a general version of the bias-corrected Maximum Likelihood Estimator (MLE) based on Taylor expansion.

We apply the general methodology to the problem of estimating the KL divergence between two discrete probability measures $P$ and $Q$ from empirical data in a non-asymptotic and possibly large alphabet setting. We construct minimax rate-optimal estimators for $D(P||Q)$ when the likelihood ratio is upper bounded by a constant which may depend on the support size, and show that the performance of the optimal estimator with $n$ samples is essentially that of the MLE with $n \ln n$ samples. Our estimator is adaptive in the sense that it does not require the knowledge of the support size nor the upper bound on the likelihood ratio. We show that the general methodology results in minimax-rate-optimal estimators for other divergences as well, such as the Hellinger distance and the $\chi^2$-divergence. Our approach refines the Approximation methodology recently developed for the construction of near minimax estimators of functionals of high-dimensional parameters, such as entropy, Rényi entropy, mutual information and distance and the $\chi^2$-divergence. Our approach refines the Approximation methodology recently developed for the construction of near minimax estimators of functionals of high-dimensional parameters, such as entropy, Rényi entropy, mutual information and distance and the $\chi^2$-divergence. Our approach refines the Approximation methodology recently developed for the construction of near minimax estimators of functionals of high-dimensional parameters, such as entropy, Rényi entropy, mutual information and distance and the $\chi^2$-divergence.

Index Terms

Divergence estimation, KL divergence, multivariate approximation theory, Taylor expansion, functional estimation, maximum likelihood estimator, high dimensional statistics, minimax lower bound

I. INTRODUCTION

Given jointly independent $m$ samples from $P = (p_1, \cdots, p_S)$ and $n$ samples from $Q = (q_1, \cdots, q_S)$ over some unknown common alphabet of size $S$, consider the problem of estimating a functional of the distribution of the following form:

$$F(P, Q) = \sum_{i=1}^{S} f(p_i, q_i)$$

where $f : A \to \mathbb{R}$ is a continuous function with some $A \subset [0,1]^2$. Note that by allowing $f$ to solely depend on $p$, this problem generalizes the functional estimation problem considered in [1]. Among the most fundamental of such functionals is the $f$-divergence [2]

$$D_f(P||Q) = \int f \left( \frac{dP}{dQ} \right) dQ = \sum_{i=1}^{S} f \left( \frac{p_i}{q_i} \right) q_i \tag{2}$$

for some convex function $f$ with $f(1) = 0$. The $f$-divergence serves as the fundamental information contained in binary statistical models [3] and enjoys numerable applications in information theory [4] and statistics [5].

Among many $f$-divergences, we focus on the estimation problem of the Kullback–Leibler (KL) divergence (with $f(t) = t \ln t - t + 1$) in this paper, and the general approach naturally extends to the Hellinger distance and $\chi^2$-divergence. The KL divergence is an important measure of the discrepancy between two discrete distributions $P = (p_1, \cdots, p_S)$ and $Q = (q_1, \cdots, q_S)$, defined as [6]

$$D(P||Q) = \begin{cases} \sum_{i=1}^{S} p_i \ln \frac{p_i}{q_i} & \text{if } P \ll Q, \\ +\infty & \text{otherwise}, \end{cases} \tag{3}$$

where $P \ll Q$ denotes that the absolute continuity of $P$ with respect to $Q$. Like the entropy and mutual information [7], the KL divergence is a key information theoretic measure arising naturally in data compression [8], communications [9], probability

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theory [10], statistics [11], optimization [12], machine learning [13], [14], and many other disciplines. Throughout the paper we use the squared error loss, i.e., the risk function for any estimator $\hat{D}$ is defined as
\[
L(\hat{D}; P, Q) \triangleq E_{(P,Q)}|\hat{D} - D(P||Q)|^2.
\]
(4)
The maximum risk of an estimator $\hat{D}$, and the minimax risk in estimating $D(P||Q)$ are defined as
\[
R_{\text{maximum}}(\hat{D}; U) \triangleq \sup_{(P,Q) \in U} L(\hat{D}; P, Q),
\]
\[
R_{\text{minimax}}(U) \triangleq \inf_{\hat{D}} \sup_{(P,Q) \in U} L(\hat{D}; P, Q)
\]
(5)
respectively, where $U$ is a given collection of probability measures $(P, Q)$, and the infimum is taken over all possible estimators $\hat{D}$. We aim to obtain the minimax risk $R_{\text{minimax}}(U)$ for some properly chosen $U$.

Notations: for non-negative sequences $a, b$, we use the notation $a \lesssim b$ to denote that there exists a universal constant $C$ such that $\sup_{\gamma} \frac{a}{b} \leq C$, and $a \gtrsim b$ is equivalent to $b \lesssim a$. Notation $a \asymp b$ is equivalent to $a \lesssim b$ and $b \lesssim a$. Notation $a \gg b$ means that $\liminf_{\gamma} \frac{a}{b} = \infty$, and $a \ll b$ is equivalent to $b \gg a$. We write $a \wedge b = \min\{a, b\}$ and $a \vee b = \max\{a, b\}$. Moreover, $\text{poly}_d^n$ denotes the set of all $d$-variate polynomials of degree no more than $n$, and $E_{n}[f; I]$ denotes the distance of the function $f$ to the space $\text{poly}_d^n$ in the uniform norm $\| \cdot \|_\infty, I$ on $I \subset \mathbb{R}^d$. All logarithms are in the natural base.

A. Background and main results

There have been several attempts to estimate the KL divergence for the continuous case, see [15]-[20] and references therein. These approaches usually do not operate in the minimax framework, and focus on consistency but not rates of convergence, unless strong smoothness conditions on the densities are imposed to achieve the parametric rate (i.e., $\Theta(n^{-1})$) in mean squared error. In the discrete setting, [21] and [22] proved consistency of some specific estimators without arguing minimax optimality. We note that in the discrete case, if the alphabet size $S$ is fixed and the number of samples $m, n$ go to infinity, the standard Hájek–Le Cam theory of classical asymptotics shows that the plug-in approach is asymptotically efficient [23, Thm. 8.11, Lemma 8.14]. The key challenge we face in the discrete setting is the regime where the support size $S$ can be comparable to or even larger than the number of observations $m, n$, which classical analyses do not address.

Now we consider the estimation of KL divergence between discrete distributions in a large-alphabet setting. For the choice of $U$, it may appear natural to allow $P$ to be any distribution which is absolutely continuous with respect to $Q$ with alphabet size $S$, i.e.,
\[
U_S = \{(P, Q) : P, Q \in \mathcal{M}_S, P \ll Q\}
\]
(7)
where $\mathcal{M}_S$ denotes the set of all probability measures with support size $S$. However, in this case, it turns out to be impossible to estimate the KL divergence in the minimax sense, i.e., $R_{\text{minimax}}(U_S) = \infty$ for any configuration $(S, m, n)$ with $S \geq 2$. Intuitively, this is because that the observation from the Multinomial model depends continuously on $(P, Q)$ while the KL divergence does not at extremal points. A rigorous statement and proof of this result is given in Lemma [21] of the Appendix.

It seems natural then to consider an alternative uncertainty set with bounded likelihood ratio:
\[
U_{S,u(S)} = \{(P, Q) : P, Q \in \mathcal{M}_S, \frac{p_i}{q_i} \leq u(S), \forall i\}
\]
(8)
where $u(S) \geq 1$ is an upper bound on the likelihood ratio. Since $u(S) = 1$ results in the trivial case where $D(P||Q) \equiv 0$, throughout we will assume that $u(S) \geq c$ for some constant $c > 1$.

The main result of this paper is as follows.

**Theorem 1.** For $m \gtrsim S/\ln S$, $n \gtrsim Su(S)/\ln S$, $u(S) \gtrsim (\ln S)^2$ and $\ln S \gtrsim \ln(m \vee n)$, we have
\[
R_{\text{minimax}}(U_{S,u(S)}) \asymp \left(\frac{S}{m \ln m} + \frac{Su(S)}{n \ln n}\right)^2 + \frac{(\ln u(S))^2}{m} + \frac{u(S)}{n}.
\]
(9)
Furthermore, our estimator $\hat{D}_N$ in Section [11] achieves this bound under the Poisson sampling model, and is adaptive in the sense that it does not require knowledge of $S$ or $u(S)$.

The following corollary is a direct consequence of Theorem 1. Note that $\ln S \gtrsim \ln n$ and $n \gtrsim Su(S)/\ln S$ have already implied that $\ln S \gtrsim \ln u(S)$, and thus $\ln(Su(S)) \asymp \ln S$.

**Corollary 1.** For our KL divergence estimator, the maximum mean squared error vanishes provided that $m \gg S/\ln S$ and $n \gg Su(S)/\ln S$. Moreover, if $m \ll S/\ln S$ or $n \ll Su(S)/\ln S$, then the maximum risk of any estimator for KL divergence is bounded away from zero.
Next we consider the plug-in approach in the context of minimax rate-optimality. Since it is possible that \( \hat{p}_i > 0 \) and \( \hat{q}_i = 0 \) for some \( i \in \{1, \ldots, S\} \), where \( P_m = (\hat{p}_1, \ldots, \hat{p}_S), Q_n = (\hat{q}_1, \ldots, \hat{q}_S) \) are the respective empirical probability distributions, the direct plug-in estimate \( D(P_m \| Q_n) \) may be infinity with positive probability. Hence, we use the following modification of the direct plug-in approach: when we observe that \( \hat{p}_i > 0 \) and \( \hat{q}_i = 0 \), since naturally \( \hat{q}_i \) is an integral multiple of \( 1/n \), we manually change the value of \( \hat{q}_i \) to the closed lattice \( 1/n \) of zero. More precisely, we define

\[
Q'_n = \left( \frac{1}{n} \lor \hat{q}_1, \ldots, \frac{1}{n} \lor \hat{q}_S \right)
\]

and use the estimator \( D(P_m \| Q'_n) \) to estimate the KL divergence. Note that \( Q'_n \) may not be a probability distribution (in which case \( D(P_m \| Q'_n) \) is extended in the obvious way). The performance of this modified plug-in approach is summarized in the following theorem.

**Theorem 2.** Under the Poisson sampling model, the modified plug-in estimator \( D(P_m \| Q'_n) \) satisfies

\[
R_{\text{max}}(D(P_m \| Q'_n); U_{S,n(S)}) \lesssim \left( \frac{S}{m} + \frac{SU(S)}{n} \right)^2 + \frac{(\ln u(S))^2}{m} + \frac{u(S)}{n}.
\]

Moreover, for \( m \geq 15S \) and \( n \geq 4Su(S) \), we have

\[
R_{\text{max}}(D(P_m \| Q'_n); U_{S,n(S)}) \gtrsim \left( \frac{S}{m} + \frac{SU(S)}{n} \right)^2 + \frac{(\ln u(S))^2}{m} + \frac{u(S)}{n}.
\]

The following corollary on the minimum sample complexity is immediate.

**Corollary 2.** The worst-case mean squared error of the modified plug-in estimator \( D(P_m \| Q'_n) \) vanishes if and only if \( m \gg S \lor (\ln u(S))^2 \) and \( n \gg Su(S) \).

Hence, compared with the mean squared error or the minimum sample complexity of the modified plug-in approach, the optimal estimator enjoys a logarithmic improvement. Note that \( (\ln u(S))^2 \lesssim (\ln S)^2 \ll S \) is negligible under the condition in Theorem 1 so there is no counterpart of \( S \) in Corollary 1. Specifically, the performance of the optimal estimator with \((m, n)\) samples is essentially that of the plug-in approach with \((m \ln m, n \ln n)\) samples, which is another manifestation of the effective sample size enlargement phenomenon \( \|[1, 24] \). Note that in the KL divergence example, the modified plug-in estimator \( D(P_m \| Q'_n) \) essentially exploits the plug-in idea.

After our submission of this work to arXiv, an independent study of the same problem was presented in ISIT 2016 \( [25] \) without the construction of the optimal estimator, which was added to the full version \( [26] \) that appeared later on arXiv. Specifically, the main result (i.e., Theorem 1) was also obtained in \( [26] \), while there are some differences. First, our estimator is agnostic to both the support size \( S \) and the upper bound \( u(S) \) on the likelihood ratio, while the estimator in \( [26] \) requires both. Second, as for Theorem 2, there is an unnecessary additional term \( \frac{(\ln S)^2}{m} \) in the upper bound \( (11) \) of the plug-in approach in \( [26] \), though there is a minor difference between our choices of the plug-in estimator. Third, and most significant, \( [26] \) is dedicated exclusively to the KL divergence case, while in our paper we propose a general approximation-based methodology for the estimation of a wide class of functionals, with the estimation of KL divergence serving as the main example for concrete illustration of the concepts. As additional examples, following the general recipe in the next subsection and the later analysis, the result on estimating the \( L_1 \) distance in \( [24] \) can be recovered, and for the Hellinger distance and the \( \chi^2 \)-divergence \( [2] \)

\[
H^2(P, Q) \triangleq \frac{1}{2} \sum_{i=1}^{S} (\sqrt{P_i} - \sqrt{Q_i})^2
\]

\[
\chi^2(P, Q) \triangleq \begin{cases} 
\sum_{i=1}^{S} \frac{P_i^2}{Q_i} - 1 & \text{if } P \ll Q, \\
+\infty & \text{otherwise}
\end{cases}
\]

we can similarly obtain the following results on the optimal estimation rates in the large-alphabet setting.

**Theorem 3.** For \( m \land n \gtrsim \frac{S}{\ln S} \) and \( n \gtrsim \ln(m \lor n) \), for Hellinger distance we have

\[
\inf_{T \in \mathcal{M}_S} \sup_{P \in \mathcal{M}_S} \mathbb{E}_{P}(T) \left( \hat{T} - H^2(P, Q) \right)^2 \asymp \frac{S}{(m \land n) \ln(m \land n)} + \frac{1}{m \land n}
\]

and the estimator in Section V achieves this bound without the knowledge of \( S \) under the Poisson sampling model.

**Theorem 4.** For \( n \gtrsim \frac{(\ln u(S))^2}{\ln S}, u(S) \gtrsim (\ln S)^2 \) and \( n \gtrsim \ln(m \lor n) \), for \( \chi^2 \)-divergence we have

\[
\inf_{T} \sup_{(P, Q) \in U_{S,n(S)}} \mathbb{E}_{P,Q}(T) \left( \hat{T} - \chi^2(P, Q) \right)^2 \asymp \left( \frac{S(u(S))^2}{n \ln n} \right)^2 + \frac{(u(S))^2}{m} + \frac{(u(S))^3}{n}
\]
and the estimator in Section V achieves this bound without the knowledge of either $S$ or $u(S)$ under the Poisson sampling model.

The following corollaries on the minimum sample complexities follow directly from the previous theorems.

**Corollary 3.** For Hellinger distance over $(P, Q) \in \mathcal{M}_S \times \mathcal{M}_S$, there exists an estimator with a vanishing maximum mean squared error if and only if $m \land n \gg S^2$.

**Corollary 4.** For χ²-divergence over $(P, Q) \in \mathcal{U}_{S,u(S)}$, there exists an estimator with a vanishing maximum mean squared error if and only if $m \gg (u(S))^2$ and $n \gg \frac{S(u(S))^2}{\ln S} \lor (u(S))^3$.

### B. Approximation: the general recipe

Estimation of KL divergence belongs to a large family of functional estimation problems: consider estimating the functional $G(\theta)$ of a parameter $\theta \in \Theta \subset \mathbb{R}^p$ for an experiment $\{P_0 : \theta \in \Theta\}$. There has been a recent wave of study on functional estimation of high dimensional parameters, e.g., the scaled $\ell_1$ norm $\frac{1}{n}\sum_{i=1}^n |\theta_i|$ in the Gaussian model [27], the Shannon entropy $\sum_{i=1}^S -p_i \ln p_i$ [1], [28], [30], the mutual information [1], the power sum function $\sum_{i=1}^S p_i^\alpha$ [1], the Rényi entropy $\frac{\ln \sum_{i=1}^S p_i^\alpha}{1-\alpha}$ [31] and the $\ell_1$ distance $\sum_{i=1}^S |p_i - q_i|$ [24] in Multinomial and Poisson models. Moreover, the effective sample size enlargement phenomenon holds in all these examples: the performance of the minimax estimators with $n$ samples is essentially that of the plug-in approach with $n \ln n$ samples.

The optimal estimators in the previous examples all follow the general methodology of Approximation proposed in [1]: suppose $\hat{\theta}_n$ is a consistent estimator for $\theta$, where $n$ is the number of observations. Suppose the functional $G(\theta)$ is analytic everywhere except at $\theta \in \Theta_0$. A natural estimator for $G(\theta)$ is $G(\hat{\theta}_n)$, and we know from classical asymptotics [23, Lemma 8.14] that given the benign LAN (Local Asymptotic Normality) condition [23], $G(\hat{\theta}_n)$ is asymptotically efficient for $G(\theta)$ for $\theta \notin \Theta_0$ if $\hat{\theta}_n$ is asymptotically efficient for $\theta$. In the estimation of functionals of discrete distributions, $\Theta$ is the $S$-dimensional probability simplex, and a natural candidate for $\hat{\theta}_n$ is the empirical distribution, which is unbiased for any $\theta \in \Theta$. Then the following two-step procedure is conducted in estimating $G(\theta)$.

1. **Classify the Regime:** Compute $\hat{\theta}_n$, and declare that we are in the “non-smooth” regime if $\hat{\theta}_n$ is “close” enough to $\Theta_0$. Otherwise declare we are in the “smooth” regime;
2. **Estimate:**
   - If $\hat{\theta}_n$ falls in the “smooth” regime, use an estimator “similar” to $G(\hat{\theta}_n)$ to estimate $G(\theta)$;
   - If $\hat{\theta}_n$ falls in the “non-smooth” regime, replace the functional $G(\theta)$ in the “non-smooth” regime by an approximation $G_{\text{app}}(\theta)$ (another functional) which can be estimated without bias, then apply an unbiased estimator for the functional $G_{\text{app}}(\theta)$.

Simple as it may sound, this methodology has a few drawbacks and ambiguities. In our recent work [24], we applied this general recipe to the estimation of $\ell_1$ distance between two discrete distributions, where this recipe proves to be inadequate. In the estimation of the $\ell_1$ distance, a bivariate function $f(x,y) = |x-y|$ which is non-analytic in a segment was considered, which is completely different from the previous studies [1], [28], [31] where a univariate function analytic everywhere except a point is always taken into consideration. In particular, two more topics, i.e., multivariate approximation and localization via confidence sets, were introduced and used.

**Question 1.** What if the domain of $\hat{\theta}_n$ is different from (usually larger than) $\Theta$, the domain of $\theta$?

**Question 2.** How to determine the “non-smooth” regime? What is its size?

**Question 3.** If $\hat{\theta}_n$ falls in the “non-smooth” regime, in which region should $G_{\text{app}}(\theta)$ be a good approximation of $G(\theta)$ (e.g., the whole domain $\Theta$, or a proper neighborhood of $\hat{\theta}_n$)?

**Question 4.** If $\hat{\theta}_n$ falls in the “smooth” regime, how to construct an estimator “similar” to $G(\hat{\theta}_n)$?

Other questions, such as what type/degree of approximation $G_{\text{app}}(\theta)$ should be used, were answered in more detail in [1]. Among these questions, Question 1 is a relatively new one, where the estimation of KL divergence is the second example so far for which it has arisen, where the first example on estimating the support size of a discrete distribution [32] did not explicitly propose and answer this question. Question 2 and 3 were partially addressed in [1] and [24], but the answer to Question 2 changes in view of Question 1 and further elaborations are also necessary for Question 3. As for Question 4, the previous approaches can only handle order-one bias correction, while for some problems bias correction with an arbitrary order is proved to be necessary [33]. Before answering these questions, we begin with a formal definition of confidence set in statistical experiments, which is motivated by [24].

1 A function $f$ is analytic at a point $x_0$ if and only if its Taylor series about $x_0$ converges to $f$ in some neighborhood of $x_0$. 
**Definition 1** (Confidence set). Consider a statistical model \((P_\theta)_{\theta \in \Theta}\) and an estimator \(\hat{\theta} \in \hat{\Theta}\) of \(\theta\), where \(\Theta \subset \hat{\Theta}\). For \(r \in [0,1]\), a confidence set of significance level \(r\) is a collection of sets \(\{U(x)\}_{x \in \Theta}\), where \(U(x) \subset \Theta\) for any \(x \in \Theta\), and

\[
\sup_{\theta \in \Theta} \mathbb{P}_\theta(\theta \notin U(\hat{\theta})) \leq r.
\]  
(17)

Moreover, every confidence set of significance level \(r\) can also induce a reverse confidence set \(\{V(y)\}_{y \in \Theta}\) of significance level \(r\), where \(V(y) \triangleq \{x \in \Theta : y \in U(x)\}\) for any \(y \in \Theta\), and

\[
\sup_{\theta \in \Theta} \mathbb{P}_\theta(\hat{\theta} \notin V(\theta)) \leq r.
\]  
(18)

Intuitively, if \(\{U(x)\}_{x \in \Theta}\) is a confidence set of significance level \(r\), then after observing \(\hat{\theta}\) we can conclude that \(\theta \in U(\hat{\theta})\) with error probability at most \(r\). More precisely, for any \(\theta \in \Theta\), with probability at least \(1-r\), we can get back to \(\theta\) based on \(U(\cdot)\) after observing \(\hat{\theta}\). Conversely, with probability at least \(1-r\), we can also restrict \(\hat{\theta}\) in the region \(V(\theta)\). In other words, the true parameter \(\theta\) is localized at \(U(\hat{\theta})\), and the observation \(\hat{\theta}\) is localized at \(V(\theta)\), from which the name localization via confidence sets originates. Note that confidence set of any level exists for any statistical model \((P_\theta)_{\theta \in \Theta}\) and estimator \(\hat{\theta}\), since \(U(x) \equiv \Theta\) is always a feasible confidence set of level zero (and then \(V(y) \equiv \hat{\Theta}\)). In practice, we seek confidence sets which are as small as possible. We also remark that, apart from the confidence set used in traditional hypothesis testing where \(r\) is usually chosen to be a fixed constant (e.g., 0.01), here we allow \(r\) to decay with \(n\), e.g., \(r_n \approx n^{-A}\) with some constant \(A > 0\).

For example, in the Binomial model \(np \sim B(n,p)\) with \(\Theta = [0,1]\) and any \(\Theta \subset \hat{\Theta}\), for \(r_n \approx n^{-A}\), by measure concentration (cf. Lemma 28 in Appendix A), the collection \(\{U(x)\}_{x \in [0,1]}\) with

\[
U(x) = \Theta \cap \begin{cases} 
(0, c_1 \ln n / n) & \text{if } x \leq c_1 \ln n / n, \\
[x - \sqrt{c_1 x \ln n / n}, x + \sqrt{c_1 x \ln n / n}] & \text{if } c_1 \ln n / n < x \leq 1 
\end{cases}
\]  
(19)

is a confidence set of significance level \(r_n\) assuming the universal constant \(c_1 > 0\) is large enough, and the induced reverse confidence set is contained in

\[
V(y) = [0,1] \cap \begin{cases} 
(0, 2c_1 \ln n / n) & \text{if } y \leq 2c_1 \ln n / n, \\
y - \sqrt{2c_1 y \ln n / n}, y + \sqrt{2c_1 y \ln n / n} & \text{if } 2c_1 \ln n / n < y \leq 1 
\end{cases}
\]  
(20)

which is of a similar structure. Figure 1 gives a pictorial illustration of both the confidence set and the reverse confidence set in 2D Binomial and Gaussian models, respectively.

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**Fig. 1:** Pictorial illustration of confidence set \(U(\hat{\theta})\) and reverse confidence set \(V(\theta)\) in 2D Binomial (left panel) and Gaussian (right panel) models. In the Binomial model, \(n(p_1,p_2) \sim B(n,p_1) \times B(n,p_2)\) with \((p_1,p_2) \in \Theta, (\hat{p}_1,\hat{p}_2) \in \hat{\Theta}\) and \(\Theta \subset \hat{\Theta}\). In the Gaussian model, \(\theta \sim N(\theta,\sigma^2 I_2)\) with \(\theta \in \Theta, \hat{\theta} \in \hat{\Theta}\) and \(\Theta = \hat{\Theta}\).

Now we provide answers to these questions with the help of localization via confidence sets.

1) **Question 1.** When we consider the non-analytic region of \(G(\cdot)\), we should always stick to the domain of \(\hat{\theta}_n\) instead of that of the true parameter \(\theta\) (for the existence of \(G(\hat{\theta}_n)\)). Here we assume that \(G(\cdot)\) is well-defined on the \(\Theta \supset \hat{\Theta}\), where \(\Theta\) is the domain of \(\hat{\theta}_n\). In fact, we should distinguish the “smooth” (resp. “non-smooth”) regime of \(\theta\) and that of \(\hat{\theta}_n\); we determine the corresponding regimes of \(\theta\) first, and then localize \(\hat{\theta}_n\) since \(\theta\) cannot be observed. Hence, in the first step, to make the plug-in approach \(G(\hat{\theta}_n)\) work for the estimation of \(G(\theta)\), it must be ensured that with high probability \(\hat{\theta}_n\) does not fall into the non-analytic region of \(G(\cdot)\), which is defined over \(\Theta\) instead of \(\Theta\). As a result, the non-analytic region of \(G(\cdot)\) over the domain of \(\hat{\theta}_n\) is the correct region to consider.

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2In standard terminology in statistical testing, this is also the confidence set of level \(1 - r\).
2) Question 2: We first determine the “smooth” regime $\Theta_s$ of $\theta$. Let $\hat{\Theta}_0 \subset \hat{\Theta}$ be the non-analytic region of $G(\cdot)$ over $\hat{\Theta}$. By the previous answer to Question 1, $\Theta_s$ should be set to

$$\Theta_s \triangleq \{ \theta \in \Theta : P_\theta(\hat{\theta}_n \in \Theta_0) \leq r_n \}$$

(21)

where the convergence rate $r_n$ (e.g., $r_n \asymp n^{-A}$ for some constant $A > 0$) depends on the specific problem. Usually $r_n$ can be of any negligible order compared to the minimax risk of the estimation problem. With the help of localization via confidence sets, we can just set $\Theta_s = \Theta - \bigcup_{x \in \Theta_0} U(x)$ for any confidence set $\{U(x)\}_{x \in \Theta_0}$ of significance level $r_n$.

In fact, if $\theta \in \Theta_s$ and $\hat{\theta}_n \in \hat{\Theta}_0$, we have $U(\hat{\theta}_n) \subset \bigcup_{x \in \Theta_0} U(x) = \Theta - \Theta_s$ and thus $\theta \notin U(\hat{\theta}_n)$. As a result, by definition of the confidence set we have

$$\sup_{\theta \in \Theta_s} P_\theta(\hat{\theta}_n \notin \Theta_0) \leq \sup_{\theta \in \Theta_s} P_\theta(\theta \notin U(\hat{\theta}_n)) \leq \sup_{\theta \in \Theta} P_\theta(\theta \notin U(\hat{\theta}_n)) \leq r_n$$

(22)

as desired. By taking complement we obtain the “non-smooth” regime $\Theta_{ns} \triangleq \Theta - \Theta_s$ of $\theta$.

Since we cannot observe $\theta$, we need to determine the “smooth” regime $\Theta_s$ based on $\hat{\theta}_n$ rather than $\theta$. A natural choice is given by confidence set: $\Theta_s \triangleq \{ \theta \in \Theta : \Theta_0 \supset U(\hat{\theta}_n) \}$, i.e., $\Theta_s$ contains all observations whose confidence set for the true parameter falls into the “smooth” regime $\Theta_s$. Likewise, we can define $\Theta_{ns} \triangleq \{ \hat{\theta}_n \in \Theta : \Theta_{ns} \supset U(\hat{\theta}_n) \}$ for the “non-smooth” regime based on $\hat{\theta}_n$. Since $\Theta_s \cap \Theta_{ns} = \emptyset$, it can be easily seen that $\hat{\Theta}_s \cap \Theta_{ns} = \emptyset$ as well, but one problem is that $\Theta_{ns} \cup \Theta_{ns} \subset \Theta$, i.e., some observation $\hat{\theta}_n$ is attributed to neither the “non-smooth” regime nor the “smooth” regime.

To solve this problem, we should expand $\Theta_s$ and $\Theta_{ns}$ a little bit to ensure that $\hat{\Theta}_s$ and $\hat{\Theta}_{ns}$ form a partition of $\hat{\Theta}$. In fact, this expansion can be done in many statistical models with satisfactory measure concentration properties (e.g., in Multinomial, Poisson and Gaussian models). Specifically, for some proper $r_n^{(1)} \geq r_n^{(2)}$ of order both negligible to that of the minimax risk, there exists confidence sets $\{U_1(x)\}_{x \in \Theta_0}$ and $\{U_2(x)\}_{x \in \Theta_0}$ of significance level $r_n^{(1)}$ and $r_n^{(2)}$, respectively, such that

$$\Theta_s^{(1)} \triangleq \Theta - \bigcup_{x \in \Theta_0} U_1(x)$$

(23)

$$\Theta_s^{(2)} \triangleq \Theta - \bigcup_{x \in \Theta_0} U_2(x)$$

(24)

$$\hat{\Theta}_s \triangleq \{ \hat{\theta}_n \in \hat{\Theta} : \Theta_s^{(1)} \supset U_1(\hat{\theta}_n) \}$$

(25)

$$\hat{\Theta}_{ns} \triangleq \{ \hat{\theta}_n \in \hat{\Theta} : \Theta_{ns}^{(2)} \supset U_2(\hat{\theta}_n) \}$$

(26)

satisfy that $\hat{\Theta}_s \cup \hat{\Theta}_{ns} = \hat{\Theta}$ (by passing through subsets it does not matter if $\hat{\Theta}_s \cap \hat{\Theta}_{ns} = \emptyset$). Note that in this case we must have $\Theta_s^{(1)} \cap \Theta_{ns}^{(2)} \neq \emptyset$, i.e., there exists some $\theta$ which belongs to both the “smooth” regime and the “non-smooth” regime.

The interpretation of this approach is as follows. If the true parameter $\theta$ falls in the “smooth” regime $\Theta_s^{(1)}$, then the plug-in approach will work; conversely, if the true parameter $\theta$ falls in the “non-smooth” regime $\Theta_{ns}^{(2)}$, then the approximation idea will work. Then $\Theta_s^{(1)} \cap \Theta_{ns}^{(2)} \neq \emptyset$ implies that there exists an intermediate regime such that both the plug-in approach and the approximation approach work when $\theta$ falls into this regime. This intermediate regime is unnecessary when we are given the partial information whether $\theta \in \Theta_s^{(1)}$ or $\theta \in \Theta_{ns}^{(2)}$, but it becomes important when we need to infer this partial information based on $\hat{\theta}_n$. Our target is as follows: if the true parameter $\theta$ does not fall in the “smooth” (resp. “non-smooth”) regime, then with high probability we will also declare based on $\hat{\theta}_n$ that we are not in the “smooth” (resp. “non-smooth”) regime. Mathematically, with high probability, $\theta \in \Theta - \Theta_s^{(1)}$ implies $\hat{\theta}_n \in \hat{\Theta}_{ns}$, and $\theta \in \Theta - \Theta_{ns}^{(2)}$ implies $\hat{\theta}_n \in \hat{\Theta}_s$. Note that if $\theta \in \Theta_s^{(1)} \cap \Theta_{ns}^{(2)}$ falls in the intermediate regime, either $\hat{\theta}_n \in \hat{\Theta}_s$, or $\hat{\theta}_n \in \hat{\Theta}_{ns}$ suffices for our estimator to perform well. The key fact is that this target is fulfilled by the definition of confidence sets: if $\theta \in \Theta - \Theta_s^{(1)}$ and $\hat{\theta}_n \notin \hat{\Theta}_{ns}$, we have $\hat{\theta}_n \in \hat{\Theta}_s$, and by definition of $\Theta_s$, we have $U_1(\hat{\theta}_n) \subset \Theta_s^{(1)}$, which implies $\theta \notin U_1(\hat{\theta}_n)$. As a result,

$$\sup_{\theta \in \Theta - \Theta_s^{(1)}} P_\theta(\hat{\theta}_n \notin \hat{\Theta}_{ns}) \leq \sup_{\theta \in \Theta - \Theta_s^{(1)}} P_\theta(\theta \notin U_1(\hat{\theta}_n)) \leq \sup_{\theta \in \Theta} P_\theta(\theta \notin U_1(\hat{\theta}_n)) \leq r_n^{(1)}$$

(27)

and similarly $\sup_{\theta \in \Theta - \Theta_s^{(2)}} P_\theta(\hat{\theta}_n \notin \hat{\Theta}_s) \leq r_n^{(2)}$. Hence, we successfully localize $\theta$ via confidence sets based on $\hat{\theta}_n$ such that the true parameter $\theta$ is very likely to belong to the declared regime based on $\hat{\theta}_n$.

A pictorial illustration of this idea is shown in Figure 2.

3) Question 3: Given a confidence set $\{U(x)\}_{x \in \Theta}$ of a satisfactory significance level $r_n$, after observing $\hat{\theta}_n \in \hat{\Theta}_s$ we can always set the approximation region to be $U(\hat{\theta}_n)$. Note that $U(\hat{\theta}_n) \subset \Theta_{ns}$ by definition, and in fact $U(\hat{\theta}_n)$ can be considerably smaller than $\Theta_{ns}$, which makes it a desirable regime to approximate over rather than $\Theta_{ns}$ and is proved to be necessary in [24]. The reason why $U(\hat{\theta}_n)$ is sufficient is as follows: by definition of confidence sets we have $\sup_{\theta \in \Theta} P_\theta(\theta \in U(\hat{\theta}_n)) \leq r_n$, hence with probability at least $1 - r_n$, the approximation region $U(\hat{\theta}_n)$ based on $\hat{\theta}_n$ covers $\theta$, which allows us to operate as if $\theta$ is conditioned to be inside $U(\hat{\theta})$. Note that in order to obtain a good approximation
Fig. 2: Pictorial explanation of the “smooth” and “non-smooth” regimes based on $\theta$ and $\hat{\theta}_n$, respectively. In the above figure, we have $\Theta^{(1)} = II \cup III \cup IV$, $\Theta^{(2)} = I \cup II \cup III$, $\Theta_s = III \cup IV$, and $\Theta_{ns} = I \cup II$. In particular, $\Theta^{(1)} \cap \Theta^{(2)} = II \cup III$ is the intermediate regime, where both the plug-in and the approximation approach are performing well. For $\hat{\theta}_1 \in \Theta_{ns}$, we have $U_1(\hat{\theta}_1) \subset \Theta^{(2)}$; for $\theta_2 \in \Theta_s$, we have $U_2(\theta_2) \subset \Theta^{(1)}$.

For Binomial random variable $X \sim B(n, p)$, denote the empirical frequency by $\hat{p} = \frac{X}{n}$. Then it follows from Taylor’s theorem that

$$E[\hat{p}] - f(p) = \frac{1}{2} f''(p) \text{Var}(\hat{p}) + O\left(\frac{1}{n^2}\right) = \frac{p(1-p)}{2n} f''(p) + O\left(\frac{1}{n^2}\right)$$

(28)

where $f''(p)$ is the second-order derivative of $f$ at $p$. Hence, the bias-corrected estimator in [1] was proposed as follows:

$$f^c(\hat{p}) = f(\hat{p}) - \frac{f''(\hat{p})\hat{p}(1-\hat{p})}{2n}.$$  

(29)

However, the plug-in approach was still used for the bias-correction term in the previous estimator, which should be further corrected based on Taylor expansion again in order to achieve higher-order bias correction. Continuing this approach, the further correction still suffers from the same problem and additional corrections need to be done, and so on and so forth. As a result, the previous bias-correction fails to be generalized to high-order corrections, and a successful bias-correction approach should avoid employing the plug-in approach for bias-correction terms.

One way to avoid the plug-in approach is as follows: instead of doing Taylor expansion of $G(\hat{\theta}_n)$ near $\theta$, we employ Taylor expansion of $G(\theta)$ near $\hat{\theta}_n$ as

$$G(\theta) \approx \sum_{k=0}^{T} \frac{G^{(k)}(\hat{\theta}_n)}{k!} (\theta - \hat{\theta}_n)^k.$$  

(30)

The advantage is that, now $G^{(k)}(\hat{\theta}_n)$ is by definition an unbiased estimator of $E_\theta[G^{(k)}(\hat{\theta}_n)]$. However, the unknown $\theta$ in the RHS still prevents us from using this estimator explicitly. Fortunately, this difficulty can be overcome by the standard sample splitting approach: we split samples to obtain independent $\hat{\theta}_n^{(1)}$ and $\hat{\theta}_n^{(2)}$, both of which follow the same class of distribution (with possibly different parameters) as $\hat{\theta}_n$. We remark that sample splitting can be employed for divisible distributions, including Multinomial, Poisson and Gaussian models [36].

For example, in entropy estimation, one of the earliest investigations on reducing the bias of MLE in entropy estimation is due to Miller [34]. Interestingly, it was already observed in 1969 by Carlton [35] that Miller’s bias correction formula should only be applied when $p \gg 1/n$, which is automatically satisfied when $p$ belongs to the “smooth” regime $\left[\frac{\ln n}{n}, 1\right]$ defined in [1]. As a result, in the “smooth” regime, Miller’s idea was used in [1]. In our generalization of the “smooth” regime, by definition of $\Theta_s$, $G^{(T)}(\hat{\theta}_n)$ remains bounded with high probability for any order $T > 0$ and $\theta \in \Theta_s$. Hence, it shows that Miller’s bias-correcton approach based on Taylor expansion can also be used in general. However, Miller’s approach fails when high-order bias correction is desired, or equivalently, when $T$ is large. To see why it is the case, we take a look at the procedure considered in [1].

4) Question 4: there has been a long history of correcting the bias of the MLE based on Taylor expansion. For example, in entropy estimation, one of the earliest investigations on reducing the bias of MLE in entropy estimation is due to Miller [34].
the beginning of Section III for Poisson models. Now our bias-corrected estimator is
\[
\hat{G}_s(\hat{\theta}_n) = \sum_{k=0}^{T} \frac{G^{(k)}(\hat{\theta}_n^{(1)})}{k!} \sum_{j=0}^{k} \binom{k}{j} S_j(\hat{\theta}_n^{(2)})(-\hat{\theta}_n^{(1)})^{k-j}
\]  
(31)

where \(S_j(\hat{\theta}_n^{(2)})\) is an unbiased estimator of \(\theta^j\) (which usually exists). Now it is straightforward to show that
\[
\mathbb{E}[\hat{G}_s(\hat{\theta}_n)] - G(\theta) = \mathbb{E}_\theta \left[ \sum_{k=0}^{T} \frac{G^{(k)}(\hat{\theta}_n^{(1)})}{k!} (\theta - \hat{\theta}_n^{(1)})^k - G(\theta) \right] = O(\left( \frac{T+1}{T+1} \right)^{T+1})
\]  
(32)

i.e., the estimator in (31) achieves the bias-correction of any desired order. Although in many scenarios (those in [1], [24], [27]–[30]) no bias correction or only order-one bias correction is required in the “smooth” regime, bias correction of an arbitrary order turns out to be crucial in our recent work on the estimation of nonparametric functionals [33]. We also conjecture that this approach is crucial for the construction of the minimax rate-optimal estimator for the Rényi entropy in the large alphabet setting, which [31] did not address completely.

The answers to these questions shed light on the detailed implementation of the general recipe and give rise to the important concept of localization via confidence sets, which leads us to propose a refined two-step approach. As before, denote by \(\hat{\Theta} \supset \Theta\) the set containing all possible values of the estimator \(\hat{\theta}_n\), and by \(\hat{\Theta}_0 \subset \hat{\Theta}\) the set on which \(G(\cdot)\) is non-analytic. Let \(\{U(x)\}_{x \in \hat{\Theta}}\) be a satisfactory confidence set.

1) Classify the Regime:
- For the true parameter \(\theta\), declare that \(\theta\) is in the “non-smooth” regime if \(\theta\) is “close” enough to \(\hat{\Theta}_0\) in terms of localization via confidence sets (cf. (24)). Otherwise declare \(\theta\) is in the “smooth” regime (cf. (25));
- Compute \(\hat{\theta}_n\), and declare that we are in the “non-smooth” regime if the confidence set of \(\hat{\theta}_n\) falls into the “non-smooth” regime of \(\theta\) (cf. (26)). Otherwise declare we are in the “smooth” regime (cf. (25));

2) Estimate:
- If \(\hat{\theta}_n\) falls in the “smooth” regime, use an estimator “similar” to \(G(\hat{\theta}_n)\) to estimate \(G(\theta)\);
- If \(\hat{\theta}_n\) falls in the “non-smooth” regime, replace the functional \(G(\theta)\) in the “non-smooth” regime by an approximation \(G_{\text{app}}(\theta)\) (another functional which well approximates \(G(\theta)\) on \(U(\hat{\theta}_n)\)) which can be estimated without bias, then apply an unbiased estimator for the functional \(G_{\text{app}}(\theta)\).

In this paper, we follow the refined recipe for the construction of our optimal estimator in estimating several divergences between discrete distributions, including the KL divergence, Hellinger distance and \(\chi^2\)-divergence, where only the KL divergence will be discussed in detail. Moreover, in the estimation of KL divergence, we will encounter a new phenomenon, i.e., multivariate approximation in polytopes, which is a highly non-trivial topic in approximation theory, and will also propose a general tool to analyze the risk of the bias-corrected plug-in approach with the help of localization via confidence sets.

The rest of this paper is organized as follows. We first analyze the performance of the modified plug-in estimator and prove Theorem 2 in Section II. In Section III, we first follow the general recipe to explicitly construct our estimator for the KL divergence step by step, and show that it essentially achieves the bound in Theorem 1. Then we adopt and adapt some tricks to construct another estimator which is rate-optimal, adaptive and easier to implement. The minimax lower bound for estimating the KL divergence is proved in Section IV. For the Hellinger distance and the \(\chi^2\)-divergence, we sketch the construction of the respective minimax rate-optimal estimators in Section V. Conclusions are drawn in Section VI, and complete proofs of the remaining theorems and lemmas are provided in the appendices. The Matlab code of estimating KL divergence has been released on http://www.stanford.edu/~tsachy/index_hjw.

II. PERFORMANCE OF THE MODIFIED PLUG-IN APPROACH

In this section, we give the upper bound and the lower bound of the worst-case mean squared error via the modified plug-in approach, i.e., we prove Theorem 2. Throughout our analysis, we utilize the Poisson sampling model, i.e., each component \(X_i\) (resp. \(Y_i\)) in the histogram \(X\) (resp. \(Y\)) has distribution \(\text{Poi}(m q_i)\) (resp. \(\text{Poi}(n q_i)\)), and all coordinates of \(X\) (resp. \(Y\)) are independent. In other words, instead of drawing fixed sample sizes \(m\) and \(n\), there are i.i.d. samples from distributions \(P,Q\) of sizes \(M \sim \text{Poi}(m)\) and \(N \sim \text{Poi}(n)\), respectively. Consequently, the observed number of occurrences of each symbol are independent [37] Theorem 5.6. We note that the Poisson sampling model is essentially the same as the Multinomial model, and their minimax risks are related via Lemma 22 in Appendix A.

A. Proof of upper bounds
Recall that the empirical distribution \(Q_n\) has been modified to
\[
Q'_n = \left( \frac{1}{n} \lor \hat{q}_1, \ldots, \frac{1}{n} \lor \hat{q}_s \right)
\]  
(33)
the modified plug-in estimator $D(P_m || Q_n')$ is not the exact plug-in approach. However, it can be observed that this quantity

$$D(P_m || Q_n') = \sum_{i=1}^{S} \left[ \hat{p}_i \ln \hat{p}_i - \hat{p}_i \ln \left( \frac{1}{n} \lor \hat{q}_i \right) \right]$$

(34)
is close to the following natural plug-in estimator

$$D_1(P_m || Q_n) = \sum_{i=1}^{S} \left[ \hat{p}_i \ln \hat{p}_i - \hat{p}_i g_n(\hat{q}_i) \right],$$

(35)

where

$$g_n(q) \triangleq \left\{ \begin{array}{ll}
-(1 + \ln n) + nq & \text{if } 0 \leq q < \frac{1}{n}, \\
\ln q & \text{if } \frac{1}{n} \leq q \leq 1.
\end{array} \right.$$  

(36)

In view of this fact, we can apply the general approximation-based method in [38] to analyze the performance of the plug-in approach.

By construction it is obvious that $g_n(q)$ is continuously differentiable on $[0, 1]$, which coincides with $g(q) = \ln q$ on $[\frac{1}{n}, 1]$. Moreover, since $\hat{q}_i$ is a multiple of $\frac{1}{n}$, $g_n(\hat{q}_i)$ only differs from $\ln(\frac{1}{n} \lor \hat{q}_i)$ at $\hat{q}_i = 0$ by $- (1 + \ln n) - \ln(1/n) = 1$. Hence, we may consider the performance of the plug-in estimator $\hat{p}_i(\ln \hat{p}_i - g_n(\hat{q}_i))$ in estimating $p(\ln p - g_n(q))$, which is summarized in the following lemma.

**Lemma 1.** Let $n\hat{p} \sim \text{Poi}(mp)$ and $n\hat{q} \sim \text{Poi}(nq)$ be independent, and $p \leq u(S)/q$. Then we have

$$|E[\hat{p}(\ln \hat{p} - g_n(\hat{q}))] - p(\ln p - g_n(q))| \leq \frac{30u(S)}{n} + \frac{5 \ln 2}{m},$$

(37)

$$\text{Var}(\hat{p}(\ln \hat{p} - g_n(\hat{q}))) \leq \frac{51}{m^2} + \frac{2}{m} \left( p + p(\ln u(S))^2 + \frac{4q}{e^2} + \frac{4u(S)}{en} \right) + \frac{700u(S)}{n} \left( p + \frac{1}{m} \right).$$

(38)

In particular,

$$|E[\hat{p}(\ln \hat{p} - g_n(\hat{q}))] - p(\ln p - g_n(q))| \lesssim \frac{u(S)}{n} + \frac{1}{m},$$

(39)

$$\text{Var}(\hat{p}(\ln \hat{p} - g_n(\hat{q}))) \lesssim \frac{1}{m^2} + \frac{pu(S)}{n} + \frac{u(S)}{mn} + \frac{p(1 + \ln u(S))^2}{m} + \frac{q}{m}.$$  

(40)

Hence, by Lemma[1] we conclude that

$$|E D_1(P_m || Q_n) - D_1(P || Q)| \leq \sum_{i=1}^{S} \left| E[\hat{p}_i(\ln \hat{p}_i - g_n(\hat{q}_i))] - p_i(\ln p_i - g_n(q_i)) \right|$$

(41)

$$\lesssim \sum_{i=1}^{S} \frac{u(S)}{n} + \frac{1}{m}$$

(42)

$$= \frac{Su(S)}{n} + \frac{S}{m}$$

(43)

and

$$\text{Var}(D_1(P_m || Q_n)) = \sum_{i=1}^{S} \text{Var}(\hat{p}_i g_n(\hat{q}_i))$$

(44)

$$\lesssim \sum_{i=1}^{S} \frac{1}{m^2} + \frac{p_i u(S)}{n} + \frac{u(S)}{mn} + \frac{p_i(1 + \ln u(S))^2}{m} + \frac{q_i}{m}$$

(45)

$$\lesssim \frac{S}{m^2} + \frac{u(S)}{n} + \frac{Su(S)}{mn} + \frac{(1 + \ln u(S))^2}{m}$$

(46)

$$\lesssim \frac{S}{m^2} + \frac{u(S)}{n} + \frac{(Su(S))^2}{n^2} + \frac{1}{m^2} + \frac{(\ln u(S))^2}{m}$$

(47)

$$\lesssim \frac{S}{m^2} + \frac{u(S)}{n} + \frac{(Su(S))^2}{n^2} + \frac{(\ln u(S))^2}{m}.$$  

(48)
Combining these two inequalities yields, for any \((P, Q) \in \mathcal{U}_{S, u(S)}\),
\[
\mathbb{E}(D_1(P_m || Q_n) - D_1(P || Q))^2 = \mathbb{E}D_1(P_m || Q_n) - D_1(P || Q)^2 + \text{Var}(D_1(P_m || Q_n))
\]
\[
\lesssim \left( \frac{Su(S)}{n} + \frac{S}{m} \right)^2 + \frac{u(S)}{n} + \left( \frac{\ln u(S)}{m} \right)^2.
\]

(49)  

To prove Theorem 2, it remains to compute the difference between \(D\) and \(D_1\). By the definition of \(g_n(\cdot)\), we have
\[
\mathbb{E}|D_1(P_m || Q_n) - D(P_m || Q'_n)|^2 = \mathbb{E} \left| \sum_{i=1}^{S} \hat{p}_i \mathbb{I}(\hat{q}_i = 0) \right|^2
\]
\[
\leq S \sum_{i=1}^{S} \mathbb{E}\left| \hat{p}_i \mathbb{I}(\hat{q}_i = 0) \right|^2
\]
\[
= S \sum_{i=1}^{S} \left( \hat{p}_i^2 + \frac{\hat{p}_i}{m} e^{-nq_i} \right)
\]
\[
\leq S \sum_{i=1}^{S} \left( (u(S))^2 q_i^2 e^{-nq_i} + \frac{u(S)}{m} q_i e^{-nq_i} \right)
\]
\[
\leq S \sum_{i=1}^{S} \left( (u(S))^2 \left( \frac{2}{en} \right)^2 + \frac{u(S)}{enm} \right)
\]
\[
\lesssim \left( \frac{Su(S)}{n} + \frac{S^2 u(S)}{m} \right)
\]
\[
\lesssim \left( \frac{Su(S)}{n} + \frac{S}{m} \right)^2
\]

(50)  

(51)  

(52)  

(53)  

(54)  

(55)  

(56)  

(57)

where we have used the fact that
\[
\sup_{x \in [0, 1]} x^k e^{-nx} = \left( \frac{k}{en} \right)^k.
\]

(58)

Moreover, for any \((P, Q) \in \mathcal{U}_{S, u(S)}\),
\[
|D_1(P || Q) - D(P || Q)| \leq \sum_{i=1}^{S} p_i \left( - (\ln n + 1) + nq_i - \ln q_i \right) \mathbb{I}(q_i < \frac{1}{n})
\]
\[
\leq \sum_{i=1}^{S} p_i (1 - \ln(nq_i)) \mathbb{I}(q_i < \frac{1}{n})
\]
\[
\leq u(S) \cdot \sum_{i=1}^{S} q_i (1 - \ln(nq_i)) \mathbb{I}(q_i < \frac{1}{n})
\]
\[
\lesssim \frac{Su(S)}{n}
\]

(59)  

(60)  

(61)  

(62)

where we have used that \(\sup_{q \in [0, 1/n]} q(1 - \ln(nq)) = 1/n\). Hence, by the triangle inequality, for any \((P, Q) \in \mathcal{U}_{S, u(S)}\), we have
\[
\mathbb{E}(D(P_m || Q'_n) - D(P || Q))^2 \leq 3 \left( \mathbb{E}(D_1(P_m || Q_n) - D_1(P || Q))^2 \right.\]
\[
\left. + \mathbb{E}(D_1(P_m || Q_n) - D(P_m || Q'_n))^2 + |D_1(P || Q) - D(P || Q)|^2 \right)
\]
\[
\lesssim \left( \frac{Su(S)}{n} + \frac{S}{m} \right)^2 + \frac{u(S)}{n} + \left( \frac{\ln u(S)}{m} \right)^2
\]

(63)  

(64)

which completes the proof of the upper bound in Theorem 2.
B. Proof of lower bounds

By the bias-variance decomposition of the mean squared error, to prove that the squared term in Theorem 2 serves as a lower bound, it suffices to find some \((P,Q) \in \mathcal{U}_{S,u(S)}\) such that

\[
|\mathbb{E}_{(P,Q)}D(P_m||Q_m) - D(P||Q)| \geq \frac{S u(S)}{n} + \frac{S}{m}, \tag{65}
\]

Note that here we prove this inequality based on the Multinomial model, and then obtain the result for the Poisson sampling model via Lemma 22. The construction of \((P,Q)\) is as follows: \(P = (\frac{1}{S u(S)}, \cdots, \frac{1}{S u(S)}, 1 - \frac{S - 1}{S u(S)})\) is near-uniform. We first recall from [38] that, if \(m \geq 15S\), we have

\[
\sum_{i=1}^{S} \mathbb{E}[\hat{p}_i \ln \hat{p}_i] - p_i \ln p_i \geq \frac{S - 1}{2m} - \frac{S^2}{20m^2} - \frac{1}{12m^2}. \tag{66}
\]

Next we give a lower bound for the term \(\mathbb{E}(-\ln(\hat{q}_i \lor \frac{1}{n})) - (-\ln q_i)\) for \(q_i \geq \frac{4}{n}\). We shall use the following lemma for the approximation error of the Bernstein polynomial, which corresponds to the bias in the Multinomial model. Define the Bernstein operator \(B_n\) as follows:

\[
B_n[f](x) = \sum_{i=0}^{n} \binom{n}{i} x^i (1-x)^{n-i} \cdot f\left(\frac{i}{n}\right), \quad f \in C[0,1]. \tag{67}
\]

**Lemma 2.** [39] Let \(k \geq 4\) be an even integer. Suppose that the \(k\)-th derivative of \(f\) satisfies that \(f^{(k)} \leq 0\) on \((0,1)\), and \(Q_{k-1}\) is the Taylor polynomial of order \(k-1\) of \(f\) at some point \(x_0\). Then for \(x \in [0,1]\),

\[
f(x) - B_n[f](x) \geq Q_{k-1}(x) - B_n(Q_{k-1})(x). \tag{68}
\]

Since our modification of \(\ln(\cdot)\) is not even differentiable, Lemma 2 cannot be applied directly. However, we can consider the following function instead:

\[
h_n(x) = \begin{cases} 
-\ln n + n(x - \frac{1}{n}) - \frac{n^2}{2}(x - \frac{1}{n})^2 + \frac{n^3}{3}(x - \frac{1}{n})^3 - \frac{n^4}{4}(x - \frac{1}{n})^4 & \text{if } 0 \leq x < \frac{1}{n}, \\
\ln x & \text{if } \frac{1}{n} \leq x \leq 1.
\end{cases} \tag{69}
\]

By construction it is obvious that \(h_n(x) \in C^4[0,1]\) which coincides with \(\ln x\) on \([\frac{1}{n}, 1]\). Moreover, \(h_n(\hat{q})\) only differs from \(\ln(\frac{1}{n} \lor \hat{q})\) at zero by \(|h_n(0) + \ln n| = \frac{25}{12}\). Since \(h_n(4)(x) \leq 0\), Lemma 2 can be applied here to yield the following lemma.

**Lemma 3.** For \(\frac{4}{n} \leq x \leq 1\), we have

\[
h_n(x) - B_n[h_n](x) \geq \frac{(1-x)((n+4)x-2)}{n^2 x^2} > 0. \tag{70}
\]

Since our assumption \(n \geq 4S u(S)\) ensures that for our choice of \(Q\), \(q_i \geq \frac{4}{n}\) for any \(i\). Hence, by Lemma 3 and the concavity of \(h_n(\cdot)\), we have

\[
\sum_{i=1}^{S} [p_i \ln q_i - \mathbb{E}[\hat{p}_i h_n(\hat{q}_i)]] \geq \sum_{i=1}^{S-1} \frac{1}{S} [\ln q_i - \mathbb{E}[h_n(\hat{q}_i)]] \tag{71}
\]

\[
= \frac{S - 1}{S} \cdot \frac{(Su(S))^2}{n^2} \left(1 - \frac{1}{Su(S)}\right) \left(\frac{n + 4}{2Su(S)} - 2\right) \tag{72}
\]

\[
= \frac{(S - 1)u(S)}{2n} \left(1 - \frac{1}{Su(S)}\right). \tag{73}
\]
Now note that
\[
\sum_{i=1}^{S} \left| \mathbb{E}[\hat{p}_i h_n(\hat{q}_i)] - \mathbb{E}[\hat{p}_i \ln(\frac{1}{n} \lor \hat{q}_i)] \right| \leq \frac{25}{12} \sum_{i=1}^{S} p_i \cdot \mathbb{P}(\hat{q}_i = 0) \leq \frac{25}{12} \sum_{i=1}^{S} p_i (1 - q_i)^n \leq \frac{25}{12} u(S) \sum_{i=1}^{S} q_i (1 - q_i)^n \leq \frac{25Su(S)}{3ne^4}
\]  
where we have used the fact that
\[
\sup_{x \in [\frac{1}{3} : 1]} x(1 - x)^n = \frac{4}{n} \left(1 - \frac{4}{n}\right)^n \leq \frac{4}{ne^4}.
\]  
A combination of these two inequalities yields
\[
\sum_{i=1}^{S} \left[ \mathbb{E}[-\hat{p}_i \ln(\frac{1}{n} \lor \hat{q}_i)] - (-p_i \ln q_i) \right] \geq \sum_{i=1}^{S} [p_i \ln q_i - \mathbb{E}[\hat{p}_i h_n(\hat{q}_i)]] - \sum_{i=1}^{S} [\mathbb{E}[\hat{p}_i h_n(\hat{q}_i)] - \mathbb{E}[\hat{p}_i \ln(\frac{1}{n} \lor \hat{q}_i)]] \geq \frac{(S - 1)u(S)}{2n} \left(1 - \frac{1}{Su(S)}\right) - \frac{25Su(S)}{3ne^4}.
\]  
Hence, when \( m \geq 15S \) and \( n \geq 4Su(S) \), combining (86) and (81) gives
\[
|\mathbb{E}(P,Q)D(P_m||Q'_n) - D(P||Q)| \geq \mathbb{E}(P,Q)D(P_m||Q'_n) - D(P||Q)
\]  
which gives (65), as desired.

For the remaining terms, we remark that
\[
\sup_{(P,Q) \in \mathcal{U}_{S,m,n}(\mathbb{P})} \mathbb{E}(P,Q) \left( \hat{D} - D(P||Q) \right)^2 \geq \frac{(\ln u(S))^2}{m} + \frac{u(S)}{n}
\]  
holds for any estimator \( \hat{D} \) (and thus for the modified plug-in estimator \( D(P_m||Q'_n) \)), and we postpone the proof to Section IV. Now the proof of Theorem 2 is complete.

### III. Construction of the Optimal Estimator

We stay with the Poisson sampling model in this section. For simplicity of analysis, we conduct the classical “splitting” operation \([40]\) on the Poisson random vector \( \mathbf{X} \), and obtain three independent identically distributed random vectors \( \mathbf{X}_j = [X_{1,j}, X_{2,j}, \ldots, X_{S,j}]^T, j \in \{1, 2, 3\} \), such that each component \( X_{i,j} \) in \( \mathbf{X}_j \) has distribution \( \text{Poi}(mp_i/3) \), and all coordinates in \( \mathbf{X}_j \) are independent. For each coordinate \( i \), the splitting process generates a random sequence \( \{T_{ik}\}_{k=1}^{X_i} \), such that \( \{T_{ik}\}_{k=1}^{X_i} \sim \text{Multinomial}(X_i; 1/3, 1/3, 1/3) \), and assign \( X_{i,j} = \sum_{k=1}^{X_i} 1(T_{ik} = j) \) for \( j \in \{1, 2, 3\} \). All the random variables \( \{T_{ik}\}_{k=1}^{X_i} : 1 \leq i \leq S \) are conditionally independent given our observation \( \mathbf{X} \). The splitting operation is similarly conducted for the Poisson random vector \( \mathbf{Y} \).

For simplicity, we re-define \( m/3 \) as \( m \) and \( n/3 \) as \( n \), and denote
\[
\hat{p}_{i,j} = X_{i,j}/m, \quad \hat{q}_{i,j} = Y_{i,j}/n, \quad i \in \{1, 2, \ldots, S\}, \quad j \in \{1, 2, 3\}.
\]  
We remark that the “splitting” operation is not necessary in implementation. We also note that for independent random variables \( (X, Y) \) such that \( nX \sim \text{Poi}(m\rho), nY \sim \text{Poi}(n\rho) \),
\[
\mathbb{E} \prod_{r=0}^{k-1} (X - \frac{r}{m}) \prod_{s=0}^{l-1} (Y - \frac{s}{n}) = p^k q^l,
\]  
for any \( k, l \in \mathbb{N} \). For a proof of this fact we refer to Withers [41] Example 2.8].
A. Estimator construction

Now we apply our general recipe to construct the estimator. Note that

\[
D(P||Q) = \sum_{i=1}^{S} p_i \ln \frac{p_i}{q_i} = \sum_{i=1}^{S} p_i \ln p_i - \sum_{i=1}^{S} p_i \ln q_i = -H(P) - \sum_{i=1}^{S} p_i \ln q_i \tag{88}
\]

where \(H(P) = \sum_{i=1}^{S} -p_i \ln p_i\) is the entropy function. Hence, the optimal estimator \(\hat{H}\) for entropy [1], [28]-[30] can be used here and it remains to estimate the cross entropy \(\sum_{i=1}^{S} p_i \ln q_i\), i.e., our target is the bivariate function \(f(p, q) = p \ln q\).

We first classify the regime. For the bivariate function \(f(p, q) = p \ln q\), the entire parameter set is \(\Theta = \{(p, q) \in [0, 1]^2 : p \leq u(S)q\}\), and the function is analytic everywhere except for \(\Theta_0 = \{(0, 0)\}\). For all possible values of the estimator \((\hat{p}, \hat{q})\), we have \(\hat{\Theta} = [0, 1]^2\), and non-analytic points are \(\hat{\Theta}_0 = [0, 1] \times \{0\}\). For the confidence set of this two-dimensional Poisson model \((\hat{m}, \hat{n}) \sim \text{Poi}(mp) \times \text{Poi}(nq)\), we can set \(r_n \propto n^{-A}\) for some universal constant \(A > 0\) and use

\[
U(x, y) = \Theta \cap \left\{ \begin{array}{ll}
[0, \frac{c \ln m}{m}] & \text{if } x \leq \frac{c \ln m}{m}, \\
\left[x - \sqrt{\frac{c x \ln m}{m}}, x + \sqrt{\frac{c x \ln m}{m}}\right] & \text{if } \frac{c \ln m}{m} < x \leq 1, \\
\left[y - \sqrt{\frac{c y \ln n}{n}}, y + \sqrt{\frac{c y \ln n}{n}}\right] & \text{if } \frac{c \ln n}{n} < y \leq 1,
\end{array} \right. \tag{89}
\]

for some constant \(c > 0\). Hence, by choosing \(c = c_1/2\) and \(c = 2c_1\) respectively in [23] and [24] for some universal constant \(c_1 > 0\) to be specified later, we get the “smooth” and “non-smooth” regimes for \((p, q)\) as (for brevity we omit the superscripts in [23] and [24])

\[
\Theta_s = \Theta \cap \left\{ [0, 1] \times \left[\frac{c_1 \ln n}{2n}, 1\right] \right\} = \left\{ (p, q) \in [0, 1]^2 : \frac{c_1 \ln n}{2n} \leq q \leq 1, p \leq u(S)q \right\} \tag{90}
\]

\[
\Theta_m = \Theta \cap \left\{ [0, 1] \times [0, \frac{2c_1 \ln n}{n}] \right\} = \left\{ (p, q) \in [0, 1]^2 : 0 \leq q \leq \frac{2c_1 \ln n}{n}, p \leq u(S)q \right\}. \tag{91}
\]

Further, by [25] and [26], the ultimate “smooth” and “non-smooth” regimes are given by

\[
\hat{\Theta}_s = [0, 1] \times \left[\frac{c_1 \ln n}{n}, 1\right], \quad \hat{\Theta}_m = [0, 1] \times [0, \frac{c_1 \ln n}{n}] \tag{92}
\]

i.e., we are in the “non-smooth” regime if \(\hat{q} \leq \frac{c_1 \ln n}{n}\), and are in the “smooth” regime otherwise.

Next we construct the estimator in each regime. First, if we are in the “smooth” regime, our bias-corrected estimator [31] of order \(T = 3\) becomes

\[
T^{(3)}(\hat{q}_1, \hat{q}_2) = \sum_{k=0}^{3} \frac{g^{(k)}(\hat{q}_1)}{k!} \sum_{j=0}^{k} \binom{k}{j} S_j(\hat{q}_2)(-\hat{q}_1)^{k-j} \tag{93}
\]

\[
= \ln \hat{q}_1 + \frac{\hat{q}_2 - \hat{q}_1}{\hat{q}_1} - \frac{(\hat{q}_2 - \hat{q}_1)^2}{2\hat{q}_1^2} + \frac{3\hat{q}_2}{2\hat{q}_1^2} + \frac{(\hat{q}_2 - \hat{q}_1)^3}{3\hat{q}_1^3} - \frac{\hat{q}_2^2}{n\hat{q}_1^2} + \frac{2\hat{q}_2}{n^2\hat{q}_1^2} \tag{94}
\]

for estimating \(g(q) = \ln q\). Note that in the Poisson model \(n\hat{q} \sim \text{Poi}(nq)\), by [57] we have \(S_j(\hat{q}_2) = \prod_{k=0}^{j-1}(\hat{q}_2 - \frac{k}{n})\). Then for estimating \(f(p, q) = p \ln q\) in the “smooth” regime, our estimator becomes

\[
T(\hat{p}, \hat{q}_1) = T^{(3)}(\hat{q}_1, \hat{q}_2) = \hat{p}_1 \cdot T^{(3)}(\hat{q}_1, \hat{q}_2) = \hat{p}_1 \left( \ln \hat{q}_1 + \frac{\hat{q}_2 - \hat{q}_1}{\hat{q}_1} - \frac{(\hat{q}_2 - \hat{q}_1)^2}{2\hat{q}_1^2} + \frac{3\hat{q}_2}{2n\hat{q}_1^2} + \frac{(\hat{q}_2 - \hat{q}_1)^3}{3\hat{q}_1^3} - \frac{\hat{q}_2^2}{n^2\hat{q}_1^2} + \frac{2\hat{q}_2}{n^2\hat{q}_1^2} \right). \tag{95}
\]

To ensure that \(T_s\) is well-defined, it suffices to define an additional value of \(T_s\) (e.g., zero) when \(\hat{q}_1 = 0\). Note that sample splitting here is only used for the simplicity of analysis, and it is indeed not necessary in implementation. We can also replace \(\hat{p}_1\) with \(\frac{\hat{p}_1 + \hat{p}_2}{2}\) here to further reduce the variance.

Now consider the case where we are in the “non-smooth” regime, i.e., \(\hat{q} \leq \frac{c_1 \ln n}{n}\). By our general recipe, we should approximate \(f(p, q) = p \ln q\) in the approximation region given by the confidence set

\[
U(\hat{p}, \hat{q}) = \Theta \cap \left\{ \begin{array}{ll}
[0, \frac{2c_1 \ln m}{m}] & \text{if } \hat{p} \leq \frac{c_1 \ln m}{m}, \\
[\hat{p} - \frac{1}{2} \sqrt{c_1 \hat{p} \ln m}, \hat{p} + \frac{1}{2} \sqrt{c_1 \hat{p} \ln m}] & \text{if } \frac{c_1 \ln m}{m} < \hat{p} \leq 1.
\end{array} \right. \times [0, 4c_1 \ln n] \tag{96}
\]

As a result, we further distinguish the “non-smooth” regime into two sub-regimes depending on \(\hat{p} \leq \frac{c_1 \ln m}{m}\) or not, which by localization via confidence sets is essentially equivalent to \(p \leq \frac{c_1 \ln m}{m}\) or not.
If \( \hat{p} > \frac{c_1 \ln m}{m} \), the approximation region is given by
\[
\left\{ (p, q) \in [0, 1]^2 : \hat{p} - \frac{1}{2} \sqrt{\frac{c_1 \hat{p} \ln m}{m}} \leq p \leq \hat{p} + \frac{1}{2} \sqrt{\frac{c_1 \hat{p} \ln m}{m}}, 0 \leq q \leq \frac{4c_1 \ln n}{n}, p \leq u(S)q \right\}
\]
where the latter is a rectangle. Since \( q \) cannot hit zero in this approximation regime, and \( f(p, q) = p \ln q \) is a product of \( p \) and \( \ln q \), we can consider the best polynomial approximation of \( \ln q \) in this regime. As a result, in this regime, we use the approximation-based estimator
\[
T_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) = 1(\hat{p}_2 \geq \frac{c_1 \ln m}{3m}) \cdot \sum_{k=0}^{K} g_{K,k}(\hat{p}_2) \cdot \hat{p}_1 \prod_{j=0}^{k-1} \left( \hat{q}_1 - \frac{j}{n} \right)
\]
(98)
where
\[
\frac{K}{\prod_{k=0}^{K} g_{K,k}(\hat{p}) z^k = \arg \min_{P \in \text{poly}_K} \max_{z \in [1/4, 1]} (\hat{p}_2 - \frac{1}{2} \sqrt{\frac{c_1 \ln m}{m}}, \frac{4c_1 \ln n}{n}) |\ln z - P(z)|
\]
(99)
is the best 1D order-\( K \) polynomial approximation of \( g(q) = \ln q \), where \( K = c_2 \ln n \) with universal constant \( c_2 > 0 \) to be specified later. Note that \( \hat{p}_2 \geq \frac{c_1 \ln m}{m} \) ensures that the 1D approximation interval does not contain zero and is thus valid. We call this regime as “non-smooth” regime I.

If \( \hat{p} \leq \frac{c_1 \ln m}{m} \), the approximation region is given by
\[
R = \left\{ (p, q) \in [0, 1]^2 : 0 \leq p \leq \frac{2c_1 \ln m}{m}, 0 \leq q \leq \frac{4c_1 \ln n}{n}, p \leq u(S)q \right\}.
\]
(100)
Since \( q \) may be zero in \( R \), the usual best 1D polynomial approximation of \( g(q) = \ln q \) over this region does not work, and the best 2D polynomial approximation of \( f(p, q) = p \ln q \) should be employed here. Hence, in this regime the approximation-based estimator is
\[
T_{m,II}(\hat{p}_1, \hat{q}_1) = \sum_{k,l \geq 0, 0 < k + l \leq K} h_{K,k,l} \prod_{i=0}^{k-1} \left( \hat{p}_1 - \frac{i}{m} \right) \prod_{j=0}^{l-1} \left( \hat{q}_1 - \frac{j}{n} \right)
\]
(101)
where
\[
\frac{K}{\sum_{k,l \geq 0, 0 < k + l \leq K} h_{K,k,l} w^k z^l = \arg \min_{P \in \text{poly}_K} \max_{w,z \in \mathbb{R}} |w \ln z - P(w, z)|}
\]
(102)
is the best 2D order-\( K \) polynomial approximation of \( f(p, q) = p \ln q \) in \( R \), where \( K = c_2 \ln n \). Note that the condition \( k + l > 0 \) in the summation ensures that the estimator is zero for unseen symbols. We call this regime as “non-smooth” regime II.

In summary, we have the following estimator construction for \( \sum_{i=1}^{S} p_i \ln q_i \).

**Estimator Construction 1.** Conduct three-fold sample splitting to obtain i.i.d. samples \((\hat{p}_i, 1, \hat{p}_i, 2, \hat{p}_i, 3)\) and \((\hat{q}_i, 1, \hat{q}_i, 2, \hat{q}_i, 3)\). The estimator \( \hat{D}' \) for the cross entropy \( \sum_{i=1}^{S} p_i \ln q_i \) is constructed as follows:
\[
\hat{D}' = \sum_{i=1}^{S} \left[ \hat{T}_{m,1}(\hat{p}_i, 1, \hat{q}_i, 1; \hat{p}_i, 2, \hat{q}_i, 2) \mathbb{I}(\hat{p}_i, 3 > \frac{c_1 \ln m}{m}) + \hat{T}_{m,II}(\hat{p}_i, 1, \hat{q}_i, 1) \mathbb{I}(\hat{p}_i, 3 \leq \frac{c_1 \ln m}{m}) \right]
\]
\[
+ \hat{T}_s(\hat{p}_i, 1, \hat{q}_i, 1; \hat{p}_i, 2, \hat{q}_i, 2) \mathbb{I}(\hat{q}_i, 3 > \frac{c_1 \ln n}{n})
\]
(103)
where
\[
\hat{T}_{m,1}(x, y; x', y') \triangleq (T_{m,1}(x, y; x', y') \wedge 1) \vee (-1)
\]
(104)
\[
\hat{T}_{m,II}(x, y) \triangleq (T_{m,II}(x, y; x', y') \wedge 1) \vee (-1)
\]
(105)
\[
\hat{T}_s(x, y; x', y') \triangleq T_s(x, y; x', y') \cdot \mathbb{I}(y' \neq 0)
\]
(106)
and \( T_{m,1}, T_{m,II}, T_s \) are given by (98), (107) and (95), respectively. A pictorial illustration of three regimes and our estimator is displayed in Figure [FIG].

For the estimation of entropy, we essentially follow the estimator in [9]. Specifically, let \( L_H(x) \) be the lower part function
Fig. 3: Pictorial explanation of three regimes and our estimator for \( \sum_{i=1}^{S} p_i \ln q_i \). The point \((\hat{q}_1, \hat{p}_1)\) falls in the “smooth” regime, \((\hat{q}_2, \hat{p}_2)\) falls in the “non-smooth” regime I, and \((\hat{q}_3, \hat{p}_3)\) falls in the “non-smooth” regime II.

\[
\hat{p}_2 = \frac{1}{2} \sqrt{c_1 \ln m / m} \cdot \hat{p}_2
\]

“Smooth” regime: plug-in approach with order-three bias correction

“Non-smooth” regime II: unbiased estimate of best 2D polynomial approximation of \( p \ln q \)

“Non-smooth” regime I: unbiased estimate of best 1D polynomial approximation of \( \ln q \)

Finally, the overall estimator \( \hat{D} \) for \( D(P\|Q) \) is defined as

\[
\hat{D} = -\hat{D}' - \hat{H}
\]

where \( c_1, c_2 > 0 \) are suitably chosen universal constants.

B. Estimator analysis

In this subsection we will prove that the estimator constructed above achieves the minimax rate in Theorem 1. Recall that the mean squared error of any estimator \( \hat{D} \) in estimating \( D(P\|Q) \) can be decomposed into the squared bias and the variance as follows:

\[
\mathbb{E}_{(P,Q)}(\hat{D} - D(P\|Q))^2 = |\text{Bias}(\hat{D})|^2 + \text{Var}(\hat{D})
\]

where the bias and the variance are defined as

\[
\text{Bias}(\hat{D}) \triangleq \mathbb{E}_{(P,Q)} \hat{D} - D(P\|Q)
\]

\[
\text{Var}(\hat{D}) \triangleq \mathbb{E}_{(P,Q)}(\hat{D} - \mathbb{E}_{(P,Q)} \hat{D})^2
\]

respectively. Hence, it suffices to analyze the bias and the variance in these three regimes.

1) “Smooth” regime: First we consider the “smooth” regime where the true parameter \((p, q)\) belongs to \( \Theta_s \), i.e., \( q > \frac{c_1 \ln n}{2m} \). In this regime, the estimator we employ is the plug-in approach whose bias is corrected by Taylor expansion, e.g., (94). Recall defined in [1], and \( U_H(x) \) be defined as

\[
U_H(x) \triangleq -x \ln x + \frac{1}{2m}
\]

which gets rid of the interpolation function compared with the upper part function defined in [1]. Then the entropy estimator is defined as

\[
\hat{H} = \sum_{i=1}^{S} \left[ U_H(\hat{p}_{i,1}) \mathbb{1}(\hat{p}_{i,1} > \frac{c_1 \ln m}{m}) + L_H(\hat{p}_{i,1}) \mathbb{1}(\hat{p}_{i,1} \leq \frac{c_1 \ln m}{m}) \right].
\]
that the bias of our bias-corrected plug-in estimator can be expressed as
\[
|E_q T^{(r)}(\hat{q}_1, \hat{q}_2) - g(q)| = \left| E_q \sum_{k=0}^{r} \frac{g^{(k)}(q)}{k!} (q - \hat{q})^k - g(q) \right| \leq E_q \frac{g^{(r+1)}(\xi)}{(r+1)!} (q - \hat{q})^{k+1}
\]  
(113)

where \(nq \sim \text{Poi}(nq)\), and \(\xi \in [q \wedge \hat{q}, q \vee \hat{q}]\) depends on \(\hat{q}\). For smooth \(g(\cdot)\) with \(|g^{(r+1)}(\xi)|\) bounded everywhere, it suffices to consider \(\max_x |g^{(r+1)}(\xi)|\), the upper bound of the \((r+1)\)-th derivative. However, the reason why the plug-in approach and its bias-corrected version are both strictly suboptimal for the estimation of non-smooth functionals (e.g., the empirical entropy (38)) is that the functional \(g(\cdot)\) may have non-analytic points where the high-order derivatives may be unbounded. Hence, a direct application of the Taylor expansion does not work for a general non-smooth \(g(\cdot)\). However, now we are at the “smooth” regime (i.e., \((p, q) \in \Theta_0\), by our general recipe we know that with high probability \(\hat{q}\) will not fall into the non-analytic region \(\Theta_0\) of \(g(\cdot)\), thus \(g(\cdot)\) is sufficiently smooth on the segment connecting \(\hat{q}\) and \(q\), and \(\max_{q \wedge \hat{q} \leq \xi \leq q \vee \hat{q}} |g^{(r+1)}(\xi)|\) can be well controlled. In other words, the bias can be upper bounded with the help of localization via confidence sets.

Motivated by the previous insights, we begin with the following general lemma.

**Lemma 4.** Assume that the estimator in (31) is well-defined, \(E_0 \hat{\theta}_n^{(1)} = \theta\), and let \(\{V(\theta)\}_{\theta \in \Theta}\) be a reverse confidence set of level \(1 - \delta\) with \(\delta \in (0, 1)\). Further suppose that for any \(k = 0, \cdots, r\), the function \(H_k(\hat{\theta}_n^{(1)}, \hat{\theta}_n^{(2)})\) coincides with
\[
G_k(\hat{\theta}_n^{(1)}, \hat{\theta}_n^{(2)}) \triangleq \frac{\sum_j \sum_{k=0}^{r} \frac{G^{(k)}(\hat{\theta}_n^{(1)})}{k!} S_j(\hat{\theta}_n^{(2)})}{\sum_j \sum_{k=0}^{r} \frac{G^{(k)}(\hat{\theta}_n^{(1)})}{k!} S_j(\hat{\theta}_n^{(2)})} - \left( \frac{G^{(r+1)}(\hat{\theta}_n^{(1)})}{(r+1)!} \right) \delta_j(\hat{\theta}_n^{(2)})
\]

for any \(k = 0, 1, \cdots, r\),
\[
\text{Var}_0(H_k(\hat{\theta}_n^{(1)}, \hat{\theta}_n^{(2)})) \leq A_r \left( \delta \cdot \frac{\sum_j \sum_{k=0}^{r} \frac{G^{(k)}(\hat{\theta}_n^{(1)})}{k!} S_j(\hat{\theta}_n^{(2)})}{\sum_j \sum_{k=0}^{r} \frac{G^{(k)}(\hat{\theta}_n^{(1)})}{k!} S_j(\hat{\theta}_n^{(2)})} \cdot \text{Var}_0(S_{k-j}(\hat{\theta}_n^{(2)})) \right)
\]

and for any \(k = 0, 1, \cdots, r\),
\[
|E_0 H_k(\hat{\theta}_n^{(1)}, \hat{\theta}_n^{(2)})| \leq \left\{ \begin{array}{ll}
\frac{\sum_j \sum_{k=0}^{r} \frac{G^{(k)}(\hat{\theta}_n^{(1)})}{k!} S_j(\hat{\theta}_n^{(2)})}{\sum_j \sum_{k=0}^{r} \frac{G^{(k)}(\hat{\theta}_n^{(1)})}{k!} S_j(\hat{\theta}_n^{(2)})} \cdot \text{Var}_0(S_{k-j}(\hat{\theta}_n^{(2)})) & \text{if } k = 1, \\
\frac{\sum_j \sum_{k=0}^{r} \frac{G^{(k)}(\hat{\theta}_n^{(1)})}{k!} S_j(\hat{\theta}_n^{(2)})}{\sum_j \sum_{k=0}^{r} \frac{G^{(k)}(\hat{\theta}_n^{(1)})}{k!} S_j(\hat{\theta}_n^{(2)})} \cdot \text{Var}_0(S_{k-j}(\hat{\theta}_n^{(2)})) & \text{if } k \geq 2.
\end{array} \right.
\]

where \(G_{k,j}(x) \triangleq x^j G^{(k)}(x)\), and \(A_r > 0\) is a universal constant which depends on \(r\) only.

It can be seen from the previous lemma that the upper bounds of both the bias and the variance are very easy to compute, for we only need to calculate the finite-order derivatives of \(G(\cdot)\) and the moments of some usually well-behaved estimators (i.e., \(S_j(\hat{\theta}_n^{(2)})\)). Moreover, with the help of localization via confidence sets, all bounds only depend on the local behavior of function \(G(\cdot)\) (so we only require that \(H_k(\hat{\theta}_n^{(1)}, \hat{\theta}_n^{(2)})\) coincide with \(G_k(\hat{\theta}_n^{(1)}, \hat{\theta}_n^{(2)})\) when \(\hat{\theta}_n \in V(\theta)\)) plus a negligible term corresponding to the event that \(\hat{\theta}_n \not\in V(\theta)\). Note that this was the major difficult part in the analysis of the bias-corrected plug-in estimator in (1), whose proof is quite lengthy (over four pages in the proof of Lemma 2) and requires the explicit construction of the interpolation function in estimator construction. Note that in Lemma 4 we implicitly use the following “interpolation” idea: we essentially condition on the event that \(\hat{\theta}_n \in V(\theta)\), which is similar as we “interpolate” the function \(G(\hat{\theta}_n)\) using the rectangle window \(1(\hat{\theta}_n \in V(\theta))\) so as to prevent \(\max_{\xi} |G^{(r+1)}(\xi)|\) becoming infinity. Note that this interpolation is done only in the analysis but not in the construction of our estimator, and thus we remark that the explicit interpolation in (1) is indeed unnecessary given the implicit interpolation by localization via confidence sets. Following this idea, although \(U_{M}(\cdot)\) in (107) does not follow the same idea of our bias correction (31), the result in (1) can still be easily recovered without explicit interpolation.
Lemma 5. Let \( p \geq \frac{c_1 \ln m}{2m} \), and \( \hat{m} \sim \text{Poi}(mp) \). If \( c_1 \ln m \geq 4 \), the following inequalities hold:

\[
|\mathbb{E}U_H(\hat{p}) + p \ln p| \leq \frac{6}{c_1 \ln m} + 4m^{-c_1/24+2} \tag{118}
\]

\[
\text{Var}(U_H(\hat{p})) \leq A_0 \left( \frac{(p - \ln p)^2}{m} + 4m^{-c_1/24} \right) \tag{119}
\]

where \( A_0 \) is the universal constant appearing in Lemma 2.

Now we apply Lemma 6 to analyze the estimation performance of the bias-corrected plug-in estimator \( T^{(3)}(\hat{q}_1, \hat{q}_2) \) in (94).

In the Poisson model \( nq \sim \text{Poi}(nq) \) with \( q \geq \frac{c_1 \ln n}{2n} \), a natural reverse confidence set is given by

\[
V(q) = \left[ q - \frac{1}{2} \sqrt{\frac{c_1 q \ln n}{2n}}, q + \frac{1}{2} \sqrt{\frac{c_1 q \ln n}{2n}} \right], \quad q \geq \frac{c_1 \ln n}{2n}. \tag{120}
\]

By Lemma 28 we know that this reverse confidence set has level \( 1 - \delta \) with

\[
\delta \leq \sup_{q \geq \frac{c_1 \ln n}{2n}} \mathbb{P}_q(\hat{q} \notin V(q)) \leq \exp \left( -\frac{1}{3} \left( \frac{1}{2} \sqrt{\frac{c_1 q \ln n}{2n}} \right)^2 \right) \leq 2n^{-c_1/24} \tag{121}
\]

which can decay faster than any polynomial rate provided that \( c_1 \) is large enough. In this special case we can simplify the expressions in Lemma 6.

Lemma 6. Let \( q \geq \frac{c_1 \ln n}{2n} \), \((nq_1, nq_2) \sim \text{Poi}(nq) \times \text{Poi}(nq) \) and \( c_1 \ln n \geq 2 \), and \( g(\cdot) \) be an \((r+1)\) times differentiable function on \([\frac{c_1 \ln n}{2n}, 1]\). Suppose that for any \( k = 0, \cdots, r \), the function \( h_k(\hat{q}_1, \hat{q}_2) \) coincides with

\[
h_k(\hat{q}_1, \hat{q}_2) \triangleq \frac{g^{(k)}(\hat{q}_1)}{k!} \sum_{j=0}^{k} \binom{k}{j} S_j(\hat{q}_2)(-\hat{q}_1)^{k-j} \tag{122}
\]

whenever \( \hat{q}_1 \in V(q) \), and define \( h(\hat{q}_1, \hat{q}_2) \triangleq \sum_{k=0}^{r} h_k(\hat{q}_1, \hat{q}_2) \). Then there exists a universal constant \( B_r > 0 \) depending on \( r \) only such that

\[
|\mathbb{E}h(\hat{q}_1, \hat{q}_2) - g(q)| \leq B_r \left( \frac{q}{n} \right)^{r+1} \cdot \sup_{\xi \in [q/2, 2q]} |g^{(r+1)}(\xi)| + n^{-c_1/24} \cdot \left( |g(q)| + \sup_{q_1, q_2} |h(q_1, q_2)| \right) \tag{123}
\]

and for any \( k \leq r \),

\[
\text{Var}(h_k(\hat{q}_1, \hat{q}_2)) \leq B_r \left( n^{-c_1/24} \cdot \sup_{q_1, q_2} |h_k(q_1, q_2)| + \sum_{j=0}^{k} q^{2(k-j)} \left( \frac{q}{n} \right)^{k-j} \sup_{\xi \in [q/2, 2q]} |g^{(k-j)}(\xi)| + n^{-c_1/24} |g^{(k-j)}(q)|^2 \right)
\]

\[
+ \sum_{j=0}^{k-1} \frac{q^{2(k-j)-1}}{n} \left( \text{sup}_{\xi \in [q/2, 2q]} |g^{(k-j)}(\xi)| + n^{-c_1/24} |g^{(k-j)}(q)|^2 \right), \quad k \geq 0 \tag{124}
\]

\[
|\mathbb{E}h_k(\hat{q}_1, \hat{q}_2)| \leq B_r \left( \frac{q}{n} \right)^{k+1} \cdot \sup_{\xi \in [q/2, 2q]} |g^{(k+2)}(\xi)| + n^{-c_1/24} \cdot \left( |g(q)| + \sup_{q_1, q_2} |h(q_1, q_2)| \right), \quad k \geq 1 \tag{125}
\]

where \( g_k(\cdot) \triangleq q^k g^{(k)}(\cdot) \).

Note that due to the nice property of the Poisson model, the previous lemma greatly simplifies the expression involving \( S_j(\hat{q}) \), the unbiased estimate of the monomials functions. Moreover, if \( g^{(s)}(\cdot) \) becomes a power function of \( q \) for some \( s \), all summands in Lemma 6 with \( k \geq s \) will have the same order of magnitude and can thus be merged into one term. An interesting observation is that, if we change \( r \) to \( r+1 \) in this case, the order of the bias of our bias-corrected estimator is multiplied by \( \frac{1}{\sqrt{mq}} \), which is at most of the order of \( \frac{1}{\sqrt{ln n}} \) since \( q \geq \frac{c_1 \ln n}{2n} \). Hence, by continuing this bias correction approach, we can improve the bias of the plug-in approach by any desired logarithmic multiplicative factor.

Next we apply Lemma 4 to the bias-corrected estimator \( T_\text{g}(\hat{p}_1, \hat{p}_2, \hat{q}_2) \) in the smooth regime, where \( q \geq \frac{c_1 \ln n}{2n} \) and \( g(q) = \ln q \) satisfied the previous property (i.e., \( g'(q) = 1/q \) is a power of \( q \)).

Lemma 7. Let \( p \in [0, 1], q \geq \frac{c_1 \ln n}{2n}, p \leq u(S)q \), and Poisson random variables \( m(\hat{p}_1, \hat{p}_2) \sim \text{Poi}(mp) \times \text{Poi}(mp) \), \( n(\hat{q}_1, \hat{q}_2) \sim \text{Poi}(nq) \times \text{Poi}(nq) \) be independent. Moreover, let \( c_1 \ln m \geq 4 \) and \( c_1 \ln n \geq 4 \).
If $p \leq \frac{2c_1 \ln m}{m}$ is small, we have
\begin{equation}
|E[\tilde{T}_s(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) + L_H(\hat{p}_1)] + p \ln(p/q)| \leq \frac{192B_3u(S)}{c_1n \ln n} + 6B_3pn^{-c_1/2+3} + \frac{C}{m \ln m} + \left(\frac{c_1 \ln m}{m^2} \right)^4
\end{equation}
\begin{equation}
\text{Var}(\tilde{T}_s(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) + L_H(\hat{p}_1)) \leq \frac{2(2c_1 \ln m)^4}{m^2-8c_2 \ln 2} + 1600B_4 \left(\frac{p^2 + \frac{p}{m}}{m^2} \right) \left(\frac{125}{nq} + n^{-c_1/2+4} \right)
\end{equation}
where $B_3, C$ are universal constants given in Lemma 6 and Lemma 7, respectively. If $p \geq \frac{c_1 \ln m}{2m}$ is large, we have
\begin{equation}
|E[\tilde{T}_s(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) + U_H(\hat{p}_1)] + p \ln(p/q)| \leq \frac{192B_3u(S)}{c_1n \ln n} + 6B_3pn^{-c_1/2+3} + \frac{6}{c_1 \ln m} + 4m^{-c_1/2+4}
\end{equation}
\begin{equation}
\text{Var}(\tilde{T}_s(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) + U_H(\hat{p}_1)) \leq \frac{204}{m^2} + \frac{8}{m} \left(\frac{p + p \ln u(S)}{m} \right) + \frac{1}{c_1 \ln n} \left(\frac{125}{nq} + n^{-c_1/2+3} \right)
\end{equation}
In particular, if $c_1 > 96$ and $8c_2 \ln 2 < \epsilon \in (0, 1)$, the previous bounds imply that for $p \leq \frac{2c_1 \ln m}{m}$,
\begin{equation}
|E[\tilde{T}_s(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) + L_H(\hat{p}_1)] + p \ln(p/q)| \leq \frac{u(S)}{n \ln n} + \frac{1}{m \ln m} + \frac{p(1 + \ln u(S))^2}{m} + u(S) + pu(S)
\end{equation}
and for $p \geq \frac{c_1 \ln m}{2m}$,
\begin{equation}
|E[\tilde{T}_s(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) + L_H(\hat{p}_1)] + p \ln(p/q)| \leq \frac{u(S)}{n \ln n} + \frac{1}{m \ln m} + \frac{p(1 + \ln u(S))^2}{m} + \frac{u(S)}{m} + pu(S)
\end{equation}
Note that the variance bound given by Lemma 7 is a non-asymptotic result whose order coincides with that given by classical asymptotics, where the asymptotic variance is the leading term and can be obtained easily via the delta method. Now we use Lemma 7 to analyze the property of the overall estimator
\begin{equation}
\tilde{T}_s(\hat{p}, \hat{q}) = \tilde{T}_s(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) + L_H(\hat{p}_1) 1(\hat{p}_3 \leq \frac{c_1 \ln m}{m}) + U_H(\hat{p}_1) 1(\hat{p}_3 > \frac{c_1 \ln m}{m})
\end{equation}
in the “smooth” regime $q \geq \frac{c_1 \ln n}{2m}$, where $\hat{p}, \hat{q}$ are the vector representations of $\hat{p}_1, \hat{p}_2, \hat{p}_3$ and $\hat{q}_1, \hat{q}_2, \hat{q}_3$, respectively.

**Lemma 8.** Let $p \in [0, 1], q \geq \frac{2c_1 \ln n}{m}, p \leq u(S)q$, and $mp = m(\hat{p}_1, \hat{p}_2, \hat{p}_3) \sim \text{Poi}(mp)^3, nq = n(\hat{q}_1, \hat{q}_2, \hat{q}_3) \sim \text{Poi}(nq)^3$ be independent. Moreover, let $c_1 > 96$ and $8c_2 \ln 2 < \epsilon \in (0, 1)$, we have
\begin{equation}
|E[T_s(\hat{p}, \hat{q}) + p \ln(p/q)|] \leq \frac{1}{m \ln m} + \frac{u(S)}{n \ln n}
\end{equation}
\begin{equation}
\text{Var}(T_s(\hat{p}, \hat{q})) \leq \frac{1}{m^2 \epsilon^2} + \frac{p(1 + \ln u(S))^2}{m} + \frac{u(S)}{m} + pu(S) + \left(\frac{u(S)}{n \ln n} \right)^2.
\end{equation}
2) “Non-smooth” regime $I$: Next we consider the “non-smooth” regime $I$ where $p \geq \frac{c_1 \ln m}{2m}, q \leq \frac{2c_1 \ln n}{m}$. By construction of the approximation-based estimator $T_{m, 1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)$, when $\hat{p}_2 \geq \frac{c_1 \ln m}{3m}$ and the approximation region
\begin{equation}
\left[ \frac{1}{u(S)} \left( \frac{\hat{p}_2 - \frac{1}{2} \sqrt{\frac{c_1 \hat{p}_2 \ln m}{m}}}{\frac{4c_1 \ln n}{n}} \right), \frac{4c_1 \ln n}{n} \right]
\end{equation}
contains the true parameter $q$, the bias of this estimator is essentially the product of $p$ and the best polynomial approximation error of $\ln q$ in the previous approximation region. This approximation error can be easily obtained, for the 1D polynomial approximation is well-understood (Lemma 7 gives an upper bound for the approximation error of $\ln x$). Moreover, note that the previous event occurs if $\frac{c_1 \ln m}{3m} \leq \hat{p}_2 \leq p + \frac{1}{2} \sqrt{\frac{c_1 \hat{p}_2 \ln m}{m}}$, which holds with overwhelming probability by confidence sets. As for the variance, it suffices to bound the variance of each term of the form $\prod_{i=0}^{l} (Y_i - \frac{1}{2})$, where $nY \sim \text{Poi}(nq)$.
the so-called Charlier polynomial [42].

Hence, we have good tools for the analysis of both the bias and the variance of \( \hat{T}_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) \), which is presented in the following lemma.

**Lemma 9.** Let \( c_1 \ln m \leq p \leq u(S)q, q \leq \frac{2c_1 \ln n}{n} \), and Poisson random variables \( m(\hat{p}_1, \hat{p}_2) \sim \text{Poi}(mp) \times \text{Poi}(mp), n(\hat{q}_1, \hat{q}_2) \sim \text{Poi}(nq) \times \text{Poi}(nq) \) be independent. If \( c_1 \geq 2c_2 \) and \( c_2 \ln n \geq 1 \), we have

\[
|E[\hat{T}_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)] - p \ln q| \leq C_{\ln} p W \left( \frac{u(S)}{\ln n} \right) + 2m^{-c_1/36}(1 - p \ln q) + \frac{16c_1 u(S) \ln n}{n^{1-11c_2 \ln 2}} \left( \frac{2c_1 u(S) \ln n}{n} + \frac{1}{m} \right) \left( 42C_{\ln}^2 + (c_2 \ln n)^2 (C_{\ln}^2 + (\ln n)^2) \right)
\]

\[
\text{Var}(\hat{T}_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)) \leq \frac{16c_1 u(S) \ln n}{n^{1-11c_2 \ln 2}} \left( \frac{2c_1 u(S) \ln n}{n} + \frac{1}{m} \right) \left( 42C_{\ln}^2 + (c_2 \ln n)^2 (C_{\ln}^2 + (\ln n)^2) \right) + 2m^{-c_1/36}
\]

where \( W(\cdot) \) and \( C_{\ln} > 0 \) are given in Lemma 23. In particular, by Lemma 3 if \( c_1 > 72 \) and \( 11c_2 \ln 2 < e \in (0, 1) \), we have

\[
|E[\hat{T}_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) + U_H(\hat{p}_1)] + p \ln(p/q)| \leq \frac{1}{m \ln m} + p W \left( \frac{u(S)}{\ln n} \right) + \frac{u(S)(\ln n)^5}{m n^{1-e}} \left( \frac{u(S) \ln n}{n} + \frac{1}{m} \right)
\]

\[
\text{Var}(\hat{T}_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) + U_H(\hat{p}_1)) \leq \frac{p(1 + (\ln p)^2)}{m} + \frac{1}{m^3} + \frac{u(S)(\ln n)^5}{m n^{1-e}} \left( \frac{u(S) \ln n}{n} + \frac{1}{m} \right)
\]

We emphasize that the polynomial approximation in general multivariate case is extremely complicated. Rice [43] wrote:

“The theory of Chebyshev approximation (a.k.a. best approximation) for functions of one real variable has been understood for some time and is quite elegant. For about fifty years attempts have been made to generalize this theory to functions of several variables. These attempts have failed because of the lack of uniqueness of best approximations to functions of more than one variable.”

We also show in [24] that the non-uniqueness can cause serious trouble: some polynomial that achieves the best approximation error cannot be found in our general methodology in functional estimation. What if we relax the requirement of computing the best approximation in the multivariate case, and merely analyze the best approximation rate (i.e., the best approximation error up to a multiplicative constant)? That turns out to be extremely difficult. Ditzian and Totik [44, Chap. 12] obtained the best approximation in the multivariate case, and merely analyze the best approximation rate (i.e., the best approximation error). Ditzian and Totik [44, Chap. 12] obtained the best approximation in the multivariate case, and merely analyze the best approximation rate (i.e., the best approximation error).

3) “Non-smooth” regime II: Now we consider the “non-smooth” regime II where \( p \leq \frac{2c_1 \ln m}{m}, q \leq \frac{2c_1 \ln n}{n} \) and \( p \leq u(S)q \).

By the estimator construction, it is necessary to deal with the best 2D polynomial approximation of \( p \ln q \) in

\[
R = \left\{ (p, q) \in [0, 1]^2 : 0 \leq p \leq \frac{2c_1 \ln m}{m}, 0 \leq q \leq \frac{4c_1 \ln n}{n}, p \leq u(S)q \right\}
\]

We show in [24] that the non-uniqueness can cause serious trouble: some polynomial that achieves the best approximation error cannot be found in our general methodology in functional estimation. What if we relax the requirement of computing the best approximation in the multivariate case, and merely analyze the best approximation rate (i.e., the best approximation error up to a multiplicative constant)? That turns out to be extremely difficult. Ditzian and Totik [44, Chap. 12] obtained the best approximation in the multivariate case, and merely analyze the best approximation rate (i.e., the best approximation error).
Denoting by \( S_{d-1} \) the set of all unit vectors in \( \mathbb{R}^d \), we define the Ditzian–Totik modulus of smoothness as follows:
\[
\omega^r_K(f; t) = \sup_{e \in S_{d-1}} \sup_{x \in K} \sup_{h \leq t} |\Delta^r_{hdk}(e, x)e f(x)|.
\] (146)

The significance of this quantity is presented in the following lemma.

**Lemma 10.** [45] Let \( K \subset \mathbb{R}^d \) be a d-dimensional convex polytope and \( r = 1, 2, \cdots \). Then, for \( n \geq rd \), we have
\[
E_n[f; K] \leq M \omega^r_K(f, 1/n)
\] (147)
\[
\frac{M}{n^r} \sum_{k=0}^n (k + 1)^{r-1} E_k[f; K] \geq \omega^r_K(f, 1/n)
\] (148)

where the constant \( M \geq 0 \) only depends on \( r \) and \( d \).

Hence, Lemma 10 shows that once we compute the Ditzian–Totik modulus of smoothness \( \omega^r_K(f, 1/n) \) for \( f \), we immediately obtain an upper bound for the best polynomial approximation error. Moreover, Lemma 10 also shows that this is essentially also the lower bound. In our case, \( K = \mathbb{R}^d \), and \( f(p, q) = p \ln q \). Choosing \( r = 2 \), Lemma 24 gives an upper bound for the Ditzian–Totik modulus of smoothness. Moreover, tracing back to the proof for the simple polytope case in [44], it suffices to take the supremum in (146) over all directions \( e \) which are parallel to some edge of the simple polytope \( K \), which makes the evaluation of \( \omega^r_K(f, t) \) much simpler.

Now we are in position to bound the bias and the variance of \( \tilde{T}_{ns}(\hat{p}_1, \hat{q}_1) \), which are summarized in the following lemma.

**Lemma 11.** Let \( p \leq \frac{2c_1 \ln n}{m} \wedge u(S) q \leq \frac{2c_1 \ln n}{m} \), and Poisson random variables \( m(\hat{p}_1, \hat{p}_2) \sim \text{Poi}(mp) \times \text{Poi}(mp) \), \( n(\hat{q}_1, \hat{q}_2) \sim \text{Poi}(nq) \times \text{Poi}(nq) \) be independent. If \( c_1 \geq 2c_2 \) and \( c_2 \ln n \geq 1 \), we have
\[
|\mathbb{E}[\tilde{T}_{ns}(\hat{p}_1, \hat{q}_1)] - p \ln q| \leq \frac{2MC_0 u(S)}{n \ln n} + \frac{213 c_1^3 c_2^4 (u(S))^2 (\ln n)^4}{n^{2 - 26c_2 \ln 2}} \left( 1 + \left( 1 + \frac{\ln n}{\ln m} \right)^{2c_2 \ln n} + \left( \frac{n(\ln m + \ln n)}{mu(S) \ln n} \right)^{2c_2 \ln n} \right)
\] (149)
\[
\text{Var}(\tilde{T}_{ns}(\hat{p}_1, \hat{q}_1)) \leq \frac{213 c_1^3 c_2^4 (u(S))^2 (\ln n)^4}{n^{2 - 26c_2 \ln 2}} \left( 1 + \left( 1 + \frac{\ln n}{\ln m} \right)^{2c_2 \ln n} + \left( \frac{n(\ln m + \ln n)}{mu(S) \ln n} \right)^{2c_2 \ln n} \right).
\] (150)

where the universal constant \( M > 0 \) is given by Lemma 10 (with \( r = d = 2 \)), and the constant \( C_0 \) which only depends on \( c_1 \) is given by Lemma 24. In particular, by [45] Lemma 5, if \( \frac{n}{\ln n} \leq \frac{mu(S)}{\ln m} \), there exists some universal constant \( B > 0 \) such that
\[
|\mathbb{E}[\tilde{T}_{ns}(\hat{p}_1, \hat{q}_1)] + L_H(\hat{p}_1)] + p \ln(p/q)| \leq \frac{1}{m \ln m} + \frac{u(S)}{n \ln n} + \frac{(u(S))^2}{n^{2 - c_2 B}}
\] (151)
\[
\text{Var}(\tilde{T}_{ns}(\hat{p}_1, \hat{q}_1)) + L_H(\hat{p}_1)) \leq \frac{1}{m^{2 - c_2 B}} + \frac{(u(S))^2}{n^{2 - c_2 B}}.
\] (152)

We remark that the condition \( \frac{n}{\ln n} \leq \frac{mu(S)}{\ln m} \) can be removed later in the construction of the adaptive estimator. In fact, the reason why we need this condition here is that we use an arbitrary best 2D polynomial approximation, which is not unique in general. This point is very subtle: as was shown by the present authors in [24], not all polynomials which can achieve the best uniform approximation error can be used to construct the rate-optimal estimator. Actually, we will show in the next subsection that a special approximating polynomial can achieve the same rate without this condition. Moreover, a more careful design of the approximating polynomial should require different degrees on \( p \) and \( q \) (instead of fixing a total degree \( K = c_2 \ln n \)), but it has yet been unknown to approximation theorists that how to analyze the corresponding approximation error in general polytopes.

4) Overall performance: Now we analyze the performance of the entire estimator \( \hat{D}' \). For simplicity, we define
\[
T_{ns}(\hat{p}_1, \hat{q}_1) \triangleq (\tilde{T}_{ns}(\hat{p}_1, \hat{q}_1, \hat{q}_1; \hat{p}_1, \hat{q}_1, \hat{q}_2, \hat{q}_1)) + U_H(\hat{p}_1, \hat{q}_1))\mathbb{1}(\hat{p}_1, \hat{q}_1) \geq \frac{c_1 \ln n}{m} + (\tilde{T}_{ns}(\hat{p}_1, \hat{q}_1, \hat{q}_1) + L_H(\hat{p}_1, \hat{q}_1))\mathbb{1}(\hat{p}_1, \hat{q}_1) \leq \frac{c_1 \ln n}{m}
\] (153)
\[
\xi(\hat{p}_1, \hat{q}_1) \triangleq T_{ns}(\hat{p}_1, \hat{q}_1)\mathbb{1}(\hat{q}_1, \hat{q}_1) \leq \frac{c_1 \ln n}{n} + T_s(\hat{p}_1, \hat{q}_1)\mathbb{1}(\hat{q}_1, \hat{q}_1) \geq \frac{c_1 \ln n}{n}
\] (154)
where \( T_s \) is given in [134], and \( \hat{p}_1 = (\hat{p}_1, \hat{p}_1, \hat{p}_1) \) is the vector representation of the independent components, and similarly for \( \hat{q}_1 \). Based on the current notations, we have
\[
\hat{D} = - \sum_{i=1}^{S} \xi(\hat{p}_i, \hat{q}_i)
\] (155)
and by the independence between different symbols, we have

$$|	ext{Bias}(\hat{D})| \leq \sum_{i=1}^{S} |\text{Bias}(\xi(\hat{p}_i, \hat{q}_i))|$$  \hspace{1cm} (156)

$$\text{Var}(\hat{D}) = \sum_{i=1}^{S} \text{Var}(\xi(\hat{p}_i, \hat{q}_i)).$$  \hspace{1cm} (157)

Hence, it suffices to analyze the bias and the variance of each $\xi(\hat{p}_i, \hat{q}_i)$ separately and then add them all. Based on Lemma 9 and Lemma 11, the next lemma first analyzes the bias and the variance of $T_m(\hat{p}_i, \hat{q}_i)$.

**Lemma 12.** Let $0 \leq p \leq 1 \wedge u(S)q, 0 \leq q \leq \frac{2c_1 \ln n}{m}$, and $m\hat{p} = m(\hat{p}_1, \hat{p}_2, \hat{p}_3) \sim \text{Poi}(mp)^3$ and $n\hat{q} = n(\hat{q}_1, \hat{q}_2, \hat{q}_3) \sim \text{Poi}(nq)^3$ be independent. Moreover, we assume that $n \gtrsim u(S)$, $\frac{n}{m} \lesssim \frac{\ln u(S)}{\ln m}$, $c_1 > 72$ and $c_2(B \lor 11 \ln 2) < \epsilon \in (0, 1)$ (where $B$ is given in Lemma 7). Then,

1) when $p \leq \frac{c_1 \ln n}{2m}$,

$$|\text{Bias}(T_m(\hat{p}, \hat{q}))| \lesssim \frac{1}{m \ln m} + \frac{u(S)}{n \ln n} + \frac{(u(S))^2}{n^{2-\epsilon}},$$  \hspace{1cm} (158)

$$\text{Var}(T_m(\hat{p}, \hat{q})) \lesssim \frac{1}{m^{2-\epsilon}} + \frac{(u(S))^2}{n^{2-\epsilon}}.$$  \hspace{1cm} (159)

2) when $\frac{c_1 \ln n}{2m} < p < \frac{2c_1 \ln n}{m}$,

$$|\text{Bias}(T_m(\hat{p}, \hat{q}))| \lesssim \frac{1}{m \ln m} + pW\left(\frac{u(S)}{pn \ln n}\right) + \frac{u(S)}{n \ln n} + \frac{(u(S))^2}{n^{2-\epsilon}} + \frac{u(S)}{m^{1-\epsilon}},$$  \hspace{1cm} (160)

$$\text{Var}(T_m(\hat{p}, \hat{q})) \lesssim \frac{1}{m^{2-\epsilon}} + \frac{(u(S))^2}{n^{2-\epsilon}} + \frac{u(S)}{m^{1-\epsilon}} + pW\left(\frac{u(S)}{pn \ln n}\right)^2.$$  \hspace{1cm} (161)

3) when $p \geq \frac{2c_1 \ln n}{m}$,

$$|\text{Bias}(T_m(\hat{p}, \hat{q}))| \lesssim \frac{1}{m \ln m} + pW\left(\frac{u(S)}{pn \ln n}\right) + \frac{(u(S))^2}{n^{2-\epsilon}} + \frac{u(S)}{m^{1-\epsilon}},$$  \hspace{1cm} (162)

$$\text{Var}(T_m(\hat{p}, \hat{q})) \lesssim \frac{1}{m^{2-\epsilon}} + \frac{(u(S))^2}{n^{2-\epsilon}} + \frac{u(S)}{m^{1-\epsilon}}.$$  \hspace{1cm} (163)

Note that in Lemma 12, the condition $n \gtrsim u(S)$ is a natural requirement for the consistency of the optimal estimator in view of Theorem 1 and $\frac{n}{m} \lesssim \frac{\ln u(S)}{\ln m}$ is the additional condition in Lemma 11. Now based on Lemma 8 and Lemma 12, we are about to analyze the bias and the variance of $\xi(\hat{p}, \hat{q})$.

**Lemma 13.** Let $0 \leq p \leq 1 \wedge u(S)q, 0 \leq q \leq 1$, and $m\hat{p} = m(\hat{p}_1, \hat{p}_2, \hat{p}_3) \sim \text{Poi}(mp)^3$ and $n\hat{q} = n(\hat{q}_1, \hat{q}_2, \hat{q}_3) \sim \text{Poi}(nq)^3$ be independent. Moreover, we assume that $n \gtrsim u(S)$, $\frac{n}{m} \lesssim \frac{\ln u(S)}{\ln m}$, $c_1 > 96$ and $c_2(B \lor 11 \ln 2) < \epsilon \in (0, 1/2)$ (where $B$ is given in Lemma 7). Then,

1) when $q \leq \frac{c_1 \ln n}{2m}$,

$$|\text{Bias}(\xi(\hat{p}, \hat{q}))| \lesssim \begin{cases} \frac{1}{m \ln m} + \frac{u(S)}{n \ln n} + \frac{(u(S))^2}{n^{2-\epsilon}} & \text{if } p \leq \frac{c_1 \ln n}{2m}, \\
\frac{1}{m \ln m} + pW\left(\frac{u(S)}{pn \ln n}\right) + \frac{u(S)}{n \ln n} + \frac{(u(S))^2}{n^{2-\epsilon}} + \frac{u(S)}{m^{1-\epsilon}} & \text{if } c_1 \ln n \frac{2m}{m} < p < \frac{2c_1 \ln n}{m}, \\
\frac{1}{m^{2-\epsilon}} + \frac{(u(S))^2}{n^{2-\epsilon}} & \text{if } p \geq \frac{2c_1 \ln n}{m} \end{cases}$$  \hspace{1cm} (164)

$$\text{Var}(\xi(\hat{p}, \hat{q})) \lesssim \begin{cases} \frac{1}{m^{2-\epsilon}} + \frac{(u(S))^2}{n^{2-\epsilon}} & \text{if } p \leq \frac{c_1 \ln n}{2m}, \\
\frac{1}{m^{2-\epsilon}} + \frac{(u(S))^2}{n^{2-\epsilon}} + \frac{u(S)}{m^{1-\epsilon}} + pW\left(\frac{u(S)}{pn \ln n}\right)^2 & \text{if } \frac{c_1 \ln n}{2m} < p < \frac{2c_1 \ln n}{m}, \\
\frac{1}{m^{2-\epsilon}} + \frac{(u(S))^2}{n^{2-\epsilon}} + \frac{u(S)}{m^{1-\epsilon}} & \text{if } p \geq \frac{2c_1 \ln n}{m} \end{cases}$$  \hspace{1cm} (165)

2) when $\frac{c_1 \ln n}{2m} < q < \frac{2c_1 \ln n}{n}$,

$$|\text{Bias}(\xi(\hat{p}, \hat{q}))| \lesssim \begin{cases} \frac{1}{m \ln m} + \frac{u(S)}{n \ln n} + \frac{(u(S))^2}{n^{2-\epsilon}} & \text{if } p \leq \frac{c_1 \ln n}{2m}, \\
\frac{1}{m \ln m} + pW\left(\frac{u(S)}{pn \ln n}\right) + \frac{u(S)}{n \ln n} + \frac{(u(S))^2}{n^{2-\epsilon}} + \frac{u(S)}{m^{1-\epsilon}} & \text{if } \frac{c_1 \ln n}{2m} < p < \frac{2c_1 \ln n}{m}, \\
\frac{1}{m^{2-\epsilon}} & \text{if } p \geq \frac{2c_1 \ln n}{m} \end{cases}$$  \hspace{1cm} (166)

$$\text{Var}(\xi(\hat{p}, \hat{q})) \lesssim \begin{cases} \frac{1}{m^{2-\epsilon}} & \text{if } p \leq \frac{c_1 \ln n}{2m}, \\
\frac{1}{m^{2-\epsilon}} + \frac{(u(S))^2}{n^{2-\epsilon}} + \frac{u(S)}{m^{1-\epsilon}} + pW\left(\frac{u(S)}{pn \ln n}\right)^2 & \text{if } \frac{c_1 \ln n}{2m} < p < \frac{2c_1 \ln n}{m}, \\
\frac{1}{m^{2-\epsilon}} + \frac{(u(S))^2}{n^{2-\epsilon}} & \text{if } p \geq \frac{2c_1 \ln n}{m} \end{cases}$$  \hspace{1cm} (167)
3) when \( q \geq \frac{2\epsilon_1 \ln n}{n} \),

\[
|\text{Bias}(\hat{\xi}(\hat{\theta}, \hat{\phi}))| \lesssim \frac{1}{m \ln m} + \frac{u(S)}{n \ln n},
\]

\[
\text{Var}(\hat{\xi}(\hat{\theta}, \hat{\phi})) \lesssim \frac{1}{m^{2-\epsilon}} + \frac{p(1 + \ln u(S))^2}{m} + \frac{q}{m} + \frac{u(S)}{mn} + \frac{pu(S)}{n} + \left(\frac{u(S)}{n \ln n}\right)^2.
\]

Based on Lemma [13], we can analyze the total bias and variance of our estimator \( \hat{D} \). By differentiation, we have

\[
pW\left(\frac{u(S)}{pn \ln n}\right) \leq \frac{u(S)}{en \ln n} \tag{170}
\]

and the maximum is attained at \( p = \frac{u(S)}{en \ln n} \). Hence,

\[
|\text{Bias}(\hat{D})| \lesssim \sum_{i=1}^{S} |\text{Bias}(\hat{\xi}(\hat{\theta}_i, \hat{\phi}_i))| \lesssim \frac{S}{m \ln m} + \frac{Su(S)}{n \ln n} + \frac{S(u(S))^2}{n^{2-2\epsilon}} + \frac{su(S)}{mn^{1-\epsilon}} \tag{171}
\]

\[
\text{Var}(\hat{D}) = \sum_{i=1}^{S} \text{Var}(\xi(\hat{\theta}_i, \hat{\phi}_i)) \lesssim \frac{S}{m^{2-\epsilon}} + \frac{S(u(S))^2}{n^{2-2\epsilon}} + \frac{Su(S)}{mn^{1-2\epsilon}} + \frac{(1 + \ln u(S))^2}{m} + \frac{u(S)}{n}. \tag{172}
\]

If we further require that \( \ln S \gtrsim \ln (m \lor n) \) and \( n \gtrsim Su(S)/\ln S \), the previous results can be further upper bounded as (let \( \epsilon \to 0 \))

\[
|\text{Bias}(\hat{D})| \lesssim \frac{S}{m \ln m} + \frac{Su(S)}{n \ln n} + \left(\frac{Su(S)}{n \ln n}\right)^2 + \left(\frac{S}{m^2} + \frac{S(u(S))^2}{n^{2-2\epsilon}}\right) \tag{173}
\]

\[
\lesssim \frac{S}{m \ln m} + \frac{Su(S)}{n \ln n} + \left(\frac{Su(S)}{n \ln n}\right)^2 + \left(\frac{S}{m^2} + \frac{S(u(S))^2}{n^{2-4\epsilon}}\right) \tag{174}
\]

\[
\lesssim \frac{S}{m \ln m} + \frac{Su(S)}{n \ln n} \tag{175}
\]

\[
\text{Var}(\hat{D}) \lesssim \left(\frac{S}{m \ln m}\right)^2 + \left(\frac{Su(S)}{n \ln n}\right)^2 + \left(\frac{S}{m^2} + \frac{S(u(S))^2}{n^{2-2\epsilon}}\right) + \frac{(1 + \ln u(S))^2}{m} + \frac{u(S)}{n}. \tag{176}
\]

\[
\lesssim \left(\frac{S}{m \ln m}\right)^2 + \left(\frac{Su(S)}{n \ln n}\right)^2 + \frac{(\ln u(S))^2}{m} + \frac{u(S)}{n}. \tag{177}
\]

Hence we come to the following theorem.

**Theorem 5.** Let \( m \gtrsim \frac{S}{\ln S} \), \( n \gtrsim \frac{Su(S)}{\ln S} \), \( \ln S \gtrsim \ln (m \lor n) \) and \( \frac{n}{\ln n} \lesssim \frac{nu(S)}{\ln m} \). Then for our estimator \( \hat{D} \) in [48] constructed from the general recipe, we have

\[
\sup_{(P, Q) \in U_{1, u(S)}} \mathbb{E}_{(P, Q)} \left( \hat{D} - D(P \| Q) \right)^2 \lesssim \left( \frac{S}{m \ln m} + \frac{su(S)}{mn} \right)^2 + \left( \frac{\ln u(S))^2}{m} + \frac{u(S)}{n}. \right. \tag{178}
\]

Moreover, \( \hat{D} \) does not require the knowledge of the support size \( S \).

### C. An adaptive estimator

So far we have obtained an essentially minimax estimator via our general recipe. However, since this estimator is purely obtained from the general method, it is not surprising that it is also subject to some disadvantages. Firstly, in the estimator we do not specify the explicit form of the best 2D polynomial approximation in the “non-smooth” regime II. Although the best 1D polynomial approximation is unique and can be efficiently obtained via the Remes algorithm [47], which has been efficiently implemented in Matlab [48], the best 2D polynomial approximation is not unique and hard to compute. Moreover, as what we have remarked before, the non-uniqueness forces us to add an unnecessary condition \( \frac{n}{\ln n} \lesssim \frac{nu(S)}{\ln m} \) in Lemma [11] and thus in Theorem [5]. Secondly, although the estimator does not require the knowledge of the support size \( S \) (we remove the constant term in the polynomial approximation), but it requires the upper bound on the likelihood ratio \( u(S) \) (in the design of “non-smooth” regime I). In practice, we wish to obtain an adaptive estimator which achieves the minimax rate and is agnostic to both \( S \) and \( u(S) \). Thirdly, for the estimator construction in the “non-smooth” regime I, the approximating polynomial depends on the empirical probabilities (i.e., we cannot store the polynomials in advance), which incurs large computational complexity.

To resolve these issues, we need to apply some tricks to explicitly construct an approximating polynomial for \( f(p, q) = p \ln q \) in the “non-smooth” regime, i.e., \( q \leq \frac{1}{\epsilon_1 \ln n} \). We first suppose that there exists a 1D polynomial \( T(q) \) in \( q \) with degree \( \lesssim \ln n \) such that \( T(q) \) has the desired approximation property for \( f(p, q) = p \ln q \) in the entire “non-smooth” regime, i.e., we need not to distinguish “non-smooth” regimes I and II. We remark that either the 1D approximation or only one approximation on the entire “non-smooth” regime is not always doable in general. For example, for estimating the \( \ell_1 \) distance, it has been shown...
in [24] that not only any single approximation in the entire “non-smooth” regime will always fail to give the correct order of the approximation error, but any 1D polynomial approximation of \(|p - q|\) in \(p - q\) will also not work when both \(p\) and \(q\) are small. Nevertheless, this ambitious target can be achieved in our special example. Motivated by Lemma 9 and Lemma 11 the correct order of the approximation error is \(\frac{u(S)}{n \ln n}\), i.e., \(T(q)\) should satisfy
\[
\sup_{0 \leq q \leq \frac{2c_1 \ln n}{n}} |pT(q) - p \ln q| \lesssim \frac{u(S)}{n \ln n},
\]
(179)

Since \(p \leq u(S)q\), it suffices to have
\[
|T(q) - \ln q| \lesssim \frac{1}{qn \ln n}, \quad \forall q \in (0, \frac{2c_1 \ln n}{n}]
\]
i.e., to find a 1D polynomial approximation which satisfies the desired pointwise bound. However, it is easy to show that there exists some polynomial \(T_0(q)\) on \([0, \frac{2c_1 \ln n}{n}]\) such that \(\deg(T_0) \lesssim \ln n\)
\[
\sup_{0 \leq q \leq \frac{2c_1 \ln n}{n}} |T_0(q) - q \ln q| \lesssim \frac{1}{n \ln n}.
\]
(181)

Hence, if we remove the constant term of \(T_0(q)\) and define \(T(q) = T_0(q)/q\), then \(T(q)\) will have the desired property.

Motivated by the previous observations, we can construct an explicit estimator as follows:

**Estimator Construction 2.** Conduct three-fold sample splitting to obtain i.i.d. samples \((\hat{p}_1, \hat{p}_2, \hat{p}_3)\) and \((\hat{q}_1, \hat{q}_2, \hat{q}_3)\). The adaptive estimator \(\hat{D}_A\) for the KL divergence \(D(P\|Q)\) is
\[
\hat{D}_A = -\sum_{i=1}^{S} \left[ L_H(\hat{p}_i, \hat{q}_i) \mathbb{1}(\hat{q}_i, \hat{p}_i, \hat{p}_i, \hat{p}_i, \hat{q}_i, \hat{q}_i) \right.
\]
\[+ \hat{T}_m(\hat{p}_1, \hat{q}_1) \mathbb{1}(\hat{q}_1, \hat{p}_1, \hat{p}_1, \hat{p}_1, \hat{q}_1, \hat{q}_1), \left. \mathbb{1}(\hat{q}_1, \hat{p}_1, \hat{p}_1, \hat{p}_1, \hat{q}_1, \hat{q}_1) \right] \]
(182)

where \(\hat{T}_m\) is given by (106), \(L_H(x), U_H(x)\) are given by (1) and (108), respectively, and
\[
\hat{T}_m(x, y) = (T_m(x, y) \wedge 1) \vee (-1)
\]
(183)
\[
T_m(x, y) = \sum_{k=0}^{K} g_{K,k+1} \left( \frac{2c_1 \ln n}{n} \right)^{-k} \cdot x \prod_{\ell=0}^{k-1} \left( \frac{y}{n} \right)
\]
(184)

where the coefficients \(\{g_{K,k}\}_{k=1}^{K+1}\) are given by the best polynomial approximation of \(x \ln x\) as follows:
\[
g_{K,1} = r_{K,1} + \ln \left( \frac{2c_1 \ln n}{n} \right), \quad g_{K,k} = r_{K,k}, \quad 2 \leq k \leq K + 1
\]
(185)
\[
\sum_{k=0}^{K+1} r_{K,k} x^k = \arg \min_{P \in \text{poly}_{K+1}} \sup_{x \in [0,1]} |P(x) - x \ln x|.
\]
(186)

The parameters \(c_1, c_2 > 0\) are suitably chosen universal constants. A pictorial illustration of \(\hat{D}_A\) is displayed in Fig. 4.

Recall that the entropy estimator in [11] does not require the knowledge of \(S\), we conclude that \(\hat{D}_A\) always sets zero to unseen symbols and does not depend on \(u(S)\). In other words, the estimator \(\hat{D}\) for \(D(P\|Q)\) is agnostic to both \(S\) and \(u(S)\), and is thus adaptive. Moreover, the estimator \(\hat{D}_A\) is easy to implement in practice with near-linear computational complexity, and the coefficients \(\{g_{K,k}\}_{k=1}^{K+1}\) can be obtained offline via the Remez algorithm before observing any samples.

Now we analyze the performance of \(\hat{T}_m(\hat{p}, \hat{q})\) when \(q \leq \frac{2c_1 \ln n}{n}\).

**Lemma 14.** Let \(0 \leq p \leq u(S)q\), \(0 \leq q \leq \frac{2c_1 \ln n}{n}\), and \(m \sim \text{Poi}(mp), n \sim \text{Poi}(nq)\) be independent random variables. If \(c_1 \geq 2c_2\) and \(c_2 \ln n \geq 1\), we have
\[
|E[\hat{T}_m(\hat{p}, \hat{q})] - p \ln q| \leq \frac{C u(S)}{n \ln n} + \frac{16c_2^2}{n^3 c_2 \ln 2} (C + 2c_1 (\ln n)^3) \cdot \left( \frac{2u(S)}{c_1 mn \ln n} + \frac{4(u(S))^2}{n^2} \right),
\]
(187)
\[
\text{Var} (\hat{T}_m(\hat{p}, \hat{q})) \leq \frac{16c_2^2}{n^3 c_2 \ln 2} (C + 2c_1 (\ln n)^3) \cdot \left( \frac{2u(S)}{c_1 mn \ln n} + \frac{4(u(S))^2}{n^2} \right).
\]
(188)
where $C > 0$ is a constant which only depends on $c_1$ and $c_2$. In particular, if $11c_2 \ln 2 < \epsilon \in (0, 1)$, by \[14\] Lemma 5 we have

$$|E \tilde{T}_n(p, q) - p \ln q| \lesssim \frac{n u(S)}{n^{1-\epsilon}} + \frac{(u(S))^2}{mn^{2-\epsilon}} + \frac{u(S)}{mn^{2-\epsilon}} + \frac{u(S)}{mn^{1-\epsilon}}.$$  

(189)

Note that in Lemma \[14\] we have removed the condition $\frac{n \ln n}{mn} \lesssim m u(S)$ in Lemma \[11\]. Moreover, since the upper bounds of the bias and variance of $\tilde{T}_n$ presented in Lemma \[14\] are no worse than those in Lemma \[9\] and Lemma \[11\] by the same argument in Lemma \[12\] and Lemma \[13\] we conclude that the adaptive estimator $\hat{D}_A$ is rate-optimal, and thereby satisfies Theorem \[1\].

IV. MINIMAX LOWER BOUND

In this section, we prove the minimax lower bounds presented in Theorem \[1\]. There are two main lemmas that we employ towards the proof of the minimax lower bound. The first is the Le Cam two-point method, which helps to prove the minimax lower bound corresponding to the variance, or equivalently, the classical asymptotics. Suppose we observe a random vector $Z \in (Z, A)$ which has distribution $P_{\theta}$ where $\theta \in \Theta$. Let $\theta_0$ and $\theta_1$ be two elements of $\Theta$. Let $\hat{T} = T(Z)$ be an arbitrary estimator of a function $T(\theta)$ based on $Z$. Le Cam’s two-point method gives the following general minimax lower bound.

**Lemma 15.** [5 Sec. 2.4.2] The following inequality holds:

$$\inf_{T} \sup_{\theta \in \Theta} P_{\theta} \left( |\hat{T} - T(\theta)| \geq \frac{|T(\theta_1) - T(\theta_0)|}{2} \right) \geq \frac{1}{4} \exp \left( -D(P_{\theta_1} \| P_{\theta_0}) \right).$$  

(191)

The second lemma is the so-called method of two fuzzy hypotheses presented in Tsybakov [5]. Suppose we observe a random vector $Z \in (Z, A)$ which has distribution $P_{\theta}$ where $\theta \in \Theta$. Let $\sigma_0$ and $\sigma_1$ be two prior distributions supported on $\Theta$. Write $F_i$ for the marginal distribution of $Z$ when the prior is $\sigma_i$ for $i = 0, 1$. Let $\hat{T} = T(Z)$ be an arbitrary estimator of a function $T(\theta)$ based on $Z$. We have the following general minimax lower bound.

**Lemma 16.** [5 Thm. 2.15] Given the setting above, suppose there exist $\zeta \in \mathbb{R}$, $s > 0, 0 \leq \beta_0, \beta_1 < 1$ such that

$$\sigma_0(\theta : T(\theta) \leq \zeta - s) \geq 1 - \beta_0,$$

(192)

$$\sigma_1(\theta : T(\theta) \geq \zeta + s) \geq 1 - \beta_1.$$  

(193)
If \( V(F_1, F_0) \leq \eta < 1 \), then
\[
\inf_{\hat{T}} \sup_{\theta \in \Theta} \mathbb{P}_\theta \left( |\hat{T} - T(\theta)| \geq s \right) \geq \frac{1 - \eta - \beta_0 - \beta_1}{2},
\]
(194)
where \( F_i, i = 0, 1 \) are the marginal distributions of \( Z \) when the priors are \( \sigma_i, i = 0, 1 \), respectively.

Here \( V(P, Q) \) is the total variation distance between two probability measures \( P, Q \) on the measurable space \((Z, A)\). Concretely, we have
\[
V(P, Q) \triangleq \sup_{A \in A} |P(A) - Q(A)| = \frac{1}{2} \int |p - q| d\nu,
\]
(195)
where \( p = \frac{dp}{d\nu}, q = \frac{dq}{d\nu} \), and \( \nu \) is a dominating measure so that \( P \ll \nu, Q \ll \nu \).

By the proof of the achievability results in previous sections, we observe that \( (\frac{S}{m} m + \frac{u(S)}{n} n)^2 \) corresponds to the squared bias term, and \( \frac{(\ln S)^2}{m} + \frac{u(S)}{n} \) corresponds to the variance term. In the sequel we will also prove the minimax lower bound for the squared bias term and the variance term separately.

A. Minimax lower bound for the “variance”

First we prove that when \( n \geq u(S) \), we have
\[
\inf_{\hat{D}} \sup_{(P, Q) \in \mathcal{U}_{S, u(S)}} \mathbb{E}_{(P, Q)} \left( \hat{D} - D(P\|Q) \right)^2 \geq \frac{u(S)}{n}. \tag{196}
\]

Fix \( P = (\frac{1}{2(3-1)}, \cdots, \frac{1}{2(3-1)}, \frac{1}{2}) \). Applying Lemma 15 to our Poisson sampling model \( nq_i \sim \text{Poi}(nq_i), 1 \leq i \leq S \), we know that for feasible \( \theta_1 = P \times Q_1 = (p_1, \cdots, p_S) \times (q_1, \cdots, q_S), \theta_0 = P \times Q_0 = (p_1, \cdots, p_S) \times (q_1', \cdots, q_S') \) with \( \theta_0, \theta_1 \in \mathcal{U}_{S, u(S)} \),
\[
D(P_{\theta_1} \| P_{\theta_0}) = \sum_{i=1}^{S} D(P(\text{Poi}(mp_i) \times \text{Poi}(nq_i)) \| \text{Poi}(mp_i) \times \text{Poi}(nq_i'))),
\]
(197)
\[
= \sum_{i=1}^{S} D(P(\text{Poi}(nq_i)) \| \text{Poi}(nq_i')) \tag{198}
\]
\[
= \sum_{i=1}^{S} \sum_{k=0}^{\infty} \mathbb{P}(\text{Poi}(nq_i) = k) \cdot \left[ k \ln \frac{q_i}{q_i'} - n(q_i - q_i') \right], \tag{199}
\]
\[
= \sum_{i=1}^{S} nq_i \ln \frac{q_i}{q_i'} - n \sum_{i=1}^{S} (q_i - q_i') \tag{200}
\]
\[
= nD(Q_1 \| Q_0), \tag{201}
\]
then Markov’s inequality yields
\[
\inf_{\hat{D}} \sup_{(P, Q) \in \mathcal{U}_{S, u(S)}} \mathbb{E}_{(P, Q)} \left( \hat{D} - D(P\|Q) \right)^2 \geq \frac{[D(\theta_1) - D(\theta_0)]^2}{4} \times
\]
\[
\inf_{\hat{D}} \sup_{P \in \mathcal{M}_S} \mathbb{E} \left( |\hat{D} - D(P\|Q)| \geq \frac{|D(\theta_1) - D(\theta_0)|}{2} \right), \tag{202}
\]
\[
\geq \frac{|D(P\|Q_1) - D(P\|Q_0)|^2}{16} \exp(-nD(Q_1 \| Q_0)) \tag{203}
\]
where we are operating under the Poisson sampling model.

Fix \( \epsilon \in (0, 1/2) \) to be specified later. Letting
\[
Q_1 = \left( \frac{1}{(S-1)u(S)}, \cdots, \frac{1}{(S-1)u(S)}, \frac{1}{u(S)} - \frac{1}{u(S)} \right), \tag{204}
\]
\[
Q_0 = \left( \frac{1 + \epsilon}{(S-1)u(S)} \cdot \frac{1 - \epsilon}{(S-1)u(S)}, \cdots, \frac{1 + \epsilon}{(S-1)u(S)} \cdot \frac{1 - \epsilon}{(S-1)u(S)}, \frac{1}{u(S)} \cdot \frac{1}{u(S)} \right), \tag{205}
\]
where without loss of generality we assume that $S$ is an odd integer. Direct computation yields
\begin{equation}
D(Q_1\|Q_0) = -\frac{1}{2u(S)} \ln(1 + \epsilon) - \frac{1}{2u(S)} \ln(1 - \epsilon)
\end{equation}
\begin{equation}
= -\frac{1}{2u(S)} \ln(1 - \epsilon^2)
\end{equation}
\begin{equation}
\leq \frac{\epsilon^2}{u(S)},
\end{equation}
and
\begin{equation}
|D(P\|Q_1) - D(P\|Q_0)| \geq -\frac{1}{4} \ln(1 + \epsilon) - \frac{1}{4} \ln(1 - \epsilon)
\end{equation}
\begin{equation}
= -\frac{1}{4} \ln(1 - \epsilon^2)
\end{equation}
\begin{equation}
\geq \frac{\epsilon^2}{4}.
\end{equation}

Hence, by choosing $\epsilon = \sqrt{\frac{u(S)}{m}}$, we know that
\begin{equation}
\inf_{D} \sup_{(P,Q) \in U_{S,u(S)}} \mathbb{E}_{(P,Q)} \left( \hat{D} - D(P\|Q) \right)^2 \geq \frac{u(S)}{256en}
\end{equation}
under the Poisson sampling model. The result for the multinomial case can be obtained via Lemma [22].

Next we apply Lemma [15] to show that
\begin{equation}
\inf_{D} \sup_{(P,Q) \in U_{S,u(S)}} \mathbb{E}_{(P,Q)} \left( \hat{D} - D(P\|Q) \right)^2 \geq \frac{(\ln u(S))^2}{m}.
\end{equation}

Now fix $Q = (\frac{1}{2(S-1)u(S)}, \ldots, \frac{1}{2(S-1)u(S)}, 1 - \frac{1}{2u(S)})$, and consider
\begin{equation}
P_1 = \left( \frac{1}{2(S-1)}, \ldots, \frac{1}{2(S-1)} \right)
\end{equation}
\begin{equation}
P_0 = \left( \frac{1 - \epsilon}{2(S-1)}, \ldots, \frac{1 - \epsilon}{2(S-1)} \right)
\end{equation}
with $\epsilon \in (0, \frac{1}{2})$ to be specified later. By the same argument, for $\theta_1 = P_1 \times Q \in U_{S,u(S)}, \theta_0 = P_0 \times Q \in U_{S,u(S)}$, we have
\begin{equation}
\inf_{D} \sup_{(P,Q) \in U_{S,u(S)}} \mathbb{E}_{(P,Q)} \left( \hat{D} - D(P\|Q) \right)^2 \geq \frac{|D(P_1\|Q) - D(P_0\|Q)|^2}{16} \exp(-mD(P_1\|P_0))
\end{equation}
under the Poisson sampling model. It is straightforward to compute that
\begin{equation}
D(P_1\|P_0) = \frac{1}{2} \ln \frac{1}{1 - \epsilon} + \frac{1}{2} \ln \frac{1}{1 + \epsilon} = -\frac{1}{2} \ln(1 - \epsilon^2) \leq \frac{\epsilon^2}{4}
\end{equation}
and
\begin{equation}
|D(P_1\|Q) - D(P_0\|Q)| = \frac{1}{2} \ln u(S) + \frac{1}{2} \ln \frac{u(S)}{2u(S) - 1} - \frac{1 - \epsilon}{2} (\ln u(S) + \ln(1 - \epsilon)) - \frac{1 + \epsilon}{2} \ln \frac{(1 + \epsilon)u(S)}{2u(S) - 1}
\end{equation}
\begin{equation}
= \frac{\epsilon}{2} \ln u(S) - \frac{1 + \epsilon}{2} \ln(1 + \epsilon) - \frac{1 - \epsilon}{2} \ln(1 - \epsilon) - \frac{\epsilon}{2} \ln \frac{u(S)}{2u(S) - 1}
\end{equation}
\begin{equation}
\geq \frac{\epsilon}{2} \ln u(S).
\end{equation}

Combining these inequalities and setting $\epsilon = m^{-\frac{1}{2}}$ completes the proof of (213).

**B. Minimax lower bound for the “squared bias”**

We employ Lemma [16] to prove the minimax lower bounds corresponding to the squared bias terms. First we show that when $m \gtrsim \frac{S}{mS}$ and $u(S) \gtrsim (\ln S)^2, \ln S \gtrsim \ln m$, we have
\begin{equation}
\inf_{D} \sup_{(P,Q) \in U_{S,u(S)}} \mathbb{E}_{(P,Q)} \left( \hat{D} - D(P\|Q) \right)^2 \gtrsim \left( \frac{S}{m \ln m} \right)^2.
\end{equation}
In fact, by choosing $Q$ to be the uniform distribution, the estimation of KL divergence reduces to the estimation of entropy of discrete distribution $P$, subject to an additional constraint $p_i \leq u(S)q_i = u(S)/n$ for all $i = 1, \cdots, S$. Since in the proof of the minimax lower bound in \cite{30}, all $p_i$ satisfy that $p_i \lesssim \frac{\ln m}{m}$, and our assumption implies

$$p_i \lesssim \frac{\ln m}{m} \lesssim \frac{(\ln S)^2}{S} \lesssim \frac{u(S)}{S}, \tag{222}$$

i.e., the additional condition is automatically satisfied. Hence, we can operate as if we do not have the additional condition, and \cite{30} gives

$$\inf_{D} \sup_{(P,Q) \in \mathcal{U}_{S,u(S)}} E_{(P,Q)} \left( \hat{D} - D(P\|Q) \right)^2 \gtrsim \left( \frac{S}{m \ln S} \right)^2 \left( \frac{S}{m \ln m} \right)^2. \tag{223}$$

where we have used the condition $m \gtrsim \frac{S}{\ln S}$ and $\ln S \gtrsim \ln m$ to give $\ln S \approx \ln m$ here.

Now we are about the prove that when $m \gtrsim \frac{S}{\ln S}, n \gtrsim \frac{Su(S)}{\ln S}$ and $u(S) \gtrsim (\ln S)^2$, $\ln S \gtrsim \ln n$, we have

$$\inf_{D} \sup_{(P,Q) \in \mathcal{U}_{S,u(S)}} E_{(P,Q)} \left( \hat{D} - D(P\|Q) \right)^2 \gtrsim \frac{Su(S)^2}{n \ln n}. \tag{224}$$

We begin with a lemma to construct two measures with matching moments and large difference on the functional value, which corresponds to the duality between function space and measure space.

**Lemma 17.** \cite{1, Lemma 10, Lemma 12} For any bounded interval $I \subset \mathbb{R}$, positive integer $K > 0$ and continuous function $f$ on $I$, there exist two probability measures $\nu_0$ and $\nu_1$ supported on $I$ such that

1. $\int t^j \nu_I(dt) = \int t^j \nu_0(dt)$, for all $l = 0, 1, 2, \cdots, L$;
2. $\int f(t) \nu_I(dt) = \int f(t) \nu_0(dt) = 2E_K[f; I]$.

Recall that $E_K[f; I]$ is the distance in the uniform norm on $I$ from the function $f(x)$ to the space spanned by $\{1, x, \cdots, x^K\}$.

Based on Lemma 17, we choose $I = \left[ \frac{1}{n \ln n}, \frac{d_1 \ln n}{n} \right], K = d_2 \ln n$ with universal constants $d_1, d_2 > 0$ to be specified later, and $f(x) = \ln x$. The following lemma presents a lower bound of the approximation error $E_K[f; I]$.

**Lemma 18.** \cite{30} For $K = d_2 \ln n$, $I = \left[ \frac{1}{n \ln n}, \frac{d_1 \ln n}{n} \right]$ and $f(x) = \ln x$, we have

$$E_K[f; I] \geq c'.$$ \tag{225}

where the constant $c' > 0$ only depends on $d_1, d_2$.

Define $\mu \triangleq \int t \nu_I(dt) = \int t \nu_0(dt)$, by construction we have $\mu \leq \frac{d_1 \ln n}{n}$. Now the two fuzzy hypotheses $\sigma_0, \sigma_1$ in Lemma 16 are constructed as follows: for each $i = 0, 1, \sigma_i$ fixes

$$P = \left( \frac{u(S)}{n \ln n}, \cdots, \frac{u(S)}{n \ln n}, 1 - \frac{(S - 1)u(S)}{n \ln n} \right),$$ \tag{226}

and assigns $\nu_i^{S-1}$ to the vector $(q_1, \cdots, q_{S-1})$, and fixes $q_S = 1 - (S - 1)\mu$. Note that by assumption,

$$S \mu \lesssim \frac{S \ln n}{n} \lesssim \frac{(\ln S)^2}{u(S)} \lesssim 1$$

thus $q_S$ takes positive value and is thus valid under proper parameter configurations. Moreover, it is straightforward to verify that $(P, Q) \in \mathcal{U}_{S,u(S)}$ with probability one under $\sigma_i$. Since under $\sigma_i$, $Q$ may not form a probability measure, we consider the set of approximate probability vectors

$$\mathcal{U}_{S,u(S)}(\epsilon) \triangleq \left\{(P, Q) : P \in \mathcal{M}_S, \sum_{i=1}^{S} q_i - 1 < \epsilon, p_i \leq u(S)q_i, \forall i \right\},$$ \tag{228}

with parameter $\epsilon \in (0, 1)$ to be specified later. Further define the minimax under the Poisson sampling model for estimating $D(P\|Q)$ with $(P, Q) \in \mathcal{U}_{S,u(S)}(\epsilon)$ as

$$R_P(S, m, n, u(S), \epsilon) \triangleq \inf_{(P,Q) \in \mathcal{U}_{S,u(S)}(\epsilon)} \sup_{D(P,Q) \in \mathcal{U}_{S,u(S)}(\epsilon)} E_{(P,Q)} \left( \hat{D} - D(P\|Q) \right)^2.$$ \tag{229}

The equivalence between $R_P(S, m, n, u(S), \epsilon)$ and $R(S, m, n, u(S))$ defined in \cite{30} is established in the following lemma.

**Lemma 19.** For any $S, m, n \in \mathbb{N}$ and $\epsilon \in (0, 1/2)$, we have

$$R(S, m, n, u(S)) \geq \frac{1}{2} R_P(S, 2m, 2n, \frac{u(S)}{1 + \epsilon} \epsilon - (\ln u(S))^2 \left( \exp(-\frac{m}{4}) + \exp(-\frac{n}{4}) \right) - 2\epsilon^2.$$ \tag{230}
Then condition $\sigma_i$ on the event

$$E_i \triangleq \mathcal{U}_{S,u(S)}(\epsilon) \cap \left\{ (P, Q) : \frac{1}{S} \sum_{j=1}^{S} \left| \ln q_j - \mathbb{E}_{\epsilon_i} \ln q_j \right| \leq \frac{E_K[f; I]}{2} \right\}, \quad i = 0, 1$$

(231)

and define the conditional probability distribution as

$$\pi_i(\cdot) \triangleq \frac{\sigma_i(\cdot \cap E_i)}{\sigma_i(E_i)}, \quad i = 0, 1.$$

(232)

By setting

$$d_1 = 1, \quad d_2 = 10e, \quad \epsilon = \frac{S}{n \ln n}$$

(233)

we have

$$\sigma_i(\mathcal{U}_{S,u(S)}(\epsilon)^c) = \sigma_i \left( \sum_{j=1}^{S} q_j - 1 \geq \epsilon \right) \leq \frac{1}{e^2} \sum_{j=1}^{S-1} \text{Var}_{\epsilon_i}(q_j) \leq \frac{1}{e^2} \sum_{j=1}^{S-1} \mathbb{E}_{\epsilon_i}(q_j^2) \leq \frac{S}{e^2} \left( \frac{d_1 \ln n}{n} \right)^2 = \frac{d_1^2 (\ln n)^4}{S} \rightarrow 0$$

(234)

and by Lemma [18],

$$\sigma_i \left( \frac{1}{S} \sum_{j=1}^{S} (\ln q_j - \mathbb{E}_{\epsilon_i} \ln q_j) \right) \geq \frac{E_K[f; I]}{2} \leq \frac{4}{(e^2)^2} \sum_{j=1}^{S-1} \text{Var}_{\epsilon_i}(\ln q_j) \leq \frac{4}{(e^2)^2} \frac{(\ln(n\ln n))^2}{S} \lesssim \frac{(\ln S)^2}{S} \rightarrow 0. \quad (235)$$

Hence, by the union bound,

$$\sigma_i(E_i^c) \leq \sigma_i(\mathcal{U}_{S,u(S)}(\epsilon)^c) + \pi_i \left( \frac{1}{S} \sum_{j=1}^{S} (\ln q_j - \mathbb{E}_{\epsilon_i} \ln q_j) \geq \frac{E_K[f; I]}{2} \right) \rightarrow 0. \quad (236)$$

Denote by $F_i, G_i$ the marginal probability under prior $\pi_i$ and $\sigma_i$, respectively, for each $i = 0, 1$. Now by the triangle inequality and [1] Lemma 11, we have

$$V(F_0, F_1) \leq V(F_0, G_0) + V(G_0, G_1) + V(G_1, F_1) \leq \sigma_0(E_0^c) + V(G_0, G_1) + \sigma_1(E_1^c) \leq \sigma_0(E_0^c) + \frac{S}{n^6} + \sigma_1(E_1^c) \rightarrow 0. \quad (237) \quad (238) \quad (239) \quad (240)$$

Moreover, by the definition of $\pi_i$, the first two conditions of Lemma [16] hold with $\beta_0 = \beta_1 = 0$ for

$$\zeta = H(P) - \frac{(S - 1) u(S)}{n \ln n} \cdot \mathbb{E}_{\nu_i}(\ln q) + \mathbb{E}_{\nu_i}(\ln q) - \left( 1 - \frac{(S - 1) u(S)}{n \ln n} \right) \ln (1 - (S - 1) \mu) \quad (241)$$

$$s = \frac{(S - 1) u(S)}{n \ln n} \cdot \mathbb{E}_{\nu_i}(\ln q) - \mathbb{E}_{\nu_i}(\ln q) - 2 \cdot \frac{E_K[f; I]}{2} = \frac{(S - 1) u(S)}{n \ln n} \cdot \frac{E_K[f; I]}{2} \gtrsim \frac{Su(S)}{n \ln n} \quad (242)$$

Hence, by Lemma [16] we conclude that

$$R_P(S, m, n, u(S), \epsilon) \gtrsim s^2 \gtrsim \left( \frac{Su(S)}{n \ln n} \right)^2 \quad (243)$$

and the desired bound [224] follows from Lemma [19].

Hence, the combination of [196], [213], [221] and [224] yields that when $u(S) \gtrsim (\ln S)^2, n \gtrsim \frac{Su(S)}{m \ln m}, m \gtrsim \frac{S}{m \ln S}$ and $\ln S \gtrsim \ln (m \lor n)$, we have

$$\inf_{\hat{D}} \sup_{(P, Q) \in \mathcal{U}_{S,u(S)}} \mathbb{E}_{(P, Q)} \left( \hat{D} - D(P \| Q) \right)^2 \gtrsim \left( \frac{Su(S)}{n \ln n} \right)^2 + \left( \frac{S}{m \ln m} \right)^2 + \frac{(u(S))^2}{m} + \frac{u(S)}{n} \quad (244)$$

and the proof of Theorem [1] is complete.

V. OPTIMAL ESTIMATORS FOR HELLMINGER DISTANCE AND $\chi^2$-DIVERGENCE

Having analyzed the minimax rate-optimal estimator for the KL divergence thoroughly, in this section we apply the general recipe to other divergence functions, i.e., the Hellinger distance and the $\chi^2$-divergence. Specifically, we explicitly construct the minimax rate-optimal estimators for the Hellinger distance and the $\chi^2$-divergence, and sketch the proof of the achievability...
part in Theorem 3 and 4. For brevity, we omit the complete proof and remark that it can be obtained in a similar fashion as in the analysis of the KL divergence.

A. Optimal estimator for the Hellinger distance

For the Hellinger distance, the bivariate function of interest is \( f(p, q) = (\sqrt{p} - \sqrt{q})^2 \). We first classify the regime. In this case, \( \Theta = \hat{\Theta} = [0, 1]^2 \), and the non-analytic regime is

\[
\hat{\Theta}_0 = \{ (p, q) \in [0, 1]^2 : p = 0 \text{ or } q = 0 \}. 
\]  
(245)

Based on the confidence sets in Poisson models, the “smooth” and “non-smooth” regimes for \( (p, q) \) can obtained via (23) and (24) as

\[
\Theta_s = ([0, 1] \times [c_1 \ln n \frac{1}{2n}, 1]) \cup ([c_2 \ln m \frac{1}{2m}, 1] \times [0, 1])
\]
(246)

\[
\Theta_{ns} = ([0, 1] \times [0, c_1 \ln n \frac{1}{n}]) \cup ([0, c_2 \ln m \frac{1}{m}] \times [0, 1])
\]
(247)

where \( c_1 > 0 \) is some universal constant. Further, by (25) and (26), we obtain the “smooth” and “non-smooth” regimes based on observations \( (\hat{p}, \hat{q}) \) as

\[
\hat{\Theta}_s = ([0, 1] \times [c_1 \ln n \frac{1}{n}, 1]) \cup ([c_1 \ln m \frac{1}{n}, 1] \times [0, 1])
\]
(248)

\[
\hat{\Theta}_{ns} = ([0, 1] \times [0, c_1 \ln n \frac{1}{n}]) \cup ([0, c_1 \ln m \frac{1}{n}] \times [0, 1])
\]
(249)

Next we estimate the quantity \( f(p, q) = (\sqrt{p} - \sqrt{q})^2 \) in each regime. In the “smooth” regime where \( p \geq \frac{c_1 \ln m}{m} \) and \( q \geq \frac{c_1 \ln n}{n} \), we simply employ the plug-in approach with no bias correction:

\[
T_s(\hat{p}, \hat{q}) = (\sqrt{\hat{p}} - \sqrt{\hat{q}})^2.
\]
(250)

In the “non-smooth” regime, by symmetry it suffices to consider the case where \( p \leq \frac{c_1 \ln m}{m} \). Now we need to find a proper polynomial \( P(p, q) \) to approximate \( f(p, q) = (\sqrt{p} - \sqrt{q})^2 \). We recall that the degree of the approximating polynomial \( P(p, q) \) is determined by the bias-variance tradeoff, and we will have the following result after careful analysis:

- when \( \hat{q} \geq \frac{c_1 \ln n}{n} \), the resulting polynomial \( P(p, q) \) should be of degree \( c_2 \ln n \) on \( p \) and of degree 0 on \( q \);
- when \( \hat{q} < \frac{c_1 \ln n}{n} \), the resulting polynomial \( P(p, q) \) should be of degree \( c_2 \ln m \) on \( p \) and of degree \( c_2 \ln n \) on \( q \).

Now we explicitly give the expression of \( P(p, q) \) in both cases in terms of the following best approximating polynomial of \( \sqrt{x} \):

\[
Q_K(x) = \sum_{k=0}^{K} a_{K,k} x^k \triangleq \min_{Q \in \text{poly}_{k} } \max_{z \in [0,1]} |Q(z) - \sqrt{z}|.
\]
(251)

Recall that we use the sample splitting technique to determine the approximation region and approximate the functional, respectively, i.e., the approximation region is based on \((\hat{p}_2, \hat{q}_2)\), while the polynomial is evaluated using \((\hat{p}_1, \hat{q}_1)\). Hence,

- when \( \hat{q} \geq \frac{c_1 \ln n}{n} \), the approximation region is \([0, 2c_1 \ln m \frac{1}{m}] \times [\hat{q}_2 - \sqrt{c_1 \ln n} \frac{1}{n}, \hat{q}_2 + \sqrt{c_1 \ln n} \frac{1}{n}]\), and by the degree requirements of \( P(p, q) \), a natural choice is \( P(p, q) = \sqrt{\Delta m} Q_{K_m} (\frac{p}{\Delta m}) \cdot \sqrt{\Delta n} Q_{K_n} (\frac{q}{\Delta n}) \) with \( K_m = c_2 \ln m, \Delta_m = 2c_1 \ln m \); and \( K_n = c_2 \ln n, \Delta_n = 2c_1 \ln n \).
- when \( \hat{q} < \frac{c_1 \ln n}{n} \), the approximation region is \([0, 2c_1 \ln m \frac{1}{m}] \times [0, 2c_1 \ln n \frac{1}{n}]\), and by the degree requirements of \( P(p, q) \), a natural choice is \( P(p, q) = \sqrt{\Delta m} Q_{K_m} (\frac{p}{\Delta m}) \cdot \sqrt{\Delta n} Q_{K_n} (\frac{q}{\Delta n}) \) with \( K_m = c_2 \ln m, \Delta_m = 2c_1 \ln m \) and \( K_n = c_2 \ln n, \Delta_n = 2c_1 \ln n \).

In summary, the estimator is constructed as follows.

Estimator Construction 3. Conduct three-fold sample splitting to obtain i.i.d. samples \((\hat{p}_{i1}, \hat{p}_{i2}, \hat{p}_{i3})\) and \((\hat{q}_{i1}, \hat{q}_{i2}, \hat{q}_{i3})\). The estimator \( \tilde{T} \) for the Hellinger distance \( H^2(P, Q) \) is given by

\[
\tilde{T} = 1 - \frac{S}{m,n} \left( \sqrt{\hat{p}_{i2}} 1(\hat{p}_{i3} \geq \frac{c_1 \ln m}{m}) + \hat{R}_m(\hat{p}_{i1}, 1(\hat{p}_{i3} < \frac{c_1 \ln m}{m})) \right) \left( \sqrt{\hat{q}_{i2}} 1(\hat{q}_{i3} \geq \frac{c_1 \ln n}{n}) + \hat{R}_n(\hat{q}_{i1}, 1(\hat{q}_{i3} < \frac{c_1 \ln n}{n})) \right)
\]
(252)

where for \( l = m, n \)

\[
\hat{R}_l(x) \triangleq (R_l(x) \wedge 1) \vee (-1)
\]
(253)

\[
R_l(x) \triangleq \sum_{k=0}^{c_2 \ln l} a_{c_2 \ln l,k} \left( \frac{2c_1 \ln l}{l} \right)^{-k+\frac{1}{2}} \prod_{j=0}^{k-1} (x-j \frac{l}{l})
\]
(254)
The previous estimator does not require the knowledge of \( S \) since it assigns zero to unseen symbols (we remove the constant term in the expression of \( R_1(x) \)). Note that since the Hellinger distance \( H^2(P, Q) = 1 - \sum_{i=1}^{\infty} \sqrt{p_i q_i} \) enjoys a natural separation in its variables \((p_i, q_i)\), the pair \((p_i, q_i)\) is also separated in our resulting estimator. Moreover, in our estimator construction we can also merge \((\hat{p}_i, 1)\) and \((\hat{q}_i, 2)\) to result in a two-fold sample splitting.

Now we analyze the bias of the previous estimator. When \( p < \frac{2c_1 \ln m}{m} \) is small, by [31] Lemma 17, we know that

\[
|\text{ER}_m(\hat{p}) - \sqrt{p}| = |\sqrt{\Delta_m Q_K(\frac{p}{\Delta_m})} - \sqrt{p}| \lesssim \frac{\sqrt{\Delta_m}}{K_m^2} \lesssim \frac{1}{\sqrt{m \ln m}}.
\]  

(255)

When \( p \geq \frac{2c_1 \ln m}{m} \) is large, by Lemma 6 with \( r = 0 \) we know that

\[
|\text{ER}_m(\hat{p}) - \sqrt{p}| \lesssim \frac{P}{m} \sup_{\xi \in [p/2, \infty]} \frac{d^2 \sqrt{\xi}}{d\xi^2} \lesssim \frac{1}{m \sqrt{p}} \lesssim \frac{1}{\sqrt{m \ln m}}.
\]  

(256)

Hence, the total bias of \( \hat{P} \) can be upper bounded as

\[
|\text{Bias}(\hat{P})| \lesssim \sum_{i=1}^{S} \left( \frac{\sqrt{q_i}}{m \ln m} + \frac{\sqrt{p_i}}{\sqrt{n \ln n}} \right) \leq \sqrt{S \ln m} + \sqrt{\frac{S}{m \ln m}} \lesssim \sqrt{S (m \wedge n) \ln(m \wedge n)}
\]  

(257)

as shown in Theorem [3]. The variance can also be obtained in a similar fashion, and we omit the details.

**B. Optimal estimator for the \( \chi^2 \)-divergence**

For the \( \chi^2 \)-divergence \( \chi^2(P, Q) \) over \( \mathcal{U}_{S, u(S)} \), the bivariate function of interest is \( f(p, q) = \frac{p^2}{q} \). We first classify the regime. Since this function shares very similar analytic properties as the function \( p \ln q \) used in the KL divergence case, and our parameter set \( \mathcal{U}_{S, u(S)} \) remains the same, here the “smooth” and “non-smooth” regimes are also given by

\[
\hat{\Theta}_s = [0, 1] \times \left[ \frac{c_1 \ln n}{n}, 1 \right]
\]

(258)

\[
\hat{\Theta}_m = [0, 1] \times \left[ 0, \frac{c_1 \ln n}{n} \right]
\]

(259)

with some universal constant \( c_1 > 0 \).

Next we estimate \( f(p, q) = \frac{p^2}{q} \) in each regime. In the “smooth” regime where \( q \geq \frac{c_1 \ln n}{n} \), we seek to correct the bias of the plug-in estimator \( 1/\hat{q} \) in estimating \( 1/q \). Based on our general bias correction technique [31], we simply use the following order-three bias correction:

\[
\hat{T}^{(3)}(\hat{q}_1, \hat{q}_2) = \frac{1}{\hat{q}_1} - \frac{\hat{q}_2 - \hat{q}_1}{\hat{q}_1^2} + \frac{(\hat{q}_2 - \hat{q}_1)^2}{\hat{q}_1^3} - \frac{4\hat{q}_2}{n\hat{q}_1^4} - \frac{(\hat{q}_2 - \hat{q}_1)^3}{\hat{q}_1^4} + \frac{3\hat{q}_2^2}{n\hat{q}_1^5} - \frac{6\hat{q}_2}{n^2\hat{q}_1^6}.
\]  

(260)

Since \( p^2 \) admits an unbiased estimate \( \hat{p}(\hat{p} - \frac{1}{m}) \) in the Poisson model \( m\hat{p} \sim \text{Poi}(mp) \), the overall estimator in the “smooth” regime is given by

\[
\hat{T}_s(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) = \hat{p}_1 \left( \hat{p}_1 - \frac{1}{m} \right) \cdot \hat{T}^{(3)}(\hat{q}_1, \hat{q}_2) \cdot 1(\hat{q}_1 \neq 0)
\]

(261)

\[
= \hat{p}_1 \left( \hat{p}_1 - \frac{1}{m} \right) \cdot \left( \frac{1}{\hat{q}_1} - \frac{\hat{q}_2 - \hat{q}_1}{\hat{q}_1^2} + \frac{(\hat{q}_2 - \hat{q}_1)^2}{\hat{q}_1^3} - \frac{4\hat{q}_2}{n\hat{q}_1^4} - \frac{(\hat{q}_2 - \hat{q}_1)^3}{\hat{q}_1^4} + \frac{3\hat{q}_2^2}{n\hat{q}_1^5} - \frac{6\hat{q}_2}{n^2\hat{q}_1^6} \right) \cdot 1(\hat{q}_1 \neq 0).
\]

(262)

In the “non-smooth” regime, as is in the KL divergence case, we can further distinguish into “non-smooth” regime I and “non-smooth” regime II and employ best polynomial approximation in these regimes, respectively. However, motivated by the adaptive estimator \( \hat{D}_\lambda \) for the KL divergence where a single polynomial approximation is enough, we wonder whether or not it is also the case in the estimation of \( \chi^2 \)-divergence. Specifically, we seek a polynomial \( Q_K(q) \) of degree \( K \) on \([0, \Delta_n]\) such that the following quantity

\[
\sup_{q \in [0, \Delta_n]} q^2 \left| \frac{1}{q} - Q_K(q) \right|
\]

(263)

is as small as possible, where \( \Delta_n = \frac{2c_1 \ln n}{n} \). In other words, we seek to approximate the linear function \( q \) using \( q^2, \cdots, q^{K+2} \) on \([0, \Delta_n]\). Fortunately, this task can be done with the help of the Chebyshev polynomial, and we summarize the result in the following lemma.
Lemma 20. Let \( T_K(x) = \cos(K \arccos x) \) be the degree-\( K \) Chebyshev polynomial on \([-1, 1]\). Then

\[
Q_K(x) = (-1)^K \frac{T_{2(K+2)}(\sqrt{x/\Delta_n}) - (-1)^{K+2} - 2(K + 2)^2 x/\Delta_n}{2(K + 2)^2(x/\Delta_n)^2}
\]  

(264)
is a degree-\( K \) polynomial such that

\[
\sup_{x \in (0, \Delta_n]} x^2 \left| \frac{1}{x} - Q_K(x) \right| = \frac{\Delta_n}{(K + 2)^2}.
\]

On the other hand, using the Ditzian–Totik modulus of smoothness and Lemma \([10]\) (or by Chebychev’s alternating theorem since \( \{x^2, x^3, \cdots \} \) satisfies the Haar condition \([49]\)), it is not hard to prove that no other degree-\( K \) polynomial can achieve an approximation error of order \( o(\Delta_n^2) \). Hence, the polynomial \( Q_K \) defined in Lemma 20 achieves the rate-optimal uniform approximation error.

Motivated by Lemma 20, define \( \hat{Q}_K(x) \) be another polynomial such that \( \mathbb{E}[\hat{Q}_K(q)] = Q_K(q) \) for \( n \hat{q} \sim \text{Poi}(nq) \). Now in the “non-smooth” regime, we choose \( K = c_2 \ln n \), and use the following estimator:

\[
\hat{T}_m(\hat{p}_1, \hat{q}_1) = \hat{p}_1 \left( \hat{p}_1 - \frac{1}{m} \right) \cdot \hat{Q}_K(\hat{q}_1).
\]

(266)

In summary, we have arrived at the following estimator construction.

**Estimator Construction 4.** Conduct three-fold sample splitting to obtain i.i.d. samples \((\hat{p}_1, \hat{p}_2, \hat{p}_3) \) and \((\hat{q}_1, \hat{q}_2, \hat{q}_3) \). The estimator \( \hat{T} \) for \( \chi^2 \)-divergence \( \chi^2(P, Q) \) is given by

\[
\hat{T} = \sum_{i=1}^{S} \left( \hat{T}_s(\hat{p}_{i,1}, \hat{q}_{i,1}; \hat{p}_{i,2}, \hat{q}_{i,2}) \mathbb{I}(\hat{q}_{i,1} > c_1 \ln n/n) + \hat{T}_m(\hat{p}_{i,1}, \hat{q}_{i,1}) \mathbb{I}(\hat{q}_{i,1} < c_1 \ln n/n) \right) - 1
\]

(267)

where

\[
\hat{T}_m(x, y) \triangleq (\hat{T}_m(x, y) \wedge 1) \lor (-1)
\]

(268)

and \( \hat{T}_s(x, y; x', y'), \hat{T}_m(x, y) \) are given by (262) and (266), respectively, and \( c_1, c_2 > 0 \) are some suitably chosen universal constants.

By construction, the previous estimator does not require the knowledge of \( S \) nor \( u(S) \), and is thus adaptive. For the analysis of its performance, when \( q < c_1 \ln n/n \) is small, with the help of Lemma 20 we know that

\[
\left| \mathbb{E}[\hat{T}_m(\hat{p}_1, \hat{q}_1) - \frac{p^2}{q}] \right| = \left| p^2 Q(q) - \frac{p^2}{q} \right| \leq (u(S))^2 q^2 \left| Q(q) - \frac{1}{q} \right| \lesssim \frac{(u(S))^2}{n \ln n}.
\]

(269)

Moreover, for \( q \geq c_1 \ln n/n \) is large, applying Lemma 6 with \( r = 3 \) yields

\[
\left| \mathbb{E}[\hat{T}_s(\hat{p}_{1,1}; \hat{q}_{1,1}; \hat{p}_{2,1}; \hat{q}_{2,1}) - \frac{p^2}{q}] \right| = \left| p^2 \mathbb{E}[\hat{T}^{(3)}(\hat{q}_{1,2}, \hat{q}_{2,2}) - 1] \right| \lesssim p^2 \cdot \left( \frac{q}{n} \right)^2 \left| \frac{d^4}{d \xi^4} \right| \sup_{\xi \in [q/2, 2q]} \left| d^4(\xi^{-1}) \right| \lesssim \frac{p^2}{n^2 q^3} \lesssim \frac{(u(S))^2}{n^2 q} \lesssim \frac{(u(S))^2}{n \ln n}.
\]

(270)

Hence, the total bias of the previous estimator can be upper bounded as

\[
|\text{Bias}(\hat{T})| \lesssim \sum_{i=1}^{S} \frac{(u(S))^2}{n \ln n} = \frac{S(u(S))^2}{n \ln n}
\]

(271)

which coincides with the term in Theorem 4. The variance can be dealt with analogously, and we omit the lengthy proofs.

**VI. Conclusions and Future Work**

We proposed a general and detailed methodology for the construction of minimax rate-optimal estimators for low-dimensional functionals of high-dimensional parameters, especially when the functional of interest is non-smooth in some part of its domain. We elaborate on the insights of [1] which shows that the bias is the dominating term in the estimation of functionals and approximation is the key for an efficient bias reduction, and find an interesting interplay between the functional itself and the statistical model. Specifically, we show that the “smooth” and “non-smooth” regimes are determined by both the non-analytic region of the underlying functional which is only related to the smoothness of the functional, and the confidence sets given by concentration of measures which solely depend on the statistical model. Moreover, in the “non-smooth” regime, the approximation region is determined by the confidence sets, while the approximation error is determined by the smoothness of the functional in this region. Our general recipe is based on the interplay between these two factors, and successfully yields the minimax rate-optimal estimators for various divergences including KL divergence, Hellinger distance and \( \chi^2 \)-divergence.
We have also explored the ideas behind the polynomial approximation and the plug-in approach in bias reduction. For polynomial approximation, the uniform approximation error corresponds to the bias of the resulting estimator, and thus the best approximating polynomials are usually used. We remark that it is a highly non-trivial task and remains open in general to obtain and analyze the best polynomial approximation error for multivariate functionals, while for some special cases (e.g., general polytopes, balls and spheres) there are powerful tools from approximation theory. The plug-in approach corrects the bias with the help of high-order Taylor expansions, which only works for the region where the functional is analytic. For bias correction of the plug-in approach, in this paper we propose a general unbiased estimator of the Taylor series up to an arbitrary order.

Following [1], this paper presents another second step towards a general theory of functional estimation. Despite our progress, the interplay between the smoothness of the functional and the statistical model has yet to be completely revealed, and the choice of the approximating polynomial in the “non-smooth” regime has thus far required functional-specific “tricks”. An ambitious but worthy goal is to establish a general explanation of the effective sample size enlargement phenomenon in the parametric case, and to find the counterpart in the estimation of non-smooth nonparametric functionals beyond the insights provided by [33, 50].

APPENDIX A

AUXILIARY LEMMAS

We first prove that the worst-case mean squared error of any estimator is infinity if we allow to choose any $P$ which is absolutely continuous with respect to $Q$.

Lemma 21. Let $\mathcal{U}_S = \{(P, Q) : P, Q \in \mathcal{M}_S, P \ll Q\}$. Then for any configuration $(S, m, n)$ with $S \geq 2$, we have

$$R_{\text{minimax}}(\mathcal{U}_S) = \infty. \quad (272)$$

The next lemma relates the minimax risk under the Poisson sampling model and that under the Multinomial model. We define the minimax risk for Multinomial model with $(m, n)$ observations with $(P, Q) \in \mathcal{U}_{S,u(S)}$ for estimating the KL divergence $D(P\|Q)$ as

$$R(S, m, n, u(S)) \triangleq \inf_{\hat{D}} \sup_{(P, Q) \in \mathcal{U}_{S,u(S)}} E_{\text{Multinomial}} \left( \hat{D} - D(P\|Q) \right)^2, \quad (273)$$

and the counterpart for the Poisson sampling model as

$$R_P(S, m, n, u(S)) \triangleq \inf_{\hat{D}} \sup_{(P, Q) \in \mathcal{U}_{S,u(S)}} E_{\text{Poisson}} \left( \hat{D} - D(P\|Q) \right)^2. \quad (274)$$

Lemma 22. The minimax risks under the Poisson sampling model and the Multinomial model are related via the following inequalities:

$$R_P(S, 2m, 2n, u(S)) - (\ln u(S))^2 \left( \exp\left(-\frac{m}{4}\right) + \exp\left(-\frac{n}{4}\right) \right) \leq R(S, m, n, u(S)) \leq 4R_P(S, \frac{m}{2}, \frac{n}{2}, u(S)). \quad (275)$$

The next lemma gives the approximation properties of $\ln x$.

Lemma 23. There exists a universal constant $C_{\ln} > 0$ such that for any $0 < a < b$,

$$E_n[\ln x; [a, b]] \leq C_{\ln} W\left( \frac{b}{an^2} \right) \equiv C_{\ln} \cdot \begin{cases} \frac{b}{an^2} & b \leq \text{can}^2, \\ \ln\left( \frac{b}{an^2} \right) & b > \text{can}^2. \end{cases} \quad (276)$$

Lemma 24. For $f(p, q) = p \ln q$ and the region $R$ given in [143], there exists a universal constant $C_0$ only depending on $c_1$ such that

$$\omega^2_R(f, \frac{1}{K}) \leq C_0 \cdot \frac{u(S) \ln n}{K^2 n}. \quad (277)$$

The following lemma gives an upper bound for the second moment of the unbiased estimate of $(p - q)^j$ in Poisson model.

Lemma 25. Suppose $nX \sim \text{Poi}(np), p \geq 0, q \geq 0$. Then, the estimator

$$g_{j, q}(X) \triangleq \sum_{k=0}^{j} \binom{j}{k} (-q)^{j-k} \prod_{h=0}^{k-1} \left( X - \frac{h}{n} \right) \quad (278)$$
is the unique unbiased estimator for $(p - q)^j$, $j \in \mathbb{N}$, and its second moment is given by

$$
E[g_{j,q}(X)^2] = \sum_{k=0}^{j} \binom{j}{k}^2 (p - q)^{2(j-k)} \frac{b^k k!}{n^k}
$$

assuming $p > 0$, \hfill (279)

where $L_m(x)$ stands for the Laguerre polynomial with order $m$, which is defined as:

$$
L_m(x) = \sum_{k=0}^{m} \binom{m}{k} (-x)^k
$$

If $M \geq \frac{n(p-q)^2}{p} \vee j$, we have

$$
E[g_{j,q}(X)^2] \leq \left( \frac{2M^2 p^2}{n} \right)^j.
$$

In order to bound the coefficients of best polynomial approximations, we need the following result by Qazi and Rahman [52, Thm. E] on the maximal coefficients of polynomials on a finite interval.

**Lemma 26.** Let $p_n(x) = \sum_{j=0}^{n} a_j x^j$ be a polynomial of degree at most $n$ such that $|p_n(x)| \leq 1$ for $x \in [-1,1]$. Then, $|a_{n-2\nu}|$ is bounded above by the modulus of the corresponding coefficient of $T_n$ for $\mu = 0, 1, \ldots, [n/2]$, and $|a_{n-1-2\mu}|$ is bounded above by the modulus of the corresponding coefficient of $T_{n-1}$ for $\mu = 0, 1, \ldots, [(n-1)/2]$. Here $T_n(x)$ is the $n$-th Chebyshev polynomial of the first kind.

Moreover, it is shown in Cai and Low [27, Lemma 2] that all of the coefficients of Chebyshev polynomial $T_{2m}(x)$, $m \in \mathbb{Z}_+$ are upper bounded by $2^{3m}$. Hence, we can obtain the following result when the approximation interval is not centered at zero.

**Lemma 27.** Let $p_n(x) = \sum_{j=0}^{n} a_j x^j$ be a polynomial of degree at most $n$ such that $|p_n(x)| \leq A$ for $x \in [a, b]$, where $a + b \neq 0$. Then

$$
|a_{\nu}| \leq 2^{n/2} A \left\lfloor \frac{a + b}{2} \right\rfloor^{-\nu} \left( \left\lfloor \frac{b + a}{b - a} \right\rfloor + 1 \right)^n, \quad \nu = 0, \ldots, n.
$$

The following lemma gives some tail bounds for Poisson and Binomial random variables.

**Lemma 28.** [53, Exercise 4.7] If $X \sim \text{Poi}(\lambda)$ or $X \sim \text{B}(n, \frac{1}{n})$, then for any $\delta > 0$, we have

$$
\mathbb{P}(X \geq (1 + \delta)\lambda) \leq \left( \frac{e^\delta}{(1 + \delta)^{1+\delta}} \right)^\lambda \leq e^{-\delta^2 \lambda/3} \vee e^{-\delta \lambda/3}
$$

$$
\mathbb{P}(X \leq (1 - \delta)\lambda) \leq \left( \frac{e^{-\delta}}{(1 - \delta)^{1-\delta}} \right)^\lambda \leq e^{-\delta^2 \lambda/2}.
$$

The following lemmas deal with the upper bound of the variance in different scenarios.

**Lemma 29.** For independent random variables $X, Y$ with finite second moment, we have

$$
\text{Var}(XY) = (\mathbb{E}Y)^2 \text{Var}(X) + (\mathbb{E}X)^2 \text{Var}(Y) + \text{Var}(X)\text{Var}(Y).
$$

**Lemma 30.** [27, Lemma 4] Suppose $\mathbb{1}(A)$ is an indicator random variable independent of $X$ and $Y$, then

$$
\text{Var}(X \mathbb{1}(A) + Y \mathbb{1}(A^c)) = \text{Var}(X)\mathbb{P}(A) + \text{Var}(Y)\mathbb{P}(A^c) + (\mathbb{E}X - \mathbb{E}Y)^2\mathbb{P}(A)\mathbb{P}(A^c).
$$

**Lemma 31.** [27, Lemma 5] For any two random variables $X$ and $Y$,

$$
\text{Var}(X \land Y) \leq \text{Var}(X) + \text{Var}(Y).
$$

In particular, for any random variable $X$ and any constant $C$,

$$
\text{Var}(X \land C) \leq \text{Var}(X).
$$
A. Proof of Lemma

**Proof of Main Lemmas**

First we give an upper bound of \(\text{Var}(g_n(\hat{q}))\) for \(n\hat{q} \sim \text{Poi}(nq)\). Note that \(g_n(q)\) is continuously differentiable on \([0, 1]\), we have

\[
\text{Var}(g_n(\hat{q})) \leq \mathbb{E}(g_n(\hat{q}) - g_n(q))^2
\]

\[
= \mathbb{E}(g_n(\hat{q}) - g_n(q))^2 \mathbb{I}(\hat{q} \geq \frac{q}{2}) + \mathbb{E}(g_n(\hat{q}) - g_n(q))^2 \mathbb{I}(\hat{q} < \frac{q}{2})
\]

\[
= \mathbb{E}[g_n'(\xi_1)^2(\hat{q} - q)^2 \mathbb{I}(\hat{q} \geq \frac{q}{2}) + \mathbb{E}[g_n'(\xi_2)^2(\hat{q} - q)^2 \mathbb{I}(\hat{q} < \frac{q}{2})]
\]

\[
\leq \sup_{\xi_1 \in (0, 1]} |g_n'(\xi_1)|^2 \cdot \mathbb{E}(\hat{q} - q)^2 + \sup_{\xi_2 \in (0, 1]} |g_n'(\xi_2)| \cdot q^2 \mathbb{P}(\hat{q} < \frac{q}{2})
\]

\[
\leq \frac{4}{q^2} \cdot \frac{q}{n} + n^2 \cdot q^2 e^{-nq/8}
\]

\[
\leq \frac{4}{nq} + \frac{n^2 \cdot q^2 e^{-nq}}{q}
\]

\[
\leq \frac{700}{nq}
\]

where in the previous steps we have used Lemma 28 and the fact

\[
q^k e^{-cnq} \leq \left(\frac{k}{ecn}\right)^k
\]

for any \(q \in [0, 1]\).

Now we are ready to bound the bias. By independence and the triangle inequality, we have

\[
|\mathbb{E}[\hat{q} g_n(\hat{q})] - p g_n(q)| = p \mathbb{E}[g_n(\hat{q}) - g_n(q)]
\]

\[
\leq u(S) q |\mathbb{E}[g_n(\hat{q}) - g_n(q)]|
\]

\[
\leq u(S) \left(\mathbb{E}[\hat{q}g_n(\hat{q})] - q g_n(q)\right) + |\mathbb{E}[(\hat{q} - q)g_n(\hat{q})]|.
\]

We bound these two terms separately. For the first term, it can be obtained similar to 38 (via the second-order Ditzian–Totik modulus of smoothness defined in 44) that

\[
|\mathbb{E}[\hat{q}g_n(\hat{q})] - q g_n(q)| \leq \frac{5 \ln 2}{n}
\]

for any \(q \in [0, 1]\). For the second term, first note that \(\mathbb{E}[\hat{q}] = q\), we have

\[
|\mathbb{E}[(\hat{q} - q)g_n(\hat{q})]| = |\mathbb{E}[(\hat{q} - q)(g_n(\hat{q}) - g_n(q))]|.
\]

Hence, by the Cauchy-Schwartz inequality and the previous bound on \(\text{Var}(g_n(\hat{q}))\), we have

\[
|\mathbb{E}[(\hat{q} - q)g_n(\hat{q})]|^2 \leq \mathbb{E}[\hat{q} - q]^2 \cdot \mathbb{E}[g_n(\hat{q}) - g_n(q)]^2
\]

\[
= \mathbb{E}[\hat{q} - q]^2 \cdot \text{Var}(g_n(\hat{q}))
\]

\[
\leq \frac{q}{n} \cdot \frac{700}{nq}
\]

\[
= \frac{700}{n^2}.
\]

A combination of these two inequalities yields the bias bound

\[
|\mathbb{E}[\hat{q}g_n(\hat{q})] - p g_n(q)| \leq u(S) \left(\frac{5 \ln 2}{n} + \sqrt{\frac{700}{n}}\right) \leq \frac{30u(S)}{n}
\]

which together with \(|\mathbb{E}[\hat{p} \ln \hat{p}] - p \ln p| \leq \frac{5 \ln 2}{n}\) in 38 yields the desired bias bound.

Next we bound the variance as follows:

\[
\text{Var}(\hat{p}(\ln \hat{p} - g_n(\hat{q}))) \leq \mathbb{E}[\hat{p}(\ln \hat{p} - g_n(\hat{q})) - p(\ln p - g_n(q)]^2
\]

\[
\leq 3 \left(\mathbb{E}[\hat{p}(\ln \hat{p} - \ln p)]^2 + \mathbb{E}[\hat{p}(g_n(\hat{q}) - g_n(q)]^2 + \mathbb{E}[(\hat{p} - p)(\ln p - g_n(q)]^2\right)
\]

\[
\equiv 3(A_1 + A_2 + A_3)
\]
We bound $A_1, A_2, A_3$ separately. To bound $A_1$, we further decompose $A_1$ as

$$A_1 = \mathbb{E}[(\hat{p}(\ln \hat{p} - \ln p))^2 \mathbb{1}(\hat{p} \leq p) + \mathbb{E}[(\hat{p}(\ln \hat{p} - \ln p))^2 \mathbb{1}(\hat{p} > p) \mathbb{1}(p \geq \frac{1}{m})] + \mathbb{E}[(\hat{p}(\ln \hat{p} - \ln p))^2 \mathbb{1}(\hat{p} > p) \mathbb{1}(p < \frac{1}{m})] \leq B_1 + B_2 + B_3 \tag{311}$$

where

$$B_1 \leq \mathbb{E} \left[ \sup_{\xi \geq \hat{p}} |\hat{p} - \hat{p}|^2 \mathbb{1}(\hat{p} \leq p) \right] \leq \mathbb{E} |\hat{p} - p|^2 = \frac{p}{m} \tag{313}$$

$$B_2 \leq \mathbb{E} \left[ \sup_{\xi \geq p} |\hat{p} - \hat{p}|^2 \mathbb{1}(\hat{p} > p) \mathbb{1}(p \geq \frac{1}{m}) \right] \leq \frac{\mathbb{E}[\hat{p}^2 (\hat{p} - p)^2]}{p^2} \mathbb{1}(p \geq \frac{1}{m}) \tag{314}$$

$$= \left( \frac{1}{m^2p} + \frac{5}{m^2} + \frac{p}{m} \right) \mathbb{1}(p \geq \frac{1}{m}) \leq \frac{6}{m^2} + \frac{p}{m}. \tag{315}$$

Upper bounding $B_3$ requires more delicate analysis. First note that by differentiation with respect to $p$, for any $k \geq 1$ we have

$$\sup_{p \leq \frac{1}{m}} \frac{(mp)^k}{k!} \frac{k^2}{m^2} (\ln \frac{k}{mp})^2 \leq \sup_{p \leq \frac{1}{m}} \frac{(mp)^k}{k!} \frac{k^2}{m^2} (2 + \ln \frac{k}{mp})^2 \leq \frac{(2 + \ln k)^2}{k!} \frac{k^2}{m^2} \tag{316}$$

Hence, expanding the expectation of $B_3$ yields

$$B_3 = \sum_{k=1}^{\infty} e^{-mp} \frac{(mp)^k}{k!} \frac{k^2}{m^2} (\ln \frac{k}{mp})^2 \mathbb{1}(p < \frac{1}{m}) \leq \frac{1}{m^2} \sum_{k=1}^{\infty} \frac{k^2 (2 + \ln k)^2}{k!} < \frac{45}{m^2} \tag{318}$$

where the infinite sum converges to

$$\sum_{k=1}^{\infty} \frac{k^2 (2 + \ln k)^2}{k!} \approx 44.17 < 45. \tag{319}$$

Hence, $A_1$ can be upper bounded as

$$A_1 = B_1 + B_2 + B_3 \leq \frac{51}{m^2} + \frac{2p}{m}. \tag{320}$$

As for $A_2$, since we have proved that $\mathbb{E}(g_n(\hat{q}) - g_n(q))^2 \leq \frac{700}{nq}$, by independence we have

$$A_2 \leq \mathbb{E}(\hat{p}^2) \left(\frac{700}{nq} \right) = \left(\frac{p^2 + \frac{p}{m}}{\sqrt{n}}\right) \leq \frac{700u(S)}{\sqrt{n}} \left(p + \frac{1}{m}\right). \tag{321}$$

For $A_3$, it is clear that

$$A_3 = \frac{p}{m} (\ln p - g_n(q))^2 \leq \frac{2p}{m} \left(\frac{\ln p}{q}^2 + (g_n(q) - \ln q)^2\right) \leq \frac{2}{m} \left(p(\ln u(S))^2 + \frac{4q}{e^2} + \frac{4u(S)}{en}\right) \tag{322}$$

where we have used the fact that for $p \leq u(S)q$,

$$p(\ln \frac{p}{q})^2 \leq p(\ln u(S))^2 \vee \frac{4q}{e^2} \leq p(\ln u(S))^2 + \frac{4q}{e^2} \tag{323}$$

$$p(g_n(q) - \ln q)^2 \leq p(1 - \ln(nq))^2 \mathbb{1}(\frac{1}{n} < q) \leq u(S)q(1 - \ln(nq))^2 \mathbb{1}(\frac{1}{n} < q) \leq \frac{4u(S)}{en}. \tag{324}$$

A combination of the upper bounds of $A_1, A_2, A_3$ yields

$$\text{Var}(\hat{p}(\ln \hat{p} - g_n(\hat{q}))) \leq \frac{51}{m^2} + \frac{2}{m} \left(p + p(\ln u(S))^2 + \frac{4q}{e^2} + \frac{4u(S)}{en}\right) + \frac{700u(S)}{\sqrt{n}} \left(p + \frac{1}{m}\right). \tag{325}$$

The proof is complete. □
B. Proof of Lemma 3
Braess and Sauer [39, Prop. 4] showed the following equalities for the Bernstein polynomials:

\[ B_n[(x-x_0)^2](x_0) = \frac{x_0(1-x_0)}{n} \]  
(326)

\[ B_n[(x-x_0)^3](x_0) = \frac{x_0(1-x_0)(1-2x_0)}{n^2} \]  
(327)

Hence, choosing \( x_0 = x \), we have

\[ Q_3(x) - B_n[Q_3](x) = \frac{1}{x^2} \cdot \frac{x(1-x)}{n} - \frac{2}{x^3} \cdot \frac{x(1-x)(1-2x)}{n^2} = \frac{(1-x)((n+4)x-2)}{n^2x^2} \]  
(328)

Then the desired inequality is a direct result of Lemma 2.

C. Proof of Lemma 4
For the first statement, define the remainder term of the Taylor expansion as

\[ R(\hat{\theta}^{(1)}) \triangleq \sum_{k=0}^{r} \frac{G^{(k)}(\hat{\theta}^{(1)})}{k!} (\theta - \hat{\theta}^{(1)})^k - G(\theta) \]  
(329)

and denote by \( E \) the event that \( \hat{\theta}^{(1)} \in V(\theta) \). By the definition of reverse confidence sets, \( \mathbb{P}(E^c) \leq \delta \), and

\[ |\mathbb{E}_\theta H(\hat{\theta}^{(1)}, \hat{\theta}^{(2)}) - G(\theta)| \leq |\mathbb{E}_\theta (H(\hat{\theta}^{(1)}, \hat{\theta}^{(2)}) - G(\theta))1(E)| + |\mathbb{E}_\theta (H(\hat{\theta}^{(1)}, \hat{\theta}^{(2)}) - G(\theta))1(E^c)| \]  
(330)

\[ \leq |\mathbb{E}_\theta (G^{(r)}(\hat{\theta}^{(1)}, \hat{\theta}^{(2)}) - G(\theta))1(E)| + \delta \cdot \left( |G(\theta)| + \sup_{\theta_1, \theta_2 \in \theta} |H(\theta_1, \theta_2)| \right) \]  
(331)

\[ = |\mathbb{E}_\theta R(\hat{\theta}^{(1)})1(E)| + \delta \cdot \left( |G(\theta)| + \sup_{\theta_1, \theta_2 \in \theta} |H(\theta_1, \theta_2)| \right) \]  
(332)

\[ \leq \frac{\mathbb{E}_\theta |\hat{\theta}^{(1)} - \theta|^{r+1}1(E)}{(r+1)!} \cdot \sup_{\theta \in V(\theta)} |G^{(r+1)}(\theta)| + \delta \cdot \left( |G(\theta)| + \sup_{\theta_1, \theta_2 \in \theta} |H(\theta_1, \theta_2)| \right) \]  
(333)

\[ \leq \frac{\mathbb{E}_\theta |\hat{\theta}^{(1)} - \theta|^{r+1}}{(r+1)!} \cdot \sup_{\theta \in V(\theta)} |G^{(r+1)}(\theta)| + \delta \cdot \left( |G(\theta)| + \sup_{\theta_1, \theta_2 \in \theta} |H(\theta_1, \theta_2)| \right). \]  
(334)

As for the variance of \( H_k(\hat{\theta}^{(1)}, \hat{\theta}^{(2)}) \) with \( k \geq 0 \), we first note by triangle inequality that

\[ \text{Var}_\theta(H_k(\hat{\theta}^{(1)}, \hat{\theta}^{(2)})) \leq 2\text{Var}_\theta(H_k(\hat{\theta}^{(1)}, \hat{\theta}^{(2)})1(E)) + 2\text{Var}_\theta(H_k(\hat{\theta}^{(1)}, \hat{\theta}^{(2)})1(E^c)) \]  
(335)

\[ \leq 2\text{Var}_\theta(G_k(\hat{\theta}^{(1)}, \hat{\theta}^{(2)})1(E)) + 2\delta \cdot \sup_{\theta_1, \theta_2 \in \theta} |H_k(\theta_1, \theta_2)|^2. \]  
(336)

Hence, it suffices to upper bound \( \text{Var}_\theta(G_k(\hat{\theta}^{(1)}, \hat{\theta}^{(2)})1(E)) \). Note that \( G_k(\hat{\theta}^{(1)}, \hat{\theta}^{(2)}) \) is a linear combination of terms of the form \( G^{(k)}(\hat{\theta}^{(1)})(\hat{\theta}^{(1)})^{k-j}S_j(\hat{\theta}^{(2)}) \) with \( 0 \leq j \leq k \), we employ the triangle inequality again to reduce the problem of bounding the total variance to bounding the variance of individual terms. By independence and Lemma 29 it further suffices to upper bound \( |\mathbb{E}_\theta G^{(k)}(\hat{\theta}^{(1)})(\hat{\theta}^{(1)})^{k-j}1(E)| \) and \( \text{Var}_\theta(G^{(k)}(\hat{\theta}^{(1)})(\hat{\theta}^{(1)})^{k-j}1(E)) \), respectively. In fact, defining \( G_{k,j}(\theta) = \theta^j G^{(k)}(\theta) \), by Taylor expansion again we have

\[ |\mathbb{E}_\theta G_{k,j}(\hat{\theta}^{(1)})1(E)| \leq |\mathbb{E}_\theta (G_{k,j}(\hat{\theta}^{(1)}) - G_{k,j}(\theta))1(E)| + |G_{k,j}(\theta)| \]  
(337)

\[ = |\mathbb{E}_\theta (G_{k,j}(\theta)(\hat{\theta}^{(1)} - \theta) + \frac{1}{2} G''_{k,j}(\xi)(\hat{\theta}^{(1)} - \theta)^2)1(E)| + |G_{k,j}(\theta)| \]  
(338)

\[ \leq \frac{1}{2} |\mathbb{E}_\theta G''_{k,j}(\xi)(\hat{\theta}^{(1)} - \theta)^21(E)| + |G_{k,j}(\theta)| + P(E^c) \cdot \left( G''_{k,j}(\theta)|\theta| + \sup_{\xi \in \bar{\theta}} |\hat{\theta}| \right) \]  
(339)

\[ \leq \frac{\mathbb{E}_\theta |\hat{\theta}^{(1)} - \theta|^2}{2} \cdot \sup_{\theta \in V(\theta)} |G''_{k,j}(\theta)| + |G_{k,j}(\theta)| + \delta \cdot \left( G''_{k,j}(\theta)|\theta| + \sup_{\xi \in \bar{\theta}} |\hat{\theta}| \right). \]  
(340)
and

$$\text{Var}_{\theta}(G_{k,j}(\hat{\theta}_n^{(1)})) \mathbb{1}(E) \leq \mathbb{E}_\theta(G_{k,j}(\hat{\theta}_n^{(1)})\mathbb{1}(E) - G_{k,j}(\theta))^2$$

\begin{equation}
\leq 2\mathbb{E}_\theta((G_{k,j}(\hat{\theta}_n^{(1)}) - G_{k,j}(\theta))\mathbb{1}(E))^2 + 2|G_{k,j}(\theta)|^2 \cdot \mathbb{P}(E^c)
\end{equation}

\begin{equation}
\leq 2\mathbb{E}_\theta(G_{k,j}(\xi)(\hat{\theta}_n^{(1)} - \theta)\mathbb{1}(E))^2 + 2\delta \cdot |G_{k,j}(\theta)|^2
\end{equation}

\begin{equation}
\leq 2\mathbb{E}_\theta(\hat{\theta}_n^{(1)} - \theta)^2 \cdot \sup_{\hat{\theta} \in \mathcal{V}(\theta)} |G_{k,j}(\hat{\theta})|^2 + 2\delta \cdot |G_{k,j}(\theta)|^2
\end{equation}

which establishes the desired variance bound.

Finally it remains to bound the quantity $$\mathbb{E}_\theta H_k(\hat{\theta}_n^{(1)}, \hat{\theta}_n^{(2)})$$ for $$k \geq 1$$. If $$k \geq 2$$, as above, by triangle inequality, we conclude that

\begin{equation}
\mathbb{E}_\theta H_k(\hat{\theta}_n^{(1)}, \hat{\theta}_n^{(2)}) \leq \mathbb{E}_\theta H_k(\hat{\theta}_n^{(1)}, \hat{\theta}_n^{(2)}) \mathbb{1}(E) + \delta \cdot \sup_{\theta_1, \theta_2} |H_k(\theta_1, \theta_2)|
\end{equation}

\begin{equation}
= \frac{1}{k!} \mathbb{E}_\theta G^{(k)}(\hat{\theta}_n^{(1)})(\theta - \hat{\theta}_n^{(1)})^k \mathbb{1}(E) + \delta \cdot \sup_{\theta_1, \theta_2} |H_k(\theta_1, \theta_2)|
\end{equation}

\begin{equation}
\leq \mathbb{E}_\theta(\hat{\theta}_n^{(1)} - \theta)^k \cdot \sup_{\hat{\theta} \in \mathcal{V}(\theta)} |G^{(k)}(\hat{\theta})| + \delta \cdot \sup_{\theta_1, \theta_2} |H_k(\theta_1, \theta_2)|
\end{equation}

For $$k = 1$$, we further note that $$\mathbb{E}_\theta \hat{\theta}_n^{(1)} = \theta$$, and conduct order-one Taylor expansion to yield

\begin{equation}
\mathbb{E}_\theta H_1(\hat{\theta}_n^{(1)}, \hat{\theta}_n^{(2)}) \leq \mathbb{E}_\theta G'(\hat{\theta}_n^{(1)})(\theta - \hat{\theta}_n^{(1)}) \mathbb{1}(E) + \delta \cdot \sup_{\theta_1, \theta_2} |H_1(\theta_1, \theta_2)|
\end{equation}

\begin{equation}
= \mathbb{E}_\theta (G'(\theta) + (\hat{\theta}_n^{(1)} - \theta)G''(\xi))(\theta - \hat{\theta}_n^{(1)}) \mathbb{1}(E) + \delta \cdot \sup_{\theta_1, \theta_2} |H_1(\theta_1, \theta_2)|
\end{equation}

\begin{equation}
\leq \mathbb{E}_\theta(\hat{\theta}_n^{(1)} - \theta)^2 \cdot \sup_{\hat{\theta} \in \mathcal{V}(\theta)} |G''(\hat{\theta})| + \delta \cdot \left( \sup_{\theta_1, \theta_2} |H_1(\theta_1, \theta_2)| + |G'(\theta)(|\theta| + \sup_{\hat{\theta}} |\hat{\theta}|) \right)
\end{equation}

as desired.

\[\Box\]

**D. Proof of Lemma**

Replacing $$n$$ by $$m$$, we adopt the notations of $$V(p)$$ and $$\delta$$ in (121). Denote by $$E$$ the event $$\hat{\rho} \in V(p)$$. We have

\begin{equation}
|\text{EU}_H(\hat{\rho}) + p \ln p| = \left| \mathbb{E} \left( \hat{\rho} \ln \hat{\rho} + \frac{1}{2m} \right) + p \ln p \right|
\end{equation}

\begin{equation}
\leq \mathbb{E} \left( \hat{\rho} \ln \hat{\rho} - (1 + \ln p)(\hat{\rho} - p) + \frac{(\hat{\rho} - p)^2}{2p} - \frac{(\hat{\rho} - p)^3}{6p^2} \right) + p \ln p + \frac{|\mathbb{E}(\hat{\rho} - p)^3|}{6p^2}
\end{equation}

\begin{equation}
\leq \mathbb{E} \left( \hat{\rho} \ln \hat{\rho} - (1 + \ln p)(\hat{\rho} - p) + \frac{(\hat{\rho} - p)^2}{2p} - \frac{(\hat{\rho} - p)^3}{6p^2} + p \ln p \right) \mathbb{1}(E) + \mathbb{P}(E^c) \cdot \sup_{\hat{\rho} \in [0,1]} \left(-\hat{\rho} \ln \hat{\rho} - (1 + \ln p)(\hat{\rho} - p) + \frac{(\hat{\rho} - p)^2}{2p} - \frac{(\hat{\rho} - p)^3}{6p^2} + p \ln p \right) + \frac{|\mathbb{E}(\hat{\rho} - p)^3|}{6p^2}
\end{equation}

\begin{equation}
\leq \frac{|\mathbb{E}(\hat{\rho} - p)^4|}{24} \sup_{x \in V(p)} \left( (1 - 4p\ln p + x^2 + 2) \left( \frac{1}{e} - p \ln p + 1 - \ln p + \frac{1}{2} \right) + \frac{1}{6p^2} \right) + \frac{1}{6p^2}
\end{equation}

\begin{equation}
\leq \frac{p + 3mp^2}{24m^2} \sup_{x \in V(p)} \frac{2}{x^3} + 4m^{-c_1/24 + 2} + \frac{1}{6p^2}
\end{equation}

where we have used $$mp \geq c_1 \ln m/2 \geq 2$$. Since any $$x \in V(p)$$ satisfies

\begin{equation}
x \geq p - \frac{1}{2} \sqrt{\frac{c_1 p \ln m}{2m}} \geq \frac{p}{2}
\end{equation}
by the previous inequality we have
\[
|\mathbb{E}U_H(\hat{p}) + p \ln p| \leq \frac{p + 3mp^2}{24m^3} \cdot \frac{2}{(p/2)^3} + 4m^{-c_1/24+2} + \frac{1}{6mp^2}
\]  
\[
\leq \frac{4mp^2}{24m^3} \cdot \frac{2}{(p/2)^3} + 4m^{-c_1/24+2} + \frac{1}{6pm^2}
\]  
\[
\leq \frac{3}{m^2p} + 4m^{-c_1/24+2}
\]  
\[
\leq \frac{6}{c_1m \ln m} + 4m^{-c_1/24+2}
\]
as desired.

As for the variance, since the constant bias correcting term does not affect variance, applying Lemma 4 with \(k = 0\) yields
\[
\text{Var}(U_H(\hat{p})) \leq A_0 \left(2m^{-c_1/24} \cdot 1 + \frac{p}{m} (1 - \ln(p/2))^2 + 2m^{-c_1/24} \cdot (p \ln p)^2\right)
\]  
\[
\leq A_0 \left(p(2 - \ln p)^2 / m + 4m^{-c_1/24}\right).
\]

\(\square\)

\(E.\; Proof \ of \ Lemma 6\)

The only non-trivial part in deducing the third inequality from Lemma 4 is to prove that for any \(k \in \mathbb{N}\) and \(q \geq \frac{1}{n} \)
\[
\mathbb{E}_q |\hat{q}_1 - q|^k \lesssim \left(\frac{q}{n}\right)^{\frac{k}{2}}.
\]

In fact, since \(\mathbb{E}_q \exp(s\hat{q}_1) = \exp(nq(e^{s/n} - 1))\), we have \(\mathbb{E}_q \exp(s(\hat{q}_1 - q)) = \exp(nq(e^{s/n} - 1 - s/n))\). Hence, by comparing the coefficient of \(s^k\) at both sides of
\[
\sum_{k=0}^{\infty} \frac{\mathbb{E}_q (\hat{q}_1 - q)^k}{k!} s^k = \sum_{k=0}^{\infty} \frac{(nq)^k}{k!} \left(\sum_{j=2}^{\infty} \frac{1}{j!} \left(\frac{s}{n}\right)^j\right)^k
\]
yields that for even \(k\), \(\mathbb{E}_q (\hat{q}_1 - q)^k\) can be expressed as
\[
\mathbb{E}_q (\hat{q}_1 - q)^k = \sum_{j=0}^{\frac{k}{2}} a_{k,j} \left(\frac{q}{n}\right)^j
\]
for some coefficients \(\{a_{k,j}\}_{j=0}^{k/2}\). Now for even \(k\), the desired inequality follows from the assumption \(q \geq n^{-1}\). For odd \(k\), Cauchy-Schwartz inequality yields
\[
\mathbb{E}_q |\hat{q}_1 - q|^k \leq \left(\mathbb{E}_q |\hat{q}_1 - q|^{k-1}\right)^{\frac{1}{2}} \left(\mathbb{E}_q |\hat{q}_1 - q|^{k+1}\right)^{\frac{1}{2}} \lesssim \left(\frac{q}{n}\right)^{\frac{k-1}{2} + \frac{k+1}{2}} = \left(\frac{q}{n}\right)^{\frac{k}{2}}.
\]

Hence, the third inequality follows. The first inequality also follows from this fact, Lemma 4, \(\delta \leq 2n^{-c_1/24}\) and \(V(q) \leq [\frac{q}{2}, 2q]\). Now it remains to deduce the second inequality from Lemma 4. By (87), we know that \(S_j(\hat{q}_2)\) is a linear combination of \(\frac{\hat{q}_1^{j-i}}{n^i}\) with constant coefficients and \(i = 0, 1, \cdots, j\). By the triangle inequality for the variance, it suffices to upper bound the variance of each individual term \(\frac{\hat{q}_1^{j-i}}{n^i}\). Using the same approach based on moment generating function, we conclude that for any \(k \geq 0\) and \(q \geq n^{-1}\),
\[
\text{Var}_q(\hat{q}_2^k) = \mathbb{E}_q(\hat{q}_2^k)^2 - (\mathbb{E}_q(\hat{q}_2^k))^2 \lesssim \sum_{j=0}^{2k-1} \frac{q^j}{n^{2k-j}} \lesssim \frac{q^{2k-1}}{n}.
\]

As a result, for \(0 \leq i \leq j\),
\[
\text{Var}_q(\frac{\hat{q}_2^j}{n^i}) \lesssim \frac{q^{2j-2i-1}}{n^{2i+1}} \leq \frac{q^{j-1}}{n}
\]
and thus \(\text{Var}_q(S_j(\hat{q}_2)) \lesssim \frac{q^{2j-1}}{n} \). Finally it suffices to note that for \(q \geq \frac{c_1 \ln n}{2n} \geq n^{-1}\),
\[
\mathbb{E}_q[S_j^2(\hat{q}_2)] = (\mathbb{E}_q S_j(\hat{q}_2))^2 + \text{Var}_q(S_j(\hat{q}_2)) \lesssim q^{2j} + \frac{q^{2j-1}}{n} \lesssim q^{2j}
\]
which completes the proof of the second inequality. \(\square\)
$F$. Proof of Lemma 6

To invoke Lemma 6, we remark that $g(q) = \ln q$, $r = 3$, and
\begin{align}
 h_0(\hat{q}_1, \hat{q}_2) &= \ln \hat{q}_1 \cdot 1(\hat{q}_1 \neq 0) \\
 h_1(\hat{q}_1, \hat{q}_2) &= \frac{\hat{q}_2 - \hat{q}_1}{\hat{q}_1} \cdot 1(\hat{q}_1 \neq 0) \\
 h_2(\hat{q}_1, \hat{q}_2) &= \left( -\frac{(\hat{q}_2 - \hat{q}_1)^2}{2\hat{q}_1} + \frac{\hat{q}_2}{2n\hat{q}_1} \right) \cdot 1(\hat{q}_1 \neq 0) \\
 h_3(\hat{q}_1, \hat{q}_2) &= \left( \frac{(\hat{q}_2 - \hat{q}_1)^3}{3\hat{q}_1^3} + \frac{\hat{q}_2}{n\hat{q}_1^2} - \frac{2\hat{q}_2^2}{n^2\hat{q}_1} + \frac{2\hat{q}_2}{n^2\hat{q}_1^2} \right) \cdot 1(\hat{q}_1 \neq 0).
\end{align}

Noting that $\sup_{\xi \in [g/2, 2g]} |g^{(k)}(\xi)| = |g^{(k)}(g/2)|$ for any $k \geq 1$ and $g \geq \frac{\epsilon c_1 \ln n}{2n}$, we have
\begin{align}
|\mathbb{E}T(3)(\hat{q}_1, \hat{q}_2) \cdot 1(\hat{q}_1 \neq 0) - \ln q| &\leq B_3 \left( \frac{q^2}{n^2} \cdot 6\left(\frac{q}{2}\right)^{-4} + n^{-c_1/24} \cdot (-\ln q + \ln n + n + n^2 + 2n^3) \right) \\
&\leq B_3 \left( \frac{96}{n^3q^2} + 6n^{-c_1/24+3} \right) \\
&\leq B_3 \left( \frac{192}{c_1n^2q \ln n} + 6n^{-c_1/24+3} \right)
\end{align}
and thus by independence,
\begin{align}
|\mathbb{E}[T_1(\hat{p}_1, \hat{q}_1; \hat{q}_2, \hat{q}_3)] - p \ln q| &= p|\mathbb{E}T(3)(\hat{q}_1, \hat{q}_2) \cdot 1(\hat{q}_1 \neq 0) - \ln q| \\
&\leq pB_3 \left( \frac{192}{c_1n^2q \ln n} + 6n^{-c_1/24+3} \right) \\
&\leq 192B_3n^2(S) / c_1n \ln n + 6B_3pn^{-c_1/24+3}.
\end{align}

Moreover, for any $0 \leq k \leq 3$,
\begin{align}
\text{Var}(h_k(\hat{q}_1, \hat{q}_2)) &\leq B_3 \left( n^{-c_1/24} \cdot n^3 + \sum_{j=0}^{k} q^{2(k-j)} \left( \frac{q}{n} \cdot \left( \frac{24}{q^{k-j+1}} \right)^2 + n^{-c_1/24} \cdot q^{2(j-k)} (-\ln q) \right) \right) \\
&\quad + \sum_{j=0}^{k-1} q^{2(k-j)-1} \left( \frac{q}{n} \cdot \left( \frac{24}{q^{k-j+1}} \right)^2 + n^{-c_1/24} \cdot q^{2(j-k)} (-\ln q) \right) \\
&\leq B_3 \left( \frac{576(k+1)}{nq} + \frac{2k}{nq} \cdot \left( 1 + \frac{80}{nq} \right)^2 + n^{-c_1/24} \cdot n^3 + (k+1) \ln n + 32kn^2 \right) \\
&\leq B_3 \left( \frac{12500}{nq} + 100n^{-c_1/24+3} \right)
\end{align}
where in the last step we have used the fact that $nq \geq 2$. For $1 \leq k \leq 3$, we also have
\begin{align}
|\mathbb{E}h_k(\hat{q}_1, \hat{q}_2)| &\leq B_3 \left( \frac{q}{n} \cdot \left( \frac{24}{q} \right)^{-k} \cdot 6\left(\frac{q}{2}\right)^{-k} + n^{-c_1/24} \cdot (q^{-1} + 2n^3) \right) \\
&\leq B_3 \left( \frac{48 + 3n^{-c_1/24+3}}{\ln m} \right).
\end{align}

Now we are about to bound the bias and the variance for small $p$ and large $p$, respectively. If $p \leq \frac{2c_1 \ln m}{m}$, first note that $L_H(x) = S_{K, H}(x) \wedge 1$ with $S_{K, H}(x)$ defined in [1]. It was shown in [1] Lemma 4] that
\begin{align}
|\mathbb{E}S_{K, H}(\hat{p}_1) + p \ln p| &\leq \frac{C}{m \ln m} \\
\mathbb{E}S_{K, H}^2(\hat{p}_1) &\leq m^{8c_2 \ln 2}(2c_1 \ln m)^4 / m^2
\end{align}
where we note that the constant $c_1$ in [1] corresponds to the constant $c_1/2$ in our paper. Then applying Lemma 31 we have
\begin{align}
\text{Var}(L_H(\hat{p}_1)) &\leq \text{Var}(S_{K, H}(\hat{p}_1)) \leq \mathbb{E}S_{K, H}^2(\hat{p}_1) \leq \frac{(2c_1 \ln m)^4}{m^2 - 8c_2 \ln 2}
\end{align}
and thus
\[
|\mathbb{E}L_H(\hat{p}_1) + p \ln p| \leq |\mathbb{E}S_{K,H}(\hat{p}_1) + p \ln p| + |\mathbb{E}S_{K,H}(\hat{p}_1)| \mathbb{1}(S_{K,H}(\hat{p}_1) \geq 1) \leq |\mathbb{E}S_{K,H}(\hat{p}_1)| \mathbb{1}(S_{K,H}(\hat{p}_1) \geq 1) + |\mathbb{E}S_{K,H}(\hat{p}_1)|^2 \leq \frac{C}{m \ln m} + \frac{(2c_1 \ln m)^4}{m^2 - 8c_2 \ln^2 m}.
\]

Hence, the total bias can be upper bounded as
\[
|\mathbb{E}[\hat{T}_i(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) + L_H(\hat{p}_1)] + p \ln (p/q)| \leq |\mathbb{E}[\hat{T}_i(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)] - p \ln q| + |\mathbb{E}L_H(\hat{p}_1) + p \ln p| \leq \frac{192B_3 m(S)}{c_1 n \ln n} + 6B_3 p n^{-c_1/24+3} + \frac{C}{m \ln m} + \frac{(2c_1 \ln m)^4}{m^2 - 8c_2 \ln^2 m}.
\]

As for the total variance, Lemma 29 can be used here to obtain
\[
\text{Var}(\hat{T}_i(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)) = \mathbb{E}[\hat{T}_i^2] - \mathbb{E}^2[\hat{T}_i] \leq \mathbb{E}[\hat{T}_i^3(\hat{q}_1, \hat{q}_2, \hat{q}_1)] - \mathbb{E}^2[\hat{T}_i(\hat{q}_1, \hat{q}_2)] \leq \mathbb{E}[\hat{T}_i(\hat{q}_1, \hat{q}_2)] - \mathbb{E}^2[\hat{T}_i(\hat{q}_1, \hat{q}_2)] \leq 1600B_3 \left( p^2 + \frac{p}{m} \right) \left( \frac{2500}{n^2} + 100n^{-c_1/24+3} \right) + \frac{p}{m} \left( B_3 \left( \frac{192}{c_1 n \ln n} + 6n^{-c_1/24+3} \right) - \ln q \right)^2 \leq 1600B_3 \left( p^2 + \frac{p}{m} \right) \left( \frac{125}{n^2} + n^{-c_1/24+3} \right) + \frac{p}{m} \left( B_3 \left( 48 + 6n^{-c_1/24+3} \right) - \ln q \right)^2.
\]

Now the desired variance bound follows from the triangle inequality $\text{Var}(X + Y) \leq 2(\text{Var}(X) + \text{Var}(Y))$. If $p \geq \frac{c_1 \ln m}{2mn}$, by Lemma 5 and the triangle inequality we have
\[
|\mathbb{E}[\hat{T}_i(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)] + U_H(\hat{p}_1)| + p \ln (p/q)| \leq |\mathbb{E}[\hat{T}_i(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)] - p \ln q| + |\mathbb{E}U_H(\hat{p}_1) + p \ln p| \leq \frac{192B_3 u(S)}{c_1 n \ln n} + 6B_3 p n^{-c_1/24+3} + \frac{6}{c_1 n \ln n} + 4m^{-c_1/24+2}
\]

which is the desired bias bound. As for the variance, we have
\[
\mathbb{E}[\hat{T}_i(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)] + U_H(\hat{p}_1) = -\hat{p}_1 \ln \hat{p}_1 \hat{q}_1 \cdot \mathbb{1}(\hat{q}_1 \neq 0) + \hat{p}_1 \cdot \sum k=1^3 h_k(\hat{q}_1, \hat{q}_2) + \frac{1}{2m}
\]

and the triangle inequality gives
\[
\text{Var}(\hat{T}_i(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)) + U_H(\hat{p}_1)) \leq 2\text{Var}(\hat{p}_1 \ln \hat{p}_1 \hat{q}_1 \cdot \mathbb{1}(\hat{q}_1 \neq 0)) + 2\text{Var}(\hat{p}_1 \cdot \sum k=1^3 h_k(\hat{q}_1, \hat{q}_2)) \leq 2(B_1 + B_2).
\]

Now we bound these two terms separately. For $B_1$, recall that Lemma 1 gives
\[
\text{Var}(\hat{p}_1 \ln \hat{p}_1 - g_n(\hat{q}_1))) \leq \frac{51}{m^2} + \frac{2}{m} \left( p + p(\ln u(S))^2 + \frac{4q}{e^2} + \frac{4u(S)}{en} \right) + \frac{700u(S)}{n} \left( p + \frac{1}{m} \right)
\]

and the difference between these two quantities is upper bounded by
\[
\mathbb{E}[\hat{p}_1 (g_n(\hat{q}_1) - \ln \hat{q}_1 \cdot \mathbb{1}(\hat{q}_1 \neq 0))^2 \leq (1 + \ln n)^2 \cdot \mathbb{P}(\hat{q}_1 = 0) \leq (1 + \ln n)^2 \cdot n^{-c_1/2}.
\]
As for $B_2$, Lemma \cite{29} is employed to obtain

\[
B_2 = \mathbb{E}[\hat{p}_1^2] \cdot \text{Var}(\sum_{k=1}^{3} h_k(\hat{q}_1, \hat{q}_2)) + \text{Var}(\hat{p}_1) \cdot (\mathbb{E} \sum_{k=1}^{3} h_k(\hat{q}_1, \hat{q}_2))^2
\]

\[
\leq \left( p^2 + \frac{p}{m} \right) \cdot 9B_3 \left( \frac{12500}{nq} + 100n^{-c_1/24+3} \right) + \frac{p}{m} \left( 3B_3 \left( 48 + 3n^{-c_1/24+3} \right) \right)^2
\]

\[
= 900B_3 \left( p^2 + \frac{p}{m} \right) \left( \frac{125}{nq} + n^{-c_1/24+3} \right) + \frac{9B_3^2 p}{m} \left( 48 + 3n^{-c_1/24+3} \right)^2.
\]

The desired variance bound then follows from the upper bounds of $B_1$ and $B_2$.

For the rest of the results, the only non-trivial observation is that when $p \leq \frac{2c_1 \ln m}{m}$, we have

\[
p(\ln q)^2 \leq p(-\ln p + \ln u(S))^2
\]

\[
\leq 2p(\ln p)^2 + 2p(\ln u(S))^2
\]

\[
\leq \frac{4c_1 \ln m}{m} \left( \ln \frac{m}{2c_1 \ln m} \right)^2 + 2p(\ln u(S))^2
\]

\[
\leq \frac{4c_1 (\ln m)^3}{m} + 2p(\ln u(S))^2
\]

since $p \leq u(S)q$ and $2c_1 \ln m \geq 8$.

\[\square\]

### G. Proof of Lemma \cite{8}

For simplicity, we define

\[
\overline{T}_{s,1}(\hat{p}, \hat{q}) \triangleq \hat{T}_s(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) + U_H(\hat{p}_1)
\]

\[
\overline{T}_{s,\Pi}(\hat{p}, \hat{q}) \triangleq \hat{T}_s(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) + L_H(\hat{p}_1)
\]

then

\[
\overline{T}_{s}(\hat{p}, \hat{q}) = \overline{T}_{s,1}(\hat{p}, \hat{q}) \mathbb{I}(\hat{p}_3 > \frac{c_1 \ln m}{m}) + \overline{T}_{s,\Pi}(\hat{p}, \hat{q}) \mathbb{I}(\hat{p}_3 \leq \frac{c_1 \ln m}{m}).
\]

By Lemma \cite{7} the bias can be upper bounded as

\[
|\overline{T}_{s}(\hat{p}, \hat{q}) + \ln(p/q)| \leq |\mathbb{E}\overline{T}_{s,1}(\hat{p}, \hat{q}) + \ln(p/q)| + |\mathbb{E}\overline{T}_{s,\Pi}(\hat{p}, \hat{q}) + \ln(p/q)|
\]

\[
\leq \frac{1}{m \ln m} + \frac{u(S)}{n \ln n}.
\]

As for the variance, by Lemma \cite{30} we have

\[
\text{Var}(\overline{T}_{s}(\hat{p}, \hat{q})) \leq \text{Var}(\overline{T}_{s,1}(\hat{p}, \hat{q})) + \text{Var}(\overline{T}_{s,\Pi}(\hat{p}, \hat{q})) + (\mathbb{E}\overline{T}_{s,1}(\hat{p}, \hat{q}) - \mathbb{E}\overline{T}_{s,\Pi}(\hat{p}, \hat{q}))^2
\]

\[
\leq \text{Var}(\overline{T}_{s,1}(\hat{p}, \hat{q})) + \text{Var}(\overline{T}_{s,\Pi}(\hat{p}, \hat{q})) + 2|\mathbb{E}\overline{T}_{s,1}(\hat{p}, \hat{q}) + \ln(p/q)|^2 + 2|\mathbb{E}\overline{T}_{s,\Pi}(\hat{p}, \hat{q}) + \ln(p/q)|^2
\]

\[
\leq \frac{1}{m^2 - \epsilon} + \frac{p(1 + \ln u(S))^2}{m} + \frac{q}{m} + \frac{u(S)}{mn} + \frac{pu(S)}{n} + \left( \frac{1}{m \ln m} + \frac{u(S)}{n \ln n} \right)^2
\]

\[
\leq \frac{1}{m^2 - \epsilon} + \frac{p(1 + \ln u(S))^2}{m} + \frac{q}{m} + \frac{u(S)}{mn} + \frac{pu(S)}{n} + \left( \frac{1}{m \ln m} + \frac{u(S)}{n \ln n} \right)^2
\]

\[
\leq \frac{1}{m^2 - \epsilon} + \frac{p(1 + \ln u(S))^2}{m} + \frac{q}{m} + \frac{u(S)}{mn} + \frac{pu(S)}{n} + \left( \frac{u(S)}{n \ln n} \right)^2
\]

as desired.

\[\square\]
where we have used (428) here. Since $\sum_{i=0}^{c_1 p \ln m} \leq \frac{1}{2} \sqrt{c_1 \hat{p}_2 \ln m}$, then by Lemma 28 we have

$$\mathbb{P}(E^c) \leq \mathbb{P}(\hat{p}_2 < \frac{2p}{3}) + \mathbb{P}(\hat{p}_2 > p + \frac{1}{2} \sqrt{c_1 \hat{p}_2 \ln m})$$

$$\leq \mathbb{P}(\hat{p}_2 < \frac{1}{2} \sqrt{c_1 p \ln m}) \leq \mathbb{P}(\hat{p}_2 > p + \frac{1}{2} \sqrt{c_1 p \ln m})$$

$$\leq \exp \left( -\frac{1}{2} \sqrt{c_1 \ln m} \cdot mp \right) + \exp \left( -\frac{1}{3} \sqrt{c_1 \ln m} \cdot mp \right)$$

$$\leq 2e^{-c_1 m/36}.$$ (427)

We prove Lemma 9

Now we are about to apply Lemma 27 to bound each coefficient $|g_{K,k}(\hat{p}_2)|$. Lemma 27 yields

$$|g_{K,k}(\hat{p}_2)| \leq 2^{7K/2} A \cdot \left( \frac{3c_1 \ln n}{n} \right)^{-k} (3^K + 1) \leq 2^{31K/2} A \cdot \left( \frac{3c_1 \ln n}{n} \right)^{-k}$$

Note that conditioning on the event $E$, we have $\hat{p}_2 \geq \frac{c_1 \ln m}{3m}$, and

$$0 < \frac{2p}{21u(S)} \leq \frac{1}{u(S)} \left( \hat{p}_2 - \frac{\sqrt{3}}{2} \hat{p}_2 \right) \leq \frac{1}{u(S)} \left( \hat{p}_2 - \frac{1}{2} \sqrt{c_1 \hat{p}_2 \ln m} \right) \leq \frac{p}{u(S)} \leq q \leq 2\frac{c_1 \ln n}{n}$$

Note that conditioning on $E$, we have

$$T_{n,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) = \hat{p}_1 \cdot \sum_{k=0}^{K} g_{K,k}(\hat{p}_2) \prod_{l=0}^{k-1} (\hat{q}_2 - \frac{l}{n}).$$ (432)

By construction, $\sum_{k=0}^{K} g_{K,k}(\hat{p}_2) x^k$ is the best polynomial approximation of $\ln q$ on $R$, where

$$\left[ \frac{2p}{21u(S)}, \frac{4c_1 \ln n}{n} \right] \subset R = \left[ \frac{1}{u(S)} \left( \hat{p}_2 - \frac{1}{2} \sqrt{c_1 \hat{p}_2 \ln m} \right), \frac{4c_1 \ln n}{n} \right] \supset \left[ \frac{2c_1 \ln n}{n}, \frac{4c_1 \ln n}{n} \right]$$ (433)

where we have used (428) here. Since $W(\cdot)$ in Lemma 23 is an increasing function, conditioning on $E$ the approximation error can be upper bounded as

$$\sup_{x \in R} \left| \sum_{k=0}^{K} g_{K,k}(\hat{p}_2) x^k - \ln x \right| \leq C_{\ln W} \left( \frac{4c_1 \ln n}{n} \right) \leq C_{\ln W} \left( \frac{42c_1 \ln n}{c_2^2} \cdot \frac{u(S)}{pm \ln n} \right).$$ (434)

Note that $W(x) \leq 1 \vee \ln x$, we conclude that for any $x \in \left[ \frac{2c_1 \ln n}{n}, \frac{4c_1 \ln n}{n} \right] \subset R$, we have

$$\left| \sum_{k=0}^{K} g_{K,k}(\hat{p}_2) x^k \right| \leq \sum_{k=0}^{K} g_{K,k}(\hat{p}_2) x^k \leq C_{\ln} \left( \frac{42c_1 \ln n}{c_2^2} \cdot \frac{u(S)}{pm \ln n} \right) \vee 1$$ (435)

$$\leq C_{\ln} \left( \ln \left( \frac{42c_1}{c_2^2} \cdot \frac{u(S)}{pm \ln n} \right) \vee 1 \right) + \ln n \equiv A.$$ (436)

Now we are about to apply Lemma 27 to bound each coefficient $|g_{K,k}(\hat{p}_2)|$. Lemma 27 yields

$$|g_{K,k}(\hat{p}_2)| \leq 2^{7K/2} A \cdot \frac{3c_1 \ln n}{n}^{-k} (3^K + 1) \leq 2^{31K/2} A \cdot \frac{3c_1 \ln n}{n}^{-k}$$ (437)
for any $k = 0, 1, \ldots, K = c_2 \ln n$ conditioning on $E$. Hence, by the triangle inequality,
\[ \mathbb{E}[T_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)^2 \mathbbm{1}(E)] = \mathbb{E}(\hat{p}_1^2) \cdot \mathbb{E} \left[ \sum_{k=0}^{K} g_{K,k}(\hat{p}_2) \prod_{l=0}^{k-1} (\hat{q}_2 - \frac{l}{n})^2 \mathbbm{1}(E) \right] \]
\[ \leq \mathbb{E}(\hat{p}_1^2) \cdot (K+1) \sum_{k=0}^{K} 2^{11K/2} A \cdot \left( \frac{3c_1 \ln n}{n} \right)^{-2k} \mathbb{E} \left[ \prod_{l=0}^{k-1} (\hat{q}_2 - \frac{l}{n})^2 \right] \]
\[ = 2^{11K} (K+1) A^2 \left( p^2 + \frac{p}{m} \right) \cdot \sum_{k=0}^{K} \left( \frac{3c_1 \ln n}{n} \right)^{-2k} \mathbb{E} \left[ \prod_{l=0}^{k-1} (\hat{q}_2 - \frac{l}{n})^2 \right]. \]

To evaluate the expectation, Lemma 25 with $q = 0$ is applied here to yield
\[ \mathbb{E} \left[ \prod_{l=0}^{k-1} (\hat{q}_2 - \frac{l}{n})^2 \right] \leq \left( \frac{2q(k \vee nq)}{n} \right)^k \leq \left( \frac{4c_1 q \ln n}{n} \right)^k \leq \left( \frac{3c_1 \ln n}{n} \right)^{2k} \]
thus
\[ \mathbb{E}[T_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)^2 \mathbbm{1}(E)] \leq 2^{11K} (K+1)^2 A^2 \left( p^2 + \frac{p}{m} \right) \leq 2^{11K+2} K^2 A^2 \left( p^2 + \frac{p}{m} \right). \]

By differentiation it is easy to show
\[ p \left[ \ln \left( \frac{4c_1}{c_2} \cdot \frac{u(S)}{pm \ln n} \right) \right] \leq \frac{8c_1}{c_2} \cdot \frac{u(S)}{n \ln n} \land p \leq \frac{8c_1}{c_2} \cdot \frac{u(S)}{n \ln n} + p \]
and note that $p \leq u(S)q \leq \frac{c_2 u(S) \ln n}{n}$, we have
\[ \mathbb{E}[T_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)^2 \mathbbm{1}(E)] \leq 2^{11K+3} K^2 \left( \frac{p + \frac{1}{m}}{m} \right) \cdot \frac{8c_1 C_{\ln n}}{n \ln n} + C_{\ln n}^2 p + p(\ln n)^2 \]
\[ \leq 2^{11K+3} K^2 \left( \frac{2c_1 u(S) \ln n}{n} + \frac{1}{m} \right) \cdot \frac{8c_1 C_{\ln n}}{n \ln n} \cdot \frac{u(S)}{n \ln n} + (C_{\ln n}^2 + (\ln n)^2) \cdot \frac{2c_1 u(S) \ln n}{n} \]
\[ = \frac{16c_1 u(S) \ln n}{n^{1-11c_2 \ln n}} \cdot \frac{2c_1 u(S) \ln n}{n} + \frac{1}{m} \cdot \left( \frac{42C_{\ln n}^2}{n^{1-11c_2 \ln n}} + (c_2 \ln n)^2 (C_{\ln n}^2 + (\ln n)^2) \right) \]
which together with (431) is the variance bound.

Now we start to analyze the bias of $\hat{T}_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)$. By triangle inequality,
\[ \mathbb{E} \left[ \hat{T}_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) - p \ln q \right] \leq \mathbb{E} \left[ \hat{T}_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) - p \ln q \right] \mathbbm{1}(E) + \mathbb{E} \left[ \hat{T}_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) - p \ln q \right] \mathbbm{1}(E^c) \]
\[ \leq \mathbb{E} \left[ T_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) - p \ln q \right] \mathbbm{1}(E) + \mathbb{E} \left[ \hat{T}_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) - T_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) \right] \mathbbm{1}(E^c) \]
\[ + 2m^{-c_1/36} (1 - p \ln q) \]
\[ \leq \mathbb{E} \left[ T_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) - p \ln q \right] \mathbbm{1}(E) + \mathbb{E} \left[ T_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) \mathbbm{1}(T_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) \geq 1) \mathbbm{1}(E) \right] \]
\[ + 2m^{-c_1/36} (1 - p \ln q) \]
\[ \equiv A_1 + A_2 + 2m^{-c_1/36} (1 - p \ln q). \]

Now we bound $A_1$ and $A_2$ separately. For $A_1$, since conditioning on $E$, the approximation region contains $q$, by (434) we get
\[ A_1 \leq p \mathbb{E} \left[ \sum_{k=0}^{K} g_{K,k}(\hat{p}_2)q^k \ln q \right] \mathbbm{1}(E) \leq C_{\ln n}^2 \cdot \frac{u(S)}{pn \ln n}. \]
As for $A_2$, since for any random variable $X$ with finite second moment, we have
\[ \mathbb{E}[|X|^2 \mathbbm{1}(|X| \geq 1)] \leq \mathbb{E}[|X|^2 \mathbbm{1}(|X| \geq 1)] \leq \mathbb{E}[X^2], \]
by (446) we get
\[ A_2 \leq \mathbb{E}[T_{m,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)^2 \mathbbm{1}(E)] \]
\[ \leq \frac{16c_1 u(S) \ln n}{n^{1-11c_2 \ln n}} \left( \frac{2c_1 u(S) \ln n}{n} + \frac{1}{m} \right) \left( 42C_{\ln n}^2 + (c_2 \ln n)^2 (C_{\ln n}^2 + (\ln n)^2) \right). \]

Now combining $A_1$ and $A_2$ completes the proof.
I. Proof of Lemma 11

First we bound the variance of $T_{\text{ms},\Pi}(\hat{p}_1, \hat{q}_1)$. Recall that

$$T_{\text{ms},\Pi}(\hat{p}_1, \hat{q}_1) = \sum_{k,l \geq 0, k+l \leq K} h_{K,k,l} \prod_{i=0}^{k-1} \left( \hat{p}_1 - \frac{i}{m} \right) \prod_{j=0}^{l-1} \left( \hat{q}_1 - \frac{j}{n} \right).$$

(455)

We first bound the coefficients $|h_{K,k,l}|$. It is straightforward to see that

$$\sup_{(x,y) \in R} \left| \sum_{k,l \geq 0, k+l \leq K} h_{K,k,l} x^k y^l \right| \leq 2 \sup_{(x,y) \in R} |x \ln y| \leq \frac{8c_1 u(S) \ln n}{n} \ln \left( \frac{n}{4c_1 \ln n} \right) \leq \frac{8c_1 u(S)(\ln n)^2}{n} \equiv A. \quad (456)$$

We distinguish into two cases.

1) Case I: If $\frac{\ln m}{\ln u(S)} \leq \frac{\ln n}{2}$, we have

$$R \supset \left[ 0, \frac{2c_1 \ln m}{m} \right] \times \left[ \frac{2c_1 \ln n}{n}, \frac{4c_1 \ln n}{n} \right] \triangleq R_1. \quad (457)$$

Hence, for any $(x, y) \in R_1$, we have

$$\left| \sum_{k=0}^{K} \left( \sum_{l=0}^{K-k} h_{K,k,l} y^l \right) x^k \right| \leq A. \quad (458)$$

By Lemma 27 we conclude that for any $y \in \left[ \frac{2c_1 \ln n}{n}, \frac{4c_1 \ln n}{n} \right],$

$$\left| \sum_{l=0}^{K-k} \sum_{k=0}^{K-k} h_{K,k,l} y^l \right| \leq 2^{7K/2+1} A \cdot \left( \frac{c_1 \ln m}{m} \right)^{-k}, \quad k = 0, 1, \ldots, K. \quad (459)$$

Using Lemma 27 again, we have

$$|h_{K,k,l}| \leq 2^{7(K-k)/2} \cdot 2^{7K/2+1} A \left( \frac{c_1 \ln m}{m} \right)^{-k} \cdot \left( \frac{3c_1 \ln n}{n} \right)^{-l} \cdot (3^{K-k} + 1) \quad (460)$$

$$\leq 2^{9K+1} A \left( \frac{c_1 \ln m}{m} \right)^{-k} \cdot \left( \frac{3c_1 \ln n}{n} \right)^{-l}, \quad \forall k, l \geq 0, k + l \leq K. \quad (461)$$

2) Case II: If $\frac{\ln m}{\ln u(S)} > \frac{\ln n}{2}$, define $t \triangleq p/q$, we have

$$R \supset \left\{ (t, q) : 0 \leq t \leq u(S), 0 \leq q \leq \frac{2c_1 \ln n}{n} \right\} \triangleq R_2 \quad (462)$$

and for any $(t, q) \in R_2$, we have

$$\left| \sum_{k=0}^{K} \left( \sum_{l=0}^{L-k} h_{K,k,l} t^{q+l} \right) t^k \right| = \left| \sum_{k,l \geq 0, k+l \leq K} h_{K,k,l}(qt)^k q^l \right| \leq A. \quad (463)$$

By Lemma 27 we conclude that for any $q \in \left[ 0, \frac{c_1 \ln n}{n} \right],$

$$\left| \sum_{l=0}^{L-k} \sum_{k=0}^{L-k} h_{K,k,l} t^{q+l} \right| \leq 2^{7K/2+1} A \cdot \left( \frac{u(S)}{2} \right)^{-k}. \quad (464)$$

By Lemma 27 again, we have

$$|h_{K,k,l}| \leq 2^{7K/2+1} \cdot 2^{7K/2+1} A \left( \frac{u(S)}{2} \right)^{-k} \cdot \left( \frac{c_1 \ln n}{n} \right)^{-k} \cdot \left( \frac{c_1 \ln n}{n} \right)^{-l} \cdot (3^{K-k} + 1) \quad (465)$$

$$= 2^{2K+2} A \left( \frac{c_1 u(S) \ln n}{2n} \right)^{-k} \cdot \left( \frac{c_1 \ln n}{n} \right)^{-l}, \quad \forall k, l \geq 0, k + l \leq n. \quad (466)$$

Hence, combining these two cases yields

$$|h_{K,k,l}| \leq 2^{9K+1} A \left[ \left( \frac{c_1 u(S) \ln n}{2n} \right)^{-k} + \left( \frac{c_1 \ln m}{m} \right)^{-k} \cdot \left( \frac{c_1 \ln n}{n} \right)^{-l} \right]. \quad (467)$$
Moreover, by Lemma 25 we have
\[
\mathbb{E}\left[ \prod_{i=0}^{k-1} \left( \frac{\hat{\theta}_1 - i}{m} \right)^2 \right] \leq \left( \frac{2p(k \lor m p)}{m} \right)^k \leq \left( \frac{4c_1 p (\ln n + \ln m)}{m} \right)^k \leq \left( \frac{3c_1 (\ln m + \ln n)}{m} \right)^{2k} \quad (468)
\]
\[
\mathbb{E}\left[ \prod_{j=0}^{l-1} \left( \frac{\hat{\theta}_1 - j}{n} \right)^2 \right] \leq \left( \frac{2q(l \lor n q)}{n} \right)^l \leq \left( \frac{8c_1 q \ln n}{n} \right)^l \leq \left( \frac{6c_1 \ln n}{n} \right)^{2l} \quad (469)
\]

Now by the triangle inequality and previous inequalities, we have
\[
\mathbb{E}[T_{\text{ns,II}}(\hat{\theta}_1, \hat{\theta}_1)] \leq (K + 1)^2 \sum_{k,l \geq 0, 0 < k+l \leq K} |h_{K,k,l}|^2 \mathbb{E}\left[ \prod_{i=0}^{k-1} \left( \frac{\hat{\theta}_1 - i}{m} \right)^2 \right] \mathbb{E}\left[ \prod_{j=0}^{l-1} \left( \frac{\hat{\theta}_1 - j}{n} \right)^2 \right] \quad (470)
\]
\[
\leq 2^{18K+3} (K + 1)^2 A^2 \sum_{k,l \geq 0, 0 < k+l \leq K} 6^{2l} \left( 2^{2k} \left( \frac{1 + \frac{\ln n}{\ln m}}{2} \right)^{2k} + 12^{2k} \left( \frac{\ln m + \ln n}{\mu(S) \ln n} \right)^{2k} \right) \quad (471)
\]
\[
\leq 2^{18K+12} 2^{2K} (K + 1)^2 A^2 \left( 1 + \left( 1 + \frac{\ln n}{\ln m} \right)^{2K} + \left( \frac{\ln m + \ln n}{\mu(S) \ln n} \right)^{2K} \right) \quad (472)
\]
\[
\leq 2^{26K+7} K^4 A^2 \left( 1 + \left( 1 + \frac{\ln n}{\ln m} \right)^{2K} + \left( \frac{\ln m + \ln n}{\mu(S) \ln n} \right)^{2K} \right) \quad (473)
\]

Hence, by Lemma 31 we get
\[
\text{Var}(\hat{T}_{\text{ns,II}}(\hat{\theta}_1, \hat{\theta}_1)) \leq \text{Var}(T_{\text{ns,II}}(\hat{\theta}_1, \hat{\theta}_1)) \leq \mathbb{E}[T_{\text{ns,II}}(\hat{\theta}_1, \hat{\theta}_1)]^2 \leq 2^{26K+7} K^4 A^2 \left( 1 + \left( 1 + \frac{\ln n}{\ln m} \right)^{2K} + \left( \frac{\ln m + \ln n}{\mu(S) \ln n} \right)^{2K} \right) \quad (474)
\]
which is the desired variance bound.

As for the bias, Lemma 10 and Lemma 24 give
\[
|\mathbb{E}[T_{\text{ns,II}}(\hat{\theta}_1, \hat{\theta}_1)] - p \ln q| \leq E_K[p \ln q; R] + |h_{K,0,0}| \leq 2E_K[p \ln q; R] \leq 2MC_0^2 \left( \frac{\ln q}{\mu(S)} \cdot \frac{\ln n}{n} \right) \leq \frac{2MC_0}{c^2} \cdot \frac{\ln q}{\mu(S)} \cdot \frac{\ln n}{n} \quad (477)
\]
where $|h_{K,0,0}| \leq E_K[p \ln q; R]$ is obtained by setting $(p, q) = (0, 0) \in R$ in
\[
\sup_{(x,y) \in R} \left| \sum_{k,l \geq 0, 0 < k+l \leq K} h_{K,k,l} x^k y^l - x \ln y \right| \leq E_K[p \ln q; R]. \quad (478)
\]
Hence, by triangle inequality and (452), we get
\[
|\mathbb{E}[\hat{T}_{\text{ns,II}}(\hat{\theta}_1, \hat{\theta}_1)] - p \ln q| \leq |\mathbb{E}[T_{\text{ns,II}}(\hat{\theta}_1, \hat{\theta}_1)] - p \ln q| + |\mathbb{E}[T_{\text{ns,II}}(\hat{\theta}_1, \hat{\theta}_1) \mathbb{I}(|T_{\text{ns,II}}(\hat{\theta}_1, \hat{\theta}_1)| \geq 1)]| \quad (479)
\]
\[
\leq 2MC_0^2 \left( \frac{\ln q}{\ln n} + E[T_{\text{ns,II}}(\hat{\theta}_1, \hat{\theta}_1)]^2 \right) \quad (480)
\]
\[
\leq 2MC_0^2 \left( \frac{\ln q}{\ln n} + 2^{26K+7} K^4 A^2 \left( 1 + \left( 1 + \frac{\ln n}{\ln m} \right)^{2K} + \left( \frac{\ln m + \ln n}{\mu(S) \ln n} \right)^{2K} \right) \right) \quad (481)
\]
as desired.

\section*{J. Proof of Lemma 12}
We distinguish into three cases based on different values of $p$. For simplicity, we define
\[
T_{\text{ns,II}}(\hat{\theta}_1, \hat{\theta}_1) \equiv T_{\text{ns,II}}(\hat{\theta}_1, \hat{\theta}_1) + L_H(\hat{\theta}_1) \quad (482)
\]
\[
T_{\text{ns,II}}(\hat{\theta}_1, \hat{\theta}_1) \equiv T_{\text{ns,II}}(\hat{\theta}_1, \hat{\theta}_1) + L_H(\hat{\theta}_1). \quad (483)
\]
1) **Case I:** We first consider the case where \( p \leq \frac{c_1 \ln m}{2m} \). By the triangle inequality, the bias can be decomposed into

\[
\text{Bias}(T_{ns}(\hat{p}, \hat{q})) \leq \left| \mathbb{E}T_{ns}(\hat{p}_1, \hat{q}_1) + p \ln(p/q) + \mathbb{E}|T_{ns}(\hat{p}_1, \hat{q}_1)| + \mathbb{E}|T_{ns}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)| \right| \mathbb{P}(\hat{p}_3 \geq \frac{c_1 \ln m}{m})
\](484)

\[
\leq \left| \mathbb{E}T_{ns}(\hat{p}_1, \hat{q}_1) + p \ln(p/q) + 4 \cdot (e/4)^{c_1 \ln m/2} \right| + \left| \mathbb{E}|T_{ns}(\hat{p}_1, \hat{q}_1)| \right| + \left| \mathbb{E}|T_{ns}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)| \right|
\](485)

\[
\leq \frac{1}{m \ln m} + \frac{u(S)}{n \ln n} + \frac{(u(S))^2}{n^2 - c_2 B} + m - \frac{\epsilon}{4} \ln\left(4/e\right)
\](486)

\[
\leq \frac{1}{m \ln m} + \frac{u(S)}{n \ln n} + \frac{(u(S))^2}{n^2 - c_2 B}
\](487)

where we have used Lemma 11 and Lemma 28 here. Similarly, by Lemma 30 the variance can be upper bounded as

\[
\text{Var}(T_{ns}(\hat{p}, \hat{q})) \leq \text{Var}(T_{ns}(\hat{p}_1, \hat{q}_1)) + \text{Var}(T_{ns}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)) \mathbb{P}(\hat{p}_3 \geq \frac{c_1 \ln m}{m}) + \left| \mathbb{E}T_{ns}(\hat{p}_1, \hat{q}_1) + \mathbb{E}T_{ns}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) \right| \mathbb{P}(\hat{p}_3 \geq \frac{c_1 \ln m}{m})
\](488)

\[
\leq \text{Var}(T_{ns}(\hat{p}_1, \hat{q}_1)) + 2^2 \cdot (e/4)^{c_1 \ln m/2} + 4^2 \cdot (e/4)^{c_1 \ln m/2}
\](489)

\[
\leq \frac{1}{m^2 - c_2 B} + \frac{(u(S))^2}{n^2 - c_2 B} + m - \frac{\epsilon}{4} \ln\left(4/e\right)
\](490)

\[
\leq \frac{1}{m^2 - c_2 B} + \frac{(u(S))^2}{n^2 - c_2 B}
\](491)

2) **Case II:** Next we consider the case where \( \frac{c_1 \ln m}{2m} < p \leq \frac{2c_1 \ln m}{m} \). By Lemma 9 and Lemma 11 the bias can be upper bounded as

\[
\text{Bias}(T_{ns}(\hat{p}, \hat{q})) \leq \left| \mathbb{E}T_{ns}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) + p \ln(p/q) + \mathbb{E}T_{ns}(\hat{p}_1, \hat{q}_1) + p \ln(p/q) \right|
\](492)

\[
\leq \frac{1}{m \ln m} + \frac{p}{m \ln m} + \frac{u(S)(\ln n)^5}{m^{1 - 11\epsilon}} \left( \frac{u(S) \ln n}{n} + \frac{1}{m} \right) + \frac{1}{m \ln m} + \frac{u(S)}{n \ln n} + \frac{(u(S))^2}{n^2 - c_2 B}
\](493)

\[
\leq \frac{1}{m \ln m} + \frac{p}{m \ln m} + \frac{u(S)(\ln n)^5}{m^{1 - 11\epsilon}} \left( \frac{u(S) \ln n}{n} + \frac{1}{m} \right) + \frac{(u(S))^2}{n^2 - c_2 B}
\](494)

The variance is obtained by Lemma 30 as follows:

\[
\text{Var}(T_{ns}(\hat{p}, \hat{q})) \leq \text{Var}(T_{ns}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)) + \text{Var}(T_{ns}(\hat{p}_1, \hat{q}_1)) + (\mathbb{E}T_{ns}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) - \mathbb{E}T_{ns}(\hat{p}_1, \hat{q}_1))^2
\](495)

\[
\leq \frac{u(S)(\ln n)^5}{mn} + \frac{p}{m^3} + \frac{u(S)(\ln n)^5}{m^{1 - 11\epsilon}} \left( \frac{u(S) \ln n}{n} + \frac{1}{m} \right) + \frac{(m \ln m)^4}{m^{2 - c_2 B}} + \frac{u(S)}{m^{2 - c_2 B}}
\](496)

\[
\leq \frac{u(S)(\ln n)^5}{mn} + \frac{p}{m^3} + \frac{u(S)(\ln n)^5}{m^{1 - 11\epsilon}} \left( \frac{u(S) \ln n}{n} + \frac{1}{m} \right) + \frac{(m \ln m)^4}{m^{2 - c_2 B}} + \frac{u(S)}{m^{2 - c_2 B}}
\](497)

\[
\leq \frac{u(S)(\ln n)^5}{mn} + \frac{p}{m^3} + \frac{u(S)(\ln n)^5}{m^{1 - 11\epsilon}} \left( \frac{u(S) \ln n}{n} + \frac{1}{m} \right) + \frac{(m \ln m)^4}{m^{2 - c_2 B}} + \frac{u(S)}{m^{2 - c_2 B}}
\](498)

where in the last step we have used that \( n \geq u(S) \).

3) **Case III:** Finally we consider the case where \( p \geq \frac{2c_1 \ln m}{m} \). By Lemma 9 and Lemma 28

\[
\text{Bias}(T_{ns}(\hat{p}, \hat{q})) \leq \left| \mathbb{E}T_{ns}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) + p \ln(p/q) + \mathbb{E}T_{ns}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) \right| \mathbb{P}(\hat{p}_3 \leq \frac{c_1 \ln m}{m})
\](499)

\[
\leq \left| \mathbb{E}T_{ns}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2) + p \ln(p/q) + 4 \cdot e^{-c_1 \ln m/2} \right| + 4 \cdot e^{-c_1 \ln m/2}
\](500)

\[
\leq \frac{1}{m \ln m} + \frac{p}{m \ln m} + \frac{u(S)(\ln n)^5}{m^{1 - 11\epsilon}} \left( \frac{u(S) \ln n}{n} + \frac{1}{m} \right) + m - c_1/2
\](501)

\[
\leq \frac{1}{m \ln m} + \frac{p}{m \ln m} + \frac{u(S)(\ln n)^5}{m^{1 - 11\epsilon}} \left( \frac{u(S) \ln n}{n} + \frac{1}{m} \right) + m - c_1/2
\](502)
and the variance is given by Lemma 30 that

\[
\text{Var}(T_{ns}(\hat{p}, \hat{q})) \leq \text{Var}(\overline{T}_{ns,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)) + \text{Var}(\overline{T}_{ns,II}(\hat{p}_1, \hat{q}_1))\mathbb{P}(\hat{p}_3 \leq \frac{c_1 \ln m}{m}) + |\mathbb{E}\overline{T}_{ns,II} - \mathbb{E}\overline{T}_{ns,1}|^2\mathbb{P}(\hat{p}_3 \leq \frac{c_1 \ln m}{m}) \quad (503)
\]

\[
\leq \text{Var}(\overline{T}_{ns,1}(\hat{p}_1, \hat{q}_1; \hat{p}_2, \hat{q}_2)) + 2^2 \cdot e^{-\frac{c_1 \ln m}{m}} + 4^2 \cdot e^{-\frac{c_1 \ln m}{m}} \quad (504)
\]

\[
\approx \frac{u(S)(\ln n)^3}{mn} + \frac{p}{m} + \frac{1}{m^3} + \frac{u(S)(\ln n)^5}{n^{1-11c_2 \ln 2}} \left(\frac{u(S)(\ln n)}{n} + \frac{1}{m}\right) + m^{-c_1/2} \quad (505)
\]

\[
\approx \frac{1}{m^2} + \frac{(u(S))^2}{n^{2-\epsilon}} + \frac{u(S)}{mn^{1-\epsilon}}. \quad (506)
\]

A combination of these three cases completes the proof.

\[\square\]

K. Proof of Lemma 13

As in the proof of Lemma 12 we also distinguish into three cases.

1) Case I: We first consider the case where \( q \leq \frac{c_1 \ln n}{m} \). By Lemma 12 and Lemma 28

\[
|\text{Bias}(\xi(\hat{p}, \hat{q}))| \leq |\mathbb{E}T_{ns}(\hat{p}, \hat{q}) + p \ln(p/q)| + (|\mathbb{E}T_{ns,1}(\hat{p}, \hat{q})| + |\mathbb{E}T_{ns,II}(\hat{p}, \hat{q})|)\mathbb{P}(|\hat{q}_3| \geq \frac{c_1 \ln n}{n}) \quad (507)
\]

\[
\leq |\mathbb{E}T_{ns}(\hat{p}, \hat{q}) + p \ln(p/q)| + (2 + \ln n + 5n^3 + 1 + \frac{1}{2n}) + 1 \cdot (e/4)^{\frac{c_1 \ln n}{m}} \quad (508)
\]

\[
\lesssim \left(\frac{1}{m^{2-\epsilon}} + \frac{p(1 + \ln u(S))^2}{m} + \frac{q}{m} + \frac{u(S)}{mn} + \frac{p(u(S))^2}{m^3} + \frac{(u(S))^2}{m^2} \right) \cdot (e/4)^{\frac{c_1 \ln n}{m}} \quad (510)
\]

here. Similarly, by Lemma 30 the variance can be upper bounded as

\[
\text{Var}(\xi(\hat{p}, \hat{q})) \leq \text{Var}(T_{ns}(\hat{p}, \hat{q})) + |\text{Var}(T_{ns}(\hat{p}, \hat{q})) + (|\mathbb{E}T_{ns}(\hat{p}, \hat{q}) - \mathbb{E}T_{ns}(\hat{p}, \hat{q})|^2)\mathbb{P}(\hat{q}_3 \geq \frac{c_1 \ln n}{n}) \quad (511)
\]

\[
\lesssim \text{Var}(T_{ns}(\hat{p}, \hat{q})) + \left[\frac{1}{m^{2-\epsilon}} + \frac{p(1 + \ln u(S))^2}{m} + \frac{q}{m} + \frac{u(S)}{mn} + \frac{p(u(S))^2}{m^3} + \frac{(u(S))^2}{m^2} \right] \cdot (e/4)^{\frac{c_1 \ln n}{m}} \quad (512)
\]

\[
\lesssim \left(\frac{1}{m^{2-\epsilon}} + \frac{(u(S))^2}{n^{2-\epsilon}} + \frac{u(S)}{mn^{1-\epsilon}} + \frac{pW(u(S))^2}{mn^{1-\epsilon}} \right) \quad (513)
\]

2) Case II: Next we consider the case where \( \frac{c_1 \ln n}{2m} < q < \frac{2c_1 \ln n}{n} \). By Lemma 8 and Lemma 12

\[
|\text{Bias}(\xi(\hat{p}, \hat{q}))| \leq |\mathbb{E}T_{ns}(\hat{p}, \hat{q}) + p \ln(p/q)| + |\mathbb{E}T_{ns}(\hat{p}, \hat{q}) + p \ln(p/q)| \quad (514)
\]

\[
\lesssim \frac{1}{m \ln m} + \frac{u(S)}{n \ln n} + \left(\frac{1}{m \ln m} + \frac{u(S)}{n \ln n} + \frac{(u(S))^2}{n^{2-\epsilon}} \right) \cdot (e/4)^{\frac{c_1 \ln m}{2m}} \quad (515)
\]

\[
\lesssim \left(\frac{1}{m \ln m} + \frac{u(S)}{n \ln n} + \frac{(u(S))^2}{n^{2-\epsilon}} \right) \quad (516)
\]
As for the variance, Lemma 30 is used here to yield
\[
\begin{align*}
\text{Var}(\xi(\hat{\rho}, \hat{\eta})) & \leq \text{Var}(T_m(\hat{\rho}, \hat{\eta})) + \text{Var}(\overline{T}_s(\hat{\rho}, \hat{\eta})) + \|ET_m(\hat{\rho}, \hat{\eta}) - E\overline{T}_s(\hat{\rho}, \hat{\eta})\|^2 \\
& \lesssim \text{Var}(T_m(\hat{\rho}, \hat{\eta})) + \frac{1}{m^{2-\epsilon}} + \frac{p(1 + \ln u(S))^2}{m} + \frac{q}{m} + \frac{u(S)}{n} + \frac{pu(S)}{n} + \left(\frac{u(S)}{n}\right)^2 \\
& \quad + \|ET_m(\hat{\rho}, \hat{\eta}) + p\ln(p/q)|^2 + |E\overline{T}_s(\hat{\rho}_1, \hat{\eta}_1; \hat{\rho}_2, \hat{\eta}_2) + p\ln(p/q)|^2 \\
& \lesssim \frac{1}{m^2} + \frac{p(1 + \ln u(S))^2}{m} + \frac{q}{m} + \frac{pu(S)}{n} + \left(\frac{u(S)}{n}\right)^2 + \left(\frac{u(S)}{n}\right)^2 \\
& \quad + \left(\frac{u(S)}{n}\right)^2 + \left(\frac{u(S)}{n}\right)^2 + \left(\frac{u(S)}{n}\right)^2 + \left(\frac{u(S)}{n}\right)^2 \\
& \quad + \left(\frac{u(S)}{n}\right)^2 + \left(\frac{u(S)}{n}\right)^2 + \left(\frac{u(S)}{n}\right)^2 + \left(\frac{u(S)}{n}\right)^2
\end{align*}
\]
where we have used the fact that \( n \geq u(S) \) here.

3) Case III: Finally we come to the case where \( q \geq \frac{2c_1 \ln n}{n} \). By Lemma 8 and Lemma 28,
\[
\begin{align*}
\text{Bias}(\xi(\hat{\rho}, \hat{\eta})) & \leq |\text{ET}_s(\hat{\rho}, \hat{\eta}) + p\ln(p/q)| + (\text{ET}_m(\hat{\rho}, \hat{\eta}) + E|T_s(\hat{\rho}, \hat{\eta}))\|P(\hat{q}_3 \leq \frac{c_1 \ln n}{n})
\end{align*}
\]

The variance bound is obtained in a similar fashion via Lemma 30
\[
\begin{align*}
\text{Var}(\xi(\hat{\rho}, \hat{\eta})) & \leq \text{Var}(T_m(\hat{\rho}, \hat{\eta})) + \left[\text{Var}(T_m(\hat{\rho}, \hat{\eta})) + \left(E|T_m(\hat{\rho}, \hat{\eta}) - E\overline{T}_s(\hat{\rho}, \hat{\eta})\|P(\hat{q}_3 \leq \frac{c_1 \ln n}{n})
\end{align*}
\]

Combining these three cases yields the desired result.

\[\square\]

L. Proof of Lemma 74

As before, we first analyze the variance. By Lemma 20, we know that there exists some constant \( C > 0 \) such that for any \( x \in [0, \frac{2c_1 \ln n}{n}] \),
\[
\left|\sum_{k=1}^{K+1} g_{K,k} \left(\frac{2c_1 \ln n}{n}\right)^{1-k} x^k - x \ln x\right| \leq \frac{C}{n \ln n}\].
\]

By triangle inequality, for any \( x \in [0, \frac{2c_1 \ln n}{n}] \),
\[
\left|\sum_{k=1}^{K+1} g_{K,k} \left(\frac{2c_1 \ln n}{n}\right)^{1-k} x^k\right| \leq \left|\sum_{k=1}^{K+1} g_{K,k} \left(\frac{2c_1 \ln n}{n}\right)^{1-k} x^k - x \ln x\right| + |x \ln x|
\]
\[
\leq \frac{C}{n \ln n} + \frac{2c_1 \ln n}{n} \cdot \ln \frac{n}{2c_1 \ln n}
\]
\[
\leq \frac{C}{n \ln n} + \frac{2c_1 (\ln n)^2}{n} \equiv A.
\]

As a result, by Lemma 27 for any \( k = 1, \ldots, K + 1 \), we have
\[
|g_{K,k}| \left(\frac{2c_1 \ln n}{n}\right)^{1-k} \leq 2^{7k/2 + 1} A \cdot \left(\frac{c_1 \ln n}{n}\right)^{-k}.
\]
Hence, by triangle inequality again and Lemma \[25\] we have

\[
\text{Var}(T_{\text{ns}}(\hat{p}, \hat{q})) \leq \mathbb{E}[T_{\text{ns}}(\hat{p}, \hat{q})^2]
\]

\[
\leq (K + 1) \sum_{k=0}^{K} |g_{K,k+1}|^2 \left( \frac{2c_1 \ln n}{n} \right)^{-2k} \cdot \mathbb{E}[(\hat{p}^2)\mathbb{E} \left[ \prod_{l=0}^{k-1} (\hat{q}^l - \frac{1}{n})^2 \right]]
\]

\[
\leq 2^{7K+2}(K + 1) A^2 \sum_{k=0}^{K} \left( \frac{c_1 \ln n}{n} \right)^{-2(2k+1)} \cdot \left( \frac{p}{m} + p^2 \right) \left( \frac{4q_c \ln n}{n} \right)^k
\]

\[
\leq 2^{11K+2}(K + 1) A^2 \sum_{k=0}^{K} \left( \frac{c_1 \ln n}{n} \right)^{-2} \cdot \left( \frac{p}{m} + p^2 \right)
\]

\[
\leq 2^{11K+2}(K + 1) A^2 \sum_{k=0}^{K} \left( \frac{c_1 \ln n}{n} \right)^{-2} \cdot \left( \frac{p}{m} + p^2 \right)
\]

\[
\leq 2^{11K+4}c_2^2(C + 2c_1(\ln n)^3)^2 \cdot \left( \frac{2u(S)}{c_m \ln n} + \frac{4(u(S))^2}{n^2} \right)
\]

and by Lemma \[31\] we have

\[
\text{Var}(\hat{T}_{\text{ns}}(\hat{p}, \hat{q})) \leq \text{Var}(T_{\text{ns}}(\hat{p}, \hat{q})) \leq 2^{11K+4}c_2^2(C + 2c_1(\ln n)^3)^2 \cdot \left( \frac{2u(S)}{c_m \ln n} + \frac{4(u(S))^2}{n^2} \right).
\]

As for the bias, by construction we have

\[
|\mathbb{E}[T_{\text{ns}}(\hat{p}, \hat{q}) - p \ln q]| = p \sum_{k=0}^{K} g_{K,k+1} \left( \frac{2c_1 \ln n}{n} \right)^{-k} q^k \ln q
\]

\[
\leq u(S)q \sum_{k=1}^{K+1} g_{K,k} \left( \frac{2c_1 \ln n}{n} \right)^{1-k} q^{-k} \ln q
\]

\[
= u(S) \left| \sum_{k=1}^{K+1} g_{K,k} \left( \frac{2c_1 \ln n}{n} \right)^{1-k} q^{-k} \right|
\]

\[
\leq \frac{C_u(S)}{n \ln n}.
\]

Hence, by triangle inequality and \[452\], we get

\[
|\text{Bias}(\hat{T}_{\text{ns}}(\hat{p}, \hat{q}))| \leq |\mathbb{E}[T_{\text{ns}}(\hat{p}, \hat{q}) - p \ln q] + \mathbb{E}[T_{\text{ns}}(\hat{p}, \hat{q})\mathbb{1}(|T_{\text{ns}}(\hat{p}, \hat{q})| \geq 1)]|
\]

\[
\leq \frac{C_u(S)}{n \ln n} + \mathbb{E}[T_{\text{ns}}(\hat{p}_1, \hat{q}_1)^2]
\]

\[
\leq \frac{C_u(S)}{n \ln n} + 2^{11K+4}c_2^2(C + 2c_1(\ln n)^3)^2 \cdot \left( \frac{2u(S)}{c_m \ln n} + \frac{4(u(S))^2}{n^2} \right)
\]

as desired. \[\square\]

**M. Proof of Lemma \[19\]**

Fix $\delta > 0$. Let $\hat{D}(X, Y)$ be a near-minimax estimator of $D(P\|Q)$ under the multinomial model with an upper bound $(1 + \epsilon)u(S)$ on the likelihood ratio. Note that the estimator $\hat{D}$ obtains the sample sizes $m, n$ from observations. By definition, we have

\[
\sup_{(P, Q) \in \mathcal{U}_{S,u(S)}(\epsilon)} \mathbb{E}_{\text{Multinomial}} \left( \hat{D} - D(P\|Q) \right)^2 \leq R(S, m, n, (1 + \epsilon)u(S)) + \delta.
\]

Now given $(P, Q) \in \mathcal{U}_{S,u(S)}(\epsilon)$, let $X = [X_1, \ldots, X_s]^T$ and $Y = [Y_1, \ldots, Y_s]^T$ with $(X_i, Y_i) \sim \text{Poi}(mp_i) \times \text{Poi}(nq_i)$. Write $m' = \sum_{i=1}^s X_i$ and $n' = \sum_{i=1}^s Y_i$, we use the estimator $\hat{D}(X, Y)$ to estimate $D(P\|Q)$.

Note that conditioned on $m' = M$, we have $X \sim \text{Multinomial}(M, \frac{P}{\sum_{i=1}^s p_i})$, and similarly for $Y$. Moreover, $(P, Q) \in \mathcal{U}_{S,u(S)}(\epsilon)$.
\( \mathcal{U}_{S,u(S)}(\varepsilon) \) implies that \((P, \sum_{i=1}^{S} q_i) \in \mathcal{U}_{S,(1+\varepsilon)u(S)}\) by construction. By the triangle inequality we have

\[
\frac{1}{2} R_P(S, m, n, u(S), \varepsilon) \leq \frac{1}{2} \mathbb{E}_{(P,Q)} \left( \hat{D} - D(P||Q) \right)^2 
\]

\[
\leq \mathbb{E}_{(P,Q)} \left( \hat{D} - D \left( P \left\| \frac{Q}{\sum_{i=1}^{S} q_i} \right. \right) \right)^2 + \left( D \left( P \left\| \frac{Q}{\sum_{i=1}^{S} q_i} \right. \right) - D(P||Q) \right)^2 
\]

\[
\leq \sum_{k,l=0}^{\infty} \mathbb{E}_{(P,Q)} \left( \hat{D} - D \left( P \left\| \frac{Q}{\sum_{i=1}^{S} q_i} \right. \right) \right) m' = k, n' = l \right)^2 \mathbb{P}(m' = k) \mathbb{P}(n' = l) + (\ln \sum_{i=1}^{S} q_i)^2 
\]

\[
\leq \sum_{k,l=0}^{\infty} (R(S,k,l,(1+\varepsilon)u(S)) + \delta) \mathbb{P}(m' = k) \mathbb{P}(n' = l) + 2\varepsilon^2 
\]

\[
= \sum_{k \geq \frac{m}{8}, l \geq \frac{(1-\varepsilon)n}{2}} R(S,m/2, (1-\varepsilon)n/2, (1+\varepsilon)u(S)) + (\ln((1+\varepsilon)u(S)))^2 \left( \exp(-(m/8)) + \exp(-(1-\varepsilon)n/8) \right) + \delta + 2\varepsilon^2 
\]

where we have used Lemma 28. Then the result follows from the arbitrariness of \( \delta \).

\(\square\)

**N. Proof of Lemma 20**

The properties of Chebyshev polynomials were well studied in [54]. In particular, the Chebyshev polynomial \( T_{2(K+2)}(x) \) is an even function and takes the form

\[
T_{2(K+2)}(x) = S_{2K}(x)x^4 - 2(-1)^K(K+2)^2x^2 + (-1)^K 
\]

for some even polynomial \( S_{2K}(x) \) of degree \( 2K \). Since \( |T_{2(K+2)}(x)| \leq 1 \) for any \( x \in [-1, 1] \), by triangle inequality

\[
\left| -1^K S_{2K}(x)x^4 \right|^{2(K+2)^2} - x^4 \leq \frac{|T_{2(K+2)}(x)|}{2(K+2)^2} + \frac{1}{2(K+2)^2} \leq \frac{1}{(K+2)^2}. 
\]

Now the desired result follows from the variable substitution \( y = \Delta_n x^2 \in [0, \Delta_n] \).

\(\square\)

**APPENDIX C**

**PROOF OF AUXILIARY LEMMAS**

**A. Proof of Lemma 27**

Fix \( m, n \) and an arbitrary (possibly randomized) estimator \( \hat{D} \). Denote by \( \mu \) the (possibly randomized) decision made by \( \hat{D} \) conditioning on the event \( E \) where \( m \) first symbols and no other symbols from \( P \), and \( n \) second symbols and no other symbols from \( Q \) are observed. Note that \( \mu \) is a probability measure on \( \mathbb{R} \). Choose \( P = (1, 0, \cdots, 0) \) and \( Q = (\delta, 1 - \delta, 0, \cdots, 0) \) with \( \delta \in (0, 1) \) to be specified in the sequel, then \( P \ll Q \). Hence, with probability at least \((1-\delta)^n\), the event \( E \) holds, and thus

\[
\sup_{(P,Q) \in \mathcal{E}_S} \mathbb{E}_{(P,Q)} \left( \hat{D} - D(P||Q) \right)^2 \geq (1-\delta)^n \cdot \int_{\mathbb{R}} (a - \ln(1/\delta))^2 \mu(da). 
\]

As a result, denote by \( a_{1/2} = \inf \{ a \in \mathbb{R} : \mu((-\infty, a]) \geq 1/2 \} \) a median of \( \mu \), choosing \( \delta = \frac{1}{2} \wedge \exp(-a_{1/2} - M) \) for any \( M > 0 \) yields

\[
\sup_{(P,Q) \in \mathcal{E}_S} \mathbb{E}_{(P,Q)} \left( \hat{D} - D(P||Q) \right)^2 \geq (1 - \frac{1}{2})^n \cdot \int_{(-\infty,a_{1/2}]} (a - \ln(1/\delta))^2 \mu(da) \geq \frac{M^2}{2^{n+1}}. 
\]

Letting \( M \to \infty \) yields the desired result.

\(\square\)

**B. Proof of Lemma 22**

Similar to the proof of [1] Lemma 16], we can show that

\[
R_P(S, m, n, u(S), \pi) = \sum_{k,l=0}^{\infty} R(S,k,l, u(S), \pi) \mathbb{P}(\operatorname{Poi}(m) = k) \mathbb{P}(\operatorname{Poi}(n) = l) 
\]

(556)
where $R(\cdot, \cdot, \cdot, \cdot, \pi)$ and $R_P(\cdot, \cdot, \cdot, \cdot)$ represent the Bayes error given prior $\pi$ under the Multinomial model and the Poisson sampling model, respectively. On one hand, we have

$$R_P(S, m, n, u(S), \pi) \geq \sum_{0 \leq k \leq 2m, 0 \leq l \leq 2n} R(S, k, l, u(S), \pi)P(\text{Poi}(m) = k)P(\text{Poi}(n) = l) \tag{557}$$

$$\geq R(S, 2m, 2n, u(S), \pi)P(\text{Poi}(m) \leq 2m)P(\text{Poi}(n) \leq 2n) \tag{558}$$

$$\geq \frac{1}{4}R(S, 2m, 2n, u(S), \pi) \tag{559}$$

where we have used the Markov inequality to get $P(\text{Poi}(m) \leq 2m) \geq \frac{1}{2}$ and $P(\text{Poi}(n) \leq 2n) \geq \frac{1}{2}$. On the other hand, note that $D(P\|Q) \leq \ln u(S)$ whenever $(P, Q) \in \mathcal{U}_{S,u(S)}$, by the Poisson tail bound in Lemma 23 we also have

$$R_P(S, m, n, u(S), \pi) \leq \sum_{k > m/2, l > n/2} R(S, k, l, u(S), \pi)P(\text{Poi}(m) = k)P(\text{Poi}(n) = l) \tag{560}$$

$$(\ln u(S))^2 \left( P(\text{Poi}(m) \leq \frac{m}{2}) + P(\text{Poi}(n) \leq \frac{n}{2}) \right) \tag{561}$$

$$\leq \sum_{k > m/2, l > n/2} R(S, \frac{m}{2}, \frac{n}{2}, u(S), \pi)P(\text{Poi}(m) = k)P(\text{Poi}(n) = l) + (\ln u(S))^2 \left( \exp(-\frac{m}{8}) + \exp(-\frac{n}{8}) \right) \tag{562}$$

By the minimax theorem [55], taking supremum over all priors $\pi$ yields the desired result. \hfill \square

### C. Proof of Lemma 23

We apply the general approximation theory on convex polytopes to our one-dimensional case where $[a, b]$ is an interval. Note that by polynomial scaling,

$$E_a[\ln x : [a, b]] = E_a[\ln ((b - a)x + a) : [0, 1]] = E_a[\ln(x + \frac{a}{b - a}) : [0, 1]] \tag{563}$$

it suffices to consider the function $h(x) = \ln(x + \Delta)$ defined on $[0, 1]$, where $\Delta = \frac{a}{b - a} > 0$. In this case, the second-order Ditzian–Totik modulus of smoothness in (146) is reduced to (44)

$$\omega^2_{[0,1]}(f, t) = \omega^2_{\varphi}(f, t) \triangleq \sup \left\{ \left| f(u) + f(v) - 2f \left( \frac{u + v}{2} \right) \right| : u, v \in [0, 1], |u - v| \leq 2t, \varphi \left( \frac{u + v}{2} \right) \right\} \tag{564}$$

where $\varphi(x) = \sqrt{x(1-x)}$. For the evaluation of $\omega^2_{\varphi}(h, t)$ for $t \in [0, 1]$, we write $u = r + s, v = r - s$ with $u, v \in [0, 1]$ and $0 \leq s \leq t\varphi(r)$ in the definition. Then for $\Delta > t^2$, by Taylor expansion we have

$$|h(r + s) + h(r - s) - 2h(r)| \leq 2 \sum_{k=1}^{\infty} \frac{|h^{(2k)}(r)|}{(2k)!} 2^{2k} \sum_{k=1}^{\infty} \frac{1}{k!} \frac{r^{2k}}{(\rho + \Delta)^{2k}} \leq \sum_{k=1}^{\infty} \frac{1}{k} \left( \frac{t^2r(1 - r)}{(\rho + \Delta)^2} \right)^k \tag{565}$$

By differentiation, it is easy to show that the maximum of $\frac{r(1-r)}{(\rho + \Delta)^2}$ is attained at $r = \frac{\Delta}{2\Delta + 1}$, and the corresponding maximum is $\frac{1}{4\Delta(1+\Delta)}$. Hence, by (565) we have

$$|h(r + s) + h(r - s) - 2h(r)| \leq \sum_{k=1}^{\infty} \frac{t^2}{4\Delta(1+\Delta)} \leq \frac{t^2}{4\Delta(1+\Delta)} \sum_{k=1}^{\infty} \left( \frac{1}{4} \right)^{k-1} = \frac{t^2}{3\Delta} \leq \frac{t^2}{3\Delta} \tag{566}$$

i.e., we conclude that $\omega^2_{\varphi}(h, t) \leq \frac{t^2}{3\Delta}$ when $\Delta > t^2$.

For $\Delta \leq t^2$, the concavity of $\ln(r)$ yields that the maximum-achieving pair $(u, v)$ must satisfy one of the following: (1) $u = 1$; (2) $v = 0$; (3) $s = t\varphi(r)$.

We start with the case where $s = t\varphi(r)$, then $\frac{t^2}{1+t^2} \leq r \leq \frac{1}{1+t^2}$. In this case (565) still holds, but now the maximum of $\frac{r(1-r)}{(\rho + \Delta)^2}$ is attained at $r = \frac{t^2}{1+t^2}$, and the corresponding inequality becomes

$$|h(r + s) + h(r - s) - 2h(r)| \leq \sum_{k=1}^{\infty} \frac{1}{k} \left( \frac{t^4}{(t^2 + 1 + t^2)\Delta^2} \right)^k \leq \sum_{k=1}^{\infty} \frac{1}{k} \left( \frac{t^4}{(t^2 + \Delta)^2} \right)^k \tag{567}$$

$$= -\ln \left( 1 - \frac{t^4}{(t^2 + \Delta)^2} \right) = \ln \left( \frac{(t^2 + \Delta)^2}{\Delta(\Delta + 2t^2)} \right) \leq \ln \left( \frac{2t^2 + \Delta}{\Delta} \right) \tag{568}$$

Note that this inequality only requires $r \geq \frac{t^2}{1+t^2}$, hence it also holds for the case where $u = 1$. 

\end{document}
Now we are only left with the case where $v = 0$, then $s = r$ and $r \leq \frac{t^2}{1+t^2}$. As a result,

$$|h(r + s) + h(r - s) - 2h(r)| = 2\ln(r + \Delta) - \ln(2r + \Delta) - \ln(\Delta)$$

$$= \ln \left(1 + \frac{r^2}{\Delta(2r + \Delta)}\right) \leq \ln \left(1 + \frac{r}{2\Delta}\right) \leq \ln \left(1 + \frac{t^2}{2\Delta}\right).$$

(569)

(570)

In summary, for $\Delta \leq t^2$ we can obtain that

$$\omega^2_u(h, t) \leq \ln \left(1 + \frac{2t^2}{\Delta}\right)$$

(571)

and Lemma 23 follows from the previous upper bounds on $\omega^2_u(h, n^{-1})$ and Lemma 10.

D. Proof of Lemma 24

It suffices to prove the claim for $\omega^2_T(f, 1/K)$, where $T$ is the following triangle containing $R$:

$$T \triangleq \left\{(x, y) : 0 \leq y \leq \frac{2c_1 \ln n}{n}, 0 \leq x < u(S)y\right\}.$$  

(572)

Denote by $E_1, E_2, E_3$ three edges of this triangle (excluding endpoints):

$$E_1 \triangleq \{(x, y) : 0 < x < \frac{2c_1 u(S) \ln n}{n}, y = \frac{2c_1 \ln n}{n}\}$$

(573)

$$E_2 \triangleq \{(x, y) : x = 0, 0 < y < \frac{2c_1 \ln n}{n}\}$$

(574)

$$E_3 \triangleq \{(x, y) : x = u(S)y, 0 < y < \frac{2c_1 \ln n}{n}\}.$$  

(575)

Since $|\Delta^2_{h_0 d_T(e, x, y)} f(x, y)|$ is a continuous function with respect to $(x, y, e, h) \in T \times S^1 \times [0, 1]$, which is a compact set, we can assume that $(x_0, y_0, e_0, h_0)$ achieves the supremum. Let $A, B$ be the intersection of the line $\ell$ passing through $(x_0, y_0)$ with direction $e_0$ with the triangle $T$.

If either $A$ or $B$ belongs to $E_1$, say $B \in E_1$, then for sufficiently small $\varepsilon > 0$, the line connecting $A$ and $(x_0 + \varepsilon, y_0)$ (resp. $(x_0 - \varepsilon, y_0)$) intersects $E_1$ with direction $e_1$ (resp. $e_2$). Hence, by the similarity relation in geometry, the $y$-coordinates of $(x_0, y_0) + h_0 d_T(e_0, x_0, y_0)$ and $(x_0 + \varepsilon, y_0) + h_0 d_T(e_1, x_0 + \varepsilon, y_0)$ are equal, and similarly for others. Hence, by linearity of $f(x, y) = x \ln y$ in $x$,

$$2|\Delta^2_{h_0 d_T(e_0, x_0, y_0)} f(x_0, y_0)| = |\Delta^2_{h_0 d_T(e_1, x_0 + \varepsilon, y_0)} f(x_0 + \varepsilon, y_0) + \Delta^2_{h_0 d_T(e_2, x_0 - \varepsilon, y_0)} f(x_0 - \varepsilon, y_0)|$$

$$\leq |\Delta^2_{h_0 d_T(e_1, x_0 + \varepsilon, y_0)} f(x_0 + \varepsilon, y_0) + |\Delta^2_{h_0 d_T(e_2, x_0 - \varepsilon, y_0)} f(x_0 - \varepsilon, y_0)|$$

(576)

(577)

i.e., we can always perturb $(x_0, y_0, e_0)$ such that $\ell$ does not intersect $E_1$.

Now we assume that $A = (0, y_1), B = (u(S)y_2, y_2)$ with $y_1, y_2 \in [0, \frac{2c_1 \ln n}{n}]$. If $y_2 = y_1$, then $f(x, y)$ is linear on $\ell$, and $\omega^2_T(f, 1/K)$ is zero. If $y_2 \neq y_1$, the function on $\ell$ becomes

$$h(y) = \frac{y - y_1}{y_2 - y_1} y_2 u(S) \ln y, \quad y \in [u, v]$$

(578)

where $u \triangleq y_1 \wedge y_2$ and $v \triangleq y_1 \lor y_2$. Hence, by the sub-additivity of the Ditzian–Töplitz modulus of smoothness, for $t \in [0, 1]$ we have

$$\omega^2_u(h, t) \leq \frac{y_2 u(S)}{y_2 - y_1} \cdot \omega^2_{[u, v]}(y \ln y, t) + \frac{y_1 y_2 u(S)}{|y_2 - y_1|} \cdot \omega^2_{[u, v]}(\ln y, t)$$

(579)

$$\leq u(S) v \left[\frac{\omega^2_{[u, v]}(y \ln y, t)}{v - u} + \frac{u}{v - u} \cdot \omega^2_{[u, v]}(\ln y, t)\right]$$

(580)

By the proof of Lemma 23 (where we have used $\ln(1 + x) \leq x$ when $\Delta \leq t^2$), we have

$$\omega^2_{[u, v]}(\ln y, t) \leq \frac{3t^2(v - u)}{u}.$$  

(581)

As for $\omega^2_{[u, v]}(y \ln y, t)$, we distinguish into two cases. If $v \leq 2u$, by Taylor expansion we have

$$\omega^2_{[u, v]}(y \ln y, t) \leq \sup_{y \in [u, v]} |(y \ln y)'| \cdot (v - u)^2 t^2 = \frac{(v - u)^2 t^2}{u} \leq (v - u)t^2.$$  

(582)
Otherwise, if \( v > 2u \), since it has been shown in [38] that \( \omega^2_{[0,1]}(y \ln y, t) = \frac{2u^2 \ln 2}{1 + t^2} \), by scaling \([u, v] \rightarrow [u/v, 1]\) we have
\[
\omega^2_{[u/v, 1]}(y \ln y, t) \leq v \cdot \omega^2_{[0,1]}(y \ln y, t) \leq v \cdot \omega^2_{[0,1]}(y \ln y, t) \leq 2 \ln 2 \cdot vt^2 \leq 4 \ln 2 \cdot (v - u)t^2.
\] (583)

A combination of the previous three inequalities yields
\[
\omega^2_T(f, t) \leq u(S)v \left[ \frac{4 \ln 2 \cdot (v - u)t^2}{v - u} + \frac{u}{v - u} \cdot 3t^2(v - u) \right]
\] (584)
\[
= (3 + 4 \ln 2)u(S)vt^2
\] (585)
\[
\leq \frac{(6 + 8 \ln 2)c_1 u(S) \ln n}{n} \cdot t^2
\] (586)
where we have used \( v = y_1 \vee y_2 \leq \frac{2c_1 \ln n}{n} \). Now the desired result follows directly by choosing \( t = 1/K^2 \) and \( C_0 = (6 + 8 \ln 2)c_1 \).

E. Proof of Lemma 27

First we assume that \( b = t + 1, a = t - 1, t \neq 0 \), and write
\[
p_n(x) = \sum_{\nu = 0}^{n} a_\nu x^\nu = \sum_{\nu = 0}^{n} b_\nu (x - t)^\nu.
\] (587)

By Lemma 26 and the related discussions, we know that \(|b_\nu| \leq 2^{3n/2}\) for any \( \nu = 0, \cdots, n \). Comparing coefficients yields
\[
|a_\nu| = \left| \sum_{\mu = \nu}^{n} \binom{\mu}{\nu} (-t)^{\mu - \nu} b_\mu \right|
\] (588)
\[
\leq 2^{3n/2}|t|^{-\nu} \sum_{\mu = \nu}^{n} \binom{\mu}{\nu} |t|^\mu
\] (589)
\[
\leq 2^{3n/2}|t|^{-\nu} 2^n (n + 1)(|t|^n + 1)
\] (590)
\[
\leq 2^{7n/2}|t|^{-\nu} (|t|^n + 1).
\] (591)
In the general case, the desired result is obtained by scaling.

F. Proof of Lemma 29

It is straightforward to show
\[
\text{Var}(XY) = \mathbb{E}[(XY)^2] - (\mathbb{E}[XY])^2
\] (592)
\[
= \mathbb{E}[X^2]\mathbb{E}[Y^2] - (\mathbb{E}[X])^2(\mathbb{E}[Y])^2
\] (593)
\[
= (\text{Var}(X) + (\mathbb{E}[X])^2)(\text{Var}(Y) + (\mathbb{E}[Y])^2) - (\mathbb{E}[X])^2(\mathbb{E}[Y])^2
\] (594)
\[
= \text{Var}(X)(\mathbb{E}[Y])^2 + \text{Var}(Y)(\mathbb{E}[X])^2 + \text{Var}(X)\text{Var}(Y)
\] (595)
as desired.

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