

## A Proofs for competitive formulation

### A.1 Examples of partitions

The following examples evaluate  $r_n^{\mathbb{P}}(\Delta_k)$  for the two simplest partitions.

**Example 7.** The singleton partition consists of  $|\Delta_k|$  parts, each a single distribution in  $\Delta_k$ ,

$$\mathbb{P}_{|\Delta_k|} \stackrel{\text{def}}{=} \{\{p\} : p \in \Delta_k\}.$$

An oracle-aided estimator that knows the part containing  $p$  knows  $p$ . The competitive regret of data-driven estimators is therefore the min-max regret,

$$\begin{aligned} r_n^{\mathbb{P}_{|\Delta_k|}}(\Delta_k) &= \min_q \max_{p \in \Delta_k} (r_n(q, \{p\}) - r_n(\{p\})) \\ &= \min_q \max_{p \in \Delta_k} r_n(q, p) \\ &= r_n(\Delta_k), \end{aligned}$$

where the middle equality follows as  $r_n(q, \{p\}) = r_n(q, p)$ , and  $r_n(\{p\}) = 0$ .

**Example 8.** The whole-collection partition has only one part, the whole collection  $\Delta_k$ ,

$$\mathbb{P}_1 \stackrel{\text{def}}{=} \{\Delta_k\}.$$

An estimator aided by an oracle that knows the part containing  $p$  has no additional information, hence no advantage over a data-driven estimator, and the competitive regret is 0,

$$\begin{aligned} r_n^{\mathbb{P}_1}(\Delta_k) &= \min_q \max_{P \in \{\Delta_k\}} \left( \max_{p \in P} r_n(q, p) - r_n(P) \right) \\ &= \min_q \left( \max_{p \in \Delta_k} r_n(q, p) - r_n(\Delta_k) \right) \\ &= \min_q \max_{p \in \Delta_k} (r_n(q, p)) - r_n(\Delta_k) \\ &= r_n(\Delta_k) - r_n(\Delta_k) \\ &= 0. \end{aligned}$$

The examples show that for the coarsest partition of  $\Delta_k$ , into a single part, the competitive regret is the lowest possible, 0, while for the finest partition, into singletons, the competitive regret is the highest possible,  $r_n(\Delta_k)$ .

### A.2 Proof of Equation (5)

The definition implies that if  $P' \subseteq P$  then  $r_n(P') \leq r_n(P)$ , for every distribution class  $P$  and  $P'$ . Hence for every  $q$ ,

$$\begin{aligned} r_n^{\mathbb{P}'}(q, \Delta_k) &= \max_{P' \in \mathbb{P}'} (r_n(q, P') - r_n(P')) \\ &= \max_{P \in \mathbb{P}} \max_{P' \supseteq P' \in \mathbb{P}'} (r_n(q, P') - r_n(P')) \\ &\geq \max_{P \in \mathbb{P}} \max_{P' \supseteq P' \in \mathbb{P}'} (r_n(q, P') - r_n(P)) \\ &= \max_{P \in \mathbb{P}} \left( \max_{P' \supseteq P' \in \mathbb{P}'} r_n(q, P') - r_n(P) \right) \\ &= \max_{P \in \mathbb{P}} (r_n(q, P) - r_n(P)) \\ &= r_n^{\mathbb{P}}(q, \Delta_k). \end{aligned}$$

## B Upper bounds

For a distribution  $p$  and sequence  $x^n$ , let  $p(x^n)$  be the probability of observing  $x^n$  under  $p$ . Recall that for a symbol  $x$ , we abbreviate  $p(x)$  to be  $p_x$ .

### B.1 Proof of Lemma 4

The proof uses the following result.

**Lemma 9.** For every class  $P \in \mathbb{P}_\sigma$ ,  $r_n(P) \geq \max_{p \in P} r_n^{\text{nat}}(p)$ .

*Proof.* We first show that there is an optimal estimator  $q$  that is natural. In particular, let

$$q''_y(x^n) = \frac{\sum_{p \in P} p(x^n y)}{\sum_{p' \in P} p'(x^n)}.$$

We show that  $q''_y(x^n)$  is an optimal estimator for  $P$ . Since  $q''_y(x^n) = q''_{\sigma(y)}(\sigma(x^n))$  for any permutation  $\sigma$ , the estimator achieves the same loss for every  $p \in P$ ,

$$\max_{p \in P} r_n(q'', p) = \frac{1}{k!} \sum_{p \in P} r_n(q'', p'). \quad (6)$$

For any estimator  $q$ ,

$$\begin{aligned} \max_{p \in P} \mathbb{E}[D(p||q)] &\stackrel{(a)}{\geq} \frac{1}{k!} \sum_{p \in P} \mathbb{E}_p[D(p||q)] \\ &\stackrel{(b)}{=} \frac{1}{k!} \sum_{p \in P} \sum_{x^n \in \mathcal{X}^n} \sum_{y \in \mathcal{X}} p(x^n y) \log \frac{1}{q_y(x^n)} - H(p) \\ &= \frac{1}{k!} \sum_{x^n \in \mathcal{X}^n} \sum_{y \in \mathcal{X}} \sum_{p \in P} p(x^n y) \log \frac{1}{q_y(x^n)} - H(p) \\ &\stackrel{(c)}{\geq} \frac{1}{k!} \sum_{x^n \in \mathcal{X}^n} \sum_{y \in \mathcal{X}} \sum_{p \in P} p(x^n y) \log \frac{\sum_{p' \in P} p'(x^n)}{\sum_{p'' \in P} p''(x^n y)} - H(p) \\ &= \frac{1}{k!} \sum_{p \in P} \sum_{x^n \in \mathcal{X}^n} \sum_{y \in \mathcal{X}} p(x^n y) \log \frac{1}{q''_y(x^n)} - H(p) \\ &\stackrel{(d)}{=} \frac{1}{k!} \sum_{p \in P} r_n(q'', p). \end{aligned}$$

(a) follows from the fact that maximum is larger than the average. (b) follows from the fact that every distribution in  $P$  has the same entropy. Non-negativity of KL divergence implies (c). All distributions in  $P$  has the same entropy and hence (d). Hence together with Equation (6)

$$\begin{aligned} r_n(P) &= \min_q \max_{p \in P} \mathbb{E}[D(p||q)] \\ &\geq \frac{1}{k!} \sum_{p \in P} r_n(q'', p) \\ &= \max_{p \in P} r_n(q'', p). \end{aligned}$$

Hence  $q''$  is an optimal estimator. Recall that  $n_y$  denote the number of times symbol  $y$  appears in the sequence.  $q''$  is natural as if  $n_y = n_{y'}$ , then  $q''_y(x^n) = q''_{y'}(x^n)$ . Since there is a natural estimator that achieves minimum in  $r_n(P)$ ,

$$\begin{aligned} r_n(P) &= \min_q \max_{p \in P} \mathbb{E}[D(p||q)] \\ &= \min_{q \in \mathcal{Q}^{\text{nat}}} \max_{p \in P} \mathbb{E}[D(p||q)] \\ &\geq \max_{p \in P} \min_{q \in \mathcal{Q}^{\text{nat}}} \mathbb{E}[D(p||q)] \\ &= \max_{p \in P} r_n^{\text{nat}}(p), \end{aligned}$$

where the last inequality follows from the fact that min-max is bigger than max-min.  $\square$

We can now prove Lemma 4.

*Proof of Lemma 4.*

$$\begin{aligned}
r_n^{\mathbb{P}_\sigma}(q, \Delta_k) &= \max_{P \in \mathbb{P}_\sigma} \left( \max_{p \in P} \mathbb{E}[D(p||q)] - r_n(P) \right) \\
&\stackrel{(a)}{\leq} \max_{P \in \mathbb{P}_\sigma} \left( \max_{p \in P} \mathbb{E}[D(p||q)] - \max_{p \in P} r_n^{\text{nat}}(p) \right) \\
&\stackrel{(b)}{\leq} \max_{P \in \mathbb{P}_\sigma} \max_{p \in P} (\mathbb{E}[D(p||q)] - r_n^{\text{nat}}(p)) \\
&= \max_{p \in \Delta_k} (\mathbb{E}[D(p||q)] - r_n^{\text{nat}}(p)) \\
&= r_n^{\text{nat}}(q, \Delta_k).
\end{aligned}$$

Lemma 9 implies (a). Difference of maximums is smaller than maximum of differences, hence (b).  $\square$

## B.2 Proof of Lemma 5

The proof uses the following lemma which computes the best natural estimator. For a random sequence  $X^n$ , let  $\Phi_t \stackrel{\text{def}}{=} \varphi_t(X^n)$ . Recall that  $S_t(x^n)$  is the sum of probabilities of symbols that appears  $t$  times in  $x^n$ . For notational convenience we use  $S_t$  to denote both  $S_t(x^n)$  and  $S_t(X^n)$ .

**Lemma 10.** *Let  $q_x^*(x^n) = \frac{S_{n_x}}{\varphi_{n_x}}$ , then*

$$q^* = \arg \min_{q \in \mathcal{Q}^{\text{nat}}} r_n(q, p)$$

and

$$r_n^{\text{nat}}(p) = \mathbb{E} \left[ \sum_{t=0}^n S_t \log \frac{\Phi_t}{S_t} \right] - H(p).$$

*Proof.* For a natural estimator  $q$ , if  $n_y = n_{y'}$ , then  $q_y(x^n) = q_{y'}(x^n)$ . Hence, with a slight abuse of notation let  $q_{n_y}(x^n) = q_y(x^n)$ . For a sequence  $x^n$  and estimator  $q$ ,

$$\begin{aligned}
\sum_{y \in \mathcal{X}} p_y \log \frac{1}{q_y(x^n)} - \sum_{t=0}^n S_t \log \frac{\varphi_t}{S_t} &= \sum_{t=0}^n \sum_{y: n_y=t} p_y \log \frac{1}{q_y(x^n)} - \sum_{t=0}^n S_t \log \frac{\varphi_t}{S_t} \\
&= \sum_{t=0}^n S_t \log \frac{1}{q_t(x^n)} - \sum_{t=0}^n S_t \log \frac{\varphi_t}{S_t} \\
&= \sum_{t=0}^n S_t \log \frac{S_t}{\varphi_t q_t(x^n)} \\
&\geq 0,
\end{aligned}$$

where the last inequality follows from the fact that  $\sum_{t=0}^n S_t = \sum_{t=0}^n \varphi_t q_t(x^n) = 1$  and KL divergence is non-negative. Furthermore, equality is achieved only by the estimator that assigns  $q_x^* = \frac{S_{n_x}}{\varphi_{n_x}}$ . Hence,

$$r_n^{\text{nat}}(p) = \min_{q \in \mathcal{Q}^{\text{nat}}} \mathbb{E} \left[ \sum_{y \in \mathcal{X}} p_y \log \frac{p_y}{q_y(X^n)} \right] = -H(p) + \mathbb{E} \left[ \sum_{t=0}^n S_t \log \frac{\Phi_t}{S_t} \right].$$

$\square$

*Proof of Lemma 5.* As before, with a slight abuse of notation let  $q_{n_y}(x^n) = q_y(x^n)$  for natural estimators  $q$ . For any natural estimator  $q$  and sequence  $x^n$ ,

$$\begin{aligned} \sum_{y \in \mathcal{X}} p_y \log \frac{1}{q_y(x^n)} &= \sum_{t=0}^n \sum_{y: n_y=t} p_y \log \frac{1}{q_y(x^n)} \\ &= \sum_{t=0}^n S_t \log \frac{S_t}{\varphi_t q_t(x^n)} + \sum_{t=0}^n S_t \log \frac{\varphi_t}{S_t} \\ &= \sum_{t=0}^n S_t \log \frac{S_t}{\hat{S}_t} + \sum_{t=0}^n S_t \log \frac{\varphi_t}{S_t}. \end{aligned}$$

Thus by Lemma 10,

$$\begin{aligned} r_n^{\text{nat}}(q, p) &= -H(p) + \mathbb{E} \left[ \sum_{t=0}^n S_t \log \frac{S_t}{\hat{S}_t} + \sum_{t=0}^n S_t \log \frac{\Phi_t}{S_t} \right] + H(p) - \mathbb{E} \left[ \sum_{t=0}^n S_t \log \frac{\Phi_t}{S_t} \right] \\ &= \mathbb{E} \left[ \sum_{t=0}^n S_t \log \frac{S_t}{\hat{S}_t} \right] \\ &= \mathbb{E}[D(S||\hat{S})]. \end{aligned}$$

□

### B.3 Optimality of natural estimators

We now show that exist natural estimators that achieve  $r_n^{\text{nat}}(\Delta_k)$  and  $r_n^{\mathbb{P}_\sigma}(\Delta_k)$ .

**Lemma 11.** *The exists a natural estimator  $q''$  such that*

$$r_n^{\text{nat}}(q'', \Delta_k) = r_n^{\text{nat}}(\Delta_k).$$

*Similar there exists a natural estimator  $q'$  such that*

$$r_n^{\mathbb{P}_\sigma}(q', \Delta_k) = r_n^{\mathbb{P}_\sigma}(\Delta_k).$$

*Proof.* We prove the result for  $r_n^{\text{nat}}(\Delta_k)$ . The result for  $r_n^{\mathbb{P}_\sigma}(\Delta_k)$  is similar and omitted. Let profile  $\bar{\varphi}$  of a sequence  $x^n$  be the vector of its prevalences i.e.,  $\bar{\varphi}(x^n) \stackrel{\text{def}}{=} (\varphi_0(x^n), \varphi_1(x^n), \varphi_2(x^n), \dots, \varphi_n(x^n))$ . For any optimal estimator  $q$  and sequence  $x^n y$  such that  $\bar{\varphi}(x^n) = \bar{\varphi}_n$  and  $n_y(x^n) = t$ , let

$$q''_y(x^n) = \frac{\sum_{w^n z: \bar{\varphi}(w^n) = \bar{\varphi}_n, n_z=t} q_z(w^n)}{\sum_{u^n v: \bar{\varphi}(u^n) = \bar{\varphi}_n, n_v=t} 1}.$$

$q''$  is a natural estimator as if for any sequence  $x^n$ ,  $n_y(x^n) = n_{y'}(x^n)$ , then  $q''_y(x^n) = q''_{y'}(x^n)$ . We show that  $q''$  is an optimal estimator. Observe that for any  $P \in \mathbb{P}_\sigma$

$$r_n(q, P) \stackrel{(a)}{\geq} \frac{1}{k!} \sum_{p \in P} r_n(q, p) \stackrel{(b)}{\geq} \frac{1}{k!} \sum_{p \in P} r_n(q'', p) \stackrel{(c)}{=} r_n(q'', P). \quad (7)$$

Maximum is larger than average and hence (a). Every distribution in  $P$  has the same KL loss for  $q''$  and hence (c). To prove (b), observe that

$$\begin{aligned}
\sum_{p \in P} r_n(q, p) &= \sum_{p \in P} \sum_{x^n \in \mathcal{X}^n} \sum_{y \in \mathcal{X}} p(x^n y) \log \frac{1}{q_y(x^n)} - H(p) \\
&= \sum_{x^n \in \mathcal{X}^n} \sum_{y \in \mathcal{X}} \sum_{p \in P} p(x^n y) \log \frac{1}{q_y(x^n)} - H(p) \\
&= \sum_{\bar{\varphi}_n, t} \sum_{x^n: \bar{\varphi}(x^n) = \bar{\varphi}_n} \sum_{y: n_y = t} \sum_{p \in P} p(x^n y) \log \frac{1}{q_y(x^n)} - H(p) \\
&\stackrel{(d)}{\geq} \sum_{\bar{\varphi}_n, t} \sum_{x^n: \bar{\varphi}(x^n) = \bar{\varphi}_n} \sum_{y: n_y = t} \sum_{p \in P} p(x^n y) \log \frac{\sum_{u^n, v: \bar{\varphi}(u^n) = \bar{\varphi}_n, n_v = t} 1}{\sum_{w^n, z: \bar{\varphi}(w^n) = \bar{\varphi}_n, n_z = t} q_z(w^n)} - H(p) \\
&= \sum_{\bar{\varphi}_n, t} \sum_{x^n: \bar{\varphi}(x^n) = \bar{\varphi}_n} \sum_{y: n_y = t} \sum_{p \in P} p(x^n y) \log \frac{1}{q''_y(x^n)} - H(p) \\
&= \sum_{p \in P} r_n(q'', p),
\end{aligned}$$

For all sequences  $x^n y$  with the same  $\bar{\varphi}(x^n)$  and  $n_y(x^n)$ ,  $\sum_{p \in P} p(x^n y)$  is the same. Hence, applying log-sum inequality results in (d). By Lemma 10, every  $p \in P$  has the same  $r_n^{\text{nat}}(p)$ , hence subtracting  $r_n^{\text{nat}}(p)$  from both sides of Equation (7) results in

$$\max_{p \in P} (r_n(q, p) - r_n^{\text{nat}}(p)) \geq \max_{p \in P} (r_n(q'', p) - r_n^{\text{nat}}(p)).$$

Hence for the optimal estimator  $q$ ,

$$\begin{aligned}
r_n^{\text{nat}}(\Delta_k) &= \max_{p \in \Delta_k} (r_n(q, p) - r_n^{\text{nat}}(p)) \\
&= \max_{P \in \mathbb{P}_\sigma} \left( \max_{p \in P} (r_n(q, p) - r_n^{\text{nat}}(p)) \right) \\
&\geq \max_{P \in \mathbb{P}_\sigma} \left( \max_{p \in P} (r_n(q'', p) - r_n^{\text{nat}}(p)) \right) \\
&= \max_{p \in \Delta_k} (r_n(q'', p) - r_n^{\text{nat}}(p)) \\
&= r_n(q'', \Delta_k).
\end{aligned}$$

Thus  $q''$  is an optimal estimator and furthermore it is natural, hence the lemma.  $\square$

## C Regret bounds on the Good-Turing estimator

### C.1 Preliminaries

In practice, often the Good-Turing estimator is used for small multiplicities and empirical estimators are used for large multiplicities. We analyze this estimator and bound its regret. For a symbol appearing  $t$  times, we assign probability  $q'_x = \hat{S}_t / \varphi_t$ , where  $\hat{S}_t = C_t / N$ .  $N$  is the normalization factor to ensure that  $\sum_{t=0}^{\infty} \hat{S}_t = 1$  and

$$C_t = \begin{cases} \varphi_t \cdot \frac{t}{n} & \text{if } t \geq t_0, \\ (\varphi_{t+1} + 1) \cdot \frac{t+1}{n} & \text{else.} \end{cases}$$

We set  $t_0 \propto n^{1/3}$  later. Similar to our experiments, we have modified the Good-Turing estimator to  $(\varphi_{t+1} + 1) \cdot \frac{t+1}{n}$ , thus ensuring that we never assign a non-zero probability. However, unlike our experiments, where we decided between empirical and Good-Turing estimators depending on if  $\varphi_{t+1} \geq t$ , for our proofs we just decide it based on  $t$  for convenience. We remark that in our experiments the estimator in Section 4 performed better than the one above.

Ideally we would like to analyze this estimator when the number of samples is  $n$ . However, such analysis is complicated as the number of times symbols appear are dependent, for example, they add to  $n$ . A standard approach to overcome the dependence, e.g., [29], samples the distribution a random number of times  $\sim \text{poi}(n)$ , the Poisson distribution with parameter  $n$ . Some useful properties of Poisson sampling include: (i) A symbol with probability  $p$  appears  $\text{poi}(np)$  times, (ii) The numbers of times different symbols appear are independent of each other, (iii) For any fixed  $n_0$ , conditioned on the length  $\text{poi}(n) \geq n_0$ , the distribution of the first  $n_0$  elements is identical to sampling  $p$  i.i.d. exactly  $n_0$  times. Thus, to simplify the analysis of the estimator, we assume that the number of samples is a Poisson random variable with mean  $n$ . A similar result holds with  $n$  samples.

We first relate the KL regret to a chi-squared like distance between  $S$  and  $C$ .

**Lemma 12.** *For any distribution  $p \in \Delta_k$ ,*

$$\mathbb{E}[D(S||\hat{S})] \leq \sum_{t=0}^{t_0-1} \mathbb{E} \left[ \frac{(S_t - (t+1)(\Phi_{t+1} + 1)/n)^2}{(\Phi_{t+1} + 1)(t+1)/n} \right] + \sum_{t=t_0}^{\infty} \mathbb{E} \left[ \frac{(S_t - t\Phi_t/n)^2}{\Phi_t t/n} \right].$$

*Proof.* Since  $\log(1+y) \leq y$ ,  $\sum_{t=0}^{\infty} S_t = 1$ , and  $\sum_{t=0}^{\infty} C_t = N$ ,

$$\begin{aligned} D(S||\hat{S}) &= \sum_{t=0}^{\infty} S_t \log \frac{S_t}{\hat{S}_t} \\ &= \sum_{t=0}^{\infty} S_t \log \frac{NS_t}{C_t} \\ &= \sum_{t=0}^{\infty} S_t \log \frac{S_t}{C_t} + \sum_{t=0}^{\infty} S_t \log N \\ &= \sum_{t=0}^{\infty} S_t \log \left( 1 + \frac{S_t - C_t}{C_t} \right) + \log N \\ &\leq \sum_{t=0}^{\infty} S_t \left( \frac{S_t - C_t}{C_t} \right) + \log N \\ &= \sum_{t=0}^{\infty} (S_t - C_t) \left( \frac{S_t - C_t}{C_t} \right) + \sum_{t=0}^{\infty} C_t \left( \frac{S_t - C_t}{C_t} \right) + \log N \\ &= \sum_{t=0}^{\infty} (S_t - C_t) \left( \frac{S_t - C_t}{C_t} \right) + \sum_{t=0}^{\infty} (S_t - C_t) + \log N \\ &= \sum_{t=0}^{\infty} \frac{(S_t - C_t)^2}{C_t} + 1 - N + \log N \\ &\leq \sum_{t=0}^{\infty} \frac{(S_t - C_t)^2}{C_t} \\ &= \sum_{t=0}^{t_0-1} \frac{(S_t - C_t)^2}{C_t} + \sum_{t=t_0}^{\infty} \frac{(S_t - C_t)^2}{C_t}. \end{aligned}$$

Taking expectations on both sides and substituting  $C_t$  results in the lemma.  $\square$

## C.2 Empirical estimators

All of our results including the next lemma hold for all distributions in  $\Delta_k$  and hence stated without any condition on the underlying distribution. Let  $N_x \stackrel{\text{def}}{=} n_x(X^n)$  for a random sequence  $X^n$ .

**Lemma 13.** *For any  $n$  and  $t_0$ ,*

$$\sum_{t=t_0}^{\infty} \mathbb{E} \left[ \frac{(S_t - t\Phi_t/n)^2}{t\Phi_t/n} \right] \leq \frac{1}{t_0}.$$

*Proof.*

$$\begin{aligned}
\sum_{t=t_0}^{\infty} \frac{(S_t - t\Phi_t/n)^2}{t\Phi_t/n} &\leq \sum_{t=t_0}^{\infty} \frac{(S_t - t\Phi_t/n)^2}{\Phi_t t_0/n} \\
&\stackrel{(a)}{\leq} \sum_{t=t_0}^{\infty} \sum_x 1_{N_x=t} \frac{(p_x - t/n)^2}{t_0/n} \\
&= \sum_x \sum_{t=t_0}^{\infty} 1_{N_x=t} \frac{(p_x - t/n)^2}{t_0/n} \\
&\leq \sum_x \sum_{t=0}^{\infty} 1_{N_x=t} \frac{(p_x - t/n)^2}{t_0/n}.
\end{aligned}$$

(a) follows from the fact that  $\frac{(\sum_{x=1}^m a_x)^2}{m} \leq \sum_{i=1}^m a_x^2$  for  $a_x = 1_{N_x=t}(p_x - t/n)$  and  $m = \Phi_t$ . Taking expectations on both sides,

$$\begin{aligned}
\sum_{t=t_0}^{\infty} \mathbb{E} \left[ \frac{(S_t - t\Phi_t/n)^2}{\Phi_t t/n} \right] &\leq \sum_x \frac{\mathbb{E}[\sum_{t=0}^{\infty} 1_{N_x=t}(p_x - t/n)^2]}{t_0/n} \\
&\leq \sum_x \frac{p_x/n}{t_0/n} \\
&= \frac{1}{t_0},
\end{aligned}$$

where the second inequality follows from observing that  $\mathbb{E}[\sum_{t=0}^{\infty} 1_{N_x=t}(p_x - t/n)^2]$  is the variance of a Poisson random variable with mean  $np_x$ .  $\square$

### C.3 Good-Turing estimators

To bound the regret corresponding to the Good-Turing estimator, we need few auxiliary results. The next set of equations follow from results in [13], For any  $n$  and  $t$ ,

$$\mathbb{E}[S_t] = \frac{t+1}{n} \cdot \mathbb{E}[\Phi_{t+1}]. \quad (8)$$

$$\text{Var}(S_t) \leq \frac{(t+1)(t+2)}{n^2} \cdot \mathbb{E}[\Phi_{t+2}]. \quad (9)$$

$$\mathbb{E} \left[ \left( S_t - \frac{(t+1)\Phi_{t+1}}{n} \right)^2 \right] \leq \frac{(t+1)(t+2)\mathbb{E}[\Phi_{t+2}]}{n^2} + \frac{(t+1)^2\mathbb{E}[\Phi_{t+1}]}{n^2}. \quad (10)$$

The next lemma relates  $\mathbb{E}[\Phi_{t+1}]$  to  $\mathbb{E}[\Phi_t]$ .

**Lemma 14.** *For any  $n$  and  $t \geq 1$ ,*

$$\mathbb{E}[\Phi_{t+1}] \leq \mathbb{E}[\Phi_t] \left( \frac{2}{t} \log n + \frac{t}{t+1} \right) + \frac{1}{t+1}.$$

*Proof.* Let  $r \geq \frac{t}{t+1}$ .

$$\begin{aligned}
\mathbb{E}[\Phi_{t+1}] &= \mathbb{E}\left[\sum_x 1_{N_x=t+1}\right] \\
&= \sum_x e^{-np_x} \frac{(np_x)^{t+1}}{(t+1)!} \\
&= \sum_x \frac{n}{t+1} \cdot e^{-np_x} \frac{(np_x)^t}{t!} p_x \\
&= \sum_{x: np_x \leq r(t+1)} \frac{n}{t+1} \cdot e^{-np_x} \frac{(np_x)^t}{t!} p_x + \sum_{x: np_x > r(t+1)} \frac{n}{t+1} \cdot e^{-np_x} \frac{(np_x)^t}{t!} p_x \\
&\stackrel{(a)}{\leq} r \sum_{x: np_x \leq r(t+1)} e^{-np_x} \frac{(np_x)^t}{t!} + \sum_{x: np_x > r(t+1)} \frac{n}{t+1} e^{-r(t+1)} \frac{(r(t+1))^t}{t!} p_x \\
&\leq r \sum_x e^{-np_x} \frac{(np_x)^t}{t!} + \sum_x \frac{n}{t+1} e^{-r(t+1)} \frac{(r(t+1))^t}{t!} p_x \\
&\stackrel{(b)}{\leq} r \sum_x e^{-np_x} \frac{(np_x)^t}{t!} + \sum_x \frac{n}{t+1} e^{-rt/2} p_x \\
&\leq r \mathbb{E}[\Phi_t] + \frac{n}{t+1} e^{-\frac{rt}{2}}.
\end{aligned}$$

(a) follows from the fact that second term is a decreasing as a function of  $np_x$  in the range  $[r(t+1), \infty)$ . (b) follows from the fact that

$$e^{-r(t+1)} \frac{(r(t+1))^t}{t!} = e^{-rt} r^t \cdot e^{-t} \frac{(t+1)^t}{t!} \leq e^{-rt} r^t \leq e^{-rt/2}.$$

Choosing  $r = \frac{2}{t} \log n + \frac{t}{t+1}$ , yields

$$\mathbb{E}[\Phi_{t+1}] \leq \mathbb{E}[\Phi_t] \left( \frac{2}{t} \log n + \frac{t}{t+1} \right) + \frac{1}{t+1}.$$

□

The final auxiliary lemma bounds the inverse moment of Poisson binomial distributions.

**Lemma 15.** *Let  $X_i$  for  $1 \leq i \leq n$  be Bernoulli random variables, then*

$$\mathbb{E}\left[\frac{1}{\sum_{i=1}^n X_i + 1}\right] \leq \frac{1}{\sum_{i=1}^n \mathbb{E}[X_i]}.$$

*Proof.* Let  $s_i = \mathbb{E}[X_i]$ . We show that of all tuples  $s_1, s_2, \dots, s_n$  such that  $\sum_{i=1}^n s_i = ns$ , the one that maximizes the expectation is  $s_i = s, \forall i$ . Suppose for some  $i, j$ ,  $s_i > s_j$ , we show that if we decrease  $s_i$  and increase  $s_j$  keeping the sum same, then the expectation increases. Let  $Y = 1 + \sum_{k \notin \{i, j\}} X_k$ . For any instance of  $X^n$ , taking expectation with respect to only  $X_i$  and  $X_j$ .

$$\begin{aligned}
\mathbb{E}\left[\frac{1}{X_i + X_j + Y} \mid Y\right] &= \frac{(1-s_i)(1-s_j)}{Y} + \frac{s_i(1-s_j) + (1-s_i)s_j}{Y+1} + \frac{s_i s_j}{Y+2} \\
&= \frac{1}{Y} + (s_i + s_j) \left( \frac{1}{Y+1} - \frac{1}{Y} \right) + s_i s_j \frac{2}{Y(Y+1)(Y+2)}.
\end{aligned}$$

Thus if we decrease  $s_i$  and increase  $s_j$  (keeping  $s_i + s_j$  fixed), then  $s_i s_j$  increases and hence the expectation increases. Hence the maximum occurs when  $s_i = s_j$  for all  $i, j$  and

$$\mathbb{E}\left[\frac{1}{\sum_{i=1}^n X_i + 1}\right] \leq \mathbb{E}\left[\frac{1}{Z+1}\right],$$



where  $Z$  is a binomial random variable with parameters  $n$  and  $s = \sum_{i=1}^n \mathbb{E}[X_i]/n$ .

The expectation can be bounded as

$$\begin{aligned} \mathbb{E} \left[ \frac{1}{Z+1} \right] &= \sum_{j=0}^n \frac{1}{j+1} \binom{n}{j} s^j (1-s)^{n-j} \\ &= \frac{1}{(n+1)s} \sum_{j=0}^n \binom{n+1}{j+1} s^{j+1} (1-s)^{n+1-(j+1)} \\ &\leq \frac{1}{(n+1)s} \\ &\leq \frac{1}{ns} \\ &= \frac{1}{\sum_{i=1}^n \mathbb{E}[X_i]}. \end{aligned}$$

□

Using the above lemma, we first bound the expectation of  $S_t^2/(\Phi_{t+1} + 1)$ .

**Lemma 16.** *For any  $n$  and  $t$ , if  $\mathbb{E}[\Phi_{t+1}] > 2$ , then*

$$\mathbb{E} \left[ \frac{S_t^2}{\Phi_{t+1} + 1} \right] \leq \frac{\mathbb{E}[S_t^2]}{\mathbb{E}[\Phi_{t+1}] - 1}.$$

*Proof.* We first observe that for any  $x$ ,

$$\mathbb{E}[1_{N_x=t+1}] = e^{-np_x} \frac{(np_x)^{t+1}}{(t+1)!} \leq e^{-t-1} \frac{(t+1)^{t+1}}{(t+1)!} \leq \frac{1}{e}. \quad (11)$$

Since  $S_t = \sum_x p_x 1_{N_x=t}$  and  $\Phi_{t+1} = \sum_x 1_{N_x=t+1}$ ,

$$\frac{S_t^2}{\Phi_{t+1} + 1} = \frac{\sum_x \sum_y p_x p_y 1_{N_x=t} 1_{N_y=t}}{\sum_z 1_{N_z=t+1} + 1} = \sum_x \sum_y \frac{p_x p_y 1_{N_x=t} 1_{N_y=t}}{\sum_{z: z \neq x, z \neq y} 1_{N_z=t+1} + 1},$$

where the equality follows from the fact that symbol cannot appear both  $t$  and  $t+1$  times thus only one of  $1_{N_x=t}$  and  $1_{N_x=t+1}$  can be 1. The numerator and the denominator of the terms on RHS are independent of each other, hence

$$\begin{aligned} \mathbb{E} \left[ \frac{p_x p_y 1_{N_x=t} 1_{N_y=t}}{\sum_{z: z \neq x, z \neq y} 1_{N_z=t+1} + 1} \right] &= \mathbb{E} \left[ \frac{p_x p_y 1_{N_x=t} 1_{N_y=t}}{\sum_{z: z \neq x, z \neq y} 1_{N_z=t+1} + 1} \right] \\ &= \mathbb{E} [p_x p_y 1_{N_x=t} 1_{N_y=t}] \mathbb{E} \left[ \frac{1}{\sum_{z: z \neq x, z \neq y} 1_{N_z=t+1} + 1} \right] \\ &\stackrel{(a)}{\leq} \frac{\mathbb{E} [p_x p_y 1_{N_x=t} 1_{N_y=t}]}{\sum_{z: z \neq x, z \neq y} \mathbb{E} [1_{N_z=t+1}]} \\ &\stackrel{(b)}{\leq} \frac{\mathbb{E} [p_x p_y 1_{N_x=t} 1_{N_y=t}]}{\mathbb{E} [\Phi_{t+1} - 1]}, \end{aligned}$$

(a) follows from Lemma 15 and (b) follows from Equation (11) as

$$\sum_{z: z \neq x, z \neq y} \mathbb{E}[1_{N_z=t+1}] = \sum_z \mathbb{E}[1_{N_z=t+1}] - \mathbb{E}[1_{N_x=t+1}] - \mathbb{E}[1_{N_y=t+1}] \geq \mathbb{E}[\Phi_{t+1}] - 1.$$

Summing over  $x$  and  $y$  results in the lemma. □

We now have all the tools to bound the error of the Good-Turing estimator. We divide the set of values into two groups, depending on the value of  $\mathbb{E}[\Phi_{t+1}]$ .

**Lemma 17.** For any  $n$  and  $t$  if  $\mathbb{E}[\Phi_{t+1}] \leq 2$ , then

$$\mathbb{E} \left[ \frac{(S_t - (t+1)(\Phi_{t+1} + 1)/n)^2}{(\Phi_{t+1} + 1)(t+1)/n} \right] \leq \frac{5t}{n} + \frac{4 \log n}{n} \left( \frac{t+2}{t+1} \right) + \frac{6}{n}.$$

*Proof.* Let  $Z = S_t - (t+1)\Phi_{t+1}/n$ .

$$\begin{aligned} \mathbb{E} \left[ \left( Z - \frac{t+1}{n} \right)^2 \right] &\stackrel{(a)}{=} \mathbb{E}[Z^2] + \frac{(t+1)^2}{n^2} \\ &\stackrel{(b)}{\leq} \frac{(t+1)(t+2)\mathbb{E}[\Phi_{t+2}]}{n^2} + \frac{(t+1)^2\mathbb{E}[\Phi_{t+1}]}{n^2} + \frac{(t+1)^2}{n^2} \\ &\stackrel{(c)}{\leq} 2 \frac{(t+1)(t+2)}{n^2} \cdot \left( \frac{2 \log n}{t+1} + \frac{t+1}{t+2} \right) + \frac{(t+1)(t+2)}{n^2(t+2)} + \frac{3(t+1)^2}{n^2}. \end{aligned}$$

Equation (8) implies  $Z$  is a zero mean random variable and hence (a). Equation (10) implies (b) and (c) follows by Lemma 14 and the fact that  $\mathbb{E}[\Phi_{t+1}] \leq 2$ . Hence,

$$\begin{aligned} \mathbb{E} \left[ \frac{(Z - (t+1)/n)^2}{(\Phi_{t+1} + 1)(t+1)/n} \right] &\leq \frac{\mathbb{E}[(Z - (t+1)/n)^2]}{(t+1)/n} \\ &\leq \frac{2(t+2)}{n} \cdot \left( \frac{2 \log n}{t+1} + \frac{t+1}{t+2} \right) + \frac{1}{n} + \frac{3(t+1)}{n} \\ &= \frac{5t}{n} + \frac{4 \log n(t+2)}{n(t+1)} + \frac{6}{n}. \end{aligned}$$

□

**Lemma 18.** For any  $n$  and  $t$  if  $\mathbb{E}[\Phi_{t+1}] > 2$ , then

$$\mathbb{E} \left[ \frac{(S_t - (t+1)(\Phi_{t+1} + 1)/n)^2}{(\Phi_{t+1} + 1)(t+1)/n} \right] \leq \frac{5t}{n} + \frac{4 \log n}{n} \left( \frac{t+2}{t+1} \right) + \frac{6}{n}.$$

*Proof.*

$$\frac{(S_t - (t+1)(\Phi_{t+1} + 1)/n)^2}{(\Phi_{t+1} + 1)(t+1)/n} = \frac{S_t^2}{(\Phi_{t+1} + 1)(t+1)/n} + \frac{(t+1)(\Phi_{t+1} + 1)}{n} - 2S_t.$$

Thus by Equation (8),

$$\mathbb{E} \left[ \frac{(S_t - (t+1)(\Phi_{t+1} + 1)/n)^2}{(\Phi_{t+1} + 1)(t+1)/n} \right] = \mathbb{E} \left[ \frac{S_t^2}{(\Phi_{t+1} + 1)(t+1)/n} \right] - \frac{(t+1)\mathbb{E}[\Phi_{t+1}]}{n} + \frac{t+1}{n}. \quad (12)$$

By Lemma 16 and Equations (8), (9),

$$\begin{aligned} \mathbb{E} \left[ \frac{S_t^2}{(\Phi_{t+1} + 1)(t+1)/n} \right] &\leq \frac{\mathbb{E}[S_t^2]}{\mathbb{E}[\Phi_{t+1} - 1](t+1)/n} \\ &\leq \frac{t+1}{n} \frac{\mathbb{E}[\Phi_{t+1}]^2}{\mathbb{E}[\Phi_{t+1} - 1]} + \frac{t+2}{n} \frac{\mathbb{E}[\Phi_{t+2}]}{\mathbb{E}[\Phi_{t+1} - 1]}. \end{aligned}$$

Substituting the above equation in Equation (12) and simplifying,

$$\begin{aligned} \mathbb{E} \left[ \frac{(S_t - (t+1)(\Phi_{t+1} + 1)/n)^2}{(\Phi_{t+1} + 1)(t+1)/n} \right] &\leq \frac{(t+1)\mathbb{E}[\Phi_{t+1}] + (t+2)\mathbb{E}[\Phi_{t+2}]}{n\mathbb{E}[\Phi_{t+1} - 1]} + \frac{t+1}{n} \\ &\stackrel{(a)}{\leq} 2 \frac{(t+1)\mathbb{E}[\Phi_{t+1}] + (t+2)\mathbb{E}[\Phi_{t+2}]}{n\mathbb{E}[\Phi_{t+1}]} + \frac{t+1}{n} \\ &\stackrel{(b)}{\leq} 2 \left( \frac{t+1}{n} + \frac{t+2}{n} \left( \frac{2 \log n}{t+1} + \frac{t+1}{t+2} + \frac{1}{2(t+2)} \right) \right) + \frac{t+1}{n} \\ &= \frac{5t}{n} + \frac{4 \log n}{n} \left( \frac{t+2}{t+1} \right) + \frac{6}{n}. \end{aligned}$$

Since  $\mathbb{E}[\Phi_{t+1}] \geq 2$ ,  $\mathbb{E}[\Phi_{t+1}] - 1 \geq \mathbb{E}[\Phi_{t+1}]/2$  and hence (a). Lemma 14 implies (b). □

Combining the above two lemmas results in

**Lemma 19.** *For any  $t_0 \geq 1$ ,*

$$\sum_{t=0}^{t_0-1} \mathbb{E} \left[ \frac{(S_t - (t+1)(\Phi_{t+1} + 1)/n)^2}{(\Phi_{t+1} + 1)(t+1)/n} \right] \leq \frac{5t_0^2}{2n} + \frac{4 \log n}{n} (t_0 + \log t_0 + 1) + \frac{7t_0}{2n}.$$

*Proof.* By Lemmas 17 and 18, regardless of the value of  $\mathbb{E}[\Phi_{t+1}]$ ,

$$\mathbb{E} \left[ \frac{(S_t - (t+1)(\Phi_{t+1} + 1)/n)^2}{(\Phi_{t+1} + 1)(t+1)/n} \right] \leq \frac{5t}{n} + \frac{4 \log n}{n} \left( \frac{t+2}{t+1} \right) + \frac{6}{n}.$$

Summing the above expression for  $0 \leq t \leq t_0 - 1$  results in the lemma.  $\square$

Substituting the results from Lemmas 13 and 19 in Lemma 12,

$$\mathbb{E}[D(S||\hat{S})] \leq \frac{1}{t_0} + \frac{5t_0^2}{2n} + \frac{4 \log n}{n} (t_0 + \log t_0 + 1) + \frac{7t_0}{2n}.$$

Substituting  $t_0 = n^{1/3}/5^{1/3}$  results in Theorem 1.

$$r_{\text{poi}(n)}^{\text{nat}}(q', \Delta_k) \leq \max_{p \in \Delta_k} \mathbb{E}[D(S||\hat{S})] \leq \frac{2.6}{n^{1/3}} + \frac{2.4 \log n (n^{1/3} + \log n + 1)}{n} + \frac{2.1}{n^{2/3}} \leq \frac{3 + o_n(1)}{n^{1/3}}.$$

## D Proof of Theorem 3

To lower bound  $r_n^{\mathbb{P}_\sigma}(\Delta_k)$  it is sufficient to lower bound  $r_n^{\mathbb{P}_\sigma}(\mathcal{P})$  for any subset  $\mathcal{P} \subseteq \Delta_k$ . We construct a subset  $\mathcal{P}$  by considering a set of distributions  $\{p^{\bar{v}} : \bar{v} \in \{-1, 1\}^{m-1}\}$  and all their possible permutations. The lower bound argument uses Fano's inequality and Gilbert Varshamov bounds.

We choose  $\mathcal{P}$  to be the set of distributions whose probability multiset are close to that of a distribution  $p^0$ , where  $p^0$  is defined as follows.

Let  $c$  be a sufficiently large constant. Let  $m$  be the largest odd number less than  $\min(k, (n/(c^2 \log^2 n))^{1/3})$ . Let  $p^0$  be the following distribution. For  $1 \leq i \leq m-1$ ,

$$p_i^0 = \frac{\log n}{6n} \sqrt{\frac{c^2 n}{m}} \left( \sqrt{\frac{n}{c^2 m \log^2 n}} + i \right)$$

and  $p_m^0 = 1 - \sum_{i=1}^{m-1} p_i^0$ . Observe that for all  $1 \leq i \leq m-1$ ,  $1/(6m) \leq p_i^0 \leq 1/(3m)$  and  $p_m^0 \geq 2/3$ .

We choose the close-by distributions as follows. Let  $\epsilon = \sqrt{\frac{c^*}{mn}}$ , where  $c^*$  is some sufficiently small constant. For a binary vector  $\bar{v} \in \{-1, 1\}^{m-1}$ , let  $p^{\bar{v}}$  be the distribution such that  $p_i^{\bar{v}} = p_i^0 + \bar{v}_i \epsilon$  for  $1 \leq i \leq m-1$  and  $p^{\bar{v}}(m) = 1 - \sum_{i=1}^{m-1} p_i^{\bar{v}}$ . Note that by the properties of  $p^0$  and  $\epsilon$ ,  $p^{\bar{v}}$  is a valid distribution for every  $\bar{v}$ . Let  $\mathcal{C}$  be the largest subset of  $\{-1, 1\}^{m-1}$  such that for every  $\bar{v} \in \mathcal{C}$ ,  $\sum_i \bar{v}_i = 0$  and for every pair  $\bar{v}, \bar{v}' \in \mathcal{C}$ ,  $\sum_i |\bar{v}_i - \bar{v}'_i| \geq c'(m-1)$  for some constant  $c'$ . The following variation of Gilbert Varshamov lemma lower bounds size of  $\mathcal{C}$ .

**Lemma 20.** *There exists a set of vectors  $\mathcal{C}$  over  $\{-1, 1\}^{m-1}$  of size  $2^{c'' \cdot (m-1)}$  such that the minimum hamming distance between any two vectors is  $\geq c'(m-1)$  for some universal constants  $c' > 0, c'' > 0$  and  $\sum_i \bar{v}_i = 0$  for all  $\bar{v} \in \mathcal{C}$ .*

Let  $\mathcal{P}' = \{p^{\bar{v}} : \bar{v} \in \mathcal{C}\}$  and  $P_{\bar{v}} = \{p^{\bar{v}}(\sigma(\cdot)) : \sigma \in \Sigma^{m-1}\}$  be the set of all permutations of a distribution  $p^{\bar{v}}$ , i.e., all distributions with the same multiset as  $p^{\bar{v}}$ . Let

$$\mathcal{P} = \cup_{\bar{v} \in \mathcal{C}} P_{\bar{v}}.$$

We first bound the regret of the induced permutation class  $P_{\bar{v}}$  that contains all permutations of a distribution  $p^{\bar{v}}$ .

**Lemma 21.** For every induced permutation class  $P_{\bar{v}}$ ,

$$r_n(P_{\bar{v}}) \leq \frac{1}{n}.$$

*Proof.* We prove the bound by constructing an estimator  $q$ . Consider the estimator  $q$  which sorts the multiplicities and assigns the  $i^{\text{th}}$ -frequently occurred symbol probability  $p_i^{\bar{v}}$ . Since this is a natural estimator, it occurs the same loss for all distributions in  $P_{\bar{v}}$  and hence,

$$\begin{aligned} r_n(P_{\bar{v}}) &\leq \max_{p \in P_{\bar{v}}} \mathbb{E}[D(p||q)] \\ &= \mathbb{E}[D(p^{\bar{v}}||q)] \\ &\stackrel{(a)}{\leq} \Pr(\exists i, j : N_i > N_j, p_i^{\bar{v}} < p_j^{\bar{v}}) \log n \\ &\stackrel{(b)}{\leq} \binom{m}{2} e^{-2 \log n} \log n \\ &\leq \frac{1}{n}. \end{aligned}$$

(a) follows from the fact that the estimator makes an error only if two multiplicities cross over and if it does make an error, the maximum KL divergence is at most  $\log(p_{\max}/p_{\min}) \leq \log n$ . Since probabilities for any two symbols  $i$  and  $j$  differ by at least  $\frac{\log n}{6n} \cdot \sqrt{\frac{c^2 n}{m}}$  and the probabilities themselves lie between  $1/(6m)$  and  $1/(3m)$ , by choosing a sufficiently large  $c$ , the cross over probability can be bounded by  $e^{-2 \log n}$  using the Chernoff bound and hence (b).  $\square$

We now lower bound the KL divergence between  $p^{\bar{v}}$  and  $p^{\bar{v}'}$  for every pair of vectors  $\bar{v}$  and  $\bar{v}'$ . Let the Hamming distance between two vectors  $\bar{v}$  and  $\bar{v}'$  be  $\|\bar{v} - \bar{v}'\|_1 = \sum_{i=1}^{m-1} |\bar{v}_i - \bar{v}'_i|$ .

**Lemma 22.** For two distributions  $p^{\bar{v}}$  and  $p^{\bar{v}'}$  in  $\mathcal{P}'$ ,

$$\frac{1}{8} \left( c' \sqrt{\frac{mc^*}{n}} \right)^2 \leq \frac{1}{2} \|p^{\bar{v}} - p^{\bar{v}'}\|_1^2 \leq D(p^{\bar{v}}||p^{\bar{v}'}) \leq \frac{48mc^*}{n}.$$

*Proof.*

$$\begin{aligned} D(p^{\bar{v}}||p^{\bar{v}'}) &\stackrel{(a)}{\leq} \sum_{i=1}^m \frac{(p_i^{\bar{v}} - p_i^{\bar{v}'})^2}{p_i^{\bar{v}'}} \\ &\stackrel{(b)}{\leq} 2 \sum_{i=1}^m \frac{(p_i^{\bar{v}} - p_i^{\bar{v}'})^2}{p_i^0} \\ &\leq 2 \sum_{i=1}^{m-1} \frac{(\bar{v}_i - \bar{v}'_i)^2 (\sqrt{c^*/nm})^2}{1/(6m)} \\ &\leq 12 \sum_{i=1}^{m-1} \frac{(\bar{v}_i - \bar{v}'_i)^2 c^*}{n} \\ &\leq 24 \sum_{i=1}^{m-1} \frac{|\bar{v}_i - \bar{v}'_i| c^*}{n} \\ &= \frac{24 \|\bar{v} - \bar{v}'\|_1 c^*}{n} \\ &\leq \frac{48mc^*}{n}. \end{aligned}$$

(a) follows from bounding the KL divergence by the Chi-squared distance and (b) follows from the fact that  $\epsilon \ll 1/m$ . For the lower bound,

$$\begin{aligned}
D(p^{\bar{v}} \| p^{\bar{v}'}) &\stackrel{(a)}{\geq} \frac{1}{2} \|p^{\bar{v}} - p^{\bar{v}'}\|_1^2 \\
&= \frac{1}{2} \left( \frac{\|\bar{v} - \bar{v}'\|_1 \sqrt{c^*}}{\sqrt{mn}} \right)^2 \\
&\stackrel{(b)}{\geq} \frac{1}{2} \left( \frac{c'(m-1)\sqrt{c^*}}{\sqrt{mn}} \right)^2 \\
&\stackrel{(c)}{\geq} \frac{1}{8} \left( c' \sqrt{\frac{mc^*}{n}} \right)^2,
\end{aligned}$$

where (a) follows from Pinsker's inequality, (b) follows by construction, and  $m-1 \geq 2$  and hence (c).  $\square$

We now state Fano's inequality for distribution estimation.

**Lemma 23.** *Let  $p^1, p^2, \dots, p^{r+1}$  be distributions such that  $D(p^i \| p^j) \leq \beta$  and  $\|p^i - p^j\|_1 \geq \alpha$ , for all  $i, j$ . For any estimator  $q$ ,*

$$\sup_i \mathbb{E}_i[\|p^i - q\|_1] \geq \frac{\alpha}{2} \left( 1 - \frac{n\beta + \log 2}{\log r} \right).$$

We now have all the tools for the lower bound.

*Proof of Theorem 3.* For every permutation subclass  $P_{\bar{v}}$  in  $\mathcal{P}$ , by Lemma 21

$$r_n(P_{\bar{v}}) \leq \frac{1}{n}.$$

Thus,

$$\begin{aligned}
r_n^{\mathbb{P}^\sigma}(\mathcal{P}) &= \min_q \max_{\bar{v}} \left( \max_{p \in P_{\bar{v}}} r_n(q, p) - r_n(P_{\bar{v}}) \right) \\
&\geq \min_q \max_{\bar{v}} \left( \max_{p \in P_{\bar{v}}} r_n(q, p) - \frac{1}{n} \right) \\
&= \min_q \max_{p \in \mathcal{P}} r_n(q, p) - \frac{1}{n} \\
&= \min_q \max_{p \in \mathcal{P}} \mathbb{E}[D(p \| q)] - \frac{1}{n} \\
&\stackrel{(a)}{\geq} \min_q \max_{p \in \mathcal{P}'} \mathbb{E}[D(p \| q)] - \frac{1}{n} \\
&\stackrel{(b)}{\geq} \min_q \max_{p \in \mathcal{P}'} \mathbb{E} \left[ \frac{\|p - q\|_1^2}{2} \right] - \frac{1}{n} \\
&\stackrel{(c)}{\geq} \min_q \max_{p \in \mathcal{P}'} \frac{1}{2} \mathbb{E}[\|p - q\|_1^2] - \frac{1}{n} \\
&\stackrel{(d)}{\geq} \Omega\left(\frac{m}{n}\right) - \frac{1}{n} \\
&\geq \Omega\left(\frac{m}{n}\right).
\end{aligned}$$

$\mathcal{P}' \subset \mathcal{P}$ , hence (a). (b) follows from Pinsker's inequality and (c) follows from convexity. By construction, for every pair of distributions in  $\mathcal{P}'$ ,  $\beta = D(p \| p') \leq 48c^*m/n$  and  $\alpha = \|p - p'\|_1 \geq \Omega(\sqrt{m/n})$  (Lemma 22). Furthermore by Lemma 20,  $\mathcal{P}'$  has  $r+1 = 2^{c''(m-1)}$  distributions. Setting  $c^*$  to be a sufficiently small constant and applying Lemma 23 to  $\mathcal{P}'$  with the above values of  $\alpha, \beta$ , and  $r$  results in (d). Substituting the value of  $m$  in the above equation results in the Theorem.  $\square$