The goal of this short note is to provide simple proofs for the "folklore facts" on the sample complexity of learning a discrete probability distribution over a known domain of size k to total variation distance ε , with error probability δ . Thanks to Gautam Kamath and John Wright for suggesting "someone should write this up as a note," and to Jiantao Jiao for discussions about the Hellinger case.

For a given distance measure d, we write $\Phi(d, k, \varepsilon, \delta)$ for the sample complexity of learning discrete distributions over a known domain of size k, to accuracy $\varepsilon > 0$, with error probability $\delta \in (0, 1]$. As usual, asymptotics will be taken with regard to k going to infinity, ε going to 0, and δ going to 0, in that order. Without loss of generality, we hereafter assume the domain is the set $[k] \stackrel{\text{def}}{=} \{1, \ldots, k\}$.

1 Total variation distance

Recall that $d_{\text{TV}}(p,q) = \sup_{S \subset [k]} (p(S) - q(S)) = \frac{1}{2} ||p - q||_1 \in [0,1]$ for any $p, q \in \Delta([k])$.

Theorem 1.
$$\Phi(d_{\text{TV}}, k, \varepsilon, \delta) = \Theta\left(\frac{k + \log(1/\delta)}{\varepsilon^2}\right)$$
.

We focus here on the upper bound. The lower bound can be proven, e.g., via Assouad's lemma (for the k/ε^2 term), and from the hardness of estimating the bias of a coin (k=2) with high probability (for the $\log(1/\delta)/\varepsilon^2$ term).

First proof. Consider the empirical distribution \tilde{p} obtained by drawing n independent samples s_1, \ldots, s_n from the underlying distribution $p \in \Delta([k])$:

$$\tilde{p}(i) = \frac{1}{n} \sum_{j=1}^{n} \mathbb{1}_{\{s_j = i\}}, \qquad i \in [k]$$
(1)

• First, we bound the expected total variation distance between \tilde{p} and p, by using ℓ_2 distance as a proxy:

$$\mathbb{E}[\mathbf{d}_{\mathrm{TV}}(p, \tilde{p})] = \frac{1}{2}\mathbb{E}[\|p - \tilde{p}\|_{1}] = \frac{1}{2}\sum_{i=1}^{k}\mathbb{E}[|p(i) - \tilde{p}(i)|] \leq \frac{1}{2}\sum_{i=1}^{k}\sqrt{\mathbb{E}[(p(i) - \tilde{p}(i))^{2}]}$$

the last inequality by Jensen. But since, for every $i \in [k]$, $n\tilde{p}(i)$ follows a Bin(n,p(i)) distribution, we have $\mathbb{E}\big[(p(i)-\tilde{p}(i))^2\big] = \frac{1}{n^2} \operatorname{Var}[n\tilde{p}(i)] = \frac{1}{n}p(i)(1-p(i))$, from which

$$\mathbb{E}[\mathrm{d}_{\mathrm{TV}}(p,\tilde{p})] \le \frac{1}{2\sqrt{n}} \sum_{i=1}^{k} \sqrt{p(i)} \le \frac{1}{2} \sqrt{\frac{k}{n}}$$

the last inequality this time by Cauchy–Schwarz. Therefore, for $n \geq \frac{k}{\varepsilon^2}$ we have $\mathbb{E}[d_{TV}(p, \tilde{p})] \leq \frac{\varepsilon}{2}$.

• Next, to convert this expected result to a *high probability* guarantee, we apply McDiarmid's inequality to the random variable $f(s_1, \ldots, s_n) \stackrel{\text{def}}{=} d_{\text{TV}}(p, \tilde{p})$, noting that changing any single sample cannot change its value by more than $c \stackrel{\text{def}}{=} 1/n$:

$$\Pr\left[|f(s_1,\ldots,s_n) - \mathbb{E}[f(s_1,\ldots,s_n)]| \ge \frac{\varepsilon}{2}\right] \le 2e^{-\frac{2\left(\frac{\varepsilon}{2}\right)^2}{nc^2}} = 2e^{-\frac{1}{2}n\varepsilon^2}$$

and therefore as long as $n \geq \frac{2}{\varepsilon^2} \ln \frac{2}{\delta}$, we have $|f(s_1, \ldots, s_n) - \mathbb{E}[f(s_1, \ldots, s_n)]| \leq \frac{\varepsilon}{2}$ with probability at least $1 - \delta$.

Putting it all together, we obtain that $d_{\text{TV}}(p, \tilde{p}) \leq \varepsilon$ with probability at least $1 - \delta$, as long as $n \geq \max\left(\frac{k}{\varepsilon^2}, \frac{2}{\varepsilon^2} \ln \frac{2}{\delta}\right)$.

Second proof – the "fun" one. Again, we will analyze the behavior of the empirical distribution \tilde{p} over n i.i.d. samples from the unknown p (cf. (1)) – because it is simple, efficiently computable, and it works. Recalling the definition of total variation distance, note that $d_{\text{TV}}(p,\tilde{p}) > \varepsilon$ literally means there exists a subset $S \subseteq [k]$ such that $\tilde{p}(S) > p(S) + \varepsilon$. There are 2^k such subsets, so... let us do a union bound.

Fix any $S \subseteq [k]$. We have

$$\tilde{p}(S) = \tilde{p}(i) \stackrel{(1)}{=} \frac{1}{n} \sum_{i \in S} \sum_{i=1}^{n} \mathbb{1}_{\{s_j = i\}}$$

and so, letting $X_j \stackrel{\text{def}}{=} \sum_{i \in S} \mathbb{1}_{\{s_j = i\}}$ for $j \in [n]$, we have $\tilde{p}(S) = \frac{1}{n} \sum_{j=1}^n X_j$ where the X_j 's are i.i.d. Bernoulli random variable with parameter p(S). Here comes the Chernoff bound (actually, Hoeffding, the *other* Chernoff):

$$\Pr[\tilde{p}(S) > p(S) + \varepsilon] = \Pr\left[\frac{1}{n} \sum_{j=1}^{n} X_j > \mathbb{E}\left[\frac{1}{n} \sum_{j=1}^{n} X_j\right] + \varepsilon\right] \le e^{-2\varepsilon^2 n}$$

and therefore $\Pr[\tilde{p}(S) > p(S) + \varepsilon] \leq \frac{\delta}{2^k}$ for any $n \geq \frac{k \ln 2 + \log(1/\delta)}{2\varepsilon^2}$. A union bound over these 2^k possible sets S concludes the proof:

$$\Pr[\exists S \subseteq [k] \text{ s.t. } \tilde{p}(S) > p(S) + \varepsilon] \le 2^k \cdot \frac{\delta}{2^k} = \delta$$

and we are done. Badda bing badda boom, as someone would say.

2 Hellinger distance

Recall that $d_H(p,q) = \frac{1}{\sqrt{2}} \sqrt{\sum_{i=1}^k (\sqrt{p(i)} - \sqrt{q(i)})^2} = \frac{1}{\sqrt{2}} ||p-q||_2 \in [0,1]$ for any $p,q \in \Delta([k])$. The Hellinger distance has many nice properties: it is well-suited to manipulating product distributions, its square is subadditive, and is always within a quadratic factor of the total variation distance; see, e.g., [Can15, Appendix C.2].

Theorem 2.
$$\Phi(d_H, k, \varepsilon, \delta) = \Theta\left(\frac{k + \log(1/\delta)}{\varepsilon^2}\right)$$
.

This theorem is "highly non-trivial" to establish, however; for the sake of exposition, we will show increasingly stronger bounds, starting with the easiest to establish.

Proposition 3 (Easy bound).
$$\Phi(d_H, k, \varepsilon, \delta) = O\left(\frac{k + \log(1/\delta)}{\varepsilon^4}\right)$$
, and $\Phi(d_H, k, \varepsilon, \delta) = \Omega\left(\frac{k + \log(1/\delta)}{\varepsilon^2}\right)$.

Proof. This is immediate from Theorem 1, recalling that $\frac{1}{2} d_{TV}^2 \leq d_{H}^2 \leq d_{TV}$.

Proposition 4 (More involved bound).
$$\Phi(d_H, k, \varepsilon, \delta) = O\left(\frac{k}{\varepsilon^2} + \frac{\log(1/\delta)}{\varepsilon^4}\right)$$
.

Proof. As for total variation distance, we consider the empirical distribution \widehat{p} (cf. (1)) obtained by drawing n independent samples s_1, \ldots, s_n from $p \in \Delta([k])$.

• First, we bound the expected squared Hellinger distance between \widehat{p} and p: using the simple fact that $d_{\rm H}(p,q)^2 = 1 - \sum_{i=1}^k \sqrt{p(i)q(i)}$ for any $p,q \in \Delta([k])$,

$$\mathbb{E}\left[\mathrm{d}_{\mathrm{H}}(p,\widehat{p})^{2}\right] = 1 - \sum_{i=1}^{k} \sqrt{p(i)} \cdot \mathbb{E}\left[\sqrt{\widehat{p}(i)}\right].$$

¹John Wright.

Now we would like to handle the square root inside the expectation, and of course Jensen's inequality is in the wrong direction. However, for every nonnegative r.v. X with positive expectation, letting $Y \stackrel{\text{def}}{=} X/\mathbb{E}[X]$, we have that

$$\begin{split} \mathbb{E}\Big[\sqrt{X}\Big] &= \sqrt{\mathbb{E}[X]} \cdot \mathbb{E}\Big[\sqrt{Y}\Big] = \sqrt{\mathbb{E}[X]} \cdot \mathbb{E}\Big[\sqrt{1 + (Y - \mathbb{E}[Y])})\Big] \\ &\geq \sqrt{\mathbb{E}[X]}\bigg(1 + \frac{1}{2}\mathbb{E}[Y - \mathbb{E}[Y]] - \frac{1}{6}\mathbb{E}\big[(Y - \mathbb{E}[Y])^2\big]\bigg) = \sqrt{\mathbb{E}[X]}\bigg(1 - \frac{\operatorname{Var}X}{6\mathbb{E}[X]^2}\bigg) \end{split}$$

where we used the inequality $\sqrt{1+x} \ge 1 + \frac{x}{2} - \frac{x^2}{6}$, which holds for $x \ge 0$. Since, for every $i \in [k]$, $n\widehat{p}(i)$ follows a Bin(n, p(i)) distribution, we get

$$\mathbb{E}\Big[\mathrm{d_H}(p,\widehat{p})^2\Big] \leq 1 - \frac{1}{\sqrt{n}} \sum_{i=1}^k \sqrt{p(i)} \cdot \sqrt{np(i)} \left(1 - \frac{np(i)(1 - np(i))}{6n^2p(i)^2}\right) \leq 1 - \sum_{i=1}^k p(i) \left(1 - \frac{1}{6np(i)}\right) = \frac{k}{6n}.$$

Therefore, for $n \geq \frac{k}{3\varepsilon^2}$, we have $\mathbb{E}\left[\mathrm{d_H}(p,\widehat{p})^2\right] \leq \frac{\varepsilon^2}{2}$.

• Next, to convert this expected result to a high probability guarantee, we would like to apply McDiarmid's inequality to the random variable $f(s_1, \ldots, s_n) \stackrel{\text{def}}{=} d_H(p, \widehat{p})^2$ as in the (first) proof of Theorem 1; unfortunately, changing a sample can change the value by up to $c \approx 1/\sqrt{n}$, and McDiarmid will yield only a vacuous bound.³ Instead, we will use a stronger, more involved concentration inequality:

Theorem 5 ([BLM13, Theorem 8.6]). Let $f: \mathcal{X}^n \to \mathbb{R}$ be a measurable function, and let X_1, \ldots, X_n be independent random variables taking values in \mathcal{X} . Define $Z \stackrel{\text{def}}{=} f(X_1, \ldots, X_n)$. Assume that there exist measurable functions $c_i: \mathcal{X}^n \to [0, \infty)$ such that, for all $x, y \in \mathcal{X}^n$,

$$f(y) - f(x) \le \sum_{i=1}^{n} c_i(x) \mathbb{1}_{\{x_i \ne y_i\}}$$
.

Then, setting $v \stackrel{\text{def}}{=} \mathbb{E} \sum_{i=1}^n c_i(x)^2$ and $v_{\infty} \stackrel{\text{def}}{=} \sup_{x \in \mathcal{X}^n} \sum_{i=1}^n c_i(x)^2$, we have, for all t > 0,

$$\Pr[Z \geq \mathbb{E}[Z] + t] \leq e^{-\frac{t^2}{2v}} \qquad \Pr[Z \leq \mathbb{E}[Z] - t] \leq e^{-\frac{t^2}{2v_{\infty}}}.$$

For our f above, we have, for two any different $x, y \in [k]^n$, that

$$\begin{split} f(y) - f(x) &= \frac{1}{\sqrt{n}} \sum_{i=1}^k \sqrt{p(i)} \left(\sqrt{\sum_{j=1}^n \mathbbm{1}_{\{x_j = i\}}} - \sqrt{\sum_{j=1}^n \mathbbm{1}_{\{y_j = i\}}} \right) \\ &= \frac{1}{\sqrt{n}} \sum_{i=1}^k \sqrt{p(i)} \frac{\sum_{j=1}^n (\mathbbm{1}_{\{x_j = i\}} - \mathbbm{1}_{\{y_j = i\}})}{\sqrt{\sum_{j=1}^n \mathbbm{1}_{\{x_j = i\}}} + \sqrt{\sum_{j=1}^n \mathbbm{1}_{\{y_j = i\}}}} \\ &\leq \frac{1}{\sqrt{n}} \sum_{i=1}^k \sqrt{p(i)} \frac{\sum_{j=1}^n \mathbbm{1}_{\{x_j = i\}} \mathbbm{1}_{\{y_j \neq x_j\}}}{\sqrt{\sum_{j=1}^n \mathbbm{1}_{\{x_j = i\}}}} = \sum_{j=1}^n \sqrt{\frac{p_{x_j}}{n \sum_{\ell=1}^n \mathbbm{1}_{\{x_\ell = x_j\}}}} \cdot \mathbbm{1}_{\{x_j \neq y_j\}} \,. \end{split}$$

In view of Theorem 5, we then must evaluate

$$v \stackrel{\text{def}}{=} \sum_{j=1}^{n} \mathbb{E}[c_j(X)^2] = \frac{1}{n} \sum_{j=1}^{n} \sum_{i=1}^{k} p(i)^2 \cdot \mathbb{E}\left[\frac{1}{1 + \sum_{\ell \neq j} \mathbb{1}_{\{X_\ell = i\}}}\right]$$

²And is inspired by the Tayor expansion $\sqrt{1+x}=1+\frac{x}{2}-\frac{x^2}{8}+o(x^2)$: there is *some* intuition for it.

³Try it: it's a real bummer.

where that last expectation is over $(x_{\ell})_{\ell \neq j}$ drawn from $p^{\otimes (n-1)}$. Since $\sum_{\ell \neq j} \mathbb{1}_{\{X_{\ell}=i\}}$ is Binomially distributed with parameters n-1 and p(i), we can use the simple fact that, for $N \sim \text{Bin}(r,\rho)$,

$$\mathbb{E}\left[\frac{1}{N+1}\right] = \frac{1 - (1-\rho)^{r+1}}{\rho(r+1)} \le \frac{1}{\rho(r+1)}$$

to conclude that $v \leq \frac{1}{n^2} \sum_{j=1}^n \sum_{i=1}^k p(i) = \frac{1}{n}$. By Theorem 5, we obtain

$$\Pr\left[|f(s_1,\ldots,s_n) - \mathbb{E}[f(s_1,\ldots,s_n)]| \ge \frac{\varepsilon^2}{2}\right] \le e^{-\frac{1}{8}n\varepsilon^4}$$

and therefore, as long as $n \geq \frac{8}{\varepsilon^4} \ln \frac{1}{\delta}$, we have $|f(s_1, \ldots, s_n) - \mathbb{E}[f(s_1, \ldots, s_n)]| \leq \frac{\varepsilon^2}{2}$ with probability at least $1 - \delta$.

Putting it all together, we obtain that $d_{\rm H}(p,\widehat{p})^2 \leq \varepsilon^2$ with probability at least $1-\delta$, as long as $n \geq \max(\frac{k}{3\varepsilon^2},\frac{8}{\varepsilon^4}\ln\frac{1}{\delta})$.

We finally get to the final, optimal bound:

Proof of Theorem 2. We will rely on a recent – and quite involved – result due to Agrawal [Agr19], analyzing the concentration of the empirical distribution \hat{p} in terms of its Kullback–Leibler (KL) divergence with regard to the true p,

$$\mathrm{KL}(\widehat{p} \parallel p) = \sum_{i=1}^{k} \widehat{p}(i) \ln \frac{\widehat{p}(i)}{p(i)} \in [0, \infty].$$

Observing that $d_H(p,q)^2 \le \frac{1}{2}KL(p \parallel q)$ for any distributions p,q, the aforementioned result is actually stronger than what we need:

Theorem 6 ([Agr19, Theorem 1.2]). Suppose $n \ge \frac{k-1}{\alpha}$. Then

$$\Pr[\operatorname{KL}(\widehat{p} \parallel p) \ge \alpha] \le e^{-n\alpha} \left(\frac{e\alpha n}{k-1}\right)^{k-1}.$$

In view of the above relation between Hellinger and KL, we will apply this convergence result with $\alpha \stackrel{\text{def}}{=} 2\varepsilon^2$, obtaining

$$\Pr[\,\mathrm{d_H}(\widehat{p},p) \ge \varepsilon\,] \le e^{-2n\varepsilon^2 + (k-1)\ln\frac{2\epsilon n\varepsilon^2}{k-1}}\,.$$

Fact 7. For $n \geq \frac{15}{2e} \frac{k}{\varepsilon^2}$, we have $(k-1) \ln \frac{2en\varepsilon^2}{k-1} \leq n\varepsilon^2$.

Proof. The conclusion is equivalent to $2e \cdot \ln \frac{2en\varepsilon^2}{k-1} \le \frac{2en\varepsilon^2}{k-1}$, and the conclusion follows from the fact that $x \ge 2e \ln x$ for $x \ge 15$.

This fact implies that, for $n \geq \frac{15k}{2\varepsilon^2}$, $\Pr[d_H(\widehat{p}, p) \geq \varepsilon] \leq e^{-n\varepsilon^2}$. Overall, we obtain that $d_H(p, \widehat{p}) \leq \varepsilon$ with probability at least $1 - \delta$ as long as $n \geq \max(\frac{15k}{2\varepsilon\varepsilon^2}, \frac{1}{\varepsilon^2} \ln \frac{1}{\delta})$, as desired.

3 χ^2 and Kullback—Leibler divergences

To conclude, some remarks on Kullback–Leibler (KL) and chi-squared (χ^2) divergences. Recall their definition, for $p, q \in \Delta([k])$,

$$KL(p || q) = \sum_{i=1}^{k} p(i) \ln \frac{p(i)}{q(i)}, \qquad \chi^{2}(p || q) = \sum_{i=1}^{k} \frac{(p(i) - q(i))^{2}}{q(i)}$$

both taking values in $[0, \infty]$; as well as the chain of (easily checked) inequalities

$$2d_{TV}(p,q)^{2} \le KL(p \parallel q) \le \chi^{2}(p \parallel q),$$

where the first one is Pinsker's. Importantly, KL and χ^2 divergences are unbounded and asymmetric, so the order of p and q matters a lot: for instance, it is easy to show that, without strong assumptions on the unknown distribution $p \in \Delta([k])$, the empirical estimator \widehat{p} cannot achieve $\mathrm{KL}(p \parallel \widehat{p}) < \infty$ (resp., $\chi^2(p \parallel \widehat{p}) < \infty$) with any finite number of samples. So, that's uplifting. (On the other hand, other estimators than the empirical one, e.g., add-constant estimators, do provide good learning guarantees for those distance measures: see for instance [KOPS15]).

We are going to focus here on getting $\mathrm{KL}(\widehat{p} \parallel p)$ and $\chi^2(\widehat{p} \parallel p)$ down to ε . Of course, in view of the inequalities above, the latter is at least as hard as the former, and a lower bound on both follows from that on d_{TV} : $\Omega((k + \log(1/\delta))/\varepsilon^2)$. And, behold! The result of Agrawal [Agr19] used in the proof of Theorem 2 does provide the optimal upper bound on learning in KL divergence – and it is achieved by the usual suspect, the empirical estimator:

Theorem 8. $\Phi(\mathrm{KL}, k, \varepsilon, \delta) = \Theta\left(\frac{k + \log(1/\delta)}{\varepsilon}\right)$, where by KL we refer to minimizing $\mathrm{KL}(\widehat{p} \parallel p)$.

The optimal sample complexity of learning in χ^2 as a function of k, ε, δ , however, remains open.

References

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 $^{^{4}}$ You can verify this: intuitively, the issue boils down to having to non-trivially learn even the elements of the support of p that have arbitrarily small probability.