

Lec 10: Entropic upper bounds of density estimation

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Last lecture: use covering/packing to prove statistical lower bound via Fano

This lecture: they can also prove upper bounds!

Density estimation: $X_1, \dots, X_n \stackrel{i.i.d.}{\sim} P$, where $P \in \mathcal{P}$ is an unknown distribution

target: for $D \in \{D_{KL}, TV, H^2\}$, construct an estimator $\hat{P} = \hat{P}(X^n)$ s.t.

$$\sup_{P \in \mathcal{P}} \mathbb{E}_{X^n \sim P^n} [D(P, \hat{P})] \text{ is small.}$$

Overview of results.

- KL (Yang-Barron): $\exists \hat{P}$ s.t.

$$\sup_{P \in \mathcal{P}} \mathbb{E}_P [D_{KL}(P \| \hat{P})] \lesssim \inf_{\varepsilon > 0} \left(\varepsilon^2 + \frac{1}{n} \log N_{KL}(\mathcal{P}, \varepsilon) \right)$$

- TV (Yatracos): $\exists \hat{P}$ s.t.

$$\sup_{P \in \mathcal{P}} \mathbb{E}_P [TV^2(P, \hat{P})] \lesssim \inf_{\varepsilon > 0} \left(\varepsilon^2 + \frac{1}{n} \log N_{TV}(\mathcal{P}, \varepsilon) \right)$$

- H^2 (Le Cam-Birgé): $\exists \hat{P}$ s.t.

$$\sup_{P \in \mathcal{P}} \mathbb{E}_P [H^2(P, \hat{P})] \lesssim \inf_{\varepsilon > 0} \left(\varepsilon^2 + \frac{1}{n} \log N_H(\mathcal{P}, \varepsilon) \right).$$

Example 1. For finite-dimensional models \mathcal{P} with d parameters, usually $N_D(\mathcal{P}, \varepsilon) \asymp d \log \frac{1}{\varepsilon}$.

In this case. $\inf_P \sup_P \mathbb{E}_P [D(P, \hat{P})] \lesssim \inf_{\varepsilon > 0} \left(\varepsilon^2 + \frac{d}{n} \log \frac{1}{\varepsilon} \right) \lesssim \frac{d \log n}{n}$.
(Volume bound)
usually optimal up to $\log n$ factor.

Example 2. For nonparametric classes \mathcal{P} with $N_D(\mathcal{P}, \varepsilon) \asymp \varepsilon^{-d}$.

$$\inf_P \sup_P \mathbb{E}_P [D(P, \hat{P})] \lesssim \inf_{\varepsilon > 0} \left(\varepsilon^2 + \frac{1}{n \varepsilon^d} \right) \lesssim n^{-\frac{2}{2+d}}.$$

Yang-Barron: progressive mixing / online-to-batch conversion

"Online" guarantee: similar to global Fano, let P_1, \dots, P_N be an ε -covering of \mathcal{P} , i.e.

$$\sup_{P \in \mathcal{P}} \min_{i \in [N]} D_{KL}(P \| P_i) \leq \varepsilon^2.$$

Let $Q_{X^{n+1}}$ be the average product distribution:

$$Q_{X^{n+1}} = \frac{1}{N} \sum_{i=1}^N P_i^{\otimes (n+1)}.$$

Lemma. $\sup_{P \in \mathcal{P}} D_{KL}(P^{\otimes (n+1)} \| Q_{X^{n+1}}) \leq (n+1)\varepsilon^2 + \log N.$

Pf. Similar to global Fano: for any $P \in \mathcal{P}$,

$$\begin{aligned} D_{KL}(P^{\otimes (n+1)} \| Q_{X^{n+1}}) &= \mathbb{E}_{X^{n+1} \sim P^{\otimes (n+1)}} \left[\log \frac{P^{\otimes (n+1)}(X^{n+1})}{\frac{1}{N} \sum_{i=1}^N P_i^{\otimes (n+1)}(X^{n+1})} \right] \\ &\leq \mathbb{E}_{X^{n+1} \sim P^{\otimes (n+1)}} \left[\min_{i \in [N]} \log \frac{P^{\otimes (n+1)}(X^{n+1})}{P_i^{\otimes (n+1)}(X^{n+1})} + \log N \right] \\ &\leq \min_{i \in [N]} D_{KL}(P^{\otimes (n+1)} \| P_i^{\otimes (n+1)}) + \log N \\ &\leq (n+1)\varepsilon^2 + \log N. \end{aligned}$$

□

This is called an "online" guarantee as it concerns the density estimation performance for joint distributions of $X_1, \dots, X_{n+1} \stackrel{\text{i.i.d.}}{\sim} P$.

"Online-to-batch" conversion: given $Q_{X^{n+1}}$, we can define

$$\hat{P}(x) = \frac{1}{n+1} \sum_{t=0}^n Q_{X_{t+1}=x | X^t}.$$

Note that \hat{P} is a well-defined estimator and depends on X^n . Expanding out the defn. of $Q_{X^{n+1}}$ gives

$$\hat{P}(x) = \frac{1}{n+1} \sum_{t=0}^n \frac{\frac{1}{N} \sum_{i=1}^N \left(\prod_{s \leq t} P_i(X_s) \right) P_i(x)}{\frac{1}{N} \sum_{i=1}^N \prod_{s \leq t} P_i(X_s)} \in \text{conv}(\mathcal{P})$$

"progressive mixing"

Yang-Barron result follows from the next result:

Lemma. $\mathbb{E}_P [D_{KL}(P \parallel \hat{P})] \leq \frac{1}{n+1} D_{KL}(P^{\otimes(n+1)} \parallel Q_{X^{n+1}}).$

Pf.

$$\begin{aligned} \mathbb{E}_P [D_{KL}(P \parallel \hat{P})] &= \mathbb{E}_P \left[D_{KL} \left(P \parallel \frac{1}{n+1} \sum_{t=0}^n Q_{X_{t+1} | X^t} \right) \right] \\ &\leq \frac{1}{n+1} \sum_{t=0}^n \mathbb{E}_P [D_{KL}(P \parallel Q_{X_{t+1} | X^t})] \quad (\text{convexity}) \\ &= \frac{1}{n+1} D_{KL}(P^{\otimes(n+1)} \parallel Q_{X^{n+1}}) \quad (\text{chain rule}) \end{aligned} \quad \square$$

Remarks: ① This online-to-batch conversion provides a general paradigm for converting "redundancy" bound to prediction risk bound, even beyond i.i.d. data; see more next lecture.

② The Yang-Barron estimator is often improper (i.e. $\hat{P} \in \text{conv}(\mathcal{P})$ but often $\hat{P} \notin \mathcal{P}$), and computationally hard to obtain.

Yatracos: minimum distance estimator

The TV density estimation result is a corollary of the following general result in the robust case.

Thm. Let $X_1, \dots, X_n \stackrel{\text{i.i.d.}}{\sim} P$, and Q_1, \dots, Q_N be arbitrary candidate distributions.

Then there exists an estimator \hat{P} s.t.

$$TV(P, \hat{P}) \leq 3 \min_{i \in [N]} TV(P, Q_i) + \varepsilon_n, \text{ with } \mathbb{E}[\varepsilon_n] = O\left(\frac{\log N}{n}\right).$$

Note that by choosing $\{Q_1, \dots, Q_N\}$ be an ε -covering of \mathcal{P} under TV , with $N = N_{TV}(\mathcal{P}, \varepsilon)$, this implies the density estimation result.

Next we prove the theorem using a minimum-distance estimator:

$$\hat{P} = \operatorname{argmin}_{Q \in \{Q_1, \dots, Q_N\}} \tilde{TV}(P_n, Q),$$

where $P_n = \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$ is the empirical distribution, and \tilde{TV} is a pseudo-distance.

(What if $\tilde{TV} = TV$? If Q_1, \dots, Q_N are all continuous distributions, since P_n is discrete, $TV(P_n, Q_i) = 0$ for all i , so it's not useful.)

Let's defer the choice of \tilde{TV} and proceed to the analysis. Let

$$Q^* = \operatorname{argmin}_{Q \in \{Q_1, \dots, Q_N\}} TV(P, Q).$$

Then

$$\begin{aligned} TV(\hat{P}, P) &\leq TV(\hat{P}, Q^*) + TV(Q^*, P) \\ &\stackrel{\text{hope}}{=} \tilde{TV}(\hat{P}, Q^*) + TV(Q^*, P) \\ &\leq \tilde{TV}(\hat{P}, P_n) + \tilde{TV}(P_n, Q^*) + TV(Q^*, P) \\ &\leq 2\tilde{TV}(P_n, Q^*) + TV(Q^*, P) \quad (\text{definition of } \hat{P}) \\ &\leq 2\tilde{TV}(P_n, P) + 2\tilde{TV}(P, Q^*) + TV(P, Q^*) \\ &\stackrel{\text{hope}}{\leq} 2\tilde{TV}(P_n, P) + 3TV(P, Q^*). \end{aligned}$$

To make the analysis go through, we need:

- ① $\tilde{TV}(P, Q) \leq TV(P, Q), \quad \forall P, Q$
- ② $\tilde{TV}(Q_i, Q_j) = TV(Q_i, Q_j), \quad \forall i, j \in [n]$
- ③ $\mathbb{E}[\tilde{TV}(P_n, P)^2]$ is small.

Motivated by ① + ②, we define

$$\tilde{TV}(P, Q) = \sup_{A \in \mathcal{A}} |P(A) - Q(A)|,$$

where $\mathcal{A} = \{A_{ij} : i, j \in [N]\}$ with

$$A_{ij} := \{x : Q_i(x) \geq Q_j(x)\}.$$

Then: ① is immediate as $TV(P, Q) = \sup_A |P(A) - Q(A)|$

② is also true as $TV(Q_i, Q_j) = |Q_i(A_{ij}) - Q_j(A_{ij})| \leq \tilde{TV}(Q_i, Q_j)$

③ notes that $|A| \leq \binom{N}{2}$, and for fixed A ,

$$P(|P(A) - P_n(A)| > \varepsilon) \leq 2 \exp(-2n\varepsilon^2) \text{ by Hoeffding.}$$

Therefore, a union bound over A gives

$$\begin{aligned} P(\tilde{TV}(P, P_n) > \varepsilon) &\leq 2N^2 \exp(-2n\varepsilon^2) \\ \Rightarrow E[\tilde{TV}^2(P, P_n)] &= \int_0^\infty P(\tilde{TV}^2(P, P_n) \geq r) dr \\ &\leq \int_0^\infty \min\left\{1, 2N^2 e^{-2nr}\right\} dr \\ &\leq \frac{\log(2N^2)}{2n} + \int_{\frac{\log(2N^2)}{2n}}^\infty 2N^2 e^{-2nr} dr \\ &= O\left(\frac{\log N}{n}\right). \end{aligned}$$

Remark: ① The Yatracos estimator is proper, i.e. $\hat{P} \in \mathcal{P}$.

② The above proof also shows a high-probability guarantee on $TV(\hat{P}, P)$

③ It's known that the constant 3 is not improvable if the estimator is required to be proper.

④ There are some recent interests in the computationally efficient version of Yatracos.

Le Cam-Birgé: pairwise comparison

Composite hypothesis testing.

$H_0: X_1, \dots, X_n \sim P \quad \text{with } P \in \mathcal{P}$

$H_1: X_1, \dots, X_n \sim Q \quad \text{with } Q \in \mathcal{Q}$

test: $T = T(X^n) \in \{0, 1\}$

type-I error: $\sup_{P \in \mathcal{P}} P^{(n)}(T=1)$

type-II error: $\sup_{Q \in \mathcal{Q}} Q^{(n)}(T=0)$

Lemma. $\inf_T \left(\sup_{P \in \mathcal{P}} P^{\otimes n}(T=1) + \sup_{Q \in \mathcal{Q}} Q^{\otimes n}(T=0) \right) \leq e^{-\frac{n}{2} H^2(\text{conv}(\mathcal{P}), \text{conv}(\mathcal{Q}))}$

where $H^2(\text{conv}(\mathcal{P}), \text{conv}(\mathcal{Q})) := \inf_{\substack{P \in \text{conv}(\mathcal{P}) \\ Q \in \text{conv}(\mathcal{Q})}} H^2(P, Q).$

Pf. In Lec 8 we know that

$$\begin{aligned} \text{LHS} &= 1 - \text{TV}(\text{conv}(\mathcal{P}^{\otimes n}), \text{conv}(\mathcal{Q}^{\otimes n})) \quad \left(\begin{array}{l} \mathcal{P}^{\otimes n} = \{P^{\otimes n} : P \in \mathcal{P}\} \\ \text{TV}(P, Q) = \inf_{\substack{P' \in \mathcal{P} \\ Q' \in \mathcal{Q}}} \text{TV}(P', Q') \end{array} \right) \\ &\leq 1 - \frac{H^2}{2}(\text{conv}(\mathcal{P}^{\otimes n}), \text{conv}(\mathcal{Q}^{\otimes n})) \quad (\text{TV} \geq \frac{H^2}{2}) \\ &\leq \left(1 - \frac{H^2}{2}(\text{conv}(\mathcal{P}), \text{conv}(\mathcal{Q})) \right)^n \quad (\text{next lemma}) \\ &\leq \exp\left(-\frac{n}{2} H^2(\text{conv}(\mathcal{P}), \text{conv}(\mathcal{Q}))\right) \quad \square \end{aligned}$$

Lemma. $1 - \frac{H^2}{2}(\text{conv}(\bigotimes_{i=1}^n \mathcal{P}_i), \text{conv}(\bigotimes_{i=1}^n \mathcal{Q}_i)) \leq \prod_{i=1}^n \left(1 - \frac{H^2}{2}(\text{conv}(\mathcal{P}_i), \text{conv}(\mathcal{Q}_i)) \right).$

Pf. Suffice to prove the case $n=2$. Note that

$$1 - \frac{H^2}{2}(P, Q) = 1 - \frac{1}{2} \int (\sqrt{P} - \sqrt{Q})^2 = \int \sqrt{PQ}.$$

and any $P_{X,Y} \in \text{conv}(\mathcal{P}_1 \otimes \mathcal{P}_2)$ can be written as $P_{X,Y} = \mathbb{E}_2[P_{X|Z} P_{Y|Z}]$ with $P_{X|Z} \in \mathcal{P}_1$, $P_{Y|Z} \in \mathcal{P}_2$. Then

$$\begin{aligned} 1 - \frac{H^2}{2}(P_{X,Y}, Q_{X,Y}) &= \int \sqrt{P_{X,Y} Q_{X,Y}} \\ &= \int_X \sqrt{P_X Q_X} \int_Y \underbrace{\sqrt{P_{Y|X} Q_{Y|X}}}_{= \mathbb{E}_{Z|X}[P_{Y|Z}] \in \text{conv}(\mathcal{P}_2)} \\ &\leq \int_X \underbrace{\sqrt{P_X Q_X}}_{= \mathbb{E}_2[P_{X|Z}] \in \text{conv}(\mathcal{P}_1)} \cdot \left(1 - \frac{H^2}{2}(\text{conv}(\mathcal{P}_2), \text{conv}(\mathcal{Q}_2)) \right) \\ &\leq \left(1 - \frac{H^2}{2}(\text{conv}(\mathcal{P}_1), \text{conv}(\mathcal{Q}_1)) \right) \left(1 - \frac{H^2}{2}(\text{conv}(\mathcal{P}_2), \text{conv}(\mathcal{Q}_2)) \right). \quad \square \end{aligned}$$

(Note: the same proof holds for all Rényi divergences $D_\alpha = \frac{1}{\alpha-1} \log \int P^\alpha Q^{1-\alpha}$.)

This lemma will be applied in the following setting:

$$H_0: X_1, \dots, X_n \sim P, \quad P \in B_H(P_0, \varepsilon) = \{P: H^2(P, P_0) \leq \varepsilon^2\}$$

$$H_1: X_1, \dots, X_n \sim Q, \quad Q \in B_H(Q_0, \varepsilon).$$

Corollary. If $H(P_0, Q_0) \geq 4\varepsilon$, then

$$\inf_T \left(\sup_{P \in B_H(P_0, \varepsilon)} P^{\otimes n}(T=1) + \sup_{Q \in B_H(Q_0, \varepsilon)} Q^{\otimes n}(T=0) \right) \leq e^{-\frac{n}{8} H^2(P_0, Q_0)}.$$

Pf. Since $(P, Q) \mapsto H^2(P, Q)$ is jointly convex (Lec 3), both balls $B_H(P_0, \varepsilon)$ and $B_H(Q_0, \varepsilon)$ are convex. Therefore, the result follows from

$$\begin{aligned} H(B_H(P_0, \varepsilon), B_H(Q_0, \varepsilon)) &= \inf_{\substack{P \in B_H(P_0, \varepsilon) \\ Q \in B_H(Q_0, \varepsilon)}} H(P, Q) \\ &\geq \inf_{\substack{P \in B_H(P_0, \varepsilon) \\ Q \in B_H(Q_0, \varepsilon)}} H(P_0, Q_0) - H(P, P_0) - H(Q, Q_0) \end{aligned}$$

$$\geq H(P_0, Q_0) - 2\varepsilon \geq \frac{1}{2} H(P_0, Q_0) \quad \square$$

Le Cam - Birgé pairwise comparison estimator.

Let P_1, \dots, P_N be a maximal ε -packing of \mathcal{P} under H , i.e.

$$H(P_i, P_j) \geq \varepsilon, \quad \forall i \neq j.$$

Since a maximal ε -packing is also an ε -covering,

$$\sup_{P \in \mathcal{P}} \min_{i \in [N]} H(P, P_i) \leq \varepsilon.$$

For $\delta = 4\varepsilon$ and $H(P_i, P_j) \geq \delta$, construct a test T_{ij} for

$$H_0: P \in B_H(P_i, \varepsilon) \quad \text{vs.} \quad H_1: P \in B_H(P_j, \varepsilon).$$

By the above corollary, $\exists T_{ij}$ (and $T_{ji} := 1 - T_{ij}$)

$$\sup_{P \in \mathcal{B}_H(P_i, \varepsilon)} P(T_{ij} = 1) \leq e^{-\frac{n}{8} H(P_i, P_j)^2}.$$

Now define the following estimator:

- For $i \in [N]$, let $\psi_i = \max \{ H(P_i, P_j) : T_{ij} = 1, H(P_i, P_j) \geq \delta \}$

($\psi_i = 0$ if no such j exists)

- $\hat{P} = P_{i^*}$, with $i^* = \arg\min_{i \in [N]} \psi_i$.

Thm. If $n\varepsilon^2 \geq \max\{\log N_H(\mathcal{P}, \varepsilon_n), 1\}$, then the above estimator \hat{P} with $\varepsilon = \varepsilon_n$ satisfies

$$\sup_{P \in \mathcal{P}} P(H(P, \hat{P}) > 4t\varepsilon_n) \leq Ce^{-t^2}, \quad \forall t \geq 1.$$

Consequently, $\sup_{P \in \mathcal{P}} \mathbb{E}[H^2(P, \hat{P})] = O(\varepsilon_n^2)$.

Pf. Since $\{P_1, \dots, P_N\}$ is an ε -covering, WLOG assume that $H(P, P_1) \leq \varepsilon$.

For $\delta = 4\varepsilon$ and $t \geq 1$,

$$\begin{aligned} \{H(\hat{P}, P_1) \geq t\delta\} &= \{H(P_{i^*}, P_1) \geq t\delta\} \\ &\leq \{\max\{\psi_{i^*}, \psi_1\} \geq t\delta\} \quad \left(\begin{array}{l} \text{one of } T_{1i^*} \\ \text{and } T_{i^*1} \text{ must be one} \end{array} \right) \\ &= \{\psi_1 \geq t\delta\} \quad (\psi_{i^*} \leq \psi_1) \\ &\leq \bigcup_{j: H(P_1, P_j) \geq t\delta} \{T_{1j} = 1\}. \end{aligned}$$

By a union bound,

$$P(H(\hat{P}, P_1) \geq t\delta) \leq N \cdot e^{-\frac{n}{8}(t\delta)^2} = N_H(\mathcal{P}, \varepsilon) e^{-2nt^2\varepsilon^2}.$$

Since $n\varepsilon^2 \geq \max\{1, \log N_H(\mathcal{P}, \varepsilon)\}$, this probability is at most $O(e^{-t^2})$.

Finally, $P(H(\hat{P}, P) \geq t\delta) \leq P(H(\hat{P}, P_1) \geq t\delta - \varepsilon)$. ②

Remark, ① \hat{P} is proper, i.e. $\hat{P} \in \mathcal{P}$.

② A high-probability upper bound on $H(\hat{P}, P)$ is established above.

Refinement via local entropy

It turns out that the global entropy $\log N_H(\mathcal{P}, \varepsilon)$ can be improved to a local entropy $\log N_{loc}(\mathcal{P}, \varepsilon)$, with

$$N_{loc}(\mathcal{P}, \varepsilon) = \sup_{P \in \mathcal{P}} \sup_{\eta \geq \varepsilon} N_H(B_H(P, \eta) \cap \mathcal{P}, \frac{\eta}{2}).$$

(In other words, we are using balls of radius $\frac{\eta}{2}$ to cover balls of radius η)

Example. For many d -dimensional family \mathcal{P} , we usually have

$$\log N_H(\mathcal{P}, \varepsilon) \asymp d \log \frac{1}{\varepsilon}, \quad \log N_{loc}(\mathcal{P}, \varepsilon) \asymp d.$$

Therefore, using local entropy improves the Hoeffding result from $O(\frac{d \log n}{\varepsilon})$ to $O(\frac{d}{\varepsilon})$.

Thm. The same guarantee holds for Le Cam-Birgé pairwise comparison estimator, with N_H replaced by N_{loc} .

Pf. Let $2^l \leq t < 2^{l+1}$. We decompose $\{j \in [N] : H(P_i, P_j) \geq t\delta\} \subseteq \bigcup_{k \geq l} A_k$, where

$$A_k = \{j \in [N] : 2^k \delta \leq H(P_i, P_j) < 2^{k+1} \delta\}.$$

By union bound,

$$\begin{aligned} P(H(\hat{P}, P_i) \geq t\delta) &\leq P(\psi_i \geq t\delta) \\ &\leq \sum_{k \geq l} P(2^k \delta \leq \psi_i < 2^{k+1} \delta) \\ &\leq \sum_{k \geq l} |A_k| e^{-\frac{n}{8}(2^k \delta)^2}. \end{aligned}$$

To upper bound $|A_k|$, since $\{P_1, \dots, P_N\}$ is an ε -packing,

$$|A_k| \leq M(\{P \in \mathcal{P} : 2^k \delta \leq H(P_i, P) < 2^{k+1} \delta\}, \varepsilon)$$

$$\leq M(B_H(P_i, 2^{k+1} \delta) \cap \mathcal{P}, \varepsilon)$$

$$\leq N(B_H(P_i, 2^{k+1} \delta) \cap \mathcal{P}, \frac{\varepsilon}{2})$$

$$\leq N_{loc}(\mathcal{P}, \varepsilon)^{k+3}$$

(see lemma below)

$$\begin{aligned} \Rightarrow P(H(\hat{P}, P_i) \geq t\delta) &\leq \sum_{k \geq l} e^{(k+3) \log N_{loc}(\mathcal{P}, \varepsilon) - 2n\varepsilon^2 4^k} \leq e^{-\Omega(4^l)} = e^{-\Omega(t^2)}. \\ &\quad \uparrow \\ &\quad n\varepsilon^2 \geq \max\{1, \log N_{loc}(\mathcal{P}, \varepsilon)\}. \end{aligned}$$

Lemma. For $\eta \geq \varepsilon$, $N_H(B_H(P, 2^k \eta) \cap \mathcal{P}, \frac{\eta}{2}) \leq N_{loc}(P, \varepsilon)^k$.

Pf. Induction on k . Base case $k=0$ is the definition of $N_{loc}(P, \varepsilon)$.

For the inductive step, first cover $B_H(P, 2^k \eta) \cap \mathcal{P}$ using balls of radius $2^{k-1} \eta$.

then cover each ball using small balls of radius $\frac{\eta}{2}$.

$$\Rightarrow N_K \leq N_{k-1} \cdot N_0 \leq N_{loc}(P, \varepsilon)^{k-1} \cdot N_{loc}(P, \varepsilon) = N_{loc}(P, \varepsilon)^k. \quad \square$$

Special Topic: Guest lecture by J. Qian on his recent work on
high-probability density estimation under KL.