>>> Distribution Learning

Name: Alkis Kalavasis

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Density estimation or distribution learning is the following task: given data generated from an unknown target probability distribution f^* from a known class \mathcal{F} , design/compute \hat{f} that is close to f^* .

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Example: \mathcal{F} = Gaussian in d dimensions, $f^\star = \mathcal{N}(0,\mathrm{I})$.

- * Evaluation: Sample Complexity and Computational Complexity
- * Data generated i.i.d. from f^\star
- * Our measure of closeness is the Total Variation distance

>>> TV Distance

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$$d_{TV}(P,Q) = \max_{S \in \mathcal{A}} |P(S) - Q(S)|$$

>>> Learning Distributions

If \widehat{f} is a density estimate from m samples, we define the risk of the estimator with respect to the class ${\cal F}$ as

$$\mathcal{R}_m(\widehat{f}, \mathcal{F}) = \sup_{f \in \mathcal{F}} \mathbb{E}[d_{TV}(\widehat{f}, f)]$$

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The analogue of the optimal sample complexity is the minimax risk of the class $\ensuremath{\mathcal{F}}$

$$\mathcal{R}_m(\mathcal{F}) = \inf_{\widehat{f}} \sup_{f \in \mathcal{F}} \mathbb{E}[d_{TV}(\widehat{f}, f)]$$

>>> Learning Discrete Distributions over X = [n]

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Problem: Given access to i.i.d. samples from the unknown $p \in \mathcal{F}$, output a hypothesis q s.t. $d_{TV}(p,q) < \epsilon$ w.p. $1 - \delta$. Fact: $\Theta(\frac{n + \log(1/\delta)}{\epsilon^2})$ (or $R_m(\mathcal{F}) = \sqrt{n/m}$).

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where $X_i \sim \operatorname{Be}(p(S))$ (i.i.d.)

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- * Step 3: U.B.: $\Pr[\exists S \subset [n] : \hat{p}(S) p(S) > \epsilon] \le 2^n \exp(-2\epsilon^2 m) \le \delta.$

>>> Continuous Case

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Focus on structured distribution families, e.g., parametric families.

>>> Univariate Gaussian: MLE

 $x \sim \mathcal{N}(\mu, \sigma^2)$



>>> Univariate Case

How many parameters? Can we accurately estimate them?

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How many parameters? Can we accurately estimate them? N samples from $\mathcal{N}(\mu,\sigma^2)$

Empirical mean

$$\hat{\mu} = \frac{1}{N} \sum_{i=1}^{N} x_i \to \mu$$

Empirical variance

$$\frac{1}{N}\sum_{i=1}^{N}(x_i-\hat{\mu})^2\to\sigma^2$$

 $x_1, ..., x_N \sim \mathcal{N}(\mu, \sigma^2)^{\otimes N}$

$$\begin{aligned} x_1, ..., x_N &\sim \mathcal{N}(\mu, \sigma^2)^{\otimes N} \\ \mathcal{L}(x_1, ..., x_N | \mu, \sigma^2) &= \prod_{i \in [N]} \mathcal{N}(x_i | \mu, \sigma^2) = \end{aligned}$$

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Optimize the negative log-likelihood over the space of parameters $(\mu,\sigma).$

>>> KL divergence and MLE

 θ^* true parameters, θ guess.

$$\mathrm{KL}(\mathcal{D}_{\theta^*}, \mathcal{D}_{\theta}) = \mathbb{E}_{x \sim \mathcal{D}_{\theta^*}} \left[\log \left(\frac{\mathcal{D}_{\theta^*}(x)}{\mathcal{D}_{\theta}(x)} \right) \right]$$

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$$\begin{split} \mathtt{KL}(\mathcal{D}_{\theta^*},\mathcal{D}_{\theta}) &= \mathbb{E}_{x\sim\mathcal{D}_{\theta^*}}\left[\log\left(\frac{\mathcal{D}_{\theta^*}(x)}{\mathcal{D}_{\theta}(x)}\right)\right]\\ \mathtt{L}(\mathcal{D}_{\theta^*},\mathcal{D}_{\theta}) &= \Theta(1) - \mathbb{E}_{\theta^*}[\log(\mathcal{D}_{\theta})]\\ \mathtt{stimate} \ \mathbb{E}_{x\sim\mathcal{D}_{\theta^*}}[h(x)] \ \mathtt{with} \ \frac{1}{N}\sum_{i\in[N]}h(x_i) \end{split}$$

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$$\min_{\theta \in \Theta} \widehat{\mathrm{KL}}(\mathcal{D}_{\theta^*}, \mathcal{D}_{\theta}) = \min_{\theta \in \Theta} -\frac{1}{N} \sum_{i=1}^N \log(\mathcal{D}_{\theta}(x_i)) = \max_{\theta \in \Theta} \prod_{i=1}^N \mathcal{D}_{\theta}(x_i)$$





>>> Gaussian density estimation

* d-dimensional Gaussian $\mathcal{N}(\mu, \Sigma)$, $\mu_{d \times 1}, \Sigma_{d \times d}$:

$$\mathcal{N}(\mu, \Sigma)(x) = \frac{1}{\sqrt{(2\pi)^d \mathtt{det}(\Sigma)}} \exp(-\frac{1}{2}(x-\mu)^\top \Sigma^{-1}(x-\mu)) \,.$$

* Ellipsoid: $\{x: (x-v)^{ op}A(x-v)=1\}$ where $A\succeq 0$

 \mathcal{N}_d using $O(d^2/\epsilon^2), ilde{\Omega}(d^2/\epsilon^2)$ samples.

>>> Gaussian Upper Bound via Yatracos Class

For a class ${\mathcal F}$ of functions from ${\mathbb X}$ to ${\mathbb R},$ the Yatracos class of ${\mathcal F}$ is

$$\mathcal{Y}(\mathcal{F}) = \left\{ \left\{ x \in \mathbb{X} : f_1(x) \ge f_2(x) \right\} : f_1, f_2 \in \mathcal{F} \right\}.$$

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Exercise: $d_{TV}(f_1, f_2) = ||f_1 - f_2||_{\mathcal{Y}(\mathcal{F})}$

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Exercise: $d_{TV}(f_1, f_2) = \|f_1 - f_2\|_{\mathcal{Y}(\mathcal{F})}$

(1) For any class \mathcal{F} , the sample complexity of learning \mathcal{F} is $O(\frac{\operatorname{VCdim}(\mathcal{Y}(\mathcal{F}) + \log(1/\delta))}{\epsilon^2})$. (2) Let G be a vector space of real-valued functions. Then $\operatorname{VCdim}(\{x: f(x) > 0\} : f \in G\}) \leq \dim(G)$.

Proof: $\mathcal{Y}(\mathcal{N}_d) = \{\{x : \mathcal{N}(\mu_1, \Sigma_1)(x) \ge \mathcal{N}(\mu_2, \Sigma_2)(x)\} : \mu_i, \Sigma_i\}$ and so is contained in the space $\{\{x^\top Ax + b^\top x + c > 0\} : A, b, c\}$ whose dimension is $O(d^2)$.

We assume that there is a hidden central ranking $\pi_0 \in \mathbb{S}_n$ and we define a notion of distance between permutations:

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 $d_{KT}(123, 213) = 1$ $d_{KT}(123, 312) = 2$ $d_{KT}(\pi, \pi^{-1}) = \binom{n}{2}$

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 $\Pr[\pi|\pi_0,\beta] \propto \exp(-\beta \cdot d_{KT}(\pi,\pi_0))$

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Sampling from a Mallows model, can we learn the true target ranking π_0 ?

Learning with probability at least $1-\epsilon$ using

Learning with probability at least $1 - \epsilon$ using $\Theta(\log(n/\epsilon))$ samples. In each sample, either $i \succ j$ or $j \succ i$ ______

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Count for each ordered pair i,j, the votes n_{ij} and n_{ji}

If $i \succ_{\pi_0} j$, we expect $n_{ij} - n_{ji} > 0$ due to the Mallows model Hoeffding and U.B. over $\binom{n}{2}$ pairs.

>>> Learning Coarse Gaussians

Consider a mixture of partitions π over \mathbb{R}^d and an unknown target mean μ^{\star} .

- 1. Draw a partition $\mathcal{S} \sim \pi$
- 2. Draw $x \sim \mathcal{N}(\mu^{\star}, I)$
- 3. Output the unique set $S \in \mathcal{S}$ that contains x (with distribution \mathcal{N}_{π})

Can we learn the true mean from i.i.d. samples from $\mathcal{N}_{\pi}?$

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If S is convex then the Brascamp-Lieb Inequality implies that the negative log-likelihood is convex! Beyond convexity?

>>> Ising Model and RBMs

J symmetric matrix, h external field

$$\Pr[X = x] = \frac{1}{Z} \exp(\frac{1}{2} \sum_{i,j} J_{ij} x_i x_j + \sum_i h_i x_i)$$

Ising models with hidden variables Y

$$\Pr[X = x, Y = y] \frac{1}{Z} \exp(x^{\top} Jy + \sum_{i \in [n]} h_i^1 x_i + \sum_{j \in [m]} h_j^2 y_j)$$

Ferromagnetic: $J_{ij} \ge 0, h_i^1, h_j^2 \ge 0$ How many samples from RBM to learn the structure of the bipartite graph?

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Submodular: For $S \subseteq T$

$$I_i(S \cup \{j\}) - I_i(S) \ge I_i(T \cup \{j\}) - I_i(T)$$

>>> The Algorithm

Greedy Neighborhood for i

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- 1. Set $S_0 = \emptyset$
- 2. For $t = 1, ..., d_2$: 2.1 Let $j_{t+1} = \operatorname{argmax} I_i(S_t \cup \{j\})$
 - **2.2** $S_{t+1} = S_t \cup \{j_{t+1}\}$

3. Find two-hop neighborhood $j \in S_k$ Number of samples: $\operatorname{poly}(d_2) \cdot \log(n)$