Permutation Mixtures and Empirical Bayes

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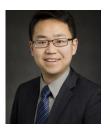


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Setup

Let P_1, \ldots, P_n be *n* probability distributions over the same space.

A permutation mixture \mathbb{P}_n :

- \rightarrow draw independent $Z_1 \sim P_1, \dots, Z_n \sim P_n$;
- \rightarrow draw a uniformly random permutation $\pi \sim \mathsf{Unif}(S_n)$;
- $\to \mathbb{P}_n$ is the joint distribution of (X_1,\ldots,X_n) with $X_i=Z_{\pi(i)}$;
- → in mathematical terms:

$$(X_1, \cdots, X_n) \sim \mathbb{E}_{\pi \sim \mathsf{Unif}(S_n)} \left[\bigotimes_{i=1}^n P_{\pi(i)} \right] \quad \mathsf{under} \ \mathbb{P}_n.$$

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An i.i.d. (mean-field) approximation \mathbb{Q}_n :

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 under \mathbb{Q}_n .

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Target of this work

Show that the i.i.d. approximation \mathbb{Q}_n to \mathbb{P}_n is accurate, i.e. the information divergence (or statistical distance) between \mathbb{P}_n and \mathbb{Q}_n is small (and ideally, independent of n)

Motivation

Later in the talk:

- ightarrow statistical and IT applications involving random permutations
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- → statistical and IT applications involving random permutations
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Bigger picture:

- → general mean-field approximation
- → information geometry of high-dimensional mixtures

A toy example

Let
$$P_1 = \cdots = P_{n/2} = \mathcal{N}(\mu, 1)$$
 and $P_{n/2+1} = \cdots = P_n = \mathcal{N}(-\mu, 1)$

- $\to \mathbb{P}_n = \nu_{\mathbb{P}} \star \mathcal{N}(0, I_n)$, where $\nu_{\mathbb{P}}$ is the distribution of n uniformly random draws from the multiset $\{-\mu, \dots, -\mu, \mu, \dots, \mu\}$ without replacement;
- $\rightarrow \mathbb{Q}_n = \nu_{\mathbb{Q}} \star \mathcal{N}(0, I_n)$, where $\nu_{\mathbb{Q}}$ is the counterpart with replacement;

$$\chi^{2}(P||Q) := \sum_{x} \frac{(p_{x} - q_{x})^{2}}{q_{x}}$$

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Our result

$$\chi^{2}(\mathbb{P}_{n}||\mathbb{Q}_{n}) = \begin{cases} O(\mu^{4}) & \text{if } \mu \leq 1, \\ O(\exp(\mu^{2})) & \text{if } \mu > 1. \end{cases}$$

- $\rightarrow \chi^2$ -divergence independent of dimension n
- \rightarrow smaller than the one-dimensional divergence $\chi^2(\mathcal{N}(\mu,1)||\mathcal{N}(-\mu,1))$
- ightarrow existing approaches fail even for this toy example

$$\chi^2(P||Q) := \sum_{x} \frac{(p_x - q_x)^2}{q_x}$$

Failure of method of moments

A powerful approach to upper bound the statistical difference between two mixtures distributions, with many recent applications [Cai and Low'11, Hardt and Price'15, Wu and Yang'20, Han et al.'20, ...]

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Idea: express the Gaussian likelihood ratio in terms of Hermite polynomials

$$\frac{\varphi(x-\theta)}{\varphi(x)} = \sum_{k=0}^{\infty} \frac{H_k(x)}{k!} \theta^k,$$

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Idea: express the Gaussian likelihood ratio in terms of Hermite polynomials

$$\frac{\varphi(x-\theta)}{\varphi(x)} = \sum_{k=0}^{\infty} \frac{H_k(x)}{k!} \theta^k,$$

so that

$$\begin{aligned} \mathsf{TV}(\mu \star \mathcal{N}(0,1), \nu \star \mathcal{N}(0,1))^2 &= \frac{1}{4} \left(\mathbb{E}_{Z \sim \mathcal{N}(0,1)} \left| \mathbb{E}_{U \sim \mu} \left[\frac{\varphi(Z - U)}{\varphi(Z)} \right] - \mathbb{E}_{V \sim \nu} \left[\frac{\varphi(Z - V)}{\varphi(Z)} \right] \right| \right)^2 \\ &= \frac{1}{4} \left(\mathbb{E}_{Z \sim \mathcal{N}(0,1)} \left| \sum_{k=0}^{\infty} \frac{H_k(Z)}{k!} \left(\mathbb{E}_{U \sim \mu} [U^k] - \mathbb{E}_{V \sim \nu} [V^k] \right) \right| \right)^2 \\ &\stackrel{\mathsf{C.S}}{\leq} \frac{1}{4} \mathbb{E}_{Z \sim \mathcal{N}(0,1)} \left(\sum_{k=0}^{\infty} \frac{H_k(Z)}{k!} \left(\mathbb{E}_{U \sim \mu} [U^k] - \mathbb{E}_{V \sim \nu} [V^k] \right) \right)^2 \\ &= \frac{1}{4} \sum_{k=0}^{\infty} \frac{\left(\mathbb{E}_{U \sim \mu} [U^k] - \mathbb{E}_{V \sim \nu} [V^k] \right)^2}{k!} \end{aligned}$$

$$\mathsf{TV}(P,Q) := \frac{1}{2} \sum_{x} |p_x - q_x|$$

Failure of method of moments (cont'd)

In general dimensions:

$$\mathsf{TV}(\nu_{\mathbb{P}} \star \mathcal{N}(0, I_n) \| \nu_{\mathbb{Q}} \star \mathcal{N}(0, I_n))^2 \leq \frac{1}{4} \sum_{\vec{\alpha} \in \mathbb{N}^n} \frac{(m_{\vec{\alpha}}(\nu_{\mathbb{P}}) - m_{\vec{\alpha}}(\nu_{\mathbb{Q}}))^2}{\vec{\alpha}!}$$

- $\rightarrow \vec{\alpha} = (\alpha_1, \dots, \alpha_n)$ is a multi-index, with $\vec{\alpha}! := \alpha_1! \cdots \alpha_n!$
- $o m_{\vec{lpha}}(\mu) := \mathbb{E}_{\vartheta \sim \mu}[\vartheta_1^{lpha_1} \cdots \vartheta_n^{lpha_n}]$ denotes the joint moment

Failure of method of moments (cont'd)

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Application to our toy example:

- \rightarrow non-zero moment difference starting from $|\vec{\alpha}|=2$, suggesting an $O(\mu^4)$ dependence
- \rightarrow however, too many cross terms in high dimensions: the total contributions of $|\vec{\alpha}|=2\ell$ are at least $\Omega_\ell(\mu^{4\ell}n^{\ell-1})$, which is growing with n for $\ell\geq 2$

Failure of method of cumulants

A recent development based on cumulants [Schramm and Wein'22]:

$$\chi^2(\nu_{\mathbb{P}}\star\mathcal{N}(0,I_n)\|\nu_{\mathbb{Q}}\star\mathcal{N}(0,I_n))\leq \sum_{\vec{x}\in\mathbb{N}^d}\frac{\kappa_{\vec{\alpha}}^2}{\vec{\alpha}!},$$

where $\kappa_{\vec{\alpha}}$ is the joint cumulant

$$\kappa_{\vec{\alpha}} = \kappa_{\nu_{\mathbb{Q}}} \left(\frac{\mathrm{d}\nu_{\mathbb{P}}}{\mathrm{d}\nu_{\mathbb{Q}}}, \vartheta_{1}, \dots, \vartheta_{1}, \vartheta_{2}, \dots, \vartheta_{2}, \dots, \vartheta_{n} \right).$$

$$\kappa(X_1,\ldots,X_n):= \tfrac{\partial^n}{\partial t_1\cdots\partial t_n}\big|_{t_1=\cdots=t_n=0}\log\mathbb{E}\left[\exp\left(\sum_{i=1}^n t_iX_i\right)\right]$$

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- → a better behavior for certain cross terms
- \to however, can show that $\kappa_{(1,\ell,0,\dots,0)} \asymp \mathcal{C}^\ell \ell!$ for odd ℓ , so summing along this subsequence gives a diverging result

Main result

Let $P_1, \ldots, P_n \in \mathcal{P}$. Define the following dimension-independent quantities:

Definition (Quantities of \mathcal{P})

- $\to \chi^2$ channel capacity: $C_{\chi^2}(\mathcal{P}) = \sup_{\rho \in \Delta(\mathcal{P})} I_{\chi^2}(P;X)$, with $P \sim \rho$ and $X \sim P$
- $\rightarrow \ \chi^2 \ \mathsf{diameter} \colon \ \mathsf{D}_{\chi^2}(\mathcal{P}) = \mathsf{sup}_{P_1,P_2 \in \mathcal{P}} \ \chi^2(P_1 \| P_2)$

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- $\rightarrow \chi^2$ diameter: $D_{\chi^2}(\mathcal{P}) = \sup_{P_1, P_2 \in \mathcal{P}} \chi^2(P_1 || P_2)$

Theorem (H., Niles-Weed'24)

$$\chi^2(\mathbb{P}_n \| \mathbb{Q}_n) \leq \min \left\{ 10 \sum_{\ell=2}^n \mathsf{C}_{\chi^2}(\mathcal{P})^\ell, (1 + \mathsf{D}_{\chi^2}(\mathcal{P}))^{1 + \mathsf{C}_{\chi^2}(\mathcal{P})} - 1 \right\}$$

- $\to \mathbb{P}_n$ is contiguous to \mathbb{Q}_n : $\chi^2(\mathbb{P}_n||\mathbb{Q}_n) = \mathcal{O}_{\mathcal{P}}(1)$ if $\mathsf{D}_{\chi^2}(\mathcal{P}) < \infty$
- \rightarrow high-probability events under the simpler product measure \mathbb{Q}_n translate to high-probability events under the mixture \mathbb{P}_n

$$I_{\chi^2}(X;Y) := \chi^2(P_{XY} || P_X P_Y)$$

Examples

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Example I (Two-component Gaussian)

$$\mathcal{P} = \{\mathcal{N}(\mu, 1), \mathcal{N}(-\mu, 1)\} \colon \mathsf{C}_{\chi^2}(\mathcal{P}) \le 1 - \mathsf{e}^{-\mu^2}, \text{ so}$$

$$\chi^2(\mathbb{P}_n || \mathbb{Q}_n) = \begin{cases} O(\mu^4) & \text{if } \mu \le 1, \\ O(\mathsf{exp}(\mu^2)) & \text{if } \mu > 1. \end{cases}$$

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Example II (Bounded Gaussian)

$$\mathcal{P} = \{\mathcal{N}(\theta,1) : |\theta| \le \mu\}\}: \ \mathsf{C}_{\chi^2}(\mathcal{P}) = O(\mu \wedge \mu^2), \mathsf{D}_{\chi^2}(\mathcal{P}) = \mathsf{exp}(O(\mu^2)), \ \mathsf{so}$$

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Applications

Permutation prior

Sequence model in statistics: observe $X_i \sim P_{\theta_i}$ with unknown $\theta = (\theta_1, \dots, \theta_n)$

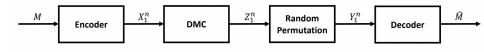
- \rightarrow statisticians would like to prove lower bounds on the estimation error of θ
- \to a prevalent strategy is to impose a prior distribution on θ , and a permutation prior is sometimes preferred: $\theta = (v_{\pi(1)}, \dots, v_{\pi(n)})$ for a known vector v and a random permutation π
- \rightarrow a key quantity in the analysis: mutual information $I(\theta; X^n)$

Our result: can pretend as if the coordinates $\theta_i \sim \frac{1}{n} \sum_{j=1}^n \delta_{v_j}$ are i.i.d.

Mutual information under a permutation prior

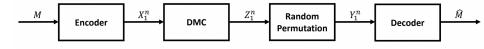
$$I_{\mathbb{Q}_n}(\theta;X^n) - \mathcal{O}_{\mathcal{P}}(1) \leq I_{\mathbb{P}_n}(\theta;X^n) \leq I_{\mathbb{Q}_n}(\theta;X^n)$$

Permutation channel



The noisy permutation channel introduced in [Makur'20]

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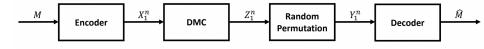


The noisy permutation channel introduced in [Makur'20]

- \rightarrow target: find the channel capacity $C_n(\mathcal{P}) = \max_{p(x^n)} I(X^n; Y^n)$
- → known achievability [Makur'20] and converse [Tang and Polyanskiy'23]:

$$C_n(\mathcal{P}) \sim \frac{\mathrm{rank}(P_{Z|X}) - 1}{2} \log n \quad \text{for discrete \mathcal{P}}.$$

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Our result: for general P, can pretend as if Y^n have independent coordinates

Converse for general permutation channels

$$C_n(\mathcal{P}) \leq \operatorname{Red}(\operatorname{conv}(\mathcal{P})^{\otimes n}) + \mathcal{O}_{\mathcal{P}}(1)$$

finite de Finetti theorems

Theorem (de Finetti)

Any exchangeable distribution $P_{X^{\infty}}$ can be written as an i.i.d. mixture:

$$P_{X^{\infty}}(x^{\infty}) = \mathbb{E}_{\theta} \left[\prod_{i=1}^{\infty} Q_{\theta}(x_i) \right].$$

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Approximately holds for exchangeable distribution P_{X^n} with finite n:

- \rightarrow [Diaconis and Freedman'80]: $\mathsf{KL}(P_{X^k} \| \mathbb{E}_{\theta}[Q_{\theta}^{\otimes k}]) \lesssim \frac{k^2}{n}$
 - o [Stam'78]: for small $|\mathcal{X}|$, $\mathsf{KL}(P_{X^k}\|\mathbb{E}_{\theta}[Q_{ heta}^{\otimes k}])\lesssim rac{|\mathcal{X}|k^2}{n(n+1-k)}$
- \rightarrow some recent refinements in [Gavalakis and Kontoyiannis'21; Johnson, Gavalakis, and Kontoyiannis'24]

Our extensions

Using the first upper bound and $C_{\chi^2}(\mathcal{P}) \leq |\mathcal{X}|$:

χ^2 -type finite de Finetti

For exchangeable distribution P_{X^n} and $k \leq n$:

$$\chi^2\left(P_{X^k}\|\mathbb{E}_{\theta}[Q_{\theta}^{\otimes k}]\right)\lesssim \frac{k^2|\mathcal{X}|^2}{n^2}\quad \text{if } k<\frac{n}{|\mathcal{X}|}.$$

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Using the second upper bound:

Noisy de Finetti

Let P_{Y^n} be the output distribution with an input exchangeable distribution P_{X^n} and a channel \mathcal{P} . Then for $k \leq n$:

$$\chi^2\left(P_{Y^k}\|\mathbb{E}_{\theta}[Q_{\theta}^{\otimes k}]\right) = \mathcal{O}_{\mathcal{P}}\left(\frac{k^2}{n^2}\right) \quad \text{if } \mathsf{D}_{\chi^2}(\mathcal{P}) < \infty.$$

Sketch of the first upper bound

Hermite basis:

$$\frac{\varphi(x-\theta)}{\varphi(x)} = \sum_{k=0}^{\infty} \frac{H_k(x)}{k!} \theta^k$$

where φ is the density of $\mathcal{N}(0,1)$.

$$(\theta_1,\ldots,\theta_n)=(\mu,\ldots,\mu,-\mu,\ldots,-\mu).$$

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Hyperbolic basis?

$$\frac{\varphi(\mathbf{x}-\theta)}{\varphi_0(\mathbf{x})} = 1 + \tanh(\mu \mathbf{x}) \frac{\theta}{\mu}, \quad \theta \in \{\pm \mu\}$$

where $\varphi_0(x) = \frac{\varphi(x-\mu) + \varphi(x+\mu)}{2}$ is the common marginal distribution of \mathbb{P}_n and \mathbb{Q}_n

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 are orthogonal in $L^2(\varphi)$

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$$\mathbb{E}[\frac{\theta}{\mu}] = 0 \text{ for } \theta \sim \mathsf{Unif}(\{\pm \mu\})$$

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Toy example: a different basis

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 are orthogonal in $L^2(\varphi)$

 $\mathbb{E}[\theta^k]$ possibly non-zero for $\theta \sim \mathsf{Unif}(\{\pm \mu\})$

Under the new basis:

$$\frac{\mathrm{d}\mathbb{P}_n}{\mathrm{d}\mathbb{O}_n}(x^n) = \mathbb{E}_{\pi} \left[\prod_{i=1}^n \frac{\varphi(x_i - \theta_{\pi(i)})}{\varphi_0(x_i)} \right] = \mathbb{E}_{\pi} \left[\right]$$

Hyperbolic basis?

$$\frac{\varphi(\mathsf{x}-\theta)}{\varphi_0(\mathsf{x})} = 1 + \tanh(\mu\mathsf{x})\frac{\theta}{\mu}, \quad \theta \in \{\pm \mu\}$$

where $\varphi_0(x) = \frac{\varphi(x-\mu) + \varphi(x+\mu)}{2}$ is the common marginal distribution of \mathbb{P}_n and \mathbb{Q}_n

$$\{1, \tanh(\mu x)\}$$
 are orthogonal in $L^2(arphi_0)$

$$\mathbb{E}[rac{ heta}{\mu}] = \mathsf{0} \,\, \mathsf{for} \,\, heta \sim \mathsf{Unif}(\{\pm \mu\})$$

$$\frac{\mathrm{d}\mathbb{P}_n}{\mathrm{d}\mathbb{Q}_n}(\mathsf{x}^n) = \mathbb{E}_\pi \left[\prod_{i=1}^n \frac{\varphi(\mathsf{x}_i - \theta_{\pi(i)})}{\varphi_0(\mathsf{x}_i)} \right] = \mathbb{E}_\pi \left[\prod_{i=1}^n \left(1 + \tanh(\mu \mathsf{x}_i) \frac{\theta_{\pi(i)}}{\mu} \right) \right]$$

$$(\theta_1,\ldots,\theta_n)=(\mu,\ldots,\mu,-\mu,\ldots,-\mu).$$

Toy example: a different basis

Hermite basis:

$$\frac{\varphi(x-\theta)}{\varphi(x)} = \sum_{k=0}^{\infty} \frac{H_k(x)}{k!} \theta^k$$

where φ is the density of $\mathcal{N}(0,1)$.

$$\{H_0(x),H_1(x),\dots\}$$
 are orthogonal in $L^2(arphi)$

$$\mathrm{d}\mathbb{P}_n$$
 , n

$$\left[\prod_{i=1}^n \frac{\varphi(\mathsf{x}_i - \theta_{\pi(i)})}{\varphi_0(\mathsf{x}_i)}\right]$$

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$$\mathbb{E}[heta^k]$$
 possibly non-zero for $heta\sim \mathsf{Unif}(\{\pm\mu\})$ $\mathbb{E}[heta^\ell]=0$ for $heta\sim \mathsf{Unif}(\{\pm\mu\})$

e new basis:
$$\frac{\mathrm{d}\mathbb{P}_n}{\mathrm{d}\mathbb{Q}_n}(x^n) = \mathbb{E}_{\pi}\left[\prod_{i=1}^n \frac{\varphi(\mathsf{x}_i - \theta_{\pi(i)})}{\varphi_0(\mathsf{x}_i)}\right] = \mathbb{E}_{\pi}\left[\prod_{i=1}^n \left(1 + \tanh(\mu \mathsf{x}_i) \frac{\theta_{\pi(i)}}{\mu}\right)\right]$$

$$= \mathbb{E}_{\pi} \left[\prod_{i=1}^{n} \left(1 + \tanh(\mu x_i) \frac{x_i}{\mu} \right) \right]$$

$$= \sum_{S \subseteq [n]} \mathbb{E}_{\pi} \left[\prod_{i \in S} \frac{\theta_{\pi(i)}}{\mu} \right] \prod_{i \in S} \tanh(\mu x_i)$$

$$\frac{\mathrm{d}\mathbb{P}_n}{\mathrm{d}\mathbb{Q}_n}(x^n) = \sum_{S \subseteq [n]} \mathbb{E}_{\pi} \left[\prod_{i \in S} \frac{\theta_{\pi(i)}}{\mu} \right] \prod_{i \in S} \tanh(\mu x_i)$$

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$$\mathbb{E}_{\mathbb{Q}_n}\left[\left(\frac{\mathrm{d}\mathbb{P}_n}{\mathrm{d}\mathbb{Q}_n}\right)^2\right] = \sum_{S \subseteq [n]} \left(\mathbb{E}_{\pi}\left[\prod_{i \in S} \frac{\theta_{\pi(i)}}{\mu}\right]\right)^2 \mathsf{C}_{\chi^2}(\mathcal{P})^{|S|}$$

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 \rightarrow the inner expectation: for $|S| = \ell$,

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→ piecing everything together:

$$\chi^2(\mathbb{P}_n\|\mathbb{Q}_n) = \mathbb{E}_{\mathbb{Q}_n}\left[\left(\frac{\mathrm{d}\mathbb{P}_n}{\mathrm{d}\mathbb{Q}_n}\right)^2\right] - 1 \leq C_{\chi^2}(\mathcal{P})^2 + C_{\chi^2}(\mathcal{P})^4 + \dots + C_{\chi^2}(\mathcal{P})^n$$

Importance of zero-mean: a Maclaurin-type inequality

For a vector $x = (x_1, \dots, x_n)$, define the elementary symmetric polynomial

$$e_{\ell}(x) := \sum_{|S|=\ell} \prod_{i \in S} x_i$$

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Theorem (Upper bound on ESPs for centered vector)

Let $\sum_{i=1}^{n} x_i = 0$ and $\sum_{i=1}^{n} |x_i|^2 = n$.

- ightarrow If $x \in \mathbb{R}^n$, then $|e_\ell(x)|^2 \leq 10 \binom{n}{\ell}$;
- \rightarrow If $x \in \mathbb{C}^n$, a weaker upper bound holds:

$$|e_{\ell}(x)|^2 \leq \frac{n^n}{\ell^{\ell}(n-\ell)^{n-\ell}} < 3\sqrt{\ell+1}\binom{n}{\ell}.$$

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- → similar problems have been recently studied in [Gopalan and Yehudayoff'14; Meka, Reingold, and Tal'19; Doron, Hatami, and Hoza'20; Tao'23]
- → best known bound due to [Tao'23]:

$$|e_{\ell}(x)|^2 \le \binom{n}{\ell}^2 \left(\frac{\ell-1}{n-1}\right)^{\ell} \le e^{\ell} \binom{n}{\ell}$$

ightarrow we crucially need to improve the base e to the best possible constant 1

Proof of the inequality

For the real case, can argue via the method of Lagrangian multipliers that the maximizer x^* is only supported on two points, i.e. it suffices to consider $x = x^{(k)}$ for some k:

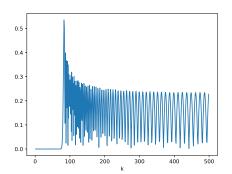
$$x^{(k)} = \left(\underbrace{\sqrt{\frac{k}{n-k}}, \dots, \sqrt{\frac{k}{n-k}}}_{n-k \text{ copies}}, \underbrace{-\sqrt{\frac{n-k}{k}}, \dots, -\sqrt{\frac{n-k}{k}}}_{k \text{ copies}}\right)$$

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However, upper bounding $|e_{\ell}(x^{(k)})|$ is still very challenging!!



The quantity $|e_{\ell}(x^{(k)})|^2/\binom{n}{\ell}$ vs. k for $n=1000, \ell=300$.

Saddle point analysis

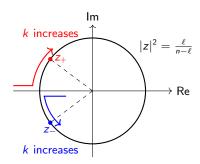
Cauchy's formula :
$$e_\ell(x) = \frac{1}{2\pi \mathrm{i}} \oint_{|z|=r} \frac{\prod_{i=1}^n (1+x_i z)}{z^\ell} \frac{\mathrm{d}z}{z}$$

Saddle point equation :
$$\frac{\ell}{z} = \sum_{i=1}^{n} \frac{x_i}{1 + x_i z}$$

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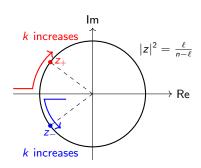


Saddle points for $x = x^{(k)}$

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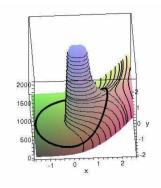


Illustration of saddle point method

Application of saddle point method

Saddle points suggest the contour choice of $\Gamma = \{z : |z| = r\}$ with $r = \sqrt{\frac{\ell}{n-\ell}}$:

$$|e_{\ell}(x)| = \left| \frac{1}{2\pi i} \oint_{\Gamma} \frac{\prod_{i=1}^{n} (1 + x_i z)}{z^{\ell}} \frac{\mathrm{d}z}{z} \right| \leq \max_{|z|=r} \left| \frac{\prod_{i=1}^{n} (1 + x_i z)}{z^{\ell}} \right|$$

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Use AM-GM:

$$\prod_{i=1}^{n} |1 + x_i z|^2 = \prod_{i=1}^{n} (1 + 2\Re(x_i z) + |x_i|^2 r^2)$$

$$\leq \left(\frac{1}{n} \sum_{i=1}^{n} (1 + 2\Re(x_i z) + |x_i|^2 r^2)\right)^n = (1 + r^2)^n.$$

This proves the inequality for the complex case.

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This proves the inequality for the complex case.

Real case: a more careful saddle point analysis for $x = x^{(k)}$.

Compound decisions in empirical Bayes

Empirical Bayes

The empirical Bayes framework [Robbins'51; '56]:

- ightarrow idea: estimate the prior distribution from data
- → lots of empirical successes but limited theoretical understanding

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A new theoretical paradigm [Hannan and Robbins'55; Greenshtein and Ritov'09]:

- \rightarrow compound decision setting: independent $X_i \sim P_{\theta_i}$, aim to estimate $\theta = (\theta_1, \dots, \theta_n)$
- → target: find an estimator with a small regret compared with powerful oracles

$$\operatorname{regret}(\widehat{\theta}) = \mathbb{E}_{\theta}[L(\theta, \widehat{\theta})] - \inf_{\widehat{\theta} \text{ oracle}} \mathbb{E}_{\theta}[L(\theta, \widehat{\theta}^{\text{oracle}})]$$

- ightarrow simple/separable oracle: $\widehat{\theta}_i^{\mathrm{S}} = f(X_i)$ for a single function f
- → permutation invariant oracle:

$$\widehat{ heta}_{\pi(i)}^{\mathrm{PI}}(X_{\pi(1)},\ldots,X_{\pi(n)}) = \widehat{ heta}_{i}^{\mathrm{PI}}(X_{1},\ldots,X_{n})$$

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Question

Do these oracles have similar estimation power?

The Gaussian case

- \rightarrow observation vector: $X^n \sim \mathcal{N}(\theta^n, I_n)$
- \rightarrow the oracle only knows the multiset $\{\theta_1,\ldots,\theta_n\}$ but not the order
- \rightarrow equivalently, θ^n follows a permutation prior on a given multiset
- → under the quadratic loss:

$$\widehat{\theta}_i^{\mathrm{S}} = \mathbb{E}[\theta_i \mid X_i], \qquad \widehat{\theta}_i^{\mathrm{PI}} = \mathbb{E}[\theta_i \mid X^n].$$

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Greenshtein and Ritov (2009)

If $|\theta_i| \leq \mu$ for all $i \in [n]$ and $\mu \geq 1$,

$$\mathbb{E}\left[\|\widehat{\theta}^{\mathrm{S}}-\widehat{\theta}^{\mathrm{PI}}\|^2\right]=e^{\textit{O}(\mu^2)}.$$

- \rightarrow an O(1) upper bound even if the vectors are *n*-dimensional
- \rightarrow can the dependence on μ be improved for large μ ?

A tight upper bound

Theorem

If
$$|\theta_i| \leq \mu$$
 for all $i \in [n]$ and $\mu \geq 1$,

$$\mathbb{E}\left[\left\|\widehat{\theta}^{\mathrm{S}}-\widehat{\theta}^{\mathrm{PI}}\right\|^{2}
ight]=O(\mu\log^{2}n).$$

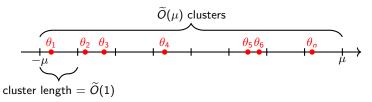
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The quantity μ represents the number of "clusters":



- $\,\rightarrow\,$ by the concentration of Gaussian, each cluster roughly corresponds to an independent subproblem
- ightarrow linear dependence on the # of clusters is tight by adding up all clusters

Application: Competitive Distribution Estimation

Competitive distribution estimation

A Poisson sequence model:

$$(N_1,\ldots,N_k)\sim \mathsf{Poi}(np_1)\otimes\cdots\otimes\mathsf{Poi}(np_k)$$

 \rightarrow n: sample size

 \rightarrow k: support size

ightarrow $p=(p_1,\ldots,p_k)$: an unknown probability vector

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- $\rightarrow p = (p_1, \dots, p_k)$: an unknown probability vector

Target of competitive distribution estimation: based on observed counts (N_1, \ldots, N_k) , devise an estimator $\hat{\rho}$ to minimize the expected regret:

$$\operatorname{regret}(\widehat{\rho}; \rho) = \mathbb{E}\left[\operatorname{KL}(\rho\|\widehat{\rho}) - \operatorname{KL}(\rho\|\widehat{\rho}^{\operatorname{PI}})\right],$$

where

$$\widehat{p}^{\mathsf{PI}} = \underset{\widehat{q}}{\mathsf{argmin}} \max_{p': \{p'\} = \{p\}} \mathbb{E}[\mathsf{KL}(p'\|\widehat{q})]$$

is the best "oracle" $\widehat{q} = \widehat{q}(N^k)$ that knows p up to permutation

"Why is Good-Turing Good"

Upper bound ([Orlitsky and Suresh'15])

A modified Good–Turing estimator $\widehat{p}^{\mathrm{MGT}}$ achieves

$$\sup_{p} \operatorname{regret}(\widehat{\rho}^{\operatorname{MGT}}; p) = \widetilde{O}\left(\min\left\{\frac{k}{n}, \frac{1}{\sqrt{n}}\right\}\right).$$

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The Good–Turing estimator \hat{p}^{GT} [Good'53]: for $N_i = y$,

$$\widehat{\rho}_i^{\mathrm{GT}} = \frac{y+1}{n} \cdot \frac{\sum_{j=1}^k \mathbb{1}(N_j = y+1)}{\sum_{j=1}^k \mathbb{1}(N_j = y)}$$

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Lower bound ([Orlitsky and Suresh'15])

$$\inf_{\widehat{p}}\sup_{p}\operatorname{regret}(\widehat{p};p)=\widetilde{O}\left(\min\left\{\frac{k}{n},\frac{1}{n^{2/3}}\right\}\right).$$

Better Good-Turing: NPMLE

A different idea based on so-called "g-modeling" [Efron'14]:

- \to think of $p_1,\ldots,p_k\stackrel{\mathrm{i.i.d.}}{\sim} G^\star$, with the empirical measure $G^\star=\frac{1}{k}\sum_{i=1}^k \delta_{p_i}$
- $\rightarrow\,$ a natural estimator is the nonparametric MLE (NPMLE):

$$\widehat{G} = \underset{G: \ \mathbb{E}_G[\rho] \leq \frac{1}{k}}{\operatorname{argmax}} \sum_{i=1}^k \log \mathbb{E}_G \left[\mathbb{P}(\operatorname{Poi}(np) = N_i) \right]$$

 \rightarrow the final estimator $\widehat{p}^{\mathrm{NPMLE}}$ mimics the separable oracle:

$$\widehat{\rho}^{\mathrm{NPMLE}} = \text{normalized version of } \big(\mathbb{E}_{\widehat{G}}[p_1 \mid \textit{N}_1], \dots, \mathbb{E}_{\widehat{G}}[p_k \mid \textit{N}_k] \big)$$

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Theorem (H., Niles-Weed, Shen, Wu, 24+)

The above estimator $\widehat{\pmb{\rho}}^{\mathrm{NPMLE}}$ achieves

$$\sup_{p} \operatorname{regret}(\widehat{\rho}^{\operatorname{NPMLE}}; p) = \widetilde{O}\left(\min\left\{\frac{k}{n}, \frac{1}{n^{2/3}}\right\}\right).$$

Regret analysis

Part I of regret: $\widehat{p}^{\mathrm{NPMLE}}$ against the separable oracle

$$\widehat{p}^{\mathrm{S}} = \text{normalized version of } (\mathbb{E}_{G^{\star}}[p_1 \mid N_1], \dots, \mathbb{E}_{G^{\star}}[p_k \mid N_k])$$

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ightarrow use the theory of NPMLE to argue that $\mathbb{E}_{\widehat{G}}[p_i \mid N_i] \approx \mathbb{E}_{G^*}[p_i \mid N_i]$

Part II of regret: separable oracle \widehat{p}^{S} against the PI oracle $\widehat{p}^{\mathrm{PI}}$

ightarrow our EB upper bound in the Poisson case gives

$$(\star) = \mathbb{E}\left[\mathrm{KL}\left(\widehat{\rho}^{\mathrm{S}} \| \widehat{\rho}^{\mathrm{PI}}\right)\right] = \frac{\widetilde{O}\left(\# \text{ of clusters in the Poisson model}\right)}{n}$$

 \rightarrow it turns out that

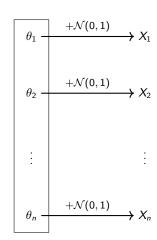
$$\#$$
 of clusters in the Poisson model $= O\left(\min\left\{k, n^{1/3}\right\}\right)$

Proof for the Gaussian case

An information-theoretic argument

→ Recall that

$$\widehat{\theta}_1^{\mathrm{S}} = \mathbb{E}[\theta_1 \mid X_1], \quad \widehat{\theta}_1^{\mathrm{PI}} = \mathbb{E}[\theta_1 \mid X^n].$$



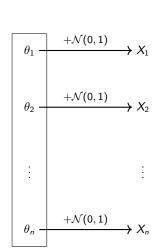
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→ Tao's inequality:

$$\mathbb{E}\left[\left(\mathbb{E}[\theta_1\mid X_1] - \mathbb{E}[\theta_1\mid X^n]\right)^2\right] = \widetilde{O}(1) \cdot I(\theta_1; X_2^n\mid X_1).$$



An information-theoretic argument

→ Recall that

$$\widehat{\theta}_1^{S} = \mathbb{E}[\theta_1 \mid X_1], \quad \widehat{\theta}_1^{PI} = \mathbb{E}[\theta_1 \mid X^n].$$

→ Tao's inequality:

$$\mathbb{E}\left[\left(\mathbb{E}[\theta_1\mid X_1] - \mathbb{E}[\theta_1\mid X^n]\right)^2\right] = \widetilde{O}(1)\cdot I(\theta_1; X_2^n\mid X_1).$$

→ A "model-free" upper bound:

$$I(heta_1; X_2^n \mid X_1) = H(heta_1 \mid X_1) - H(heta_1 \mid X^n)$$

$$\leq H(heta_1 \mid X_1) - \frac{1}{n}H(heta^n \mid X^n)$$

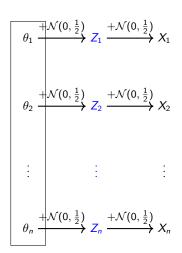
$$= H(heta_1) - \frac{H(heta^n)}{n} - \underbrace{\left(I(heta_1; X_1) - \frac{I(heta^n; X^n)}{n}\right)}_{\geq 0 \text{ as } P_{X^n \mid heta^n} = \prod_i P_{X_i \mid heta_i}}$$

$$\leq H(heta_1) - \frac{H(heta^n)}{n} = \frac{1}{n} \mathsf{KL}(P_{ heta^n} \parallel \prod P_{ heta_i})$$

 $=\widetilde{O}\left(\frac{|\operatorname{supp}(\{\theta_1,\ldots,\theta_n\})|}{n}\right)$

$$\begin{array}{c|c} \theta_1 & \xrightarrow{+\mathcal{N}(0,1)} & X_1 \\ \\ \theta_2 & \xrightarrow{+\mathcal{N}(0,1)} & X_2 \\ \\ \vdots & & \vdots \\ \\ \theta_n & \xrightarrow{+\mathcal{N}(0,1)} & X_n \end{array}$$

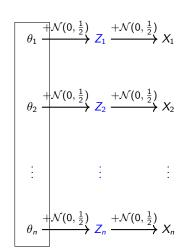
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= 2 (\mathbb{E}[Z_1 \ | X_1] - \mathbb{E}[Z_1 \ | X^n])



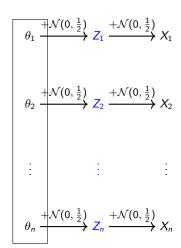
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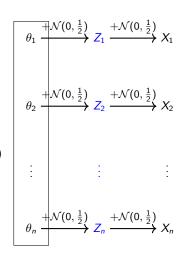
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 \rightarrow the final quantity KL($P_{Z^n} || \prod_i P_{Z_i}$) is now between a Gaussian permutation mixture and its i.i.d. approximation!



Concluding remarks

Take home messages:

- → permutations induce weak dependency, quantitatively
- $\rightarrow\,$ centered basis is preferred in the method of "moments"
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Further questions:

- \rightarrow for bounded Gaussian case, improve the χ^2 upper bound $\exp(O(\mu^3))$ to $\exp(O(\mu^2))$?
- → method of "moments" for two high-dimensional mixtures?
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Thank You!