On the tight statistical analysis of a maximum likelihood estimator based on profiles

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Maximum likelihood estimator

If
$$x \sim P_{\theta}$$
 with $\theta \in \Theta$,
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Fundamental method of parameter estimation with numerous success in:

- statistics
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"The appeal of maximum likelihood stems from its universal applicability, good mathematical properties, ..., and generally good track record as a tool in applied statistics, a record accumulated over fifty years of heavy usage."

—— [Efron, 1980]

Suboptimality of MLE under group transformation

Theorem (Cai and Low, 2011)

For $X \sim \mathcal{N}(\theta, I_p)$, it holds that

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Theorem (H., Jiao, and Weissman, 2018)

For $X=(X_1,\cdots,X_n)$ with i.i.d. $X_i\sim p=(p_1,\cdots,p_k)$, it holds that

$$\begin{split} &\inf_{\widehat{\rho}} \sup_{p} \mathbb{E}_{\rho} \| \widehat{\rho} - p \|_{1, \text{sorted}} \asymp \sqrt{\frac{k}{n \log n}} + \min \left\{ \sqrt{\frac{k}{n}}, n^{-1/3} \right\}, \\ &\sup_{p} \mathbb{E}_{p} \| p^{\text{MLE}} - p \|_{1, \text{sorted}} \asymp \sqrt{\frac{k}{n}}. \end{split}$$

Profile

A group action G on a set $\mathcal X$ partitions $\mathcal X$ into several equivalence classes: for $x,x'\in\mathcal X$,

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Definition (Profile, Orlitsky et al. 2004)

For an observation $x \in \mathcal{X}$, its profile ϕ with respect to the group action G is defined as the equivalence class of x in \mathcal{X} :

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Lemma (Hájek, 1967)

If for all $g \in G$, we have $P_{g\theta}(gx) = P_{\theta}(x)$ and $L(\theta, T) = L(g\theta, T)$, then $\phi(x)$ is "sufficient" for estimating θ under loss L.

Group action: throughout we consider the action of $G=S_p$ on \mathbb{R}^p , i.e. for $\pi\in S_p$ and $x=(x_1,\cdots,x_p)\in\mathbb{R}^p$,

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Example (permutation invariance)

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- if in addition $L(\theta, T) = L(\pi\theta, T)$, Hájek sufficiency implies that $\phi(x)$ is sufficient for estimating θ under loss L

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Example: if $x \sim P_{\theta} = \prod_{j=1}^{p} p_{\theta_j}(x_j)$:

$$\theta^{\mathsf{PMLE}} = \arg\max_{\theta} \mathbb{P}(\theta, (x_{(1)}, x_{(2)}, \cdots, x_{(p)})) = \arg\max_{\theta} \sum_{\pi \in S_{\tau}} \prod_{i=1}^{p} p_{\theta_{i}}(x_{\pi(i)})$$

• Is there an analogy between MLE and PMLE?

- How to analyze the statistical property of PMLE, where both the zeroth-order and first-order conditions look complicated?
- For permutation-invariant models, is PMLE statistically optimal in estimating permutation-invariant targets of θ ?
- Is PMLE subject to certain limitations as well?

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PMLE in discrete distribution model

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- PMLE:

$$p^{\mathsf{PMLE}} = \operatorname{arg\,max}_{p} \sum_{\pi \in S_k} \prod_{j=1}^k p_j^{h_{\pi(j)}}$$

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$$p^{\mathsf{PMLE}} = rg \max_{p} \sum_{\pi \in S_k} \prod_{j=1}^k p_j^{h_{\pi(j)}}$$

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Heuristic algorithms:

- [Orlitsky et al., 2004]: EM-type algorithm
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Provable approximate algorithms: $\mathbb{P}(\hat{p}, \phi) \geq \beta \cdot \mathbb{P}(p^{\mathsf{PMLE}}, \phi)$

- [Charikar, Shiragur, and Sidford, 2019]: $\beta = \exp(-n^{2/3} \log n)$
- [Anari et al., 2020a, 2020b]: $\beta = \exp(-\min\{\sqrt{n}, k\} \log n)$

Statistical guarantee

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A recent breakthrough:

Theorem (Acharya, Das, Orlitsky, and Suresh, 2017)

For any metric d and accuracy level $\varepsilon > 0$,

$$\sup_{p \in \mathcal{M}_k} \mathbb{P}_p(d(p^{\mathsf{PMLE}}, p) > 2\varepsilon) \leq e^{3\sqrt{n}} \cdot \inf_{\widehat{p}(\phi)} \sup_{p \in \mathcal{M}_k} \mathbb{P}_p(d(\widehat{p}, p) > \varepsilon)$$

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Corollary: as in many examples we have

$$\inf_{\widehat{p}(\phi)} \sup_{p \in \mathcal{M}_k} \mathbb{P}_p(d(\widehat{p}, p) > \varepsilon) \lesssim \exp\left(-n(\varepsilon - \varepsilon_{n,k})_+^2\right),$$

if n is the minimax sample complexity of achieving accuracy $\varepsilon/2$, the PMLE attains the rate-optimal sample complexity if $\varepsilon \gg n^{-1/4}$.

Improving the exponent

- [Charikar, Shiragur, and Sidford, 2019, Hao and Orlitsky, 2019]:
 exponent polylog(n) for a (very) restricted class of d and modified PMLE
- [Hao and Orlitsky, 2020]: distribution-dependent exponent $H_n(p)$ with $\sup_p H_n(p) \simeq \sqrt{n}$

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An open question

What is the tight exponent for the competitive analysis of the PMLE?

Main results

Result I: improved competitive analysis of PML

Theorem (H. and Shiragur, 2021)

For any metric d, accuracy level $\varepsilon>0$ and constant $c\in(0,1)$, we have

$$\sup_{p \in \mathcal{M}_k} \mathbb{P}_p(d(p^{\mathsf{PMLE}}, p) > 2\varepsilon)$$

$$\leq \exp\left(c' n^{1/3 + c}\right) \cdot \inf_{\widehat{p}} \sup_{p \in \mathcal{M}_k} \mathbb{P}_p(d(\widehat{p}, p) > \varepsilon)^{1 - c},$$

for some constant c' depending only on c.

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- exponent improved from $O(\sqrt{n})$ to $O(n^{1/3+c})$
- for any β -approximate PMLE, the competitive factor becomes $\exp(c'n^{1/3+c})/\beta$

Result II: optimality of exponent

Theorem (H., 2021)

For any $c,c',c_1,c_2>0$, there exists a metric d and accuracy level $\varepsilon>0$ such that

$$\begin{split} &\sup_{p \in \mathcal{M}_k} \mathbb{P}_p(d(p^{\mathsf{PMLE}}, p) > c_1 \varepsilon) \\ &\gg \exp\left(c' n^{1/3 - c}\right) \cdot \inf_{\widehat{p}} \sup_{p \in \mathcal{M}_k} \mathbb{P}_p(d(\widehat{p}, p) > \varepsilon)^{1 - c_2}. \end{split}$$

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- the exponent $O(n^{1/3-c})$ is not generically attainable for PMLE
- the competitive factor $\exp(O(n^{1/3}))$ is optimal and not superfluous

Result III: PMLE estimates sorted distribution optimally

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The PMLE satisfies that

$$\sup_{p \in \mathcal{M}_k} \mathbb{E}_p \| p^{\mathsf{PML}} - p \|_{1,\mathsf{sorted}} \lesssim \sqrt{\frac{k}{n \log n}} + \widetilde{O}\left(n^{-1/3} \wedge \sqrt{\frac{k}{n}}\right).$$

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- minimax rate-optimal for estimating sorted distribution
- attains optimal phase transition at $k \approx n^{1/3}$
- [Acharya et al., 2012]: requires $k \gtrsim n$
- [Hao and Orlitsky, 2019]: requires $k \gtrsim n^{0.8}$
- [Hao and Orlitsky, 2020]: requires $k \gtrsim n^{0.75}$

Application in symmetric functional estimation

Problem: Given n i.i.d. observations $X_1, \dots, X_n \sim p = (p_1, \dots, p_k)$, aim to estimate the quantity $F(p) = \sum_{i=1}^k f(p_i)$ for a given f

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Generalization: non-symmetric, multivariate and nonparametric functionals

Ad-hoc estimation

Plug-in of MLE: $\hat{F} = F(p^{\text{MLE}})$

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Supported in lots of recent literature:

- Shannon entropy (VV11a, VV11b, VV13, JVHW15, WY16)
 - Rényi entropy (AOST14, AOST17)
 - distance to uniformity (VV13, JHW18)
 - divergences (HJW16, JHW18, BZLV18)
 - nonparametrics (HJM17, HJWW17)
 - general 1-Lipschitz functional (HO19a, HO19b)
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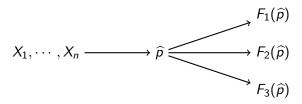
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$$X_1, \cdots, X_n \longrightarrow \widehat{p}$$

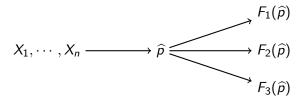
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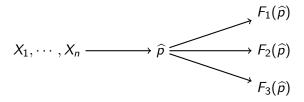
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Too good to be true? No!

Result IV: universal optimality of PMLE

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For symmetric functionals including:

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- distance to uniformity and general 1-Lipschitz functionals, the plug-in approach of the PMLE universally attains the optimal sample complexity of achieving an accuracy level $\varepsilon \gg n^{-1/3}$.
 - Proof: choose d(p,q) = |F(p) F(q)|, and construct minimax rate-optimal estimator for F

Result V: limitation of PMLE

Theorem (H., 2021)

There exists a 1-Lipschitz functional F such that

$$\sup_{p \in \mathcal{M}_k} \mathbb{E}_p |F(p^{\mathsf{PMLE}}) - F(p)| \asymp \begin{cases} \sqrt{\frac{k}{n \log n}} & \text{if } k \gg n^{1/3} \\ \sqrt{\frac{k}{n}} & \text{if } 1 \ll k \ll n^{1/3} \end{cases}$$

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• PMLE fails to be optimal when $k \ll n^{1/3}$, or equivalently, $\varepsilon \ll n^{-1/3}$

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• A larger quantity [H., Jiao, and Weissman, 2018]:

$$\inf_{\widehat{p}} \sup_{p \in \mathcal{M}_k} \mathbb{E}_p \left[\sup_{F \in \mathcal{F}_{\mathsf{Lip}}} |F(\widehat{p}) - F(p)| \right] \asymp \begin{cases} \sqrt{\frac{k}{n \log n}} & \text{if } k \gg n^{1/3} \\ \sqrt{\frac{k}{n}} & \text{if } 1 \ll k \ll n^{1/3} \end{cases}$$

Summary of approaches

	ad-hoc	LMM	PMLE
optimality	full: $\varepsilon \gg n^{-1/2}$	if $\varepsilon \gg n^{-1/3}$	iff $\varepsilon \gg n^{-1/3}$
complexity	almost linear	polynomial	polynomial*
functional independent	Х	✓	✓
asymmetric functional	✓	Х	Х
free parameter tuning	Х	Х	✓

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Tight statistical analysis of PML: optimality and limitation

Proof sketch of improved competitive analysis

Review: idea of [Acharya et al., 2017]

Notations:

- Φ_n : the set of all possible profiles with sample size n
- ϕ : a particular profile in Φ_n
- p_{ϕ} : the PMLE associated with ϕ
- $\mathbb{P}(p,\phi)$: probability of observing ϕ under the true distribution p

Review: idea of [Acharya et al., 2017]

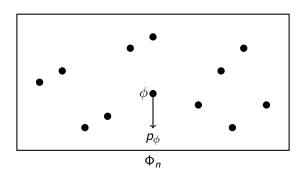
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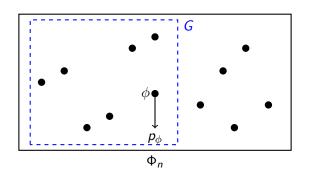
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Technical goal: using only the defining property $\mathbb{P}(p_{\phi}, \phi) \geq \mathbb{P}(p, \phi)$, find an upper bound of

$$\sup_{p\in\mathcal{M}_k}\mathbb{P}_p(d(p_\phi,p)>2\varepsilon)$$

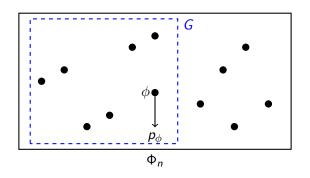
given an estimator $\widehat{p}(\phi)$ with $\sup_{p \in \mathcal{M}_k} \mathbb{P}_p(d(\widehat{p}, p) > \varepsilon) \leq \delta$.





Good profile:

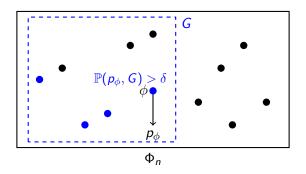
$$G = \{ \phi \in \Phi_n : d(\widehat{p}(\phi), p) \le \varepsilon \}$$



Good profile:

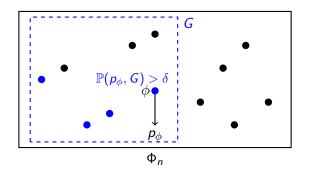
$$G = \{ \phi \in \Phi_n : d(\widehat{p}(\phi), p) \le \varepsilon \}$$

Clearly $\mathbb{P}(p,G) \geq 1 - \delta$.



Lemma

For any $\phi \in G$ satisfying $\mathbb{P}(p_{\phi}, G) > \delta$, we have $d(p_{\phi}, p) \leq 2\varepsilon$.

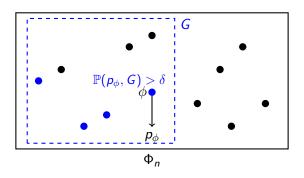


Lemma

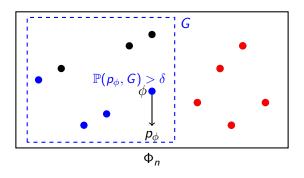
For any $\phi \in G$ satisfying $\mathbb{P}(p_{\phi}, G) > \delta$, we have $d(p_{\phi}, p) \leq 2\varepsilon$.

Proof: $\mathbb{P}(p_{\phi}, G) > \delta \Longrightarrow d(\widehat{p}(\phi'), p_{\phi}) \leq \varepsilon$ for some $\phi' \in G$. Also, definition of $G \Longrightarrow d(\widehat{p}(\phi'), p) \leq \varepsilon$.

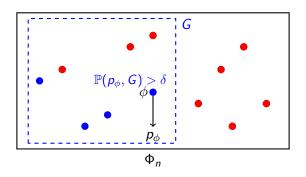




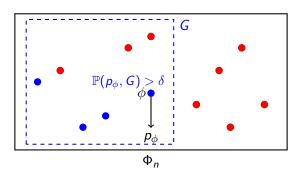
$$\mathbb{P}_p(d(p_\phi,p)>2\varepsilon)$$



$$\mathbb{P}_p(d(p_\phi, p) > 2\varepsilon) \leq \mathbb{P}(p, G^c)$$

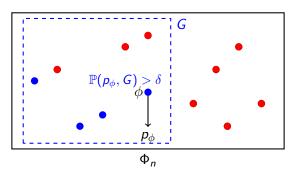


$$\mathbb{P}_p(d(p_{\phi},p) > 2\varepsilon) \leq \mathbb{P}(p,G^c) + \sum_{\phi \in G} \mathbb{P}(p,\phi)\mathbb{1}(\mathbb{P}(p_{\phi},G) \leq \delta)$$



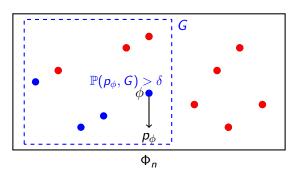
$$\begin{split} \mathbb{P}_{\rho}(d(p_{\phi}, p) > 2\varepsilon) &\leq \mathbb{P}(p, G^{c}) + \sum_{\phi \in G} \mathbb{P}(p, \phi) \mathbb{1}(\mathbb{P}(p_{\phi}, G) \leq \delta) \\ &\leq \delta + \sum_{\phi \in G} \mathbb{P}(p, \phi) \mathbb{1}(\mathbb{P}(p, \phi) \leq \delta) \end{split}$$

for $\mathbb{P}(p_{\phi},G) \geq \mathbb{P}(p_{\phi},\phi) \geq \mathbb{P}(p,\phi)$.



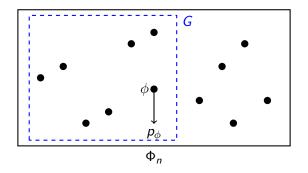
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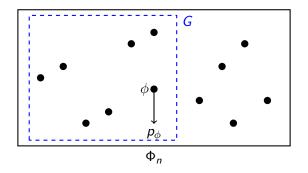


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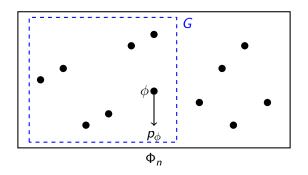


A potentially loose inequality: $\mathbb{P}(p_\phi,G) \geq \mathbb{P}(p_\phi,\phi)$ for $\phi \in G$



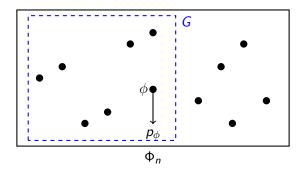
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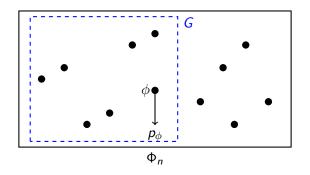


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- ullet could be tight when p_ϕ is essentially supported on ϕ
- ullet in that case, $\mathbb{P}(p_{\phi'},\phi) \ll \mathbb{P}(p_{\phi},\phi)$



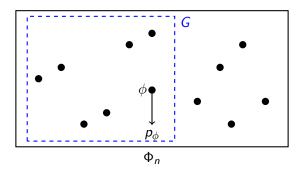
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Q: What if we could have $\mathbb{P}(p_{\phi}, \phi) \approx \mathbb{P}(p_{\phi'}, \phi)$ for all $\phi, \phi' \in G$? A: Then we are in a great shape, for if $\mathbb{P}(p_{\phi'}, G) < \delta$ for some $\phi' \in G$, then

$$\delta > \mathbb{P}(\pmb{p}_{\phi'}, \pmb{G}) = \sum_{\phi \in \pmb{G}} \mathbb{P}(\pmb{p}_{\phi'}, \phi) pprox \sum_{\phi \in \pmb{G}} \mathbb{P}(\pmb{p}_{\phi}, \phi) \geq \sum_{\phi \in \pmb{G}} \mathbb{P}(\pmb{p}, \phi) = \mathbb{P}(\pmb{p}, \pmb{G}),$$

a contradiction to $\mathbb{P}(p, G) \geq 1 - \delta$.



Idea

Improved bound if we could show certain "continuity" property of $\phi\mapsto p_\phi.$

Key covering lemma

Covering lemma

Let 0 < s < r < 1/2 be any fixed constants. There exists a discrete set of profiles $\Phi \subseteq \Phi_n$ such that:

- the new set Φ has a smaller cardinality $|\Phi| \leq \exp(n^r \log n)$;
- every profile $\phi \in \Phi_n$ could be approximated by some profile $\phi' \in \Phi$ in the following sense: for all $S \subseteq \Phi_n$,

$$\mathbb{P}(p_{\phi},S) \geq \mathbb{P}(p_{\phi'},S)^{1/(1-n^{-s})} \cdot \exp\left(-cn^{1-2r+s}\right),$$

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where c = c(r, s) > 0.

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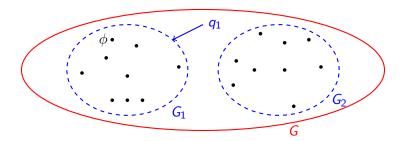
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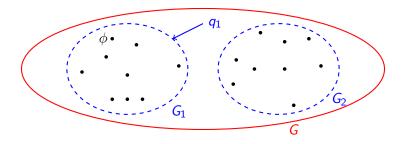
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A covering property of PML distributions $\{p_{\phi}: \phi \in \Phi_n\}$

- $r \uparrow$: the cardinality \uparrow , approximation exponent \downarrow
- $s \uparrow$: probability exponent \downarrow , multiplicative exponent \uparrow

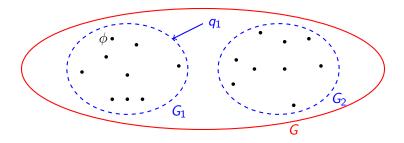




If
$$\mathbb{P}(p_{\phi}, G_1) \leq \delta$$
, then

$$\delta \geq \mathbb{P}(p_{\phi}, G_1) \geq \mathbb{P}(q_1, G_1)^{1/(1-n^{-1/8})} \cdot \exp(-cn^{3/8})$$

$$\Longrightarrow \mathbb{P}(q_1, G_1) \leq \delta^{1-o(1)} \cdot \exp(cn^{3/8})$$

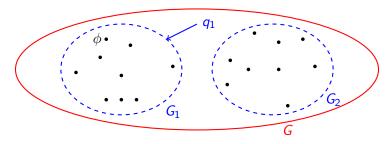


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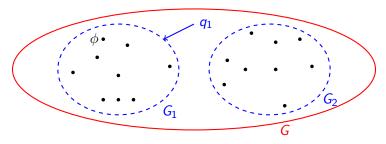
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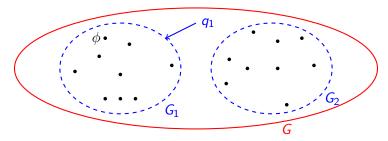
"going-down process"



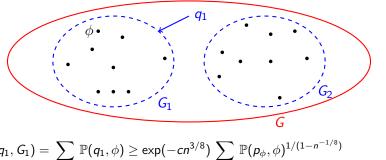
 $\mathbb{P}(q_1,G_1)$



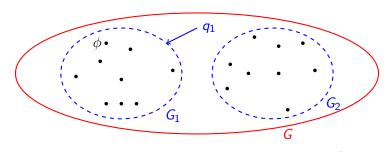
$$\mathbb{P}(q_1,\mathit{G}_1) = \sum_{\phi \in \mathit{G}_1} \mathbb{P}(q_1,\phi)$$



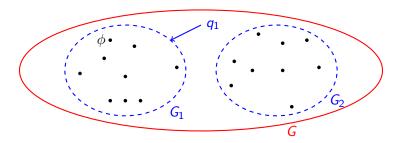
$$\mathbb{P}(q_1, \mathit{G}_1) = \sum_{\phi \in \mathit{G}_1} \mathbb{P}(q_1, \phi) \geq \exp(-\mathit{cn}^{3/8}) \sum_{\phi \in \mathit{G}_1} \mathbb{P}(p_\phi, \phi)^{1/(1 - \mathit{n}^{-1/8})}$$



$$\begin{split} \mathbb{P}(q_1,G_1) &= \sum_{\phi \in G_1} \mathbb{P}(q_1,\phi) \geq \exp(-cn^{3/8}) \sum_{\phi \in G_1} \mathbb{P}(p_\phi,\phi)^{1/(1-n^{-1/8})} \\ &\geq \exp(-cn^{3/8}) \left(\sum_{\phi \in G_1} \mathbb{P}(p_\phi,\phi) \right)^{1/(1-n^{-1/8})} \cdot |G_1|^{-n^{-1/8}/(1-n^{-1/8})} \end{split}$$

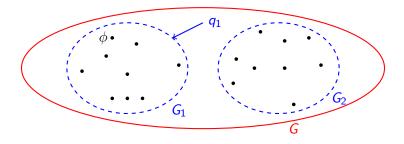


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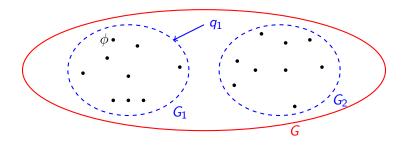


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"going-up" process



Conclusion: if
$$\mathbb{P}(p_\phi,G_1)\leq \delta$$
 for some $\phi\in G_1$, then
$$\mathbb{P}(p,G_1)\leq \delta^{1-o(1)}\cdot \exp(cn^{3/8}).$$

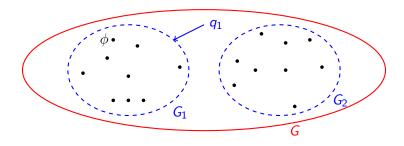


Conclusion: if $\mathbb{P}(p_{\phi}, G_1) \leq \delta$ for some $\phi \in G_1$, then

$$\mathbb{P}(p, G_1) \leq \delta^{1-o(1)} \cdot \exp(cn^{3/8}).$$

Using $|\Phi| \le \exp(n^{3/8} \log n)$, we have

$$\sum_{\phi \in G} \mathbb{P}(p,\phi) \mathbb{1}(\mathbb{P}(p_{\phi},G) \leq \delta) \leq \delta^{1-o(1)} \cdot \exp(cn^{3/8} \log n).$$



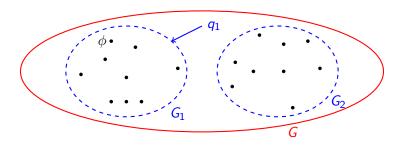
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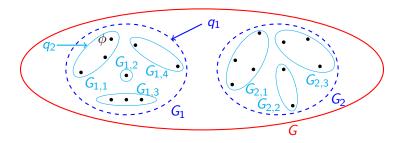
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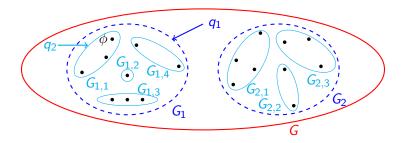
Using $|\Phi| \le \exp(n^{3/8} \log n)$, we have

$$\sum_{\phi \in G} \mathbb{P}(\rho, \phi) \mathbb{1}(\mathbb{P}(\rho_{\phi}, G) \leq \delta) \leq \delta^{1 - o(1)} \cdot \exp(cn^{3/8} \log n).$$

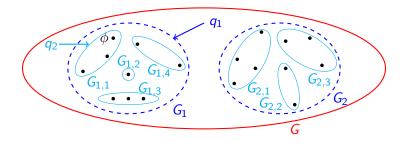
Already improves over $\exp(3\sqrt{n})!$





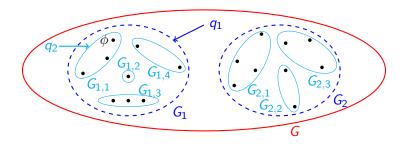


• "going-down": move along $\mathbb{P}(p_\phi, G_1) o \mathbb{P}(q_2, G_1) o \mathbb{P}(q_1, G_1)$



- "going-down": move along $\mathbb{P}(p_{\phi}, G_1) \to \mathbb{P}(q_2, G_1) \to \mathbb{P}(q_1, G_1)$
- "going-up": move along

$$\mathbb{P}(q_1, G_1)
ightarrow \sum \mathbb{P}(q_2, G_{1,1})
ightarrow \sum \sum \mathbb{P}(p_{\phi}, \phi)
ightarrow \mathbb{P}(p, G_1)$$



- "going-down": move along $\mathbb{P}(p_{\phi}, G_1) \to \mathbb{P}(q_2, G_1) \to \mathbb{P}(q_1, G_1)$
- "going-up": move along

$$\mathbb{P}(q_1, G_1)
ightarrow \sum \mathbb{P}(q_2, G_{1,1})
ightarrow \sum \sum \mathbb{P}(p_\phi, \phi)
ightarrow \mathbb{P}(p, G_1)$$

• choice of parameters: choose $(r_1, s_1), (r_2, s_2), \cdots$ to obtain exponents

$$\frac{3}{8} \rightarrow \frac{7}{20} \rightarrow \frac{15}{44} \rightarrow \cdots \rightarrow \frac{1}{3}$$

Generalization to Gaussian location model

PMLE in Gaussian location model

Theorem

For $X \sim \mathcal{N}(\theta, I_p)$, the PMLE satisfies

$$\begin{split} &\sup_{\|\theta\|_{\infty} \leq M} \mathbb{P}_{\theta}(d(\theta^{\mathsf{PMLE}}, \theta) \geq 2\varepsilon) \\ &\leq \exp\left(\widetilde{O}(p^{1/3} M^{2/3})\right) \cdot \inf_{\widehat{\theta}(\phi)} \sup_{\|\theta\|_{\infty} \leq M} \mathbb{P}_{\theta}(d(\widehat{\theta}, \theta) \geq \varepsilon)^{1 - o(1)} + \frac{1}{\operatorname{poly}(p)} \end{split}$$

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• main technical challenge: continuous values of X

Implication on sorted parameter estimation

Corollary

It holds that

$$\sup_{\|\theta\|_{\infty} \leq 1} \mathbb{E}_{\theta} \|\theta^{\mathsf{PMLE}} - \theta\|_{1,\mathsf{sorted}} \lesssim p \cdot \frac{\log\log p}{\log p}$$

 matching the minimax risk obtained in [Niles-Weed and Rigollet, 2019]

Concluding remarks

- Is there an analogy between MLE and PMLE?
 Yes MLE is rate-optimal in parameter estimation, and PMLE is rate-optimal in parameter estimation up to permutation.
- How to analyze the statistical property of PMLE, where both the zeroth-order and first-order conditions look complicated?
 Using competitive analysis.
- For permutation-invariant models, is PMLE statistically optimal in estimating permutation-invariant targets of θ ?

 Universally true when the target error is large.
- Is PMLE subject to certain limitations as well?
 Yes when the target error is small.

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Future directions:

- tightness of exponent in Gaussian location model?
- direct analysis of PMLE?
- relationships to nonparametric MLE? $\pi^{\text{NPMLE}} = \arg\max_{\pi} \sum_{i=1}^{n} \log \int p_{\theta}(x_i) \pi(d\theta)$

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Thank you!