



#### **Optimal Gaussian** Adaptive Data Analysis

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#### Joint work with Jing Lei and Steve Fienberg





#### Data analysis is conditional/adaptive



- "All inferences are conditional inferences."
  - Jonathan Taylor (via Ryan)
- "Why most published research findings are false?"
   – John Ioannidis, 2005
- "A garden of forking paths"
  Gelman and Loken, 2013

#### A model for adaptive data analysis

 $T_2$ 

 $I_3$ 

 $N(\mu_T, \Sigma)$ Data

#### **Player**

 $T_1, ..., T_k \in \mathcal{T}$ 



**Adversary** 

I have the data. I choose how to answer the questions. I have the distribution. I choose questions T.

Russo and Zou. "Controlling Bias in Adaptive Data Analysis Using Information Theory." AISTATS-2016.

## Example: Choosing classifiers

- Adversary:
  - $T_1$ : Give me a risk estimate to the optimal linear classifier using feature 1,5,7
  - T<sub>2</sub>: If the answer is greater than 0.5: give me that of feature 2,4,6. Otherwise, give me the risk of a kernel classifier using only feature 1,5,7.
- Player:
  - $\phi_{T_i}$  empirical estimates of  $T_i$  on data. Jointly distributed due to data and  $T_i$ (and  $T_i$  depends on  $T_{1:i-1}$ ,  $A_{1:i-1}$ )

### Our contribution

• Formulate the minimax problem

- Establish information-theoretic limits
  - Minimax lower bound
  - Per-instance lower bound (for natural estimators)

#### Minimax setup

- Assuming:  $\phi_{\mathcal{T}} \sim N(\mu_{\mathcal{T}}, \Sigma)$   $\Sigma_{tt} \leq \sigma^2$
- No restrictions on adversary.

How to answer all questions accurately?
 – i.e., how to minimize

$$R(A_{1:k}) = \sup_{T_{1:k}} \left[ \max_{i \in [k]} \mathbb{E}(A_i - \mu_{T_i})^2 \right]$$

#### Known estimators

- Naïve estimator:  $A_i = \phi_{T_i}$ - Achieves rate:  $\Theta(k\sigma^2)$
- Noise adding:  $A_i \sim \mathcal{N}(\phi_{T_i}, \sqrt{k\sigma^2})$ – Achieves rate:  $\Theta(\sqrt{k\sigma^2})$  (Russo and Zou, 2016)
- Can this be improved further?

#### Lower bound 1 (worst case)

• Assume  $|\mathcal{T}| = \Omega(2^k)$ 

$$\inf_{A_{1:k}} \sup_{\mathcal{D}(\phi_{\mathcal{T}})} \sup_{T_{1:k}} \left( \max_{i} \mathbb{E}[(A_{i} - \mu_{T_{i}})^{2}] \right) = \Omega(\sqrt{k\sigma^{2}})$$

• Any estimators  $A_i$  with input

$$\phi_{\mathcal{T}}, \underbrace{T_{1:i-1}, A_{1:i-1}, T_i}_{\text{data}}, \underbrace{T_i}_{\text{From prev rounds}}$$
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#### Lower bound 2 (per-Instance)

• Fix a distribution of  $\phi_{\mathcal{T}}$  that's sufficiently rich

$$\inf_{\text{Natural } A_{1:k}} \sup_{T_{1:k}} \left( \max_{i} \mathbb{E}[(A_{i} - \mu_{T_{i}})^{2}] \right) = \Omega(\sqrt{k}\sigma^{2}).$$

• Any natural estimators  $A_i$  with input



\*In the previous version of the paper: <u>https://arxiv.org/abs/1602.04287</u> The estimators are restricted to noise adding ones. New results will be on arxiv soon.

#### Summary

• Gaussian noise adding is optimal up to constant factors.

 Selection itself is often enough to impose nontrivial lower bound, even for a fixed distribution.

#### For proof details and open problems

- Talk to me at the poster!
- Thank you!

#### Supplementary slides

#### Related work

- ADA via Differential privacy (DFHPRR15, BNSSSU15, etc...)
  - Similar setting. DP is unnecessarily strong for the purpose. Need lowsensitivity.
  - We work with conditional expectations directly.
- Lower bounds via finger printing codes (Hardt, Ullman, Steinke, etc)
  - A different setting. Also, they have a computational lower bound.
  - Suboptimal rate (if we ignore differences in settings).
- Post-selection inference (Taylor, Tibshirani, Fithian, Lee, etc.)
  - The focus is to have correct confidence interval, despite selection bias.
  - Fixed procedure, lasso-like. Not adaptive.
  - We prevent finding significantly biased statistics in the first place.

#### Sign inference attack

- Choose  $T_1 = t_1, ..., T_{k-1} = t_{k-1}$ - Such that  $\phi_{t_1} \perp ... \perp \phi_{t_{k-1}}$
- Infer the signs of  $\phi_{t_1} \mu_{t_1}, ..., \phi_{t_{k-1}} \mu_{t_{k-1}}$ - using optimal classifier...
- Construct  $T_k = t_k$ 
  - Such that it's correlation with  $\phi_{t_1}, ..., \phi_{t_{k-1}}$  are proportional to the inferred signs.

Lower bound idea: Optimal obfuscation of the signs .

# Example: linear regression $y = X\beta + N(0, \sigma^2 I)$ $\hat{\beta} = (X^T X)^{-1} X^T y$

Hope to discover:

which gene is associated with heart disease?

After looking at a sequence of values:

$$\langle t_1, \hat{\beta} \rangle, \dots, \langle t_k, \hat{\beta} \rangle$$

We conclude that features indexed by  $t_k$  has the a strong association!

\* It could also be: choose a feature subset and fit a linear regression. The fitted parameters will still be jointly Gaussian.

#### Example: Hyper parameter tuning via Bayesian Optimization

- Set of d hyper parameters  $\mathcal{T} = [0,1]^d$
- Grid search is too expensive.
- Often people use sequential adaptive tuning.



## What's in common?

• In linear regression:

 $\phi_t = \langle t, \hat{\beta} \rangle$ 

 $\mu_t = \langle t, \beta \rangle$ 

$$\mathcal{T} = \left\{ t \in \mathbb{R}^d | \|t\|_2 \le 1 \right\}$$

Selection rule: exploratory • In Bayesian optimization:

 $\phi_t = \text{TestErr}(t)$ 

 $\mathcal{T} = [0, 1]^d$ 

 $\mu_t = \mathbb{E}[\text{TestErr}(t)]$  Selection rule: GP-UCB.

- In both cases:
  - $\phi_{\mathcal{T}}$  is a Gaussian Process.
  - Both sequential, but different selection rules