Statistical Estimation in Algebraically Structured Models

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Final Year Project Midterm Presentation

Outline

Introduction to Statistical Estimation

General setting: Let P be an **unknown** probability distribution on a sample space Ω. Let $X_1, X_2, \cdots, X_n$ be samples that are drawn independently and randomly from Ω according to the probability distribution P.

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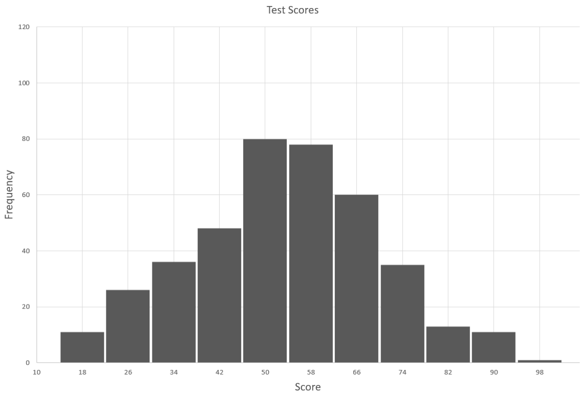
Restricted hypothesis space: In real world statistical estimation, we already have a rough idea of what the probability distribution P should look like.

Toy Example

Final exam for a large course ($\sim$ 400 students):



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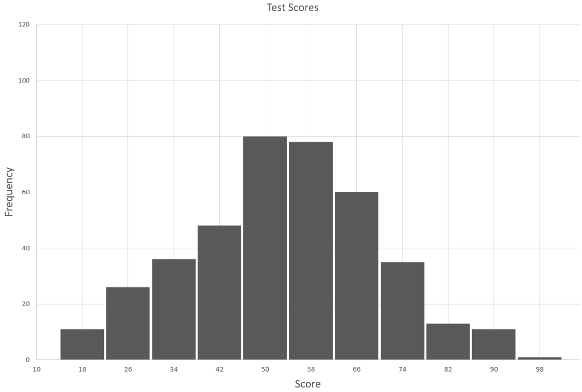

The distribution is expected to be approximately **normal.**

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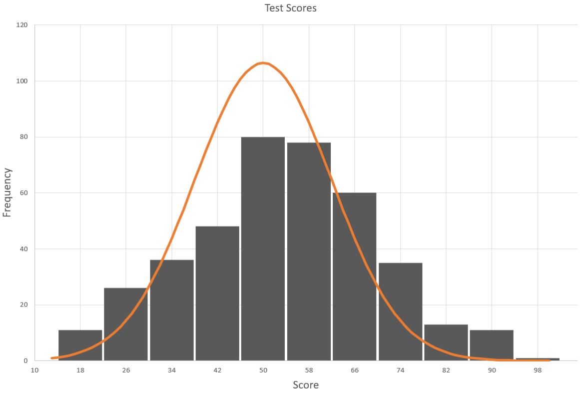
The normal distribution is completely determined by its **mean** and **variance**.



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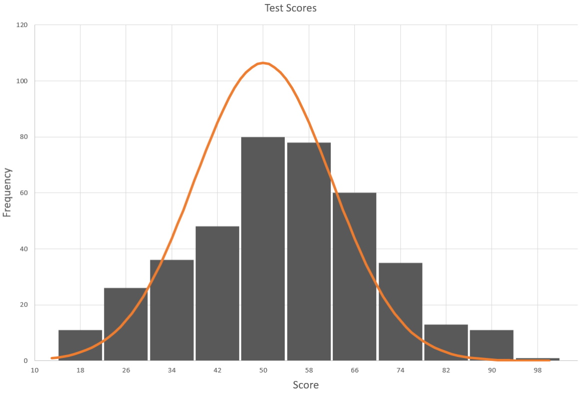

Finding the "best fit" curve on 400 samples is now simply an optimization problem in two parameters.

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Given independent samples $Y_1, \cdots, Y_n$ drawn from $\mathbb{R}^d$ according to (1), we want to recover the vector θ. This setup is known as an **algebraically structured model**.

Algebraically Structured Model

Problem Setup:

$$Y_i = G\theta + \xi$$

where $\theta \in \mathbb{R}^d, \quad G \in \mathcal{G} \subseteq O(d)$ and $\xi \sim \mathcal{N}(\mathbf{0}, \sigma^2 \boldsymbol{I}_d)$.

Additional assumption: The observations Y_i are **noisy** (i.e. $\|\theta\|^2 / \sigma^2$ is low) and precise estimates are **difficult**.

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To build an **abstract framework**, we first need some new mathematical tools.

Kullback-Leibler Divergence

Each vector $\theta \in \mathbb{R}^d$ defines a corresponding **probability distribution** P_θ according to

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If two vectors θ and ϕ define similar probability distributions, then we expect algorithms to have a hard time distinguishing between them (and vice versa).

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Answer: Statistical divergences. The **Kullback-Leibler Divergence** between two probability distributions P_θ and P_ϕ (with densities f_θ and f_ϕ respectively) is defined to be

$$D(P_\theta \parallel P_\phi) := \int_{\mathbb{R}^d} f_\theta(x) \log \frac{f_\theta(x)}{f_\phi(x)}\, dx.$$

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Gauging the performance of estimators essentially boils down to controlling the quantity $D(P_\theta \parallel P_\phi)$.

Summary Statistics

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34	84	46	22	28	45	96	59
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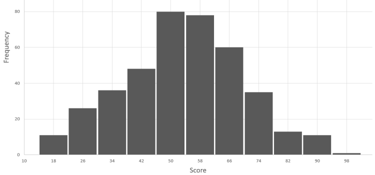

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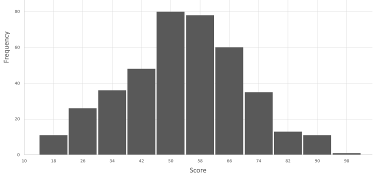

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How to **generalise** the higher moments $\mathbb{E}[X^k]$ to the multivariate setting?

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$$\mathbb{E}\left[\begin{pmatrix} Y_1 \\ \vdots \\ Y_n \end{pmatrix} \left(Y_1, \cdots, Y_n\right)\right] = \mathbb{E}[\boldsymbol{Y} \otimes \boldsymbol{Y}]$$

which is a 2-**tensor**.

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For a random vector $\boldsymbol{X} = (X_1, \cdots, X_m)$, the mth moment should be an ***m*-tensor**

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Returning to our setting, the ***m*th moment tensor** between two vectors $\theta, \phi \in \mathbb{R}^d$ is defined to be

$$\Delta_m := \mathbb{E}\big[(G\theta)^{\otimes m} - (G\phi)^{\otimes m}\big].$$

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Let $\theta, \phi \in \mathbb{R}^d$ be vectors satisfying some technical conditions. For any $k \geq 1$, there exist constants $\underline{C}$ and $\overline{C}$ such that

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This allows us to extend the **passageway:**

$$\text{Performance of Estimators} \longleftrightarrow D(P_\theta \parallel P_\phi)$$

Universal Upper and Lower Bounds

Our goal is to establish upper and lower bounds on $D(P_\theta \parallel P_\phi)$.

Bandeira-Rigollet-Weed (2017)

Let $\theta, \phi \in \mathbb{R}^d$ be vectors satisfying some technical conditions. For any $k \geq 1$, there exist constants $\underline{C}$ and $\overline{C}$ such that

$$\underline{C} \sum_{m=1}^{\infty} \frac{\|\Delta_m\|^2}{(\sqrt{3}\sigma)^{2m} m!} \leq D(P_\theta \parallel P_\phi) \leq \overline{C} \sum_{m=1}^{\infty} \frac{\|\Delta_m\|^2}{\sigma^{2m} m!}.$$

We have both an upper bound and lower bound on the KL divergence in terms of the **same quantity**.

This allows us to extend the **passageway:**

$$\text{Performance of Estimators} \longleftrightarrow D(P_\theta \parallel P_\phi) \longleftrightarrow \left\{ \|\Delta_m\| \ : \ m \in \mathbb{Z}_{\geq 1} \right\}.$$

Multi-reference Alignment

If we are able to understand how the family of moment tensors

$$\Delta_m = \mathbb{E}\left[(G\theta)^{\otimes m} - (G\phi)^{\otimes m}\right]$$

varies with θ and ϕ, it should give us a better understanding of the **fundamental difficulty** of solving the algebraically structured model.

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Further simplifications are needed to make the problem **tractable**.

Multi-reference Alignment

Define

$$\mathcal{G} := \left\{ R_\ell \;:\; 0 \leq \ell \leq d-1 \right\}.$$

where

$$R_\ell\big((\theta_1, \cdots, \theta_d)\big) := \big(\theta_{1+\ell}, \theta_{2+\ell}, \cdots, \theta_{d+\ell}\big).$$

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The **Discrete Fourier Transform** $\hat{\theta}$ of a vector $\theta \in \mathbb{R}^d$ is given by

$$\hat{\theta}_j := \frac{1}{\sqrt{d}} \sum_{k=1}^{d} e^{\frac{2\pi ijk}{d}} \theta_k, \qquad -\lfloor d/2 \rfloor \le j \le \lfloor d/2 \rfloor.$$

The Fourier Domain

By passing through the passage

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By passing through the passage

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we obtain **explicit formulas** for the moment tensors:

$$\mathbb{E}\left[(\widehat{G\theta})\right]_i = \begin{cases} \hat{\theta}_0 & \text{if } i = 0, \\ 0 & \text{otherwise.} \end{cases}$$

$$\mathbb{E}\left[(\widehat{G\theta})^{\otimes 2}\right]_{ij} = \begin{cases} |\hat{\theta}_i|^2 & \text{if } i + j = 0, \\ 0 & \text{otherwise.} \end{cases}$$

$$\vdots$$

$$\mathbb{E}\left[(\widehat{G\theta})^{\otimes m}\right]_{i_1 \cdots i_m} = \begin{cases} \hat{\theta}_{i_1}\hat{\theta}_{i_2} \cdots \hat{\theta}_{i_m} & \text{if } i_1 + \cdots + i_m = 0, \\ 0 & \text{otherwise.} \end{cases}$$

Moment Matching

$$\underline{C}\sum_{m=1}^{\infty}\frac{\|\Delta_m\|^2}{(\sqrt{3}\sigma)^{2m}m!} \leq D(P_\theta \parallel P_\phi) \leq \overline{C}\sum_{m=1}^{\infty}\frac{\|\Delta_m\|^2}{\sigma^{2m}m!}.$$

Key Idea: If the first $k-1$ moments match, then $D(P_\theta \parallel P_\phi)$ is of order $O(\sigma^{-2k})$.

Establish upper bounds: Construct two vectors θ and ϕ such that the first k moments **cancel out**.

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Key Idea: If the first $k-1$ moments match, then $D(P_\theta \parallel P_\phi)$ is of order $O(\sigma^{-2k})$.

Establish upper bounds: Construct two vectors θ and ϕ such that the first k moments **cancel out**.

Establish lower bounds: Show that no such cancellation is possible.

Moment Matching

$$\text{DC:} \qquad \mathbb{E}\left[(\widehat{G\theta})\right]_i = \begin{cases} \hat{\theta}_0 & \text{if } i = 0 \\ 0 & \text{otherwise.} \end{cases}$$

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$$\text{Bispectrum:} \qquad \mathbb{E}\left[(\widehat{G\theta})^{\otimes 3}\right]_{ijk} = \begin{cases} \hat{\theta}_i\hat{\theta}_j\hat{\theta}_k & \text{if } i + j + k = 0, \\ 0 & \text{otherwise.} \end{cases}$$

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We extend the passageway by one more step:

$$\begin{array}{c}\text{Performance of} \\ \text{Estimators}\end{array} \longleftrightarrow D(P_\theta \parallel P_\phi) \longleftrightarrow \left\{\|\Delta_m\|\right\}_{m=1}^{\infty} \longleftrightarrow \begin{array}{c}\text{Support of} \\ \hat{\theta} \text{ and } \hat{\phi}\end{array}$$

The End

Thank you for your attention.