# An Introduction to Statistical Lower Bounds for Estimation and Learning 

Part 1: Information Theory and Fano's Inequality

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Annual School on Mathematics of Data Science [Darwin, 2024]

## Information Theory

- How do we quantify "information" in data?
- Information theory [Shannon, 1948]:
- Fundamental limits of data communication



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- Information of source: Entropy
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## Principles:

- First fundamental limits without complexity constraints, then practical methods
- First asymptotic analyses, then convergence rates, finite-length, etc.
- Mathematically tractable probabilistic models


## Information Theory and Data

- Conventional view:

Information theory is a theory of communication


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- Conventional view:

Information theory is a theory of communication


- Emerging view:


## Information theory is a theory of data



- Extracting information from channel output vs. Extracting information from data


## Examples

- Information theory in machine learning and statistics:
- Statistical estimation
[Le Cam, 1973]
- Group testing
[Malyutov, 1978]
- Multi-armed bandits
- Phylogeny
[Lai and Robbins, 1985]
[Mossel, 2004]
- Sparse recovery
[Wainwright, 2009]
- Graphical model selection
- Convex optimization
[Santhanam and Wainwright, 2012]
- DNA sequencing
- Sparse PCA
- Community detection
- Matrix completion
- Ranking
- Adaptive data analysis
- Supervised learning
[Agarwal et al., 2012]
[Motahari et al., 2012]
[Birnbaum et al., 2013]
[Abbe, 2014]
[Riegler et al., 2015]
[Shah and Wainwright, 2015]
[Russo and Zou, 2015]
[Nokleby, 2016]
- Crowdsourcing
- Distributed computation
[Lahouti and Hassibi, 2016]
[Lee et al., 2018]
- Bayesian optimization
[Scarlett, 2018]
- Note: More than just using entropy / mutual information...


## Analogies

Same concepts, different terminology:

| Communication Problems | Data Problems |
| :---: | :---: |
| Feedback | Active learning / adaptivity |
| Rate-distortion theory | Approximate recovery |
| Joint source-channel coding | Non-uniform prior |
| $\ldots$ | $\ldots$ |

## Analogies

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| Communication Problems | Data Problems |
| :---: | :---: |
| Channels with feedback | Active learning / adaptivity |
| Rate distortion theory | Approximate recovery |
| Joint source-channel coding | Non-uniform prior |
| Error probability | Error probability |
| Random coding | Random sampling |
| Side information | Side information |
| Channels with memory | Statistically dependent measurements |
| Mismatched decoding | Model mismatch |
| $\ldots$ | $\ldots$ |

## Cautionary Notes

Some cautionary notes on the information-theoretic viewpoint:

- The simple models we can analyze may be over-simplified (more so than in communication)
- Compared to communication, we often can't get matching achievability/converse (often settle with correct scaling laws)
- Information-theoretic limits not (yet) considered much in practice (to my knowledge) ... but they do guide the algorithm design
- Often encounter gaps between information-theoretic limits and computation limits
- Often information theory simply isn't the right tool for the job


## Terminology: Achievability and Converse

Achievability result (example): Given $\bar{n}(\epsilon)$ data samples, there exists an algorithm achieving an "error" of at most $\epsilon$

- Estimation error: $\left\|\hat{\theta}-\theta_{\text {true }}\right\| \leq \epsilon$
- Optimization error: $f\left(x_{\text {selected }}\right) \leq \min _{x} f(x)+\epsilon$


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Converse result (example): In order to achieve an "error" of at most $\epsilon$, any algorithm requires at least $\underline{n}(\epsilon)$ data samples

## Information Measures

## Entropy

- Definition: The entropy of a discrete random variable $X$ is defined as

$$
H(X)=\sum_{x \in \mathcal{X}} P_{X}(x) \log \frac{1}{P_{X}(x)}=\mathbb{E}\left[\log \frac{1}{P_{X}(X)}\right]
$$

This is measured in bits for $\log _{2}(\cdot)$, or nats for $\log _{e}(\cdot)$.

- Interpetation: If we observe that $X=x$ then the amount of information learned is $\overline{\log \frac{1}{P_{X}(x)}}$ ( $\log \frac{1}{\rho}$ satisfies natural axioms). Entropy is the average information learned by observing $X$, or equivalently, the average uncertainty in $X$ before observing it.
- Examples: (i) If $X$ is deterministic then $H(X)=0$;
(ii) If $X \sim \operatorname{Uniform}(\mathcal{X})$ then $H(X)=\log |\mathcal{X}|$
- Source coding theorem: $H(X)$ is the fundamental limit of compression when a source emits i.i.d. symbols from $P_{X}$


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- Source coding theorem: $H(X)$ is the fundamental limit of compression when a source emits i.i.d. symbols from $P_{X}$
- Joint version: $H(X, Y)=\mathbb{E}\left[\log \frac{1}{P_{X Y}(X, Y)}\right]$; generally $H(\mathbf{X})=\mathbb{E}\left[\log \frac{1}{P_{\mathbf{X}}(\mathbf{X})}\right]$.
- Interpetation: Overall information/uncertainty in multiple variables
- Conditional version: $H(Y \mid X)=\sum_{x \in \mathcal{X}} P_{X}(x) H(Y \mid X=x)$
- Interpetation: Remaining uncertainty in $Y$ after observing $X$ (on average)
- Continuous RVs: A counterpart exists for continuous RVs, but not as "well-behaved" (can be negative, no longer invariant under 1-to-1 maps)


## Properties of Entropy

- Non-negativity:

$$
H(X) \geq 0
$$

with equality iff $X$ is deterministic

- Uniform distribution has highest entropy:

$$
H(X) \leq \log |\mathcal{X}|
$$

with equality iff $X$ is uniform

- Conditioning can't increase entropy: (on average)

$$
H(X \mid Y) \leq H(X)
$$

with equality iff $X$ and $Y$ are independent

- Chain rule:

$$
\begin{gathered}
H(X, Y)=H(X)+H(Y \mid X)=H(Y)+H(X \mid Y) \\
H\left(X_{1}, \ldots, X_{n}\right)=\sum_{i=1}^{n} H\left(X_{i} \mid X_{i-1}\right)
\end{gathered}
$$

- Tensorization / sub-additivity:

$$
H\left(X_{1}, \ldots, X_{n}\right) \leq \sum_{i=1}^{n} H\left(X_{i}\right)
$$

## Relative Entropy (KL Divergence)

- Definition: For two distributions $P$ and $Q$, the relative entropy (KL divergence) is defined as

$$
D(P \| Q)=\sum_{x} P(x) \log \frac{P(x)}{Q(x)}=\mathbb{E}_{P}\left[\log \frac{P(X)}{Q(X)}\right]
$$

- Example usage: If we draw $n$ i.i.d. samples from $Q$, the probability of getting symbol proportions $P$ is roughly $e^{-n D(P \| Q)}$ (a more general statement: Sanov's theorem)
- Key property:

$$
D(P \| Q) \geq 0
$$

with equality iff $P=Q$

- Conditional version: $D\left(P_{Y \mid X} \| Q_{Y \mid X} \mid P_{X}\right)=\sum_{X} P_{X}(x) D\left(P_{Y \mid X=x} \| Q_{Y \mid X=x}\right)$
- This also leads to a chain rule: $D\left(P_{X Y} \| Q_{X Y}\right)=D\left(P_{X} \| Q_{X}\right)+D\left(P_{Y \mid X} \| Q_{Y \mid X} \mid P_{X}\right)$
- Extends readily to continuous RVs (and beyond) while saying "well-behaved"


## Mutual Information

- Definition: The mutual information between $X$ and $Y$ is defined as

$$
\begin{aligned}
I(X ; Y) & =H(X)-H(X \mid Y) \\
& =H(Y)-H(Y \mid X) \\
& =D\left(P_{X Y} \| P_{X} \times P_{Y}\right)
\end{aligned}
$$

- Interpretation 1: $X$ has uncertainty $H(X)$, but after observing $Y$ it has remaining uncertainty $H(X \mid Y)$, so $I(X ; Y)$ is how much information $Y$ revealed about $X$.
- Interpretation 2: By the $D\left(P_{X Y} \| P_{X} \times P_{Y}\right)$ form, this measures how far $X$ and $Y$ are from being independent
- Channel coding theorem: $\max _{P_{X}} I(X ; Y)$ is the fundamental limit of communication when the communication channel is probabilistic with transition law $P_{Y \mid X}$


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- Can again have joint version, e.g., $I\left(X_{1}, X_{2} ; Y_{1}, Y_{2}\right)$, and conditional version, e.g., $I(X ; Y \mid Z)=\sum_{z} P_{Z}(z) I(X ; Y \mid Z=z)$
- Again well-behaved even for continuous variables


## Properties of Mutual Information

- Non-negativity:

$$
I(X ; Y) \geq 0
$$

with equality iff $X$ and $Y$ are independent

- Chain rule:

$$
I\left(X_{1}, X_{2} ; Y\right)=I\left(X_{1} ; Y\right)+I\left(X_{2} ; Y \mid X_{1}\right)
$$

and similarly with $n$ variables

- Tensorization: If $P_{\mathbf{Y} \mid \mathbf{X}}=\prod_{i=1}^{n} P_{Y_{i} \mid X_{i}}$, then

$$
I(\mathbf{X} ; \mathbf{Y}) \leq \sum_{i=1}^{n} I\left(X_{i} ; Y_{i}\right)
$$

(not true in general if the assumption on $P_{\mathbf{Y} \mid \mathrm{X}}$ is dropped)

- Data processing inequality: If $X \rightarrow Y \rightarrow Z$ forms a Markov chain, then

$$
I(X ; Z) \leq I(X ; Y)
$$

Similarly with more variables (e.g., $W \rightarrow X \rightarrow Y \rightarrow Z$ gives $I(W ; Z) \leq I(X ; Y))$

# Converse Bounds for Statistical Estimation via Fano's Inequality 

(Based on survey chapter https://arxiv.org/abs/1901.00555)

## Statistical Estimation

- General statistical estimation setup:
- Unknown parameter $\theta \in \Theta$
- Samples $\mathbf{Y}=\left(Y_{1}, \ldots, Y_{n}\right)$ drawn from $P_{\theta}(\mathbf{y})$
- More generally, from $P_{\theta, \mathbf{x}}$ with inputs $\mathbf{X}=\left(X_{1}, \ldots, X_{n}\right)$
- Given $\mathbf{Y}$ (and possibly $\mathbf{X}$ ), construct estimate $\hat{\theta}$



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- Goal. Minimize some loss $\ell(\theta, \hat{\theta})$
- 0-1 loss: $\ell(\theta, \hat{\theta})=\mathbf{1}\{\hat{\theta} \neq \theta\}$
- Squared $\ell_{2}$ loss: $\|\theta-\hat{\theta}\|^{2}$



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- Squared $\ell_{2}$ loss: $\|\theta-\hat{\theta}\|^{2}$
- Typical example. Linear regression
- Estimate $\theta \in \mathbb{R}^{p}$ from $\mathbf{Y}=\mathbf{X} \theta+\mathbf{Z}$



## Defining Features

- There are many properties that impact the analysis:
- Discrete $\theta$ (e.g., graph learning, sparsity pattern recovery)
- Continuous $\theta$ (e.g., regression, density estimation)
- Bayesian $\theta$ (average-case performance)
- Minimax bounds over $\Theta$ (worst-case performance)
- Non-adaptive inputs (all $X_{1}, \ldots, X_{n}$ chosen in advance)
- Adaptive inputs ( $X_{i}$ can be chosen based on $Y_{1}, \ldots, Y_{i-1}$ )
- This talk. Minimax bounds, mostly non-adaptive, first discrete and then continuous


## High-Level Steps

Steps in attaining a minimax lower bound (converse):

1. Reduce estimation problem to multiple hypothesis testing
2. Apply a form of Fano's inequality
3. Bound the resulting mutual information term
(Multiple hypothesis testing: Given samples $Y_{1}, \ldots, Y_{n}$, determine which distribution among $P_{1}(\mathbf{y}), \ldots, P_{M}(\mathbf{y})$ generated them. $M=2$ gives binary hypothesis testing.)

## Step I: Reduction to Multiple Hypothesis Testing

- Lower bound worst-case error by average over hard subset $\theta_{1}, \ldots, \theta_{M}$ :


Idea:

- Show "successful" algorithm $\hat{\theta} \Longrightarrow$ Correct estimation of $V$ (When is this true?)
- Equivalent statement: If $V$ can't be estimated reliably, then $\hat{\theta}$ can't be successful.


## Step I: Example

- Example: Suppose algorithm is claimed to return $\hat{\theta}$ such that $\|\hat{\theta}-\theta\|_{2} \leq \epsilon$

- If $\theta_{1}, \ldots, \theta_{M}$ are separated by $2 \epsilon$, then we can identify the correct $V \in\{1, \ldots, M\}$
- Note: Tension between number of hypotheses, difficulty in distinguishing them, and sufficient separation. Choosing a suitable set $\left\{\theta_{1}, \ldots, \theta_{M}\right\}$ can be challenging.


## Step II: Application of Fano's Inequality

- Standard form of Fano's inequality from textbooks: For a random variable $V$ and its estimate $\hat{V}$, defining $P_{\mathrm{e}}=\mathbb{P}[\hat{V} \neq V]$, we have

$$
H(V \mid \hat{V}) \leq H_{2}\left(P_{\mathrm{e}}\right)+P_{\mathrm{e}} \log (M-1)
$$

where $H_{2}(\alpha)=\alpha \log \frac{1}{\alpha}+(1-\alpha) \log \frac{1}{1-\alpha}$ is the entropy of $\operatorname{Bernoulli}(\alpha)$.
Intuition:

- Considering asking questions to resolve the uncertainty in $V$ given $\hat{V}$ ?.
- First ask whether the two are equal; this has uncertainty $H_{2}\left(P_{\mathrm{e}}\right)$
- When they differ, the remaining uncertainty is at most $\log (M-1)$.


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- Re-arranged and slightly weakened form for $V$ uniform over $M$ outcomes:

$$
\mathbb{P}[\hat{V} \neq V] \geq 1-\frac{I(V ; \hat{V})+\log 2}{\log M}
$$

- Intuition: Need learned information $I(V ; \hat{V})$ to be close to prior uncertainty $\log M$


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- Variations:
- Non-uniform $V$
- Approximate recovery
- Conditional version


## Step III: Bounding the Mutual Information

- The key quantity remaining after applying Fano's inequality is $I(V ; \hat{V})$
- Data processing inequality: (Based on $V \rightarrow \mathbf{Y} \rightarrow \hat{V}$ or similar)
- No inputs: $I(V ; \hat{V}) \leq I(V ; \mathbf{Y})$
- Non-adaptive inputs: $I(V ; \hat{V} \mid \mathbf{X}) \leq I(V ; \mathbf{Y} \mid \mathbf{X})$
- Adaptive inputs: $I(V ; \hat{V}) \leq I(V ; \mathbf{X}, \mathbf{Y})$


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- Adaptive inputs: $I(V ; \hat{V}) \leq I(V ; \mathbf{X}, \mathbf{Y})$
- Tensorization: (Based on conditional independence of the samples)
- No inputs: $I(V ; \mathbf{Y}) \leq \sum_{i=1}^{n} I\left(V ; Y_{i}\right)$
- Non-adaptive inputs: $I(V ; \mathbf{Y} \mid \mathbf{X}) \leq \sum_{i=1}^{n} I\left(V_{;} Y_{i} \mid X_{i}\right)$
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- Adaptive inputs: $I(V ; \mathbf{X}, \mathbf{Y}) \leq \sum_{i=1}^{n} I\left(V_{;} Y_{i} \mid X_{i}\right)$
- KL Divergence Bounds:
- $I(V ; Y) \leq \max _{v, v^{\prime}} D\left(P_{Y \mid V}(\cdot \mid v) \| P_{Y \mid V}\left(\cdot \mid v^{\prime}\right)\right)$
- $I(V ; Y) \leq \max _{V} D\left(P_{Y \mid V}(\cdot \mid v) \| Q_{Y}\right)$ for any $Q_{Y}$
- If each $P_{Y \mid V}(\cdot \mid v)$ is $\epsilon$-close to the closest $Q_{1}(\mathbf{y}), \ldots, Q_{N}(\mathbf{y})$ in KL divergence, then $I(V ; Y) \leq \log N+\epsilon$
- (Similarly with conditioning on $X$ )


# Discrete Example 1 

Group Testing

## Group Testing



## Group Testing



- Goal:

Given test matrix $\mathbf{X}$ and outcomes $\mathbf{Y}$, recover item vector $\beta$

- Sample complexity: Required number of tests $n$


## Information Theory and Group Testing



- Information-theoretic viewpoint:
$S$ : Defective set
$\mathbf{X}_{S}$ : Columns indexed by $S$



## Information Theory and Group Testing

- Example formulation of general result:

Number of tests

Mutual Information
(Information learned from measurements)

## Converse via Fano's Inequality

- Reduction to multiple hypothesis testing: Trivial! Set $V=S$.


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- Application of Fano's Inequality:

$$
\mathbb{P}[\hat{S} \neq S] \geq 1-\frac{I(S ; \hat{S} \mid \mathbf{X})+\log 2}{\log \binom{p}{k}}
$$

where $p=(\#$ items $)$ and $k=(\#$ defectives $)$.

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where $p=(\#$ items $)$ and $k=$ (\#defectives).

- Bounding the mutual information:
- Data processing inequality: $I(S ; \hat{S} \mid \mathbf{X}) \leq I(\mathbf{U} ; \mathbf{Y})$ where $\mathbf{U}$ are pre-noise outputs
- Tensorization: $I(\mathbf{U} ; \mathbf{Y}) \leq \sum_{i=1}^{n} I\left(U_{i} ; Y_{i}\right)$
- Capacity bound: $I\left(U_{i} ; Y_{i}\right) \leq C$ if outcome passed through channel of capacity $C$


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- Capacity bound: $I\left(U_{i} ; Y_{i}\right) \leq C$ if outcome passed through channel of capacity $C$
- Final result:

$$
n \leq \frac{\log \binom{p}{k}}{C}(1-\epsilon) \Longrightarrow \mathbb{P}[\hat{S} \neq S] \nrightarrow 0
$$

## Illustration of Bounds

Noiseless bounds:


## Noisy bounds:



## Illustration of Bounds

## Noiseless bounds:



## Noisy bounds:



- Other Implications:
- Adaptivity and approximate recovery:
- No gain at low sparsity levels
- Significant gain at high sparsity levels
- Information-theoretically optimal non-adaptive algorithms are now known


## Discrete Example 2

Graphical Model Selection

## Graphical Model Representations of Joint Distributions

## Motivating example:

- In a population of $p$ people, let

$$
Y_{i}=\left\{\begin{array}{ll}
1 & \text { person } i \text { is infected } \\
-1 & \text { person } i \text { is healthy, }
\end{array} \quad i=1, \ldots, p\right.
$$

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$$

- Example models:

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- Joint distribution for a given graph $G=(V, E)$ :

$$
\mathbb{P}\left[\left(Y_{1}, \ldots, Y_{p}\right)=\left(y_{1}, \ldots, y_{p}\right)\right]=\frac{1}{Z} \exp \left(\sum_{(i, j) \in E} \lambda_{i j} y_{i} y_{j}\right)
$$

## Graphical Model Selection: Illustration

- A larger example from [Abbe and Wainwright, ISIT Tutorial 2015]:
- Example graphs:

| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

- Sample images (Ising model):



## Graphical Model Selection: Illustration

- A larger example from [Abbe and Wainwright, ISIT Tutorial 2015]:
- Example graphs:

| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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## Graphical Model Selection: Illustration

- A larger example from [Abbe and Wainwright, ISIT Tutorial, 2015]:
- Example graphs:

- Sample images (Ising model):

- Goal: Identify graph given $n$ independent samples


## Graphical Model Selection: Definition

## General problem statement.

- Given $n$ i.i.d. samples of $\left(Y_{1}, \ldots, Y_{p}\right) \sim P_{G}$, recover the underlying graph $G$
- Applications: Statistical physics, social and biological networks
- Error probability:

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## Assumptions.

- Distribution class:
- Ising model

$$
P_{G}\left(x_{1}, \ldots, x_{p}\right)=\frac{1}{Z} \exp \left(\sum_{(i, j) \in E} \lambda_{i j} x_{i} x_{j}\right)
$$

- Gaussian model

$$
\left(X_{1}, \ldots, X_{p}\right) \sim \mathcal{N}(\mu, \boldsymbol{\Sigma})
$$

where $\left(\boldsymbol{\Sigma}^{-1}\right)_{i j} \neq 0 \Longleftrightarrow(i, j) \in E$ [Hammersley-Clifford theorem]

- Graph class:
- Bounded-edge (at most $k$ edges total)
- Bounded-degree (at most $d$ edges out of each node)


## Information-Theoretic Viewpoint

- Information-theoretic viewpoint:



## Converse via Fano's Inequality

- Reduction to multiple hypothesis testing: Let $G$ be uniform on hard subset $\mathcal{G}_{0} \subseteq \mathcal{G}$
- Ideally many graphs (lots of graphs to distinguish)
- Ideally close together (harder to distinguish)


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- Bounding the mutual information:
- Data processing inequality: $I(G ; \hat{G}) \leq I(G ; \mathbf{Y})$
- Tensorization: $I(G ; \mathbf{Y}) \leq \sum_{i=1}^{n} I\left(G ; Y_{i}\right)$
- KL divergence bound: Bound $I\left(G ; Y_{i}\right) \leq \max _{G} D\left(P_{Y \mid G}(\cdot \mid G) \| Q_{Y}\right)$ case-by-case


## Graph Ensembles

- Graphs that are difficult to distinguish from the empty graph:


0 0

- Reveals $n=\Omega\left(\frac{1}{\lambda^{2}} \log p\right)$ necessary condition with "edge strength" $\lambda$ and $p$ nodes


## Graph Ensembles

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0

## 0

- Reveals $n=\Omega\left(\frac{1}{\lambda^{2}} \log p\right)$ necessary condition with "edge strength" $\lambda$ and $p$ nodes
- Graphs that are difficult to distinguish from the complete (sub-)graph:

- Reveals $n=\Omega\left(e^{\lambda d}\right)$ necessary condition with "edge strength" $\lambda$ and degree $d$


## Upper vs. Lower Bounds

- Example results with maximal degree $d$, edge strength $\lambda$ (slightly informal):
- (Converse) $n=\Omega\left(\max \left\{\frac{1}{\lambda^{2}}, e^{\lambda d}\right\} \log p\right) \quad$ [Santhanam and Wainwright, 2012]
- (Achievability) $n=O\left(\max \left\{\frac{1}{\lambda^{2}}, e^{\lambda d}\right\} d \log p\right)$ [Santhanam and Wainwright, 2012]
- (Early Practical) $n=O\left(d^{2} \log p\right)$ but extra assumptions that are hard to cerify
[Ravikumar/Wainwright/Lafferty, 2010]
- (Further Practical) $n=O\left(\frac{d^{2} \lambda^{\lambda d}}{\lambda^{2}} \log p\right)$
[Klivans/Meka 2017]
[Wu/Sanghavi/Dimakis 2018]
- (Near-Optimality in Many Regimes)
- Ising models
- Gaussian models
[Lokhov/Vuffray/Misra/Chertkov, 2018] [Misra/Vuffray/Lokhov, 2020]

What About Continuous-Valued Estimation?

## Statistical Estimation

- General statistical estimation setup:
- Unknown parameter $\theta \in \Theta$
- Samples $\mathbf{Y}=\left(Y_{1}, \ldots, Y_{n}\right)$ drawn from $P_{\theta}(\mathbf{y})$
- More generally, from $P_{\theta, \mathbf{x}}$ with inputs $\mathbf{X}=\left(X_{1}, \ldots, X_{n}\right)$
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- Goal. Minimize some loss $\ell(\theta, \hat{\theta})$
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- Squared $\ell_{2}$ loss: $\|\theta-\hat{\theta}\|^{2}$
- Typical example. Linear regression
- Estimate $\theta \in \mathbb{R}^{p}$ from $\mathbf{Y}=\mathbf{X} \theta+\mathbf{Z}$



## Minimax Risk

- Since the samples are random, so is $\hat{\theta}$ and hence $\ell(\theta, \hat{\theta})$
- So seek to minimize the average loss $\mathbb{E}_{\theta}[\ell(\theta, \hat{\theta})]$.
- Note: $\mathbb{E}_{\theta}$ and $\mathbb{P}_{\theta}$ denote averages w.r.t. $\mathbf{Y}$ when the true parameter is $\theta$.


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- Approach: Lower bound worst-case error by average over hard subset $\theta_{1}, \ldots, \theta_{M}$ :



## General Lower Bound via Fano's Inequality

- To get a meaningful result, need a sufficiently "well-behaved" loss function. Subsequently, focus on loss functions of the form

$$
\ell(\theta, \hat{\theta})=\Phi(\rho(\theta, \hat{\theta}))
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where $\rho\left(\theta, \theta^{\prime}\right)$ is some metric, and $\Phi(\cdot)$ is some non-negative and increasing function (e.g., $\ell(\theta, \hat{\theta})=\|\theta-\hat{\theta}\|^{2}$ )

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- Claim. Fix $\epsilon>0$, and let $\left\{\theta_{1}, \ldots, \theta_{M}\right\}$ be a finite subset of $\Theta$ such that

$$
\rho\left(\theta_{v}, \theta_{v^{\prime}}\right) \geq \epsilon, \quad \forall v, v^{\prime} \in\{1, \ldots, M\}, v \neq v^{\prime} .
$$

Then, we have

$$
\mathcal{M}_{n}(\Theta, \ell) \geq \Phi\left(\frac{\epsilon}{2}\right)\left(1-\frac{I(V ; \mathbf{Y})+\log 2}{\log M}\right)
$$

where $V$ is uniform on $\{1, \ldots, M\}$, and $I(V ; \mathbf{Y})$ is with respect to $V \rightarrow \theta_{V} \rightarrow \mathbf{Y}$.

## Proof of General Lower Bound

- Using Markov's inequality:

$$
\begin{aligned}
\sup _{\theta \in \Theta} \mathbb{E}_{\theta}[\ell(\theta, \hat{\theta})] & \geq \sup _{\theta \in \Theta} \Phi\left(\epsilon_{0}\right) \mathbb{P}_{\theta}\left[\ell(\theta, \hat{\theta}) \geq \Phi\left(\epsilon_{0}\right)\right] \\
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$$

- Hence,

$$
\begin{aligned}
\sup _{\theta \in \Theta} \mathbb{P}_{\theta}\left[\rho(\theta, \hat{\theta}) \geq \frac{\epsilon}{2}\right] & \geq \max _{v=1, \ldots, M} \mathbb{P}_{\theta_{v}}\left[\rho\left(\theta_{v}, \hat{\theta}\right) \geq \frac{\epsilon}{2}\right] \\
& \geq \max _{v=1, \ldots, M} \mathbb{P}_{\theta_{v}}[\hat{V} \neq v] \\
& \geq \frac{1}{M} \sum_{v=1, \ldots, M} \mathbb{P}_{\theta_{v}}[\hat{V} \neq v] \\
& \geq 1-\frac{I(V ; \mathbf{Y})+\log 2}{\log M}
\end{aligned}
$$

where the final step uses Fano's inequality.

## Local Approach

- General bound: If $\rho\left(\theta_{v}, \theta_{v^{\prime}}\right) \geq \epsilon$ for all $v, v^{\prime}$ then

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Resulting bound:

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- Resulting bound:

$$
\mathcal{M}_{n}(\Theta, \ell) \geq \Phi\left(\frac{\epsilon_{\mathrm{p}}}{2}\right)\left(1-\frac{\log N_{\mathrm{KL}, n}^{*}\left(\Theta, \epsilon_{\mathrm{c}, n}\right)+\epsilon_{\mathrm{c}, n}+\log 2}{\log M_{\rho}^{*}\left(\Theta, \epsilon_{\mathrm{p}}\right)}\right)
$$

- $M_{\rho}^{*}\left(\Theta, \epsilon_{\mathrm{p}}\right)$ : No. $\epsilon$-separated $\theta$ we can pack into $\Theta$ (packing number)
- $N_{\mathrm{KL}, n}^{*}\left(\Theta, \epsilon_{\mathrm{C}, n}\right)$ : No. $\epsilon_{\mathrm{c}, n}$-size KL divergence balls to cover $\mathcal{P}_{Y}$ (covering number)


# Continuous Example 1 

Sparse Linear Regression

## Sparse Linear Regression

- Linear regression model $\mathbf{Y}=\mathbf{X} \theta+\mathbf{Z}$ :

- Feature matrix $\mathbf{X}$ is given, noise is i.i.d. $N\left(0, \sigma^{2}\right)$
- Coefficients are sparse - at most $k$ non-zeros


## Converse via Fano's Inequality

- Reduction to hyp. testing: Fix $\epsilon>0$ and restrict to sparse vectors of the form

$$
\theta=(0,0,0, \pm \epsilon, 0, \pm \epsilon, 0,0,0,0,0, \pm \epsilon, 0)
$$

- Total number of such sequences $=2^{k}\binom{p}{k} \approx \exp \left(k \log \frac{p}{k}\right)($ if $k \ll p)$
- Choose a "well separated" subset of size $\exp \left(\frac{k}{4} \log \frac{p}{k}\right)$ (Gilbert-Varshamov)
- Well-separated: Non-zero entries differ in at least $\frac{k}{8}$ indices


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- Application of Fano's inequality:
- Using the general bound given previously:

$$
\mathcal{M}_{n}(\Theta, \ell) \geq \frac{k \epsilon^{2}}{32}\left(1-\frac{I(V ; \mathbf{Y} \mid \mathbf{X})+\log 2}{\frac{k}{4} \log \frac{p}{k}}\right)
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- Bounding the mutual information:
- By a direct calculation, $I(V ; \mathbf{Y} \mid \mathbf{X}) \leq \frac{\epsilon^{2}}{2 \sigma^{2}} \cdot \frac{k}{\rho}\|\mathbf{X}\|_{F}^{2}$ (Gaussian noise) [Actually extra steps (e.g., matrix Bernstein) needed when using Fano's inequality with exact recovery. But an "approximate recovery" version avoids it.]
- Substitute and choose $\epsilon$ to optimize the bound: $\epsilon^{2}=\frac{\sigma^{2} p \log \frac{p}{k}}{2\|\mathbf{X}\|_{F}^{2}}$


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- Substitute and choose $\epsilon$ to optimize the bound: $\epsilon^{2}=\frac{\sigma^{2} p \log \frac{p}{k}}{2\|\mathbf{X}\|_{F}^{2}}$
- Final result: If $\|\mathbf{X}\|_{F}^{2} \leq n p \Gamma$, then $\mathbb{E}\left[\|\theta-\hat{\theta}\|_{2}^{2}\right] \leq \delta$ requires $n \geq \frac{c \sigma^{2}}{\Gamma \delta} \cdot k \log \frac{p}{k}$


## Upper vs. Lower Bounds

- Recap of model: $\mathbf{Y}=\mathbf{X} \theta+\mathbf{Z}$, where $\theta$ is $k$-sparse
- Lower bound: If $\|\mathbf{X}\|_{F}^{2} \leq n p \Gamma$, achieving $\mathbb{E}\left[\|\theta-\hat{\theta}\|_{2}^{2}\right] \leq \delta$ requires $n \leq \frac{c \sigma^{2}}{\Gamma \delta} \cdot k \log \frac{p}{k}$
- Upper bound: If $\mathbf{X}$ is a zero-mean random Gaussian matrix with power $\Gamma$ per entry, then we can achieve $\mathbb{E}\left[\|\theta-\hat{\theta}\|_{2}^{2}\right] \leq \delta$ using at most $n \geq \frac{c^{\prime} \sigma^{2}}{\Gamma \delta} \cdot k \log \frac{p}{k}$ samples
- Maximum-likelihood estimation suffices
- Tighter lower bounds could potentially be obtained under additional restrictions on $\mathbf{X}$


# Continuous Example 2 

Convex Optimization

## Stochastic Convex Optimization

- A basic optimization problem

$$
\mathbf{x}^{\star}=\operatorname{argmin}_{x \in D} f(x)
$$

For simplicity, we focus on the $1 D$ case $D \subseteq \mathbb{R}$ (extensions to $\mathbb{R}^{d}$ are possible)

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$$

For simplicity, we focus on the 1 D case $D \subseteq \mathbb{R}$ (extensions to $\mathbb{R}^{d}$ are possible)

- Model:
- Noisy samples: When we query $x$, we get a noisy value and noisy gradient:

$$
Y=f(x)+Z, \quad Y^{\prime}=f^{\prime}(x)+Z^{\prime}
$$

where $Z \sim N\left(0, \sigma^{2}\right)$ an $Z^{\prime} \sim N\left(0, \sigma^{2}\right)$

- Adaptive sampling: Chosen $X_{i}$ may depend on $Y_{1}, \ldots, Y_{i-1}$


## Stochastic Convex Optimization

- A basic optimization problem

$$
\mathbf{x}^{\star}=\operatorname{argmin}_{x \in D} f(x)
$$

For simplicity, we focus on the 1 D case $D \subseteq \mathbb{R}$ (extensions to $\mathbb{R}^{d}$ are possible)

- Model:
- Noisy samples: When we query $x$, we get a noisy value and noisy gradient:

$$
Y=f(x)+Z, \quad Y^{\prime}=f^{\prime}(x)+Z^{\prime}
$$

where $Z \sim N\left(0, \sigma^{2}\right)$ an $Z^{\prime} \sim N\left(0, \sigma^{2}\right)$

- Adaptive sampling: Chosen $X_{i}$ may depend on $Y_{1}, \ldots, Y_{i-1}$
- Function classes: Convex, strongly convex, Lipschitz, self-concordant, etc.
- We will focus on the class of strongly convex functions
- Strong convexity: $f(x)-\frac{c}{2} x^{2}$ is a convex function for some $c>0$ (we set $c=1$ )


## Performance Measure and Minimax Risk

- After sampling $n$ points, the algorithm returns a final point $\hat{x}$
- The loss incurred is $\ell_{f}(\hat{x})=f(\hat{x})-\min _{x \in \mathcal{X}} f(x)$, i.e., the gap to the optimum
- For a given class of functions $\mathcal{F}$, the minimax risk is given by

$$
\mathcal{M}_{n}(\mathcal{F})=\inf _{\hat{X}} \sup _{f \in \mathcal{F}} \mathbb{E}_{f}\left[\ell_{f}(\hat{X})\right]
$$

## Reduction to Multiple Hypothesis Testing

- The picture remains the same:

- Successful optimization $\Longrightarrow$ Successful identification of $V$


## General Minimax Lower Bound

- Claim 1. Fix $\epsilon>0$, and let $\left\{f_{1}, \ldots, f_{M}\right\} \subseteq \mathcal{F}$ be a subset of $\mathcal{F}$ such that for each $x \in \mathcal{X}$, we have $\ell_{f_{v}}(x) \leq \epsilon$ for at most one value of $v \in\{1, \ldots, M\}$. Then we have

$$
\begin{equation*}
\mathcal{M}_{n}(\mathcal{F}) \geq \epsilon \cdot\left(1-\frac{I(V ; \mathbf{X}, \mathbf{Y})+\log 2}{\log M}\right) \tag{1}
\end{equation*}
$$

where $V$ is uniform on $\{1, \ldots, M\}$, and $I(V ; \mathbf{X}, \mathbf{Y})$ is w.r.t $V \rightarrow f_{V} \rightarrow(\mathbf{X}, \mathbf{Y})$.

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- Claim 2. In the special case $M=2$, we have

$$
\begin{equation*}
\mathcal{M}_{n}(\mathcal{F}) \geq \epsilon \cdot H_{2}^{-1}(\log 2-I(V ; \mathbf{X}, \mathbf{Y})) \tag{2}
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where $H_{2}^{-1}(\cdot) \in[0,0.5]$ is the inverse binary entropy function.

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- Proof is like with estimation, starting with Markov's inequality:

$$
\sup _{f \in \mathcal{F}} \mathbb{E}_{f}\left[\ell_{f}(\hat{X})\right] \geq \sup _{f \in \mathcal{F}} \epsilon \cdot \mathbb{P}_{f}\left[\ell_{f}(\hat{X}) \geq \epsilon\right] .
$$

- Proof for $M=2$ uses a (somewhat less well-known) form of Fano's inequality for binary hypothesis testing


## Strongly Convex Class: Choice of Hard Subset

- Reduction to hyp. testing. In 1D, it suffices to choose just two similar functions!
- (Becomes $2^{\text {constant } \times d}$ in $d$ dimensions)



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- Reduction to hyp. testing. In 1D, it suffices to choose just two similar functions!
- (Becomes $2^{\text {constant } \times d}$ in $d$ dimensions)

- The precise functions:

$$
\begin{gathered}
f_{v}(x)=\frac{1}{2}\left(x-x_{v}^{*}\right)^{2}, \quad v=1,2, \\
x_{1}^{*}=\frac{1}{2}-\sqrt{2 \epsilon^{\prime}} \quad x_{2}^{*}=\frac{1}{2}+\sqrt{2 \epsilon^{\prime}}
\end{gathered}
$$

## Analysis

- Application of Fano's Inequality. As above,

$$
\mathcal{M}_{n}(\mathcal{F}) \geq \epsilon \cdot H_{2}^{-1}(\log 2-I(V ; \mathbf{X}, \mathbf{Y}))
$$

- Approach: $H_{2}^{-1}(\alpha) \geq \frac{1}{10}$ if $\alpha \geq \frac{\log 2}{2}$
- How few samples ensure $I(V ; \mathbf{X}, \mathbf{Y}) \leq \frac{\log 2}{2}$ ?


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- Bounding the Mutual Information. Let $P_{Y}, P_{Y^{\prime}}$ be the observation distributions (function and gradient), and $Q_{Y}, Q_{Y^{\prime}}$ similar but with $f_{0}(x)=\frac{1}{2} x^{2}$. Then:

$$
D\left(P_{Y} \times P_{Y^{\prime}} \| Q_{Y} \times Q_{Y^{\prime}}\right)=\frac{\left(f_{1}(x)-f_{0}(x)\right)^{2}}{2 \sigma^{2}}+\frac{\left(f_{1}^{\prime}(x)-f_{0}^{\prime}(x)\right)^{2}}{2 \sigma^{2}}
$$

- Simplifications: $\left(f_{1}(x)-f_{0}(x)\right)^{2} \leq\left(\epsilon+\sqrt{\frac{\epsilon}{2}}\right)^{2} \leq 2 \epsilon$ and $\left(f_{1}^{\prime}(x)-f_{0}^{\prime}(x)\right)^{2}=2 \epsilon$
- With some manipulation, $I(V ; \mathbf{X}, \mathbf{Y}) \leq \frac{\log 2}{2}$ when $\epsilon=\frac{\sigma^{2} \log 2}{4 n}$


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- With some manipulation, $I(V ; \mathbf{X}, \mathbf{Y}) \leq \frac{\log 2}{2}$ when $\epsilon=\frac{\sigma^{2} \log 2}{4 n}$
- Final result: $\mathcal{M}_{n}(\mathcal{F}) \geq \frac{\sigma^{2} \log 2}{40 n}$


## Upper vs. Lower Bounds

- Lower bound for 1D strongly convex functions: $\mathcal{M}_{n}(\mathcal{F}) \geq c \frac{\sigma^{2}}{n}$
- Upper bound for 1D strongly convex functions: $\mathcal{M}_{n}(\mathcal{F}) \leq c^{\prime} \frac{\sigma^{2}}{n}$
- Achieved by stochastic gradient descent
- Analogous results (and proof techniques) known for $d$-dimensional functions, additional Lipschitz assumptions, etc. [Raginsky and Rakhlin, 2011]


# Continuous Example 3 

Density Estimation

## Density Estimation Example

- An example density estimation problem:
- Goal: Estimate the density $f$ given $n$ i.i.d. samples
- Here we consider random variables defined on $[0,1]$, and consider the class $\mathcal{F}_{\eta, \Gamma}$ of density functions satisfying the following:

$$
f(y) \geq \eta, \forall y \in[0,1], \quad\|f\|_{\mathrm{TV}} \leq \Gamma
$$

where $\|f\|_{\mathrm{TV}}=\sup _{L} \sup _{0 \leq x_{1} \leq \ldots \leq x_{L} \leq 1} \sum_{l=2}^{L}\left(f\left(x_{l}\right)-f\left(x_{l-1}\right)\right)$.

- We measure performance via the $\ell_{2}^{2}$-loss:

$$
\ell(f, \hat{f})=\|f-\hat{f}\|_{2}^{2}=\int_{0}^{1}(f(x)-\hat{f}(x))^{2} d x
$$

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$$

- Claim: For constant $\eta$ and $\Gamma$, attaining $\mathcal{M}_{n}(\eta, \Gamma) \leq \delta$ requires $n \geq c\left(\frac{1}{\delta}\right)^{3 / 2}$.
- This scaling is tight; a matching upper bound is known
- The proof uses the global packing/covering approach
- See our survey introductory guide to Fano's inequality for this specific example, or Yang/Barron's original paper for many more classes


## Limitations and Generalizations

## Limitations and Generalizations

- Limitations of Fano's Inequality.
- Non-asymptotic weakness
- Often hard to tightly bound mutual information in adaptive settings
- Restriction to KL divergence
- Other useful measures: Total variation, Hellinger distance, $\chi^{2}$-divergence, etc.
- Generalizations of Fano's Inequality.
- Non-uniform V
- More general $f$-divergences
- Continuous $V$
[Han/Verdú, 1994]
[Guntuboyina, 2011]
[Duchi/Wainwright, 2013]
(This list is certainly incomplete!)


## Example: Difficulties in Adaptive Settings

- A simple search problem: Find the (only) biased coin using few flips

- Heavy coin $V \in\{1, \ldots, M\}$ uniformly at random
- Selected coin at time $i=1, \ldots, n$ is $X_{i}$, observation is $Y_{i} \in\{0,1\}$ (1 for heads)


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- Since $X_{i}$ and $V$ are independent, can show $I\left(V ; Y_{i} \mid X_{i}\right) \lesssim \frac{\epsilon^{2}}{M}$
- Substituting into Fano's inequality gives the requirement $n \gtrsim \frac{M \log M}{\epsilon^{2}}$


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- Substituting into Fano's inequality gives the requirement $n \gtrsim \frac{M \log M}{\epsilon^{2}}$
- Adaptive setting:
- Nuisance to characterize $I\left(V ; Y_{i} \mid X_{i}\right)$, as $X_{i}$ depends on $V$ due to adaptivity!
- Worst-case bounding only gives $n \gtrsim \frac{\log M}{\epsilon^{2}}$
- Next lecture: An alternative tool that gives $n \gtrsim \frac{M}{\epsilon^{2}}$


## Conclusion

- Information theory as a theory of data:



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- Approach highlighted in this talk:
- Reduction to multiple hypothesis testing
- Application of Fano's inequality
- Bounding the mutual information


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- Approach highlighted in this talk:
- Reduction to multiple hypothesis testing
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- Examples:
- Group testing
- Graphical model selection
- Sparse regression
- Convex optimization
- ...and many more!


## Tutorial Chapter

- Tutorial Chapter: "An Introductory Guide to Fano's Inequality with Applications in Statistical Estimation" [S. and Cevher, 2019]
https://arxiv.org/abs/1901.00555
(Chapter in 2021 book Information-Theoretic Methods in Data Science, Cambridge University Press)

