Permutation Methods for Comparing Distributions

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Outline of this talk

(1) Introduction to Hypothesis Testing

(2) Permutation Tests

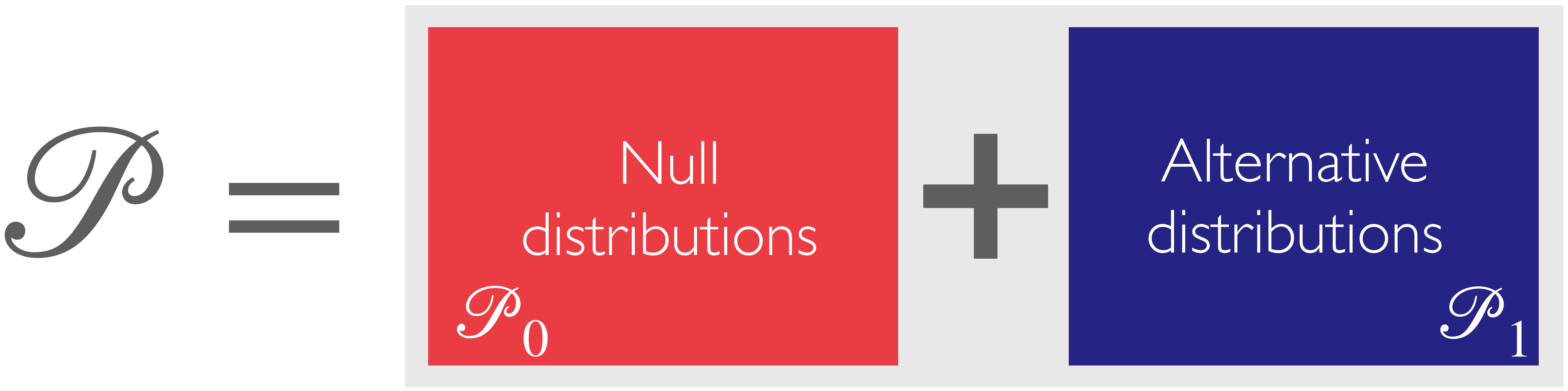
(3) Methods: Regression and Classification-based Approaches

(4) Theory: Power Analysis

(5) Summary

Recap: Statistical Hypothesis Testing

- Consider a class of distributions $\mathscr{P} = \mathscr{P}_0 \cup \mathscr{P}_1$



Recap: Statistical Hypothesis Testing

- Consider a class of distributions $\mathscr{P} = \mathscr{P}_0 \cup \mathscr{P}_1$

$$\mathscr{P} = \boxed{\text{Null distributions } \mathscr{P}_0} + \boxed{\text{Alternative distributions } \mathscr{P}_1}$$

- Given $X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} P \in \mathscr{P}$, **our goal** is to determine

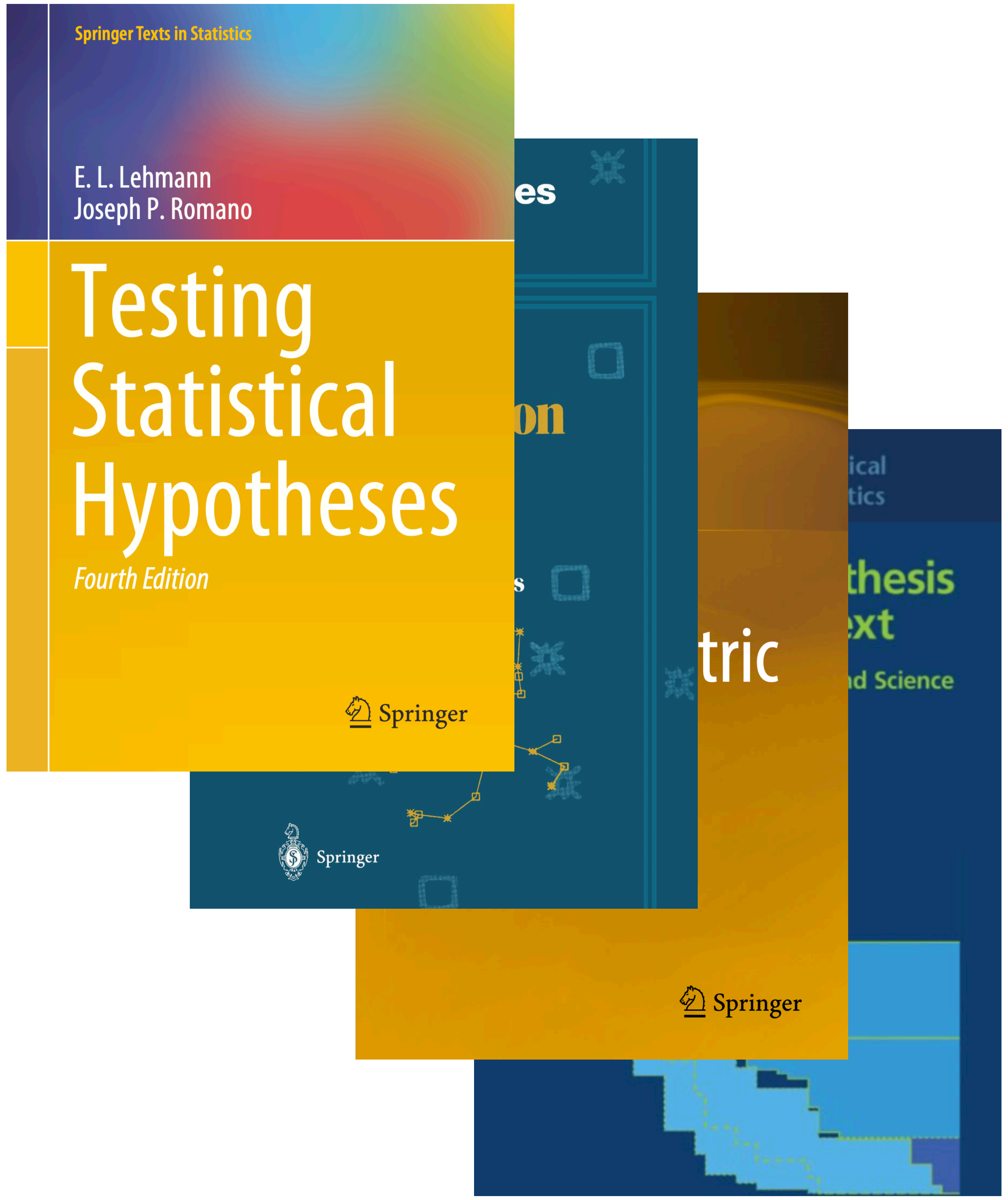
$$H_0 : P \in \mathscr{P}_0 \quad \text{versus} \quad H_1 : P \in \mathscr{P}_1$$

Recap: Statistical Hypothesis Testing

Examples include

- Mean testing
- Covariance testing
- Testing for regression models
- Two-sample testing
- Independence testing

$$\vdots$$



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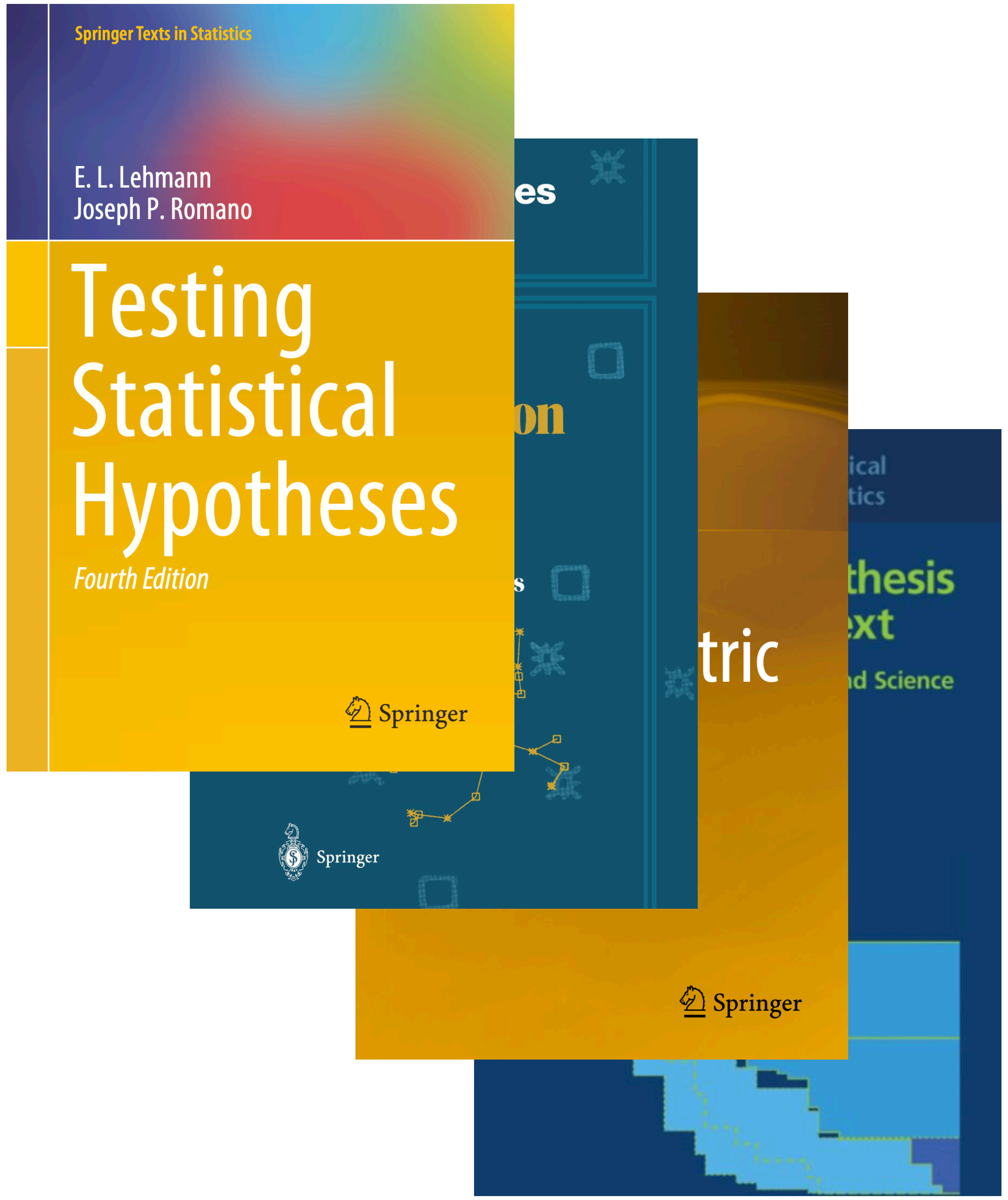
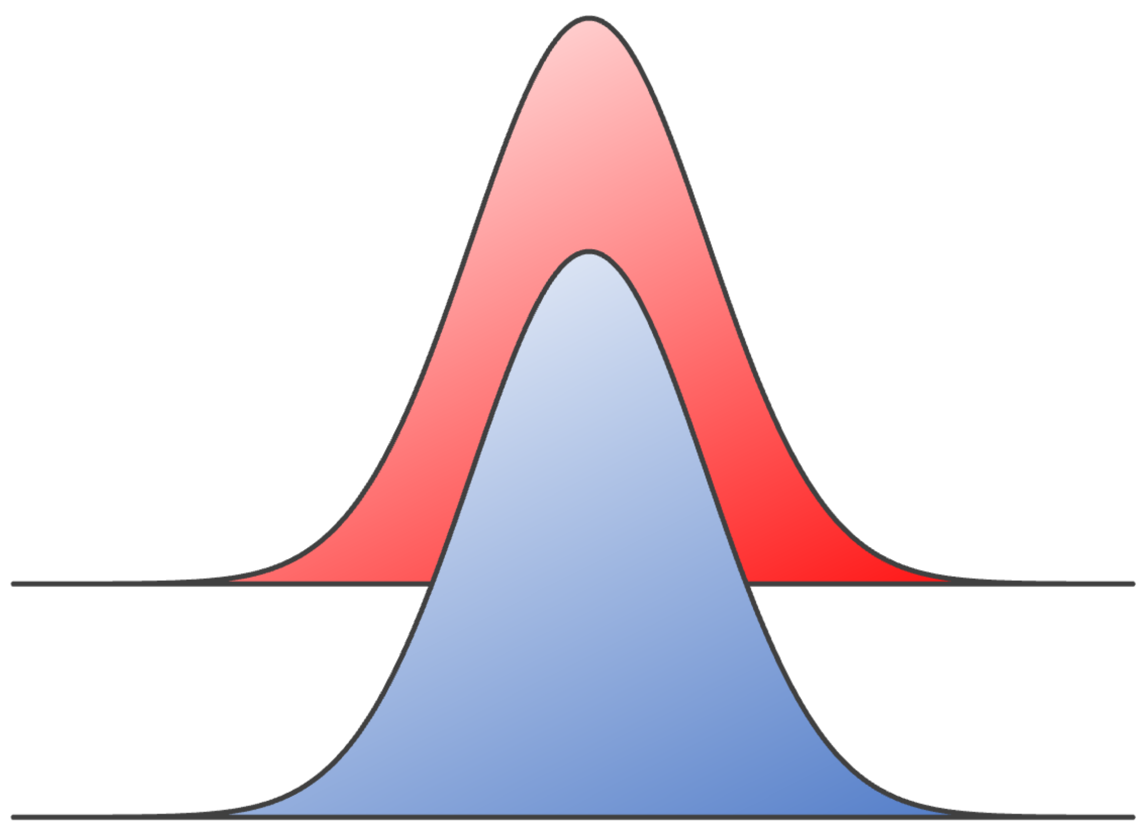


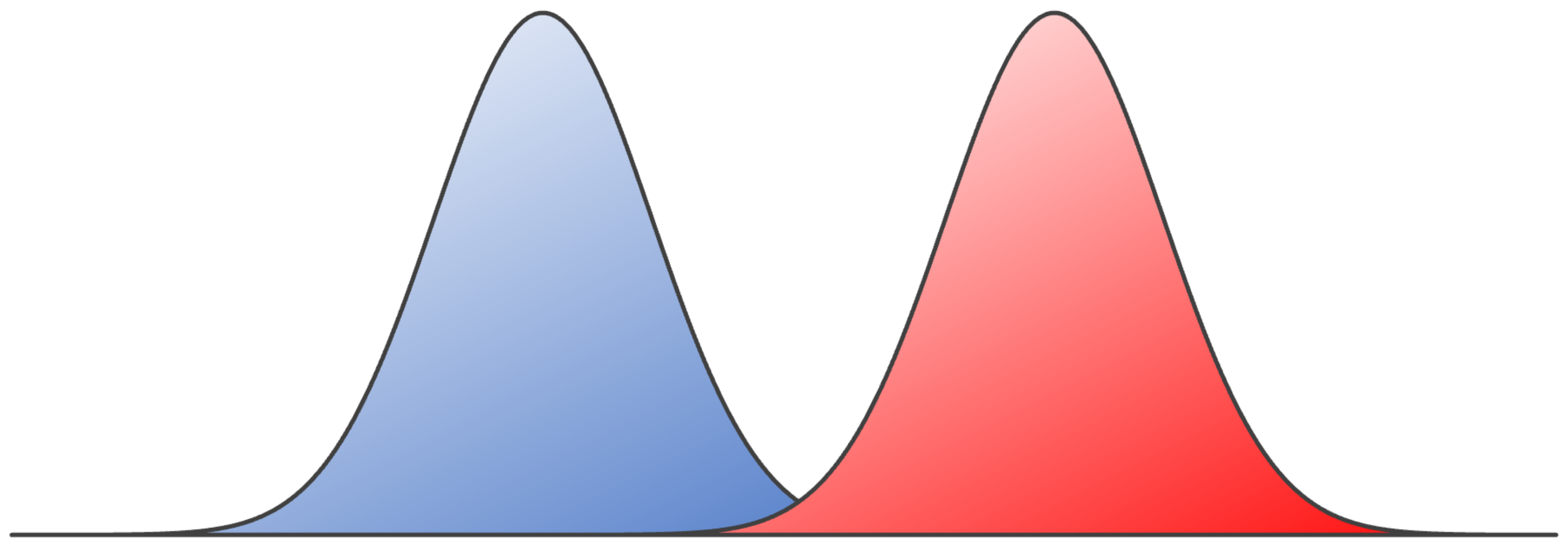
Two-Sample Problem

- Given $\{X_1, \ldots, X_n\} \overset{\text{i.i.d.}}{\sim} P_X$ and $\{Y_1, \ldots, Y_m\} \overset{\text{i.i.d.}}{\sim} Q_Y$ we want to test whether



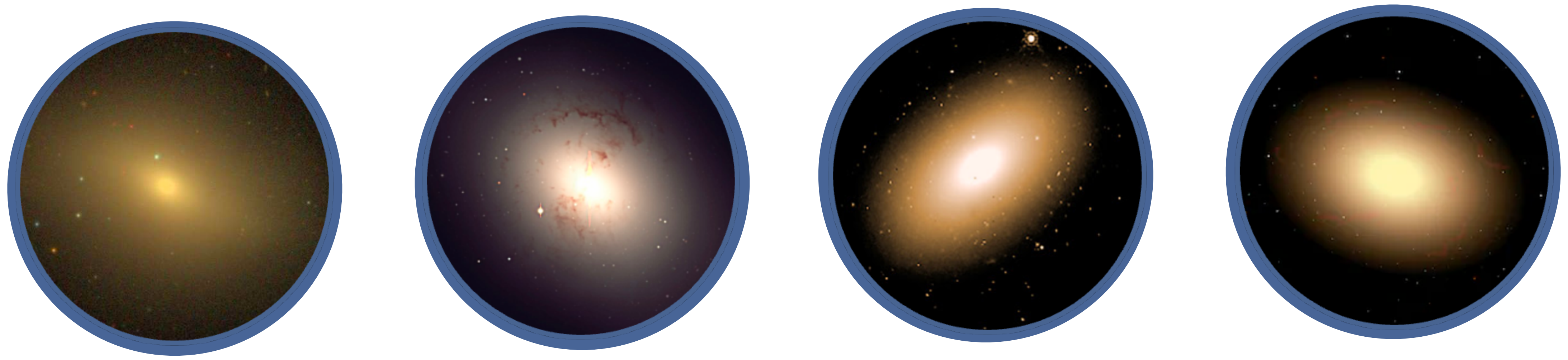
$H_0 : P_X = Q_Y$

versus



$H_1 : P_X \neq Q_Y$

Applications: Astronomy



High-mass versus Low-mass galaxies

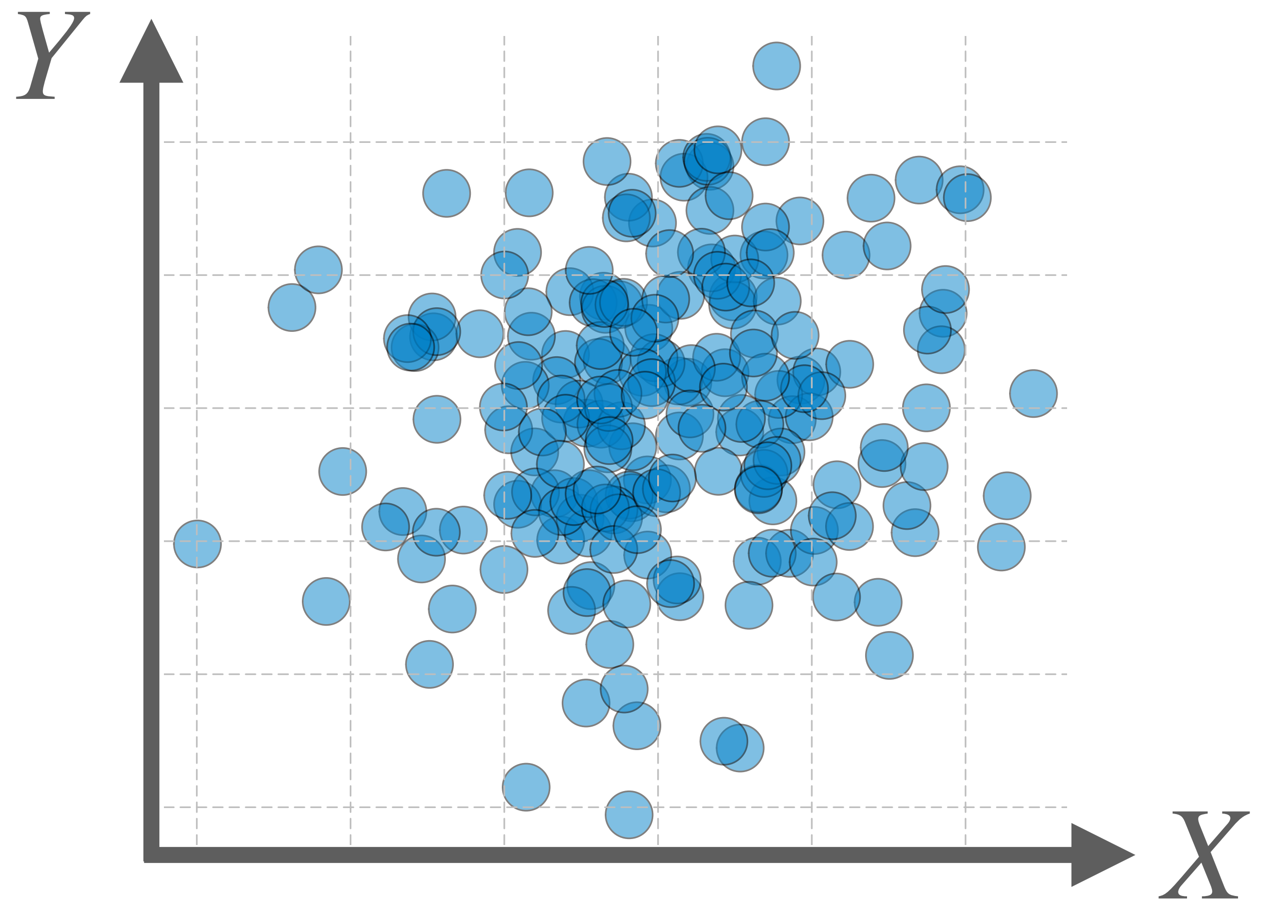
Applications: Machine Learning

$\sim P_{\text{real}}$

$\sim Q_{\text{artificial}}$

Independence Testing Problem

- Given $\{(X_1, Y_1), \ldots, (X_n, Y_n)\} \overset{\text{i.i.d.}}{\sim} P_{X,Y}$
  we want to test whether



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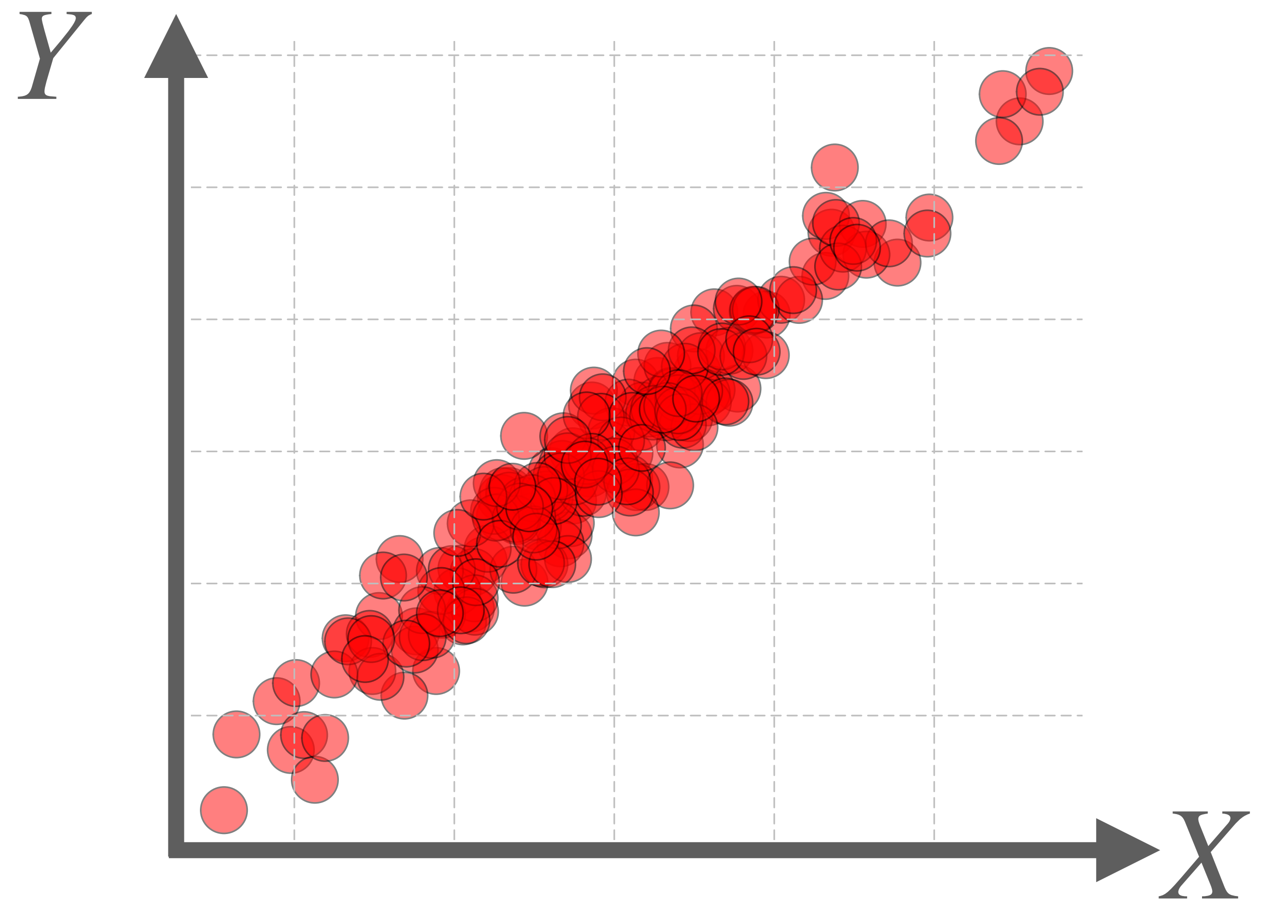

$H_1 : P_{X,Y} \neq P_X P_Y$

Applications: Multimodal Learning

X	Y
	The image shows a brown horse with a white blaze on its face, trotting in an open grassy field.
	The image shows a majestic tiger resting on the grass, accompanied by a young tiger cub.
	The image depicts a bald eagle in mid-flight, soaring through the sky with its wings fully spread.

Recap: Statistical Hypothesis Testing

- To tackle the testing problem, we construct a test function

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- We reject the null if $\phi = 1$ and accept the null if $\phi = 0$

- There are two types of error we care about

(Uniform) **Type I error:** $\sup_{P \in \mathcal{P}_0} \mathbb{P}_P(\phi = 1)$

(Uniform) **Type II error:** $\sup_{P \in \mathcal{P}_1} \mathbb{P}_P(\phi = 0)$

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Recap: Statistical Hypothesis Testing

- Frequently, the **Type I error** is more **serious** than the **Type II error**
- Hence we **first** control the **Type I error** by level α
- And then try to **minimize** the **Type II error** (or maximize the power)

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Recap: Statistical Hypothesis Testing

A typical way of constructing a test function

Step 1

Compute a test statistic

e.g.,

$$T_n = \frac{\overline{X} - \mu_0}{s/\sqrt{n}}$$

$$\chi_n^2 = \sum_k \frac{(O_k - E_k)^2}{E_k}$$

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Step II

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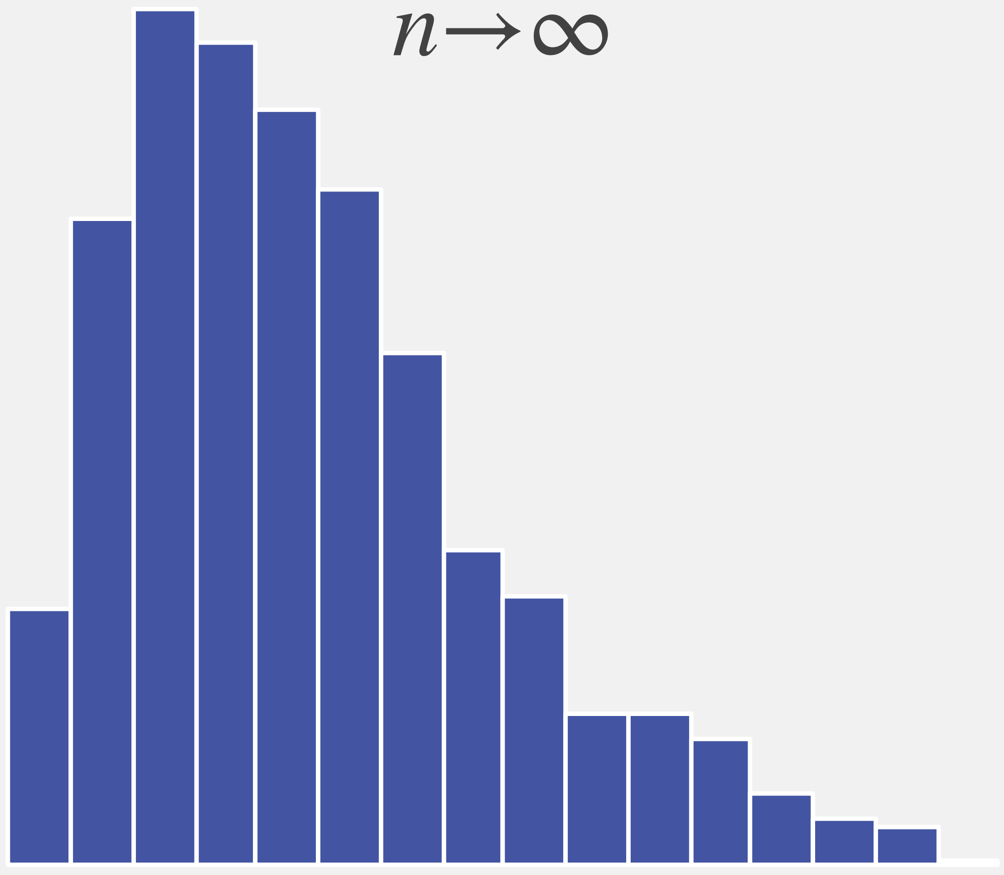
$$\lim_{n\to\infty} \mathbb{P}(T_n \leq t)$$



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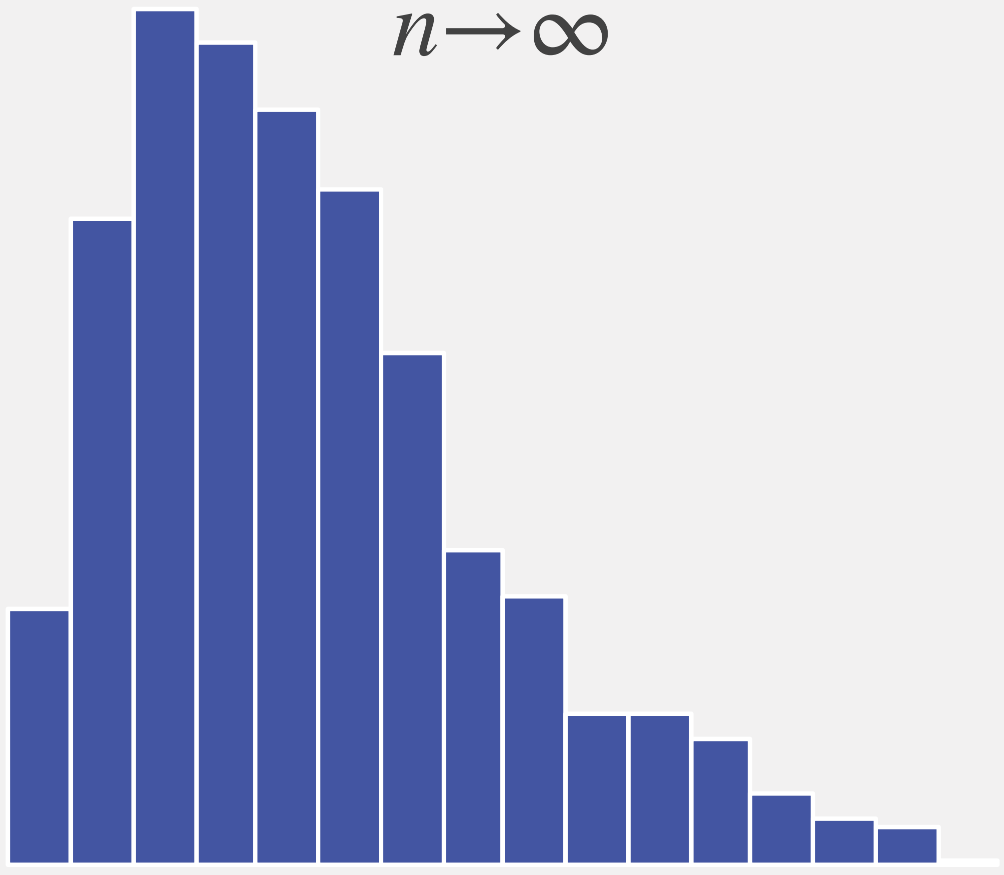
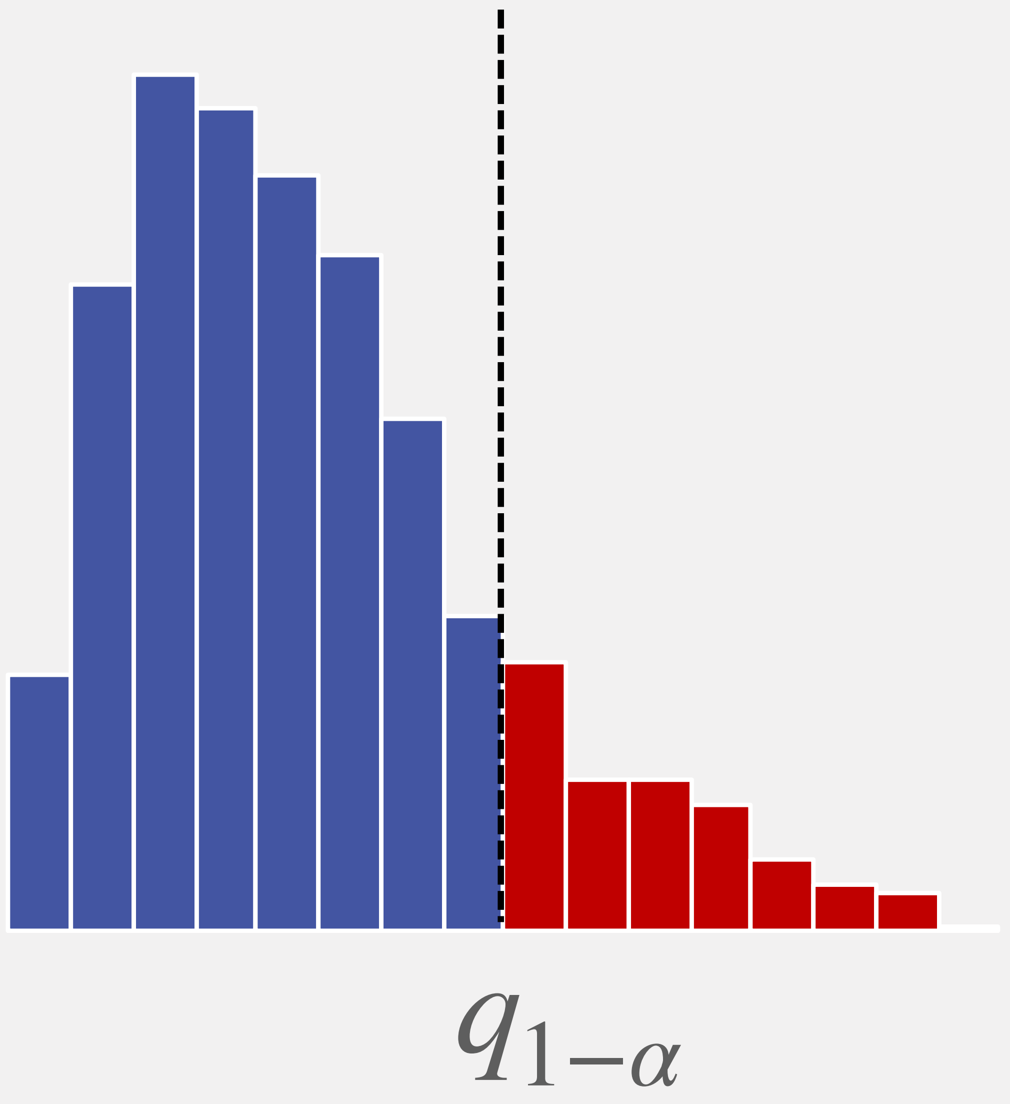


Step III

Reject H_0 if $T_n > q_{1-\alpha}$



New Challenges

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- Modern data are often **large**, **high-dimensional** **and** **complex**
- Classical **asymptotic** approaches suffer from
    - Inflated type I error
    - Suboptimal power
    - Strong assumptions

Example: χ^2-statistic in high-dimensions

Observed values

	Cat	Dog	Lion	Duck
Male	O_{11}	O_{12}	O_{13}	O_{14}
Female	O_{21}	O_{22}	O_{23}	O_{24}

Question:

Is there a significant association between gender and favorite animals?

H_0 : Gender $\perp\!\!\!\perp$ Favorite Animals

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$\Rightarrow$

Pearson's chi-squared test

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$$\chi^2 = \sum_{i=1}^{\ell_1} \sum_{j=1}^{\ell_2} \frac{(O_{ij} - E_{ij})^2}{E_{ij}}$$

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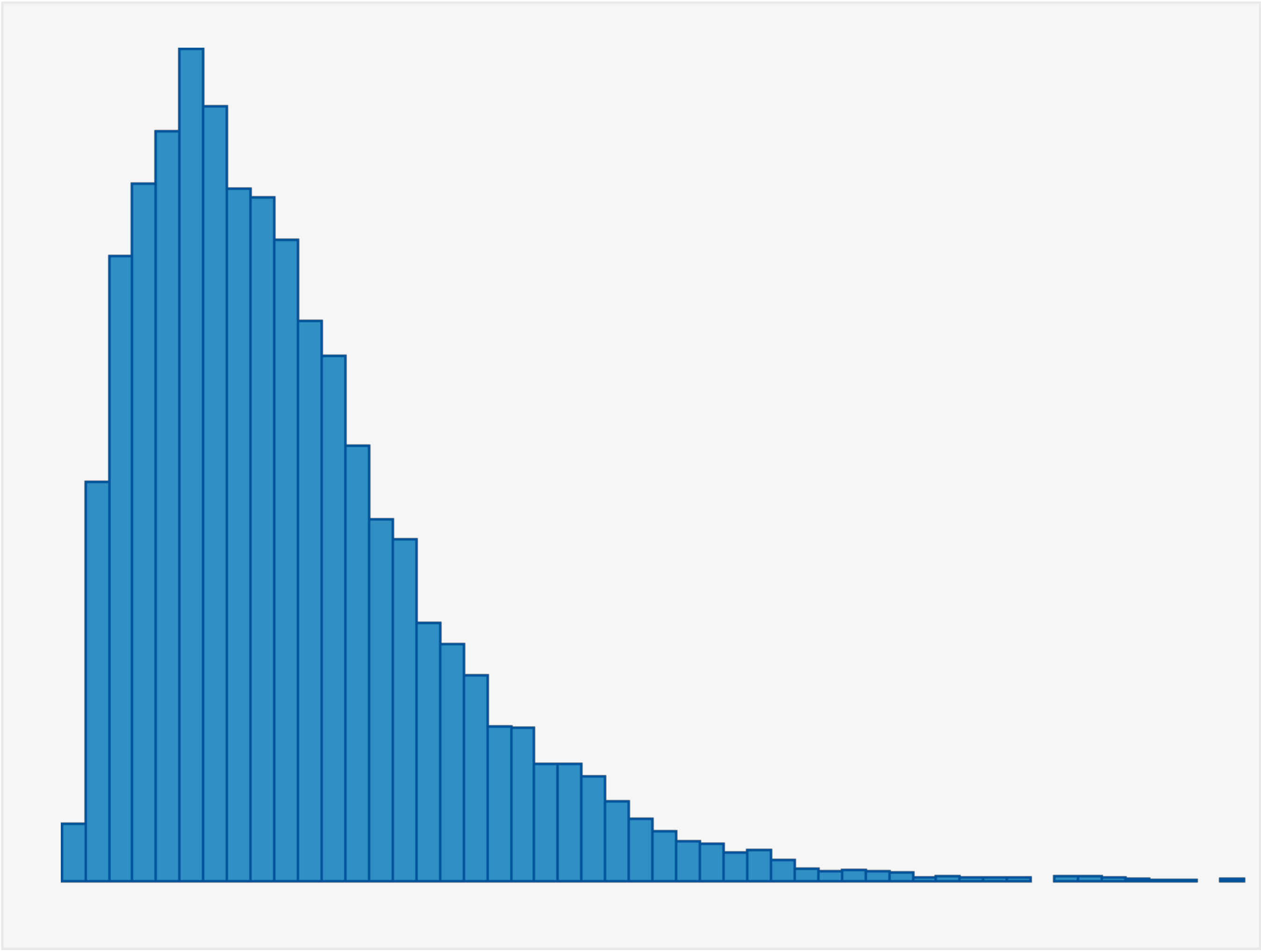
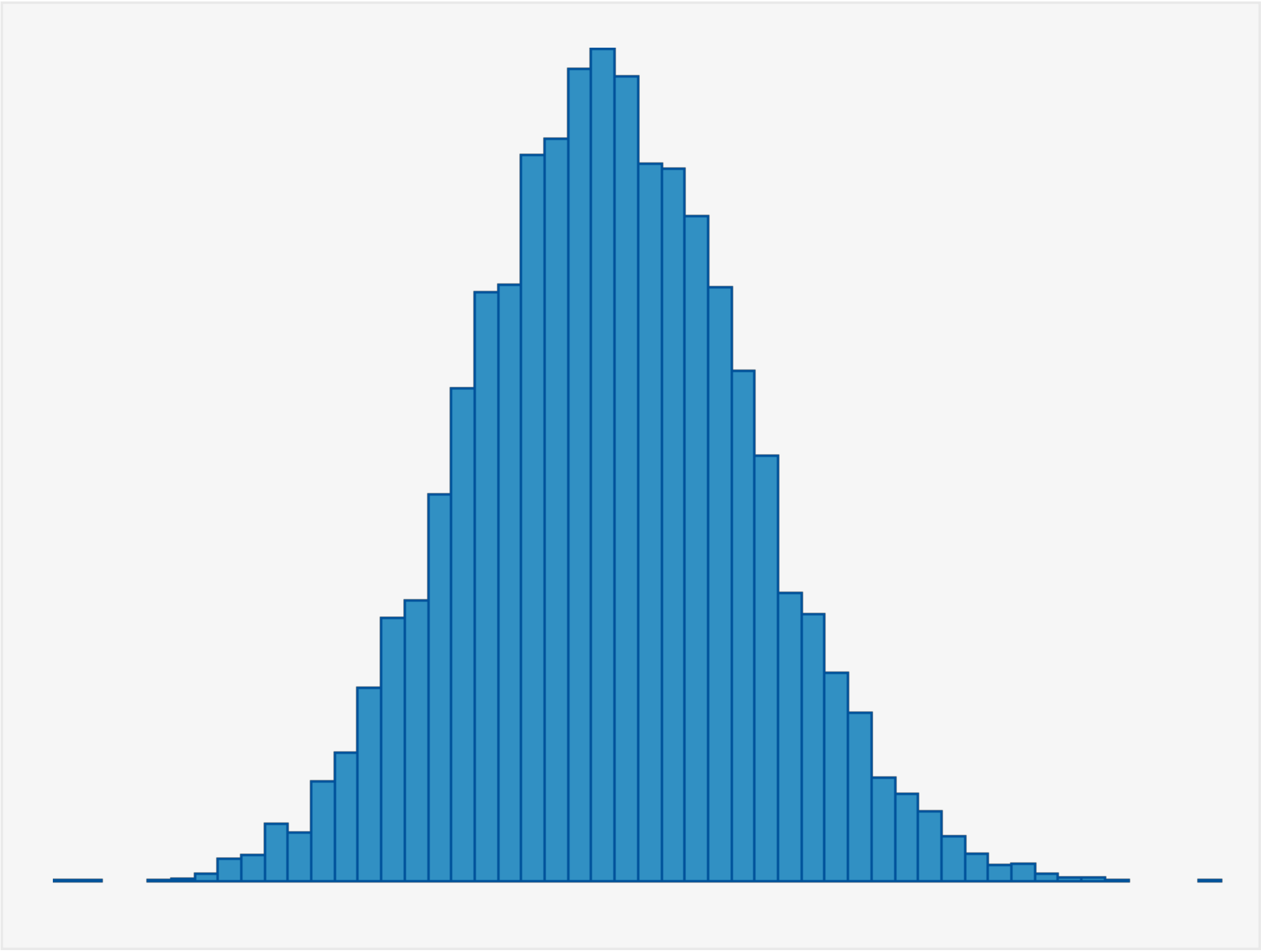
Classical asymptotic theory shows that under H_0

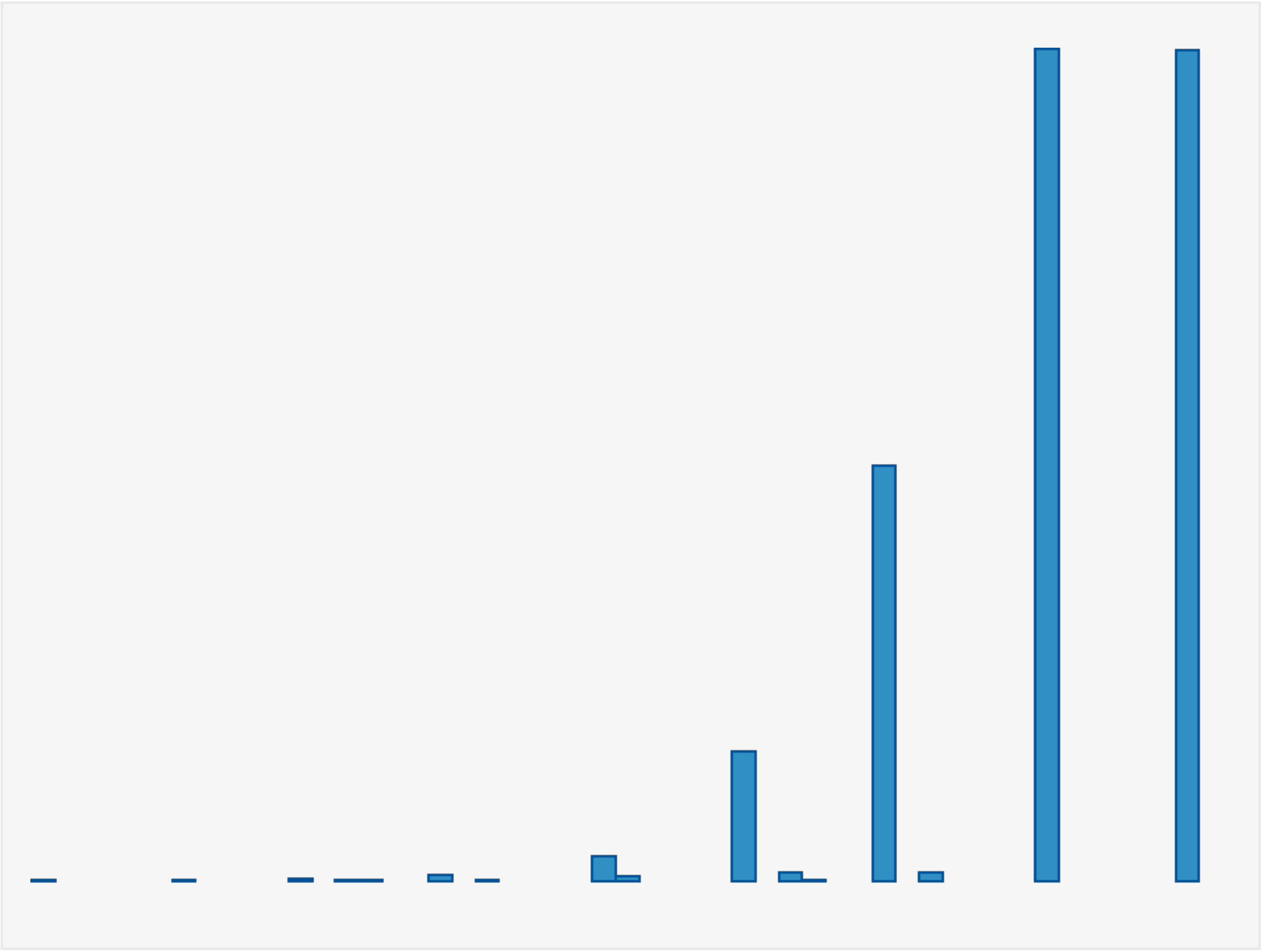
$$\boxed{\chi^2 = \sum_{i=1}^{\ell_1} \sum_{j=1}^{\ell_2} \frac{(O_{ij} - E_{ij})^2}{E_{ij}}} \quad \overset{approx.}{\sim} \quad \text{Chi-squared distribution with } (\ell_1 - 1)(\ell_2 - 1) \text{ d.f.}$$

Example: χ^2-statistic in high-dimensions

Histograms of χ^2-statistic for testing independence based on $n = 100$







$\approx$ Chi-square

$\ell_1 = \ell_2 = 3$

$\approx$ Gaussian

$\ell_1 = \ell_2 = 50$

$\approx$ Discrete

$\ell_1 = \ell_2 = 10{,}000$

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Common keyword

"Permutation tests"

- Freeman, **Kim**, Lee (2019, **MNRAS**)
- **Kim**, Lee, Lei (2019, **EJS**)
- **Kim**, Balakrishnan, Wasserman (2021, **AoS**)
- **Kim**, Balakrishnan, Wasserman (2022, **AoS**)
- **Kim**, Ramdas, Singh, Wasserman (2021, **AoS**)
- **Kim** (2021, **Bernoulli**)
- Schrab, **Kim**, Guedj, Gretton (2022, **NeurIPS**)
- **Kim**, Neykov, Balakrishnan, Wasserman (2022, **AoS**)
- Schrab, **Kim**, Albert, Laurent, Guedj, Gretton (2023, **JMRL**)
- **Kim**, Neykov, Balakrishnan, Wasserman (2023, *submitted*)
- **Kim**, Schrab (2024, *submitted*)
- Schrab, **Kim** (2024, *submitted*)
- Choi, **Kim** (2024, *submitted*)

Permutation tests

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For i = 1 to B

Sample $\{X_1, \ldots, X_n\}$

a. Permute: $X_{\pi_1}, \ldots, X_{\pi_n}$

b. Compute: T_i^π

Compare T_n with $\{T_1^\pi, \ldots, T_B^\pi\}$

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Compare T_n with $\{T_1^\pi, \ldots, T_B^\pi\}$

- Permutation p-value: $$p_{\text{perm}} = \frac{1}{B+1}\left\{1 + \sum_{i=1}^{B} \mathbb{1}(T_i^\pi \geq T_n)\right\}$$

(Reject the null when $p_{\text{perm}} \leq \alpha$)

Key features of permutation tests

$$\sup_{P \in \mathscr{P}_0} \mathbb{P}_P(p_{\text{perm}} \le \alpha) \le \alpha \quad \begin{cases} \text{for any } \alpha \in (0,1) \\ \text{for any } n \ge 1 \end{cases}$$

Class of all null distributions

- **Uniform**, **non-asymptotic** type I error control

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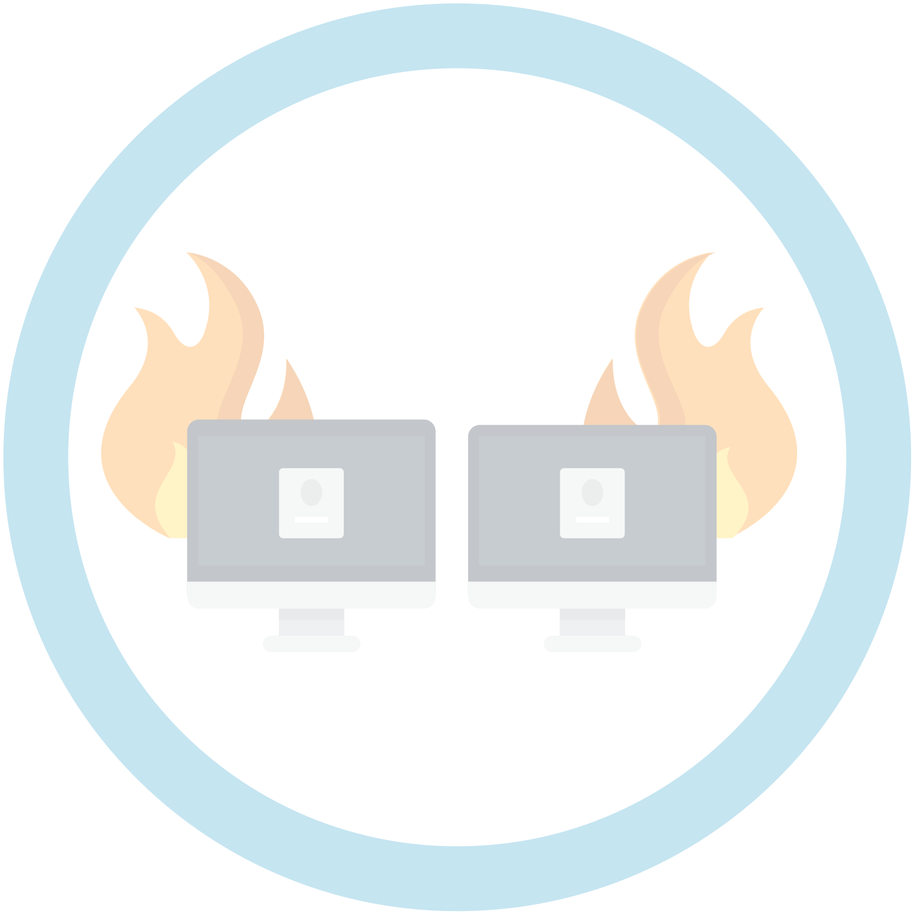
Class of all null distributions

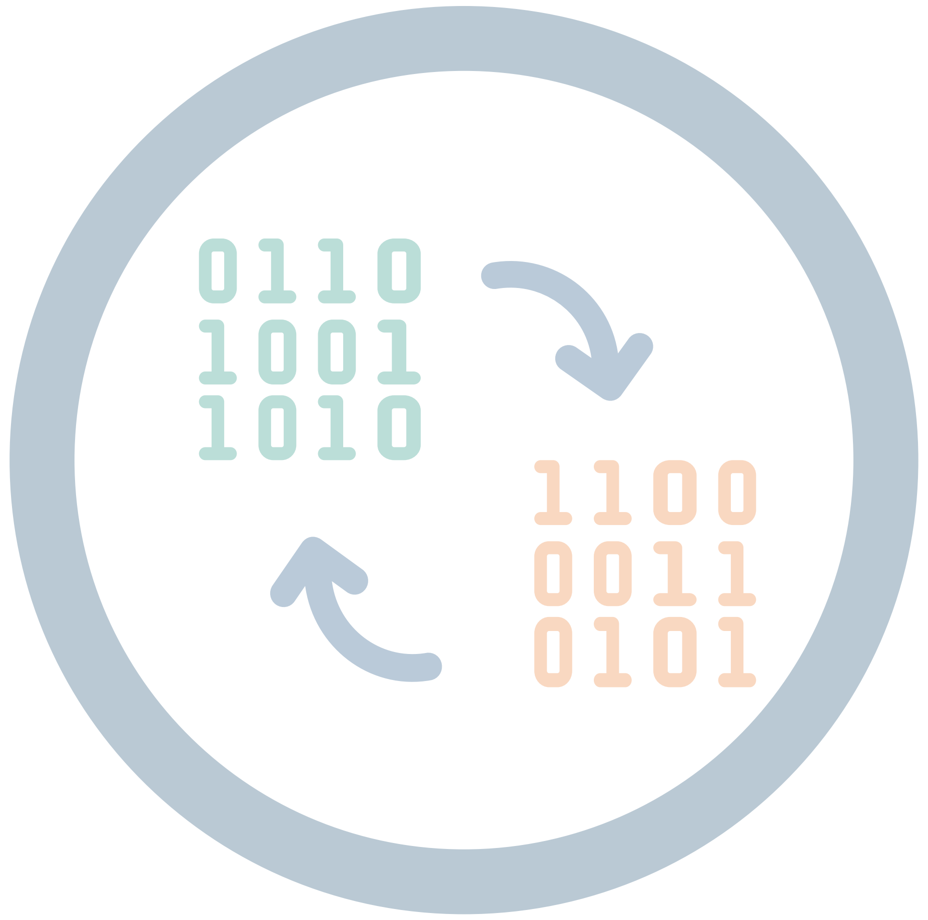
- **Uniform**, **non-asymptotic** type I error control
- **Distribution-free** for any type of test statistics
- It does not depend on **unspecified constants**
- All we need is $\{X_1, \ldots, X_n\}$ are **exchangeable** under the null

Three main challenges of the permutation approach

Power Analysis



Computational Complexity



Non-exchangeable Data

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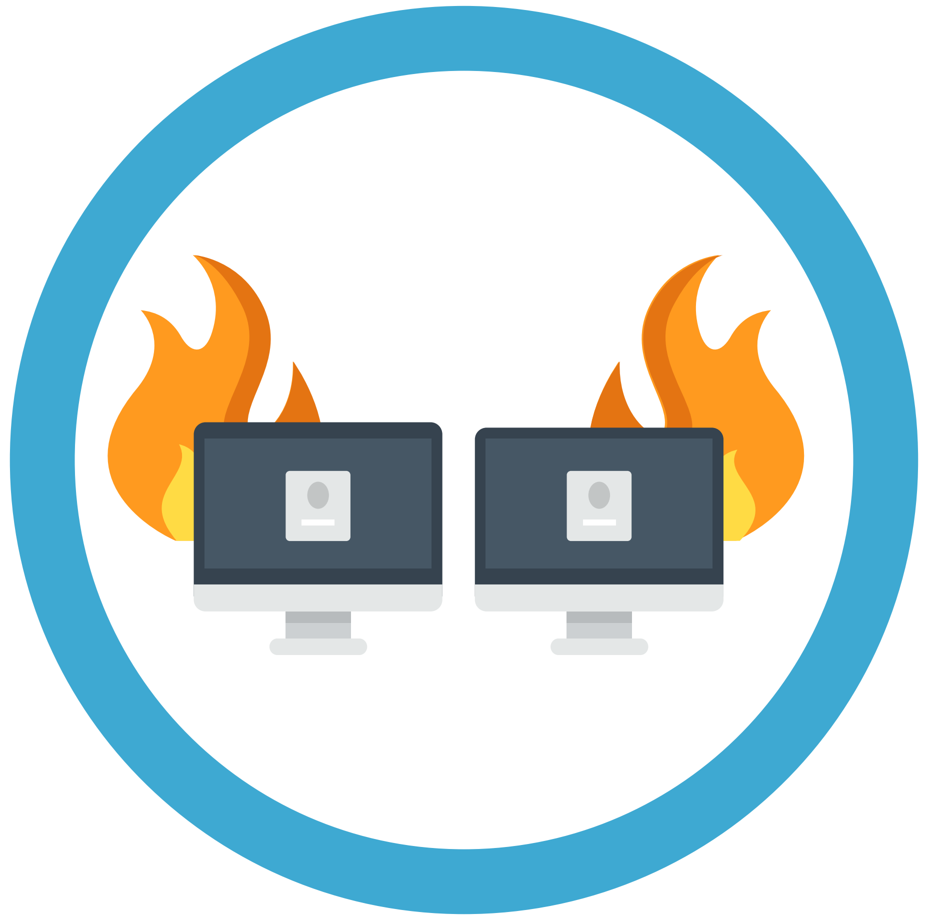

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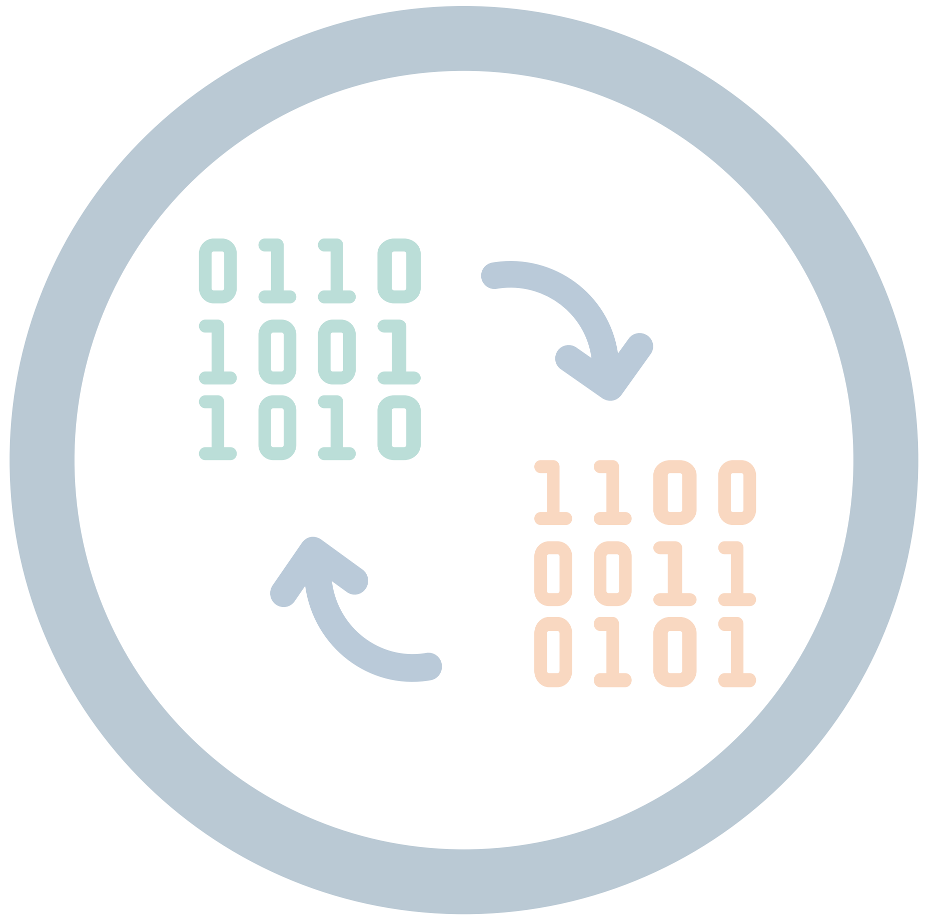

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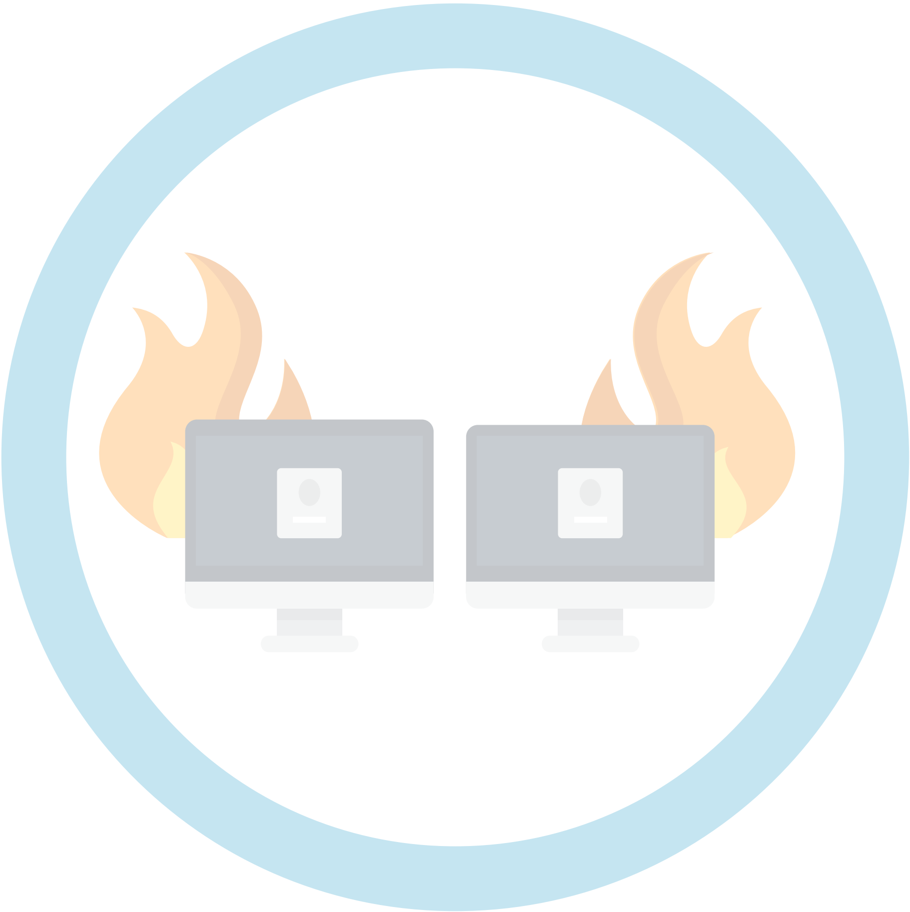

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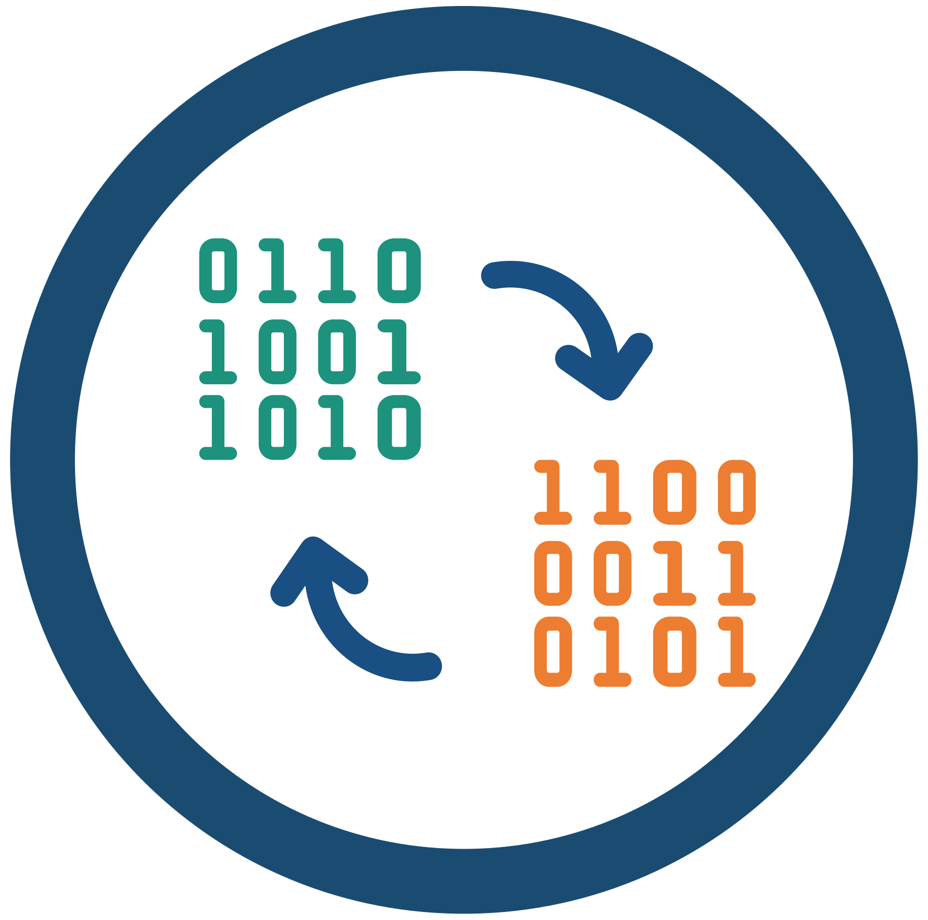

Non-exchangeable Data

Part 1. Methodological Contributions

Part II. Theoretical Contributions

Electronic Journal of Statistics
Vol. 13 (2019) 5253–5305
ISSN: 1935-7524
https://doi.org/10.1214/19-EJS1648

Global and local two-sample tests via regression

Ilmun Kim, Ann B. Lee, and Jing Lei

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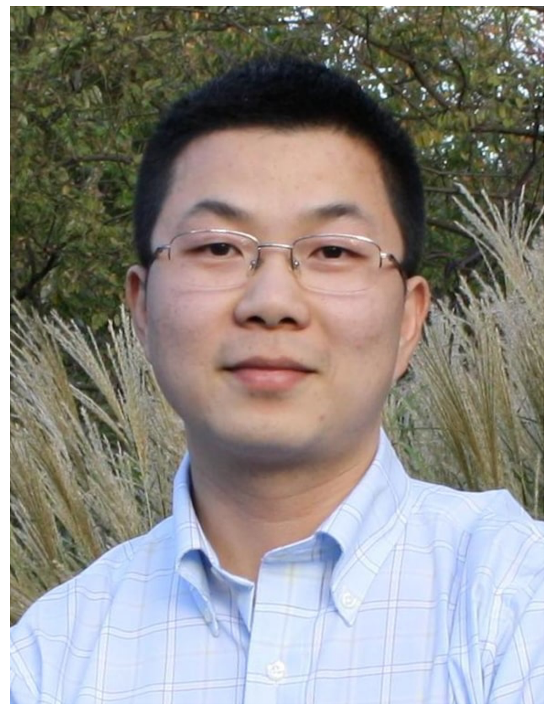
5000 Forbes Avenue
Pittsburgh, PA 15213

Ann Lee
(CMU)



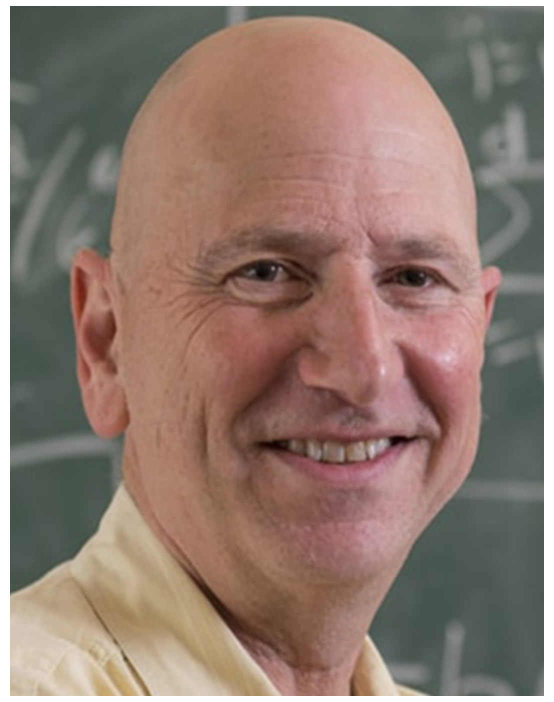
Jing Lei
(CMU)

The Annals of Statistics
2021, Vol. 49, No. 1, 411–434
https://doi.org/10.1214/20-AOS1962

CLASSIFICATION ACCURACY AS A PROXY FOR TWO-SAMPLE TESTING

BY ILMUN KIM[1,*], AADITYA RAMDAS[1,†], AARTI SINGH[1,‡] AND LARRY WASSERMAN[1,§]

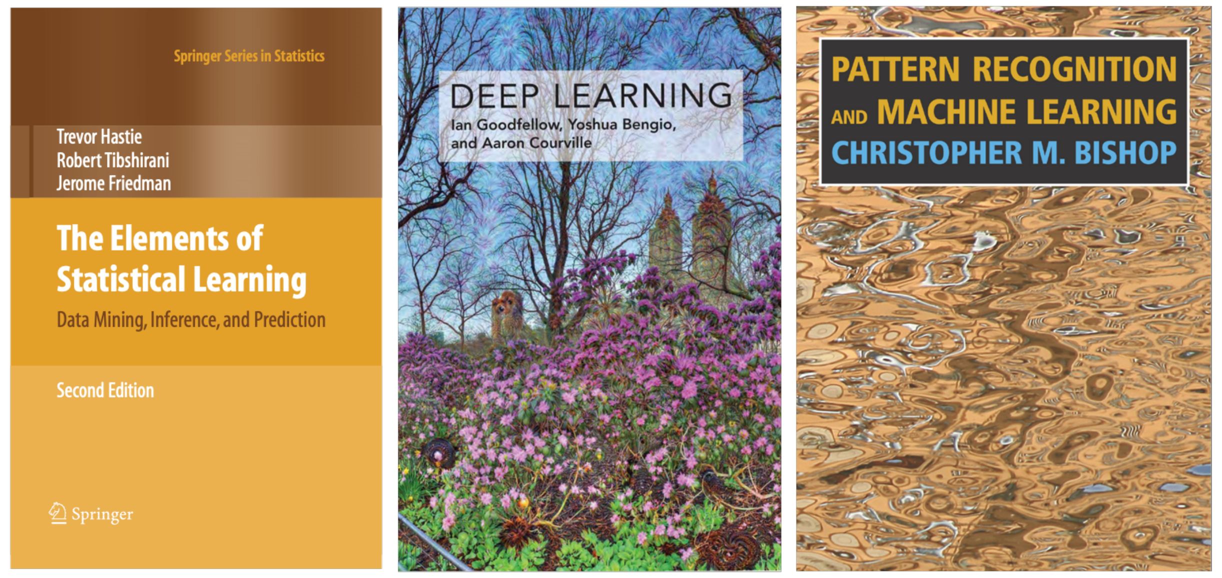
Aaditya Ramdas
(CMU)



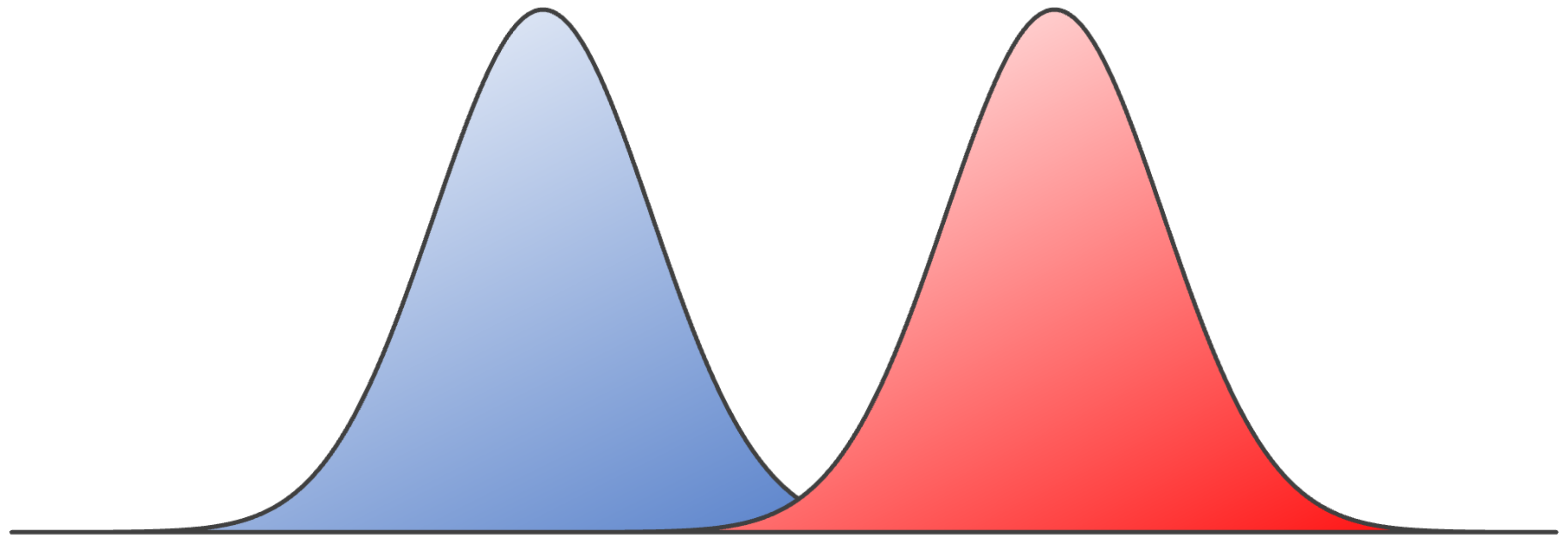
Larry Wasserman
(CMU)

Aarti Singh
(CMU)

We propose a flexible framework for two-sample testing



Classification/Regression



Two-sample test

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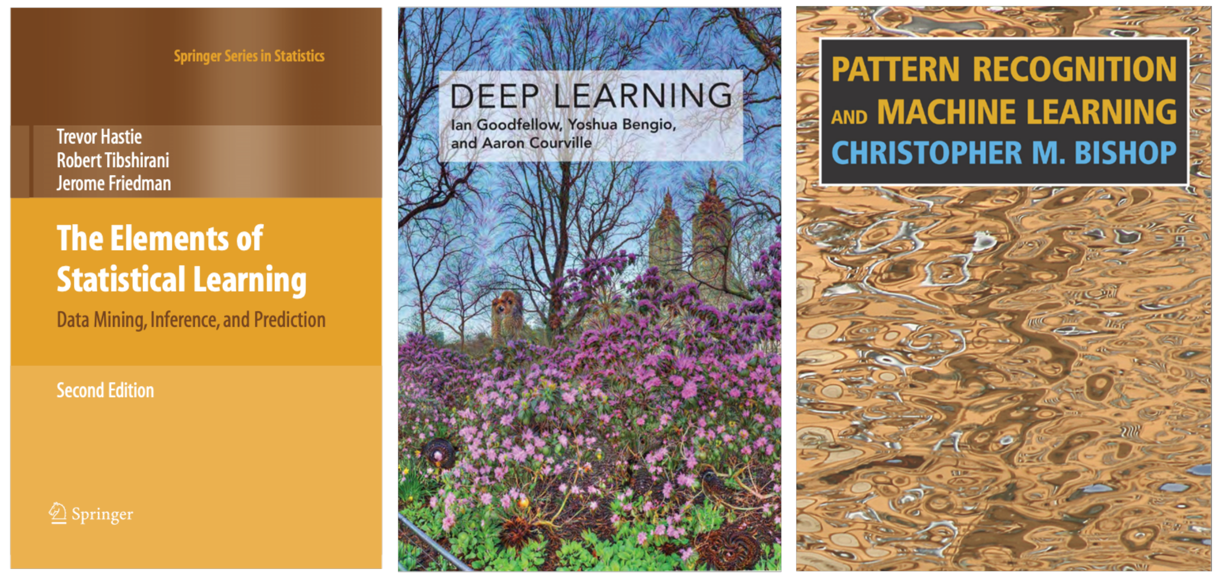

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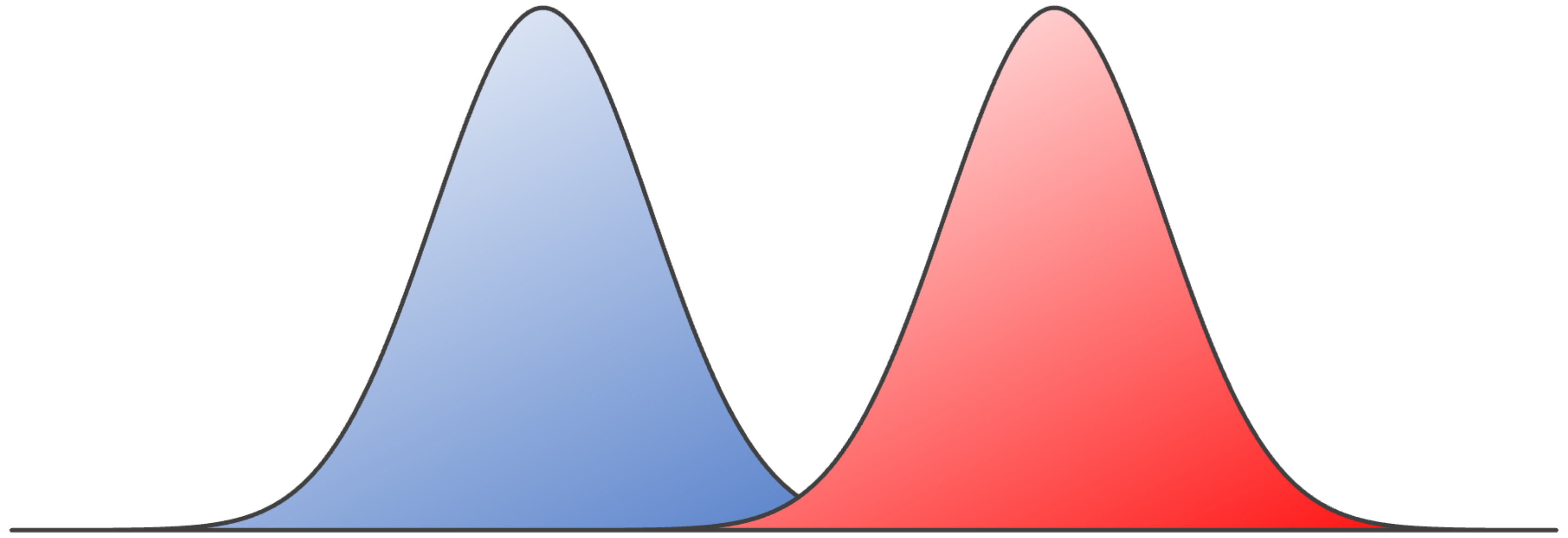

Two-sample test

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- Permutation tests present a **valid** p-value for **any** test statistic
- We can take advantage of **modern** algorithms in machine learning

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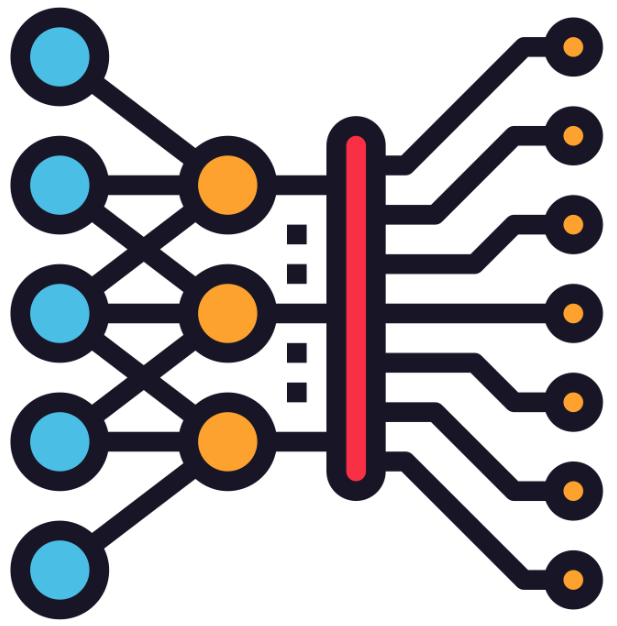
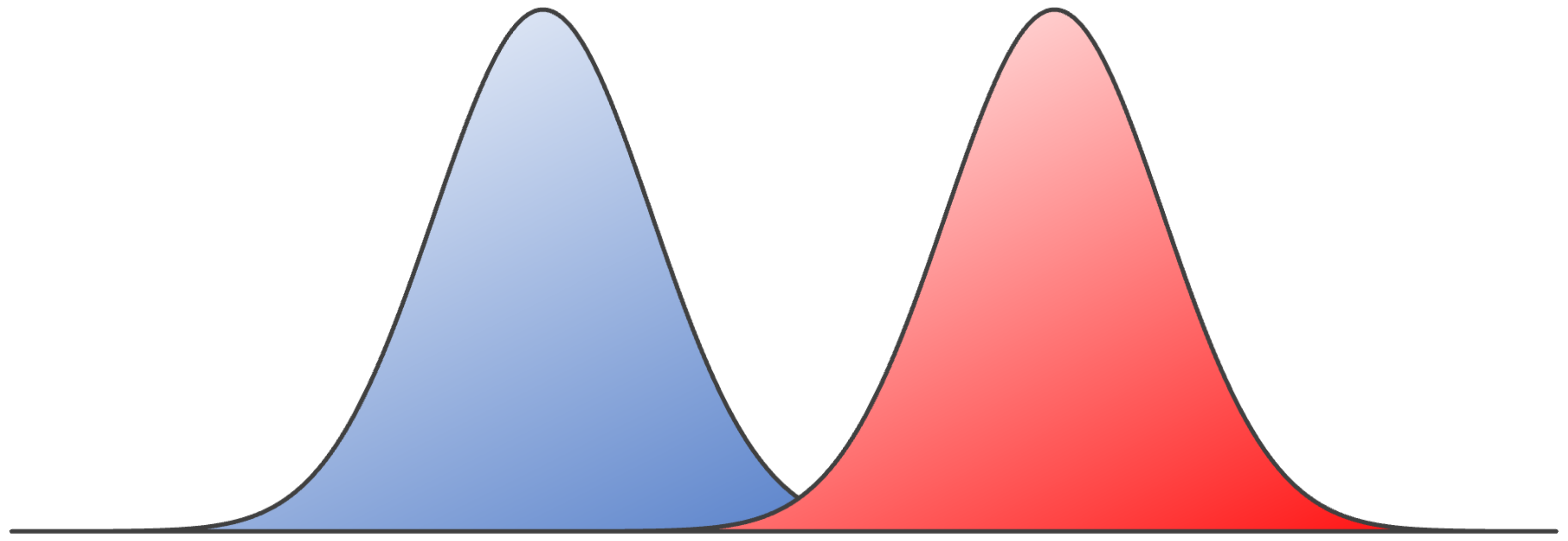


Neural networks



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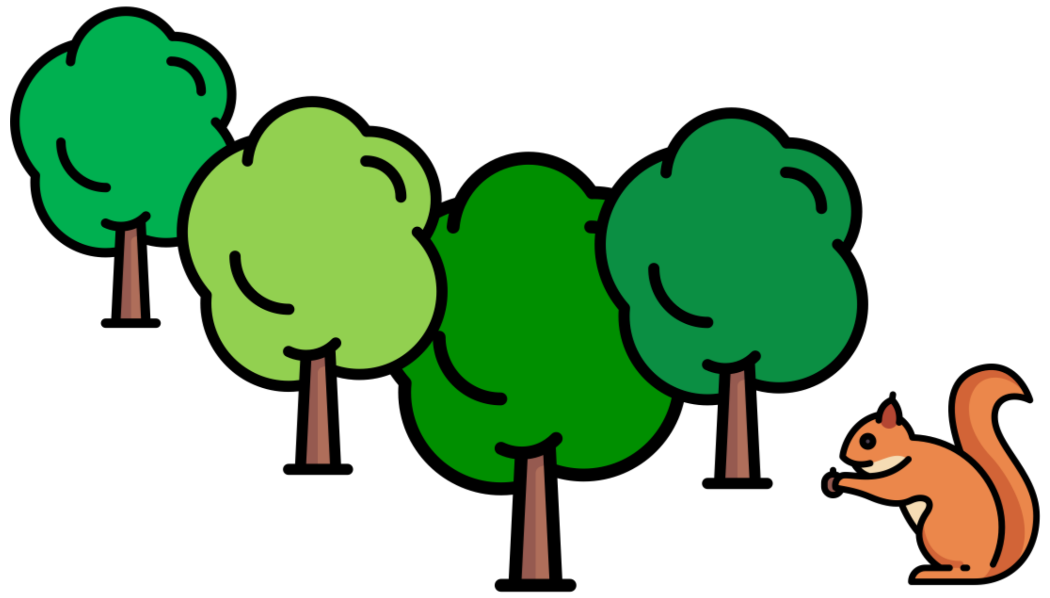
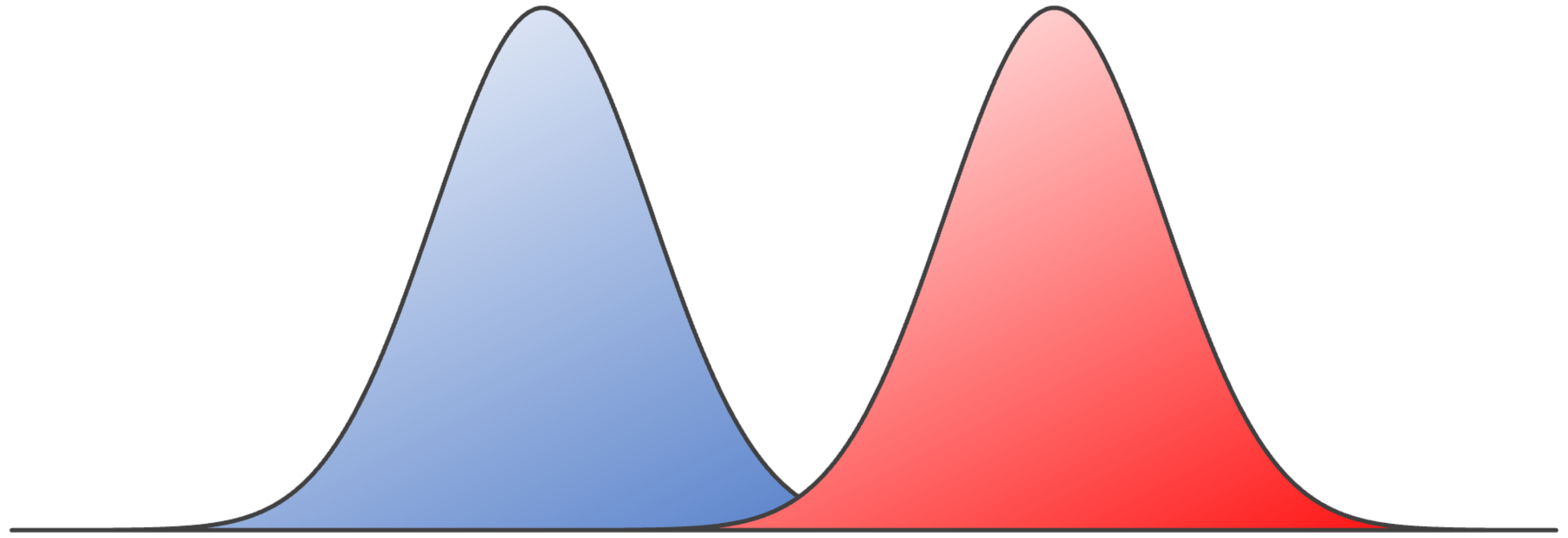


Random forests



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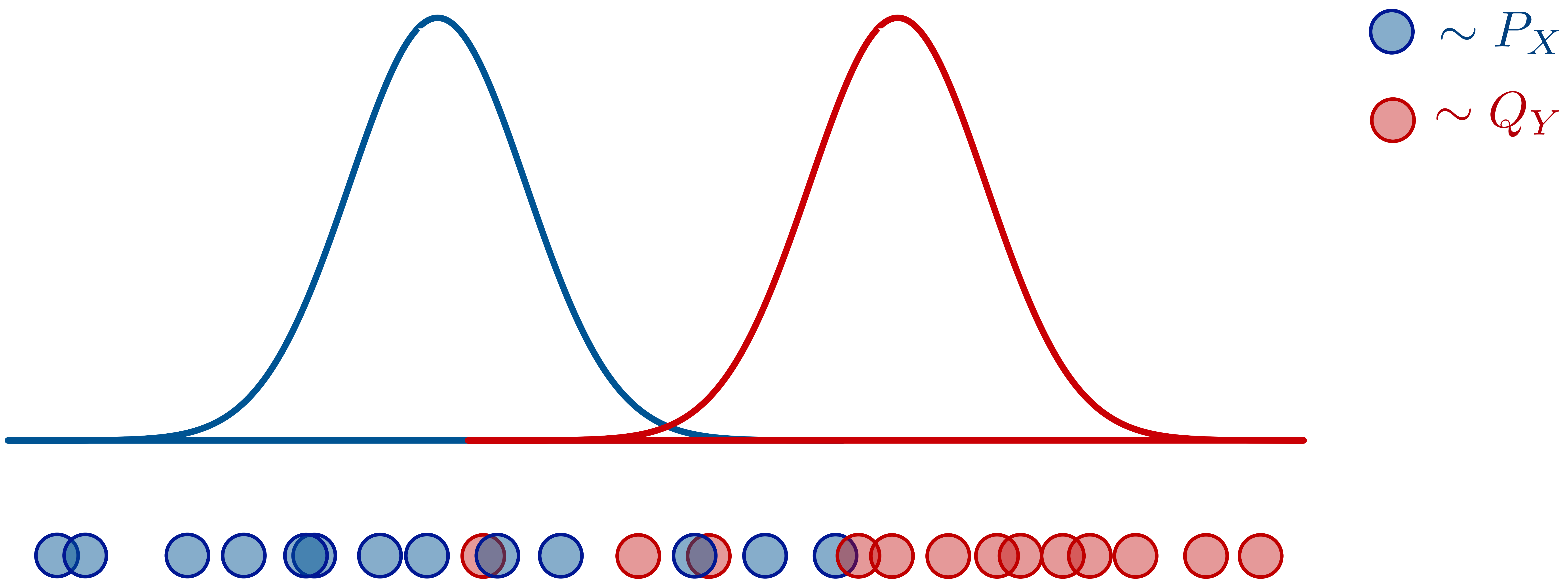
Regression-based two-sample test



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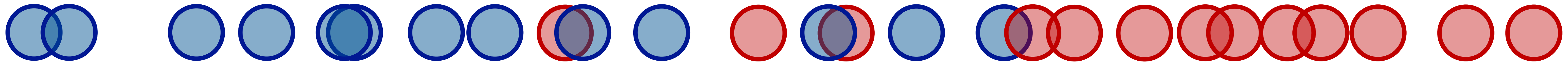

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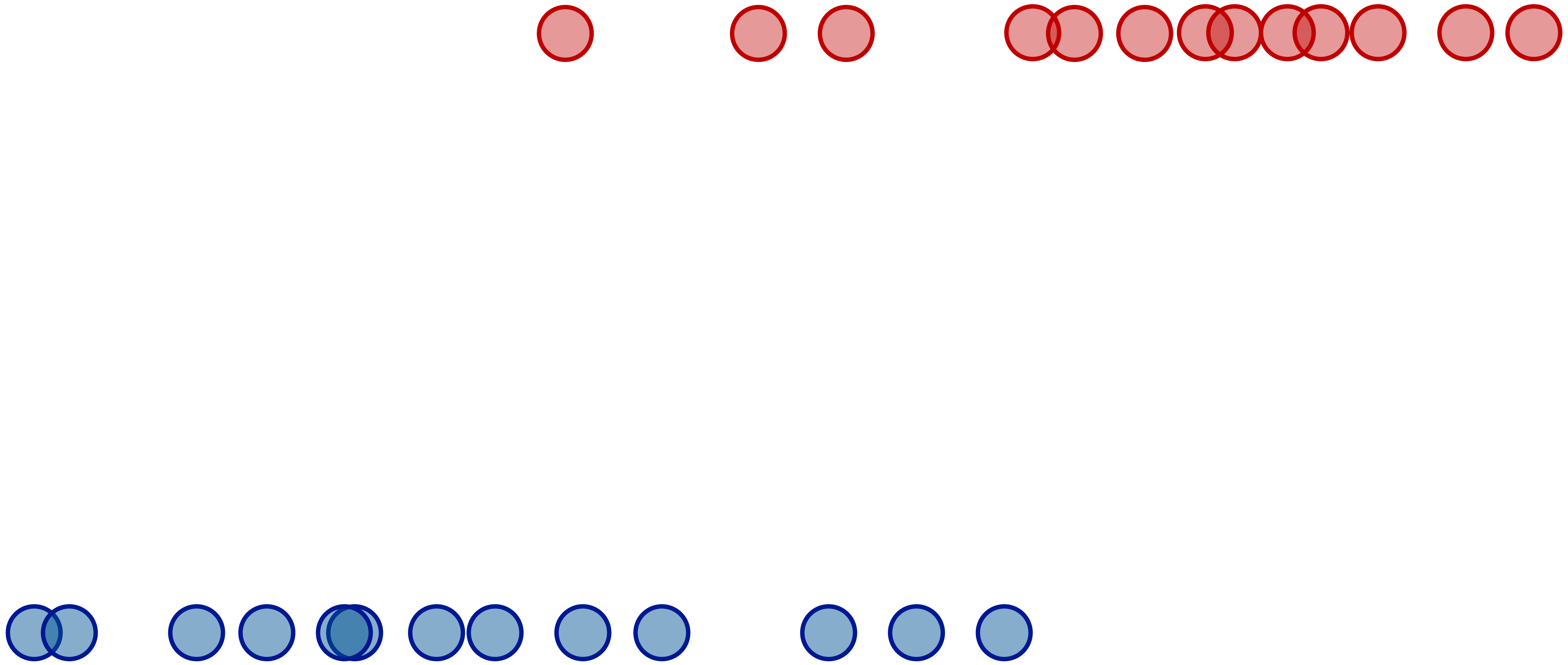

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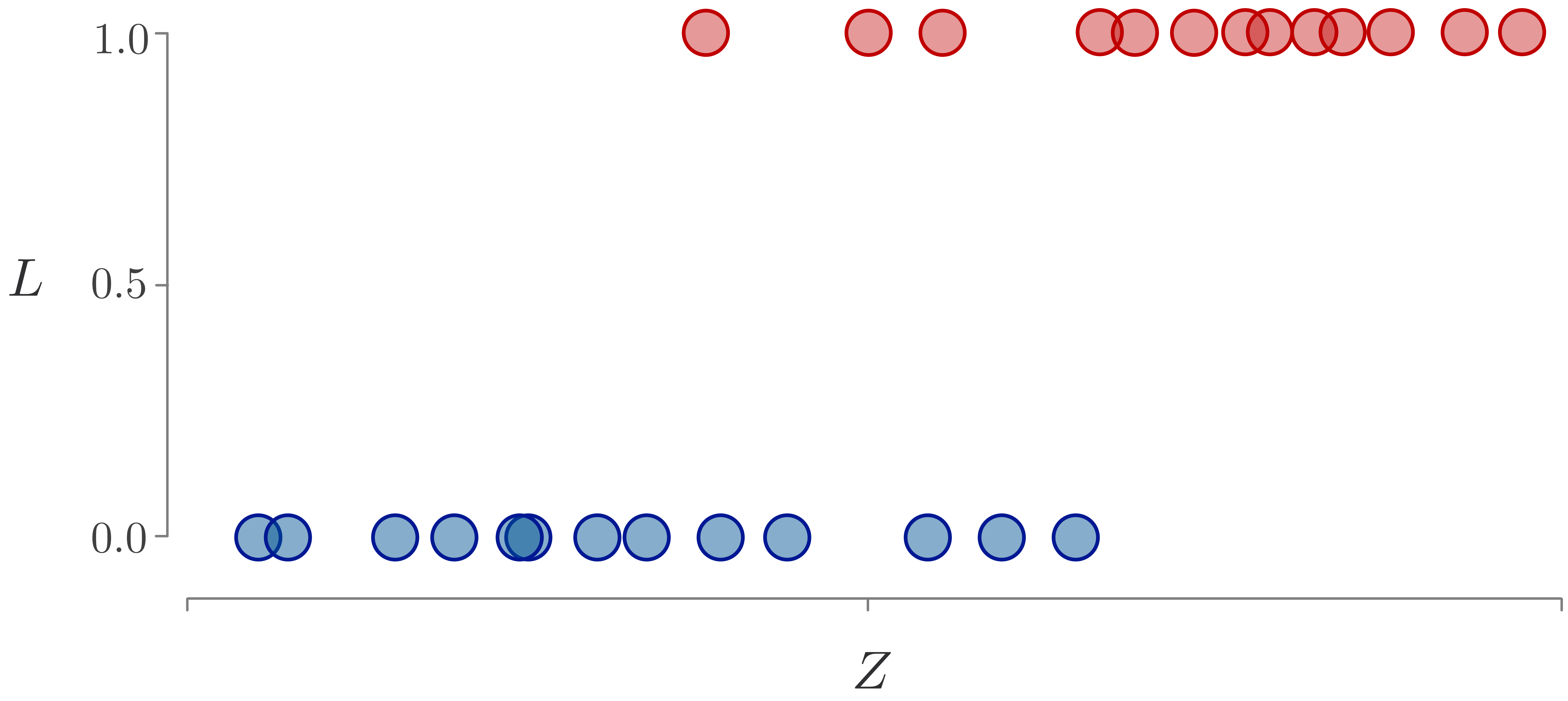

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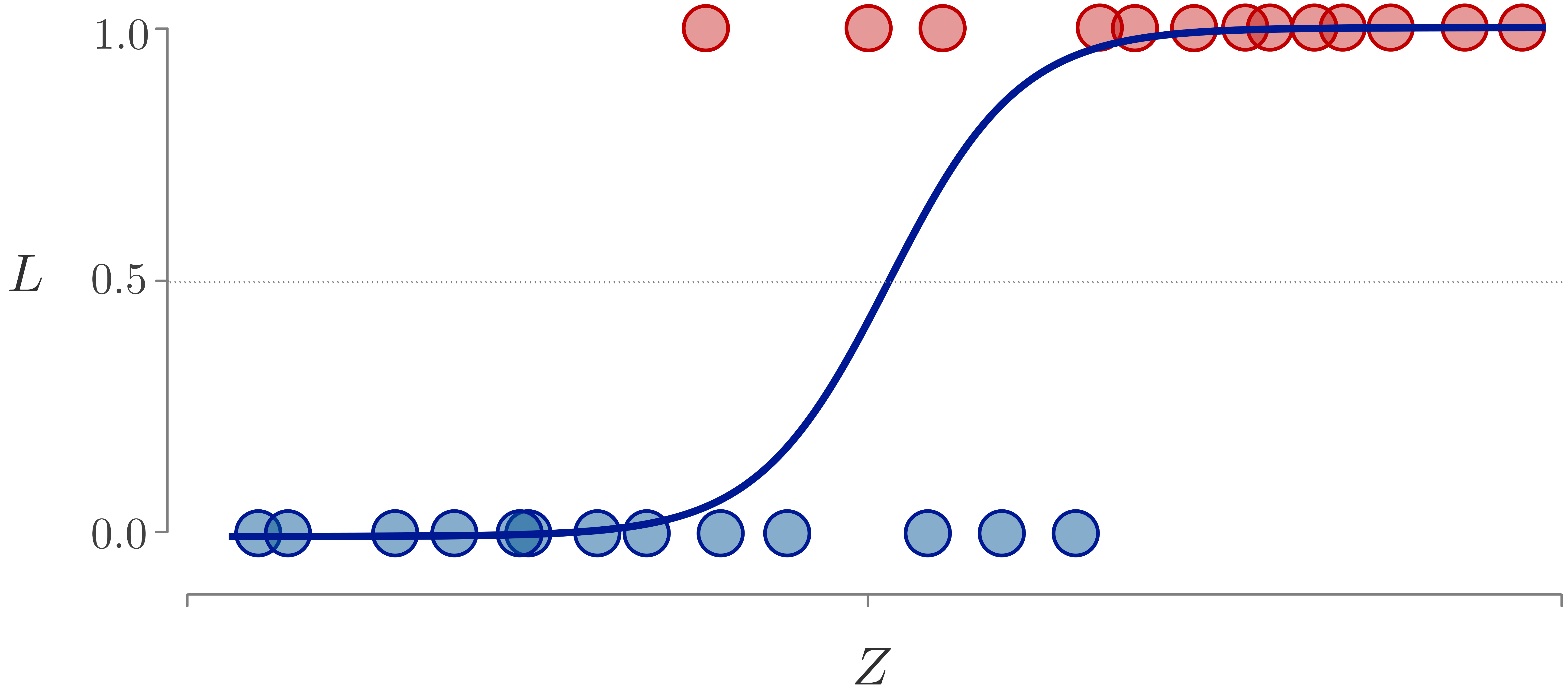
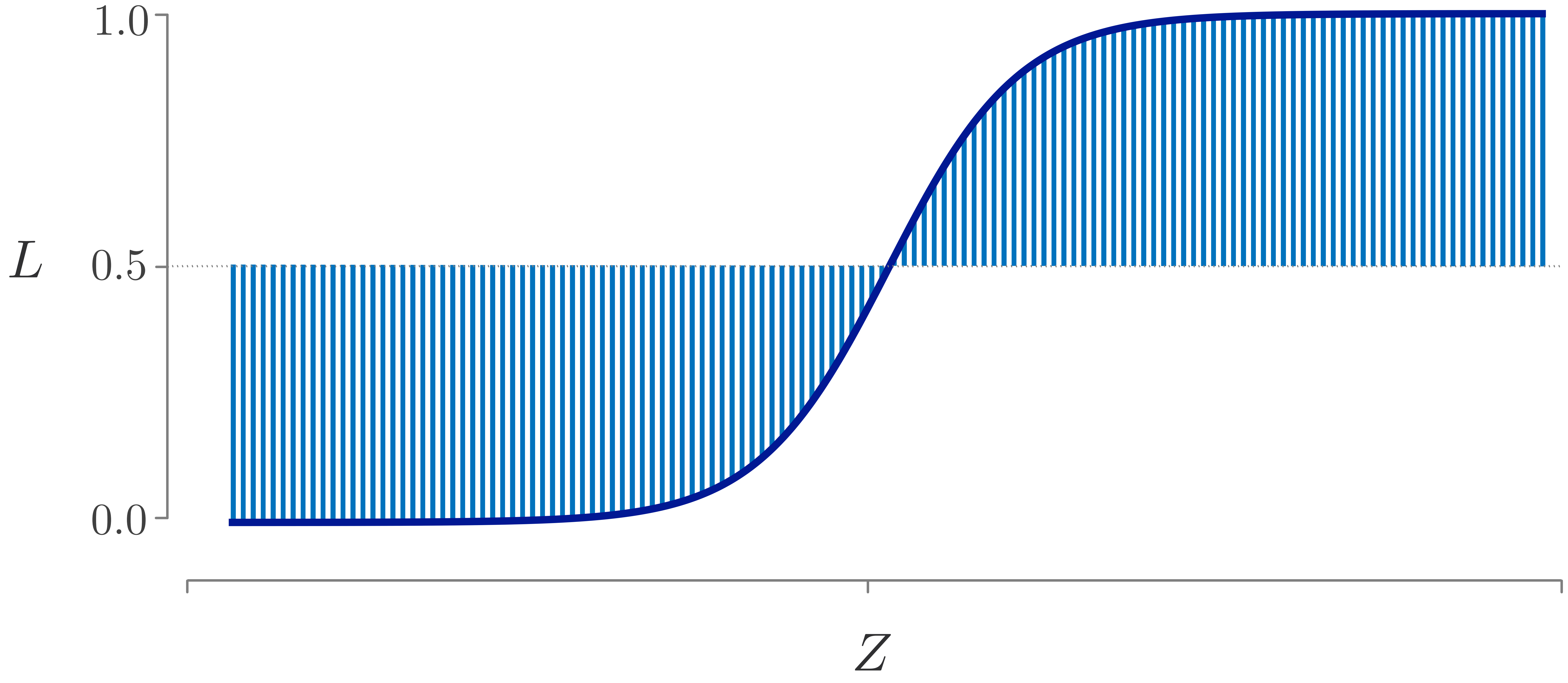


Regression-based two-sample test



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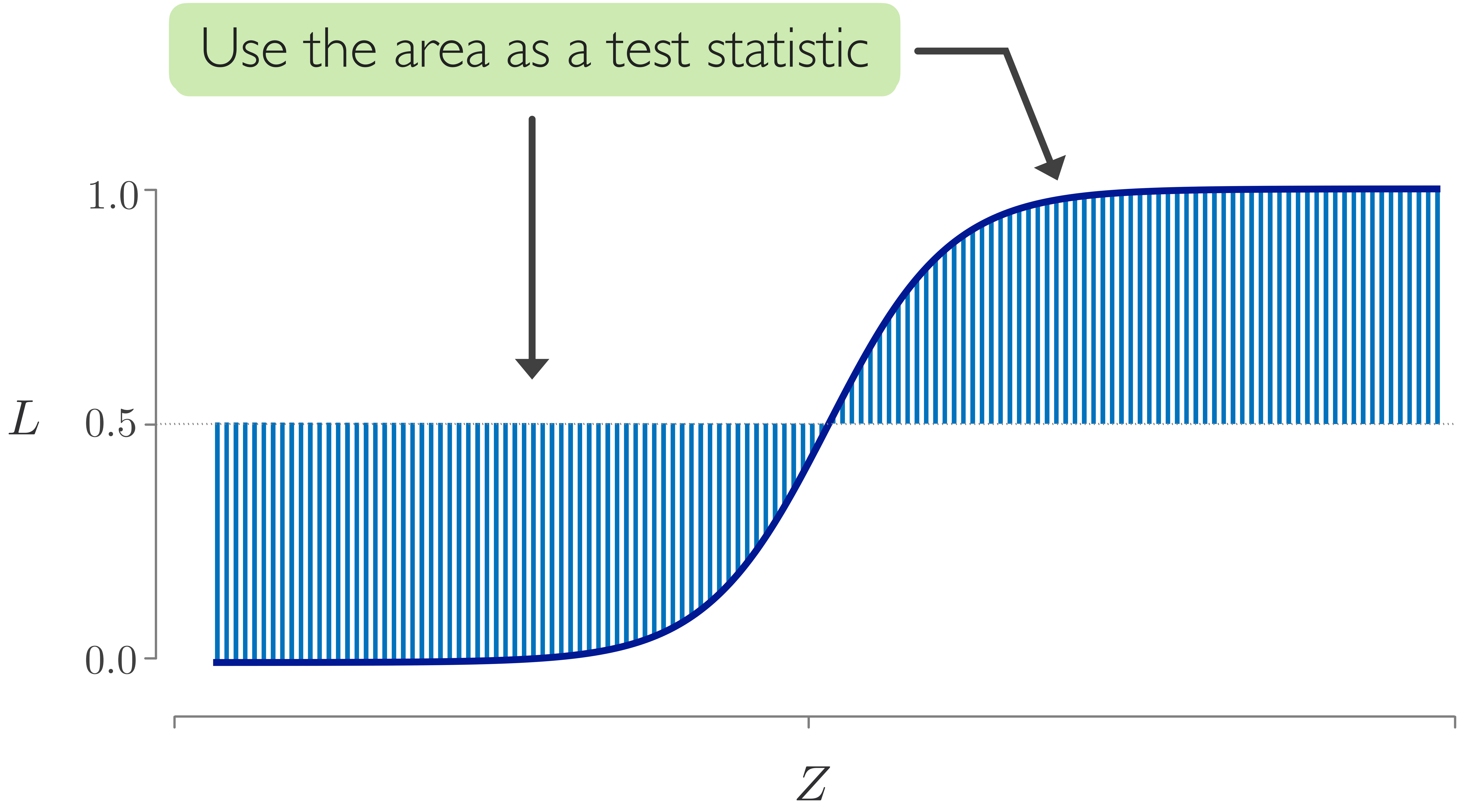
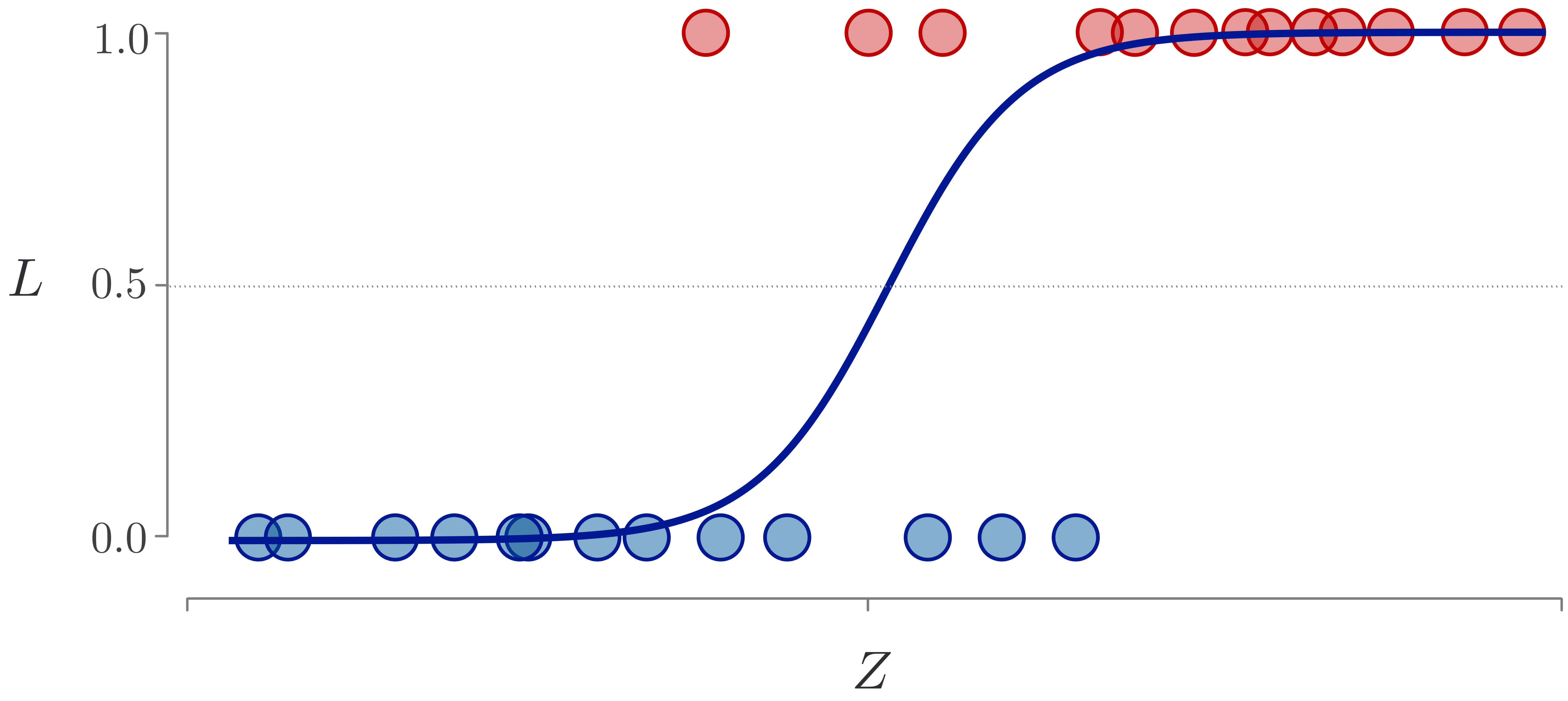


Classification accuracy-based two-sample test



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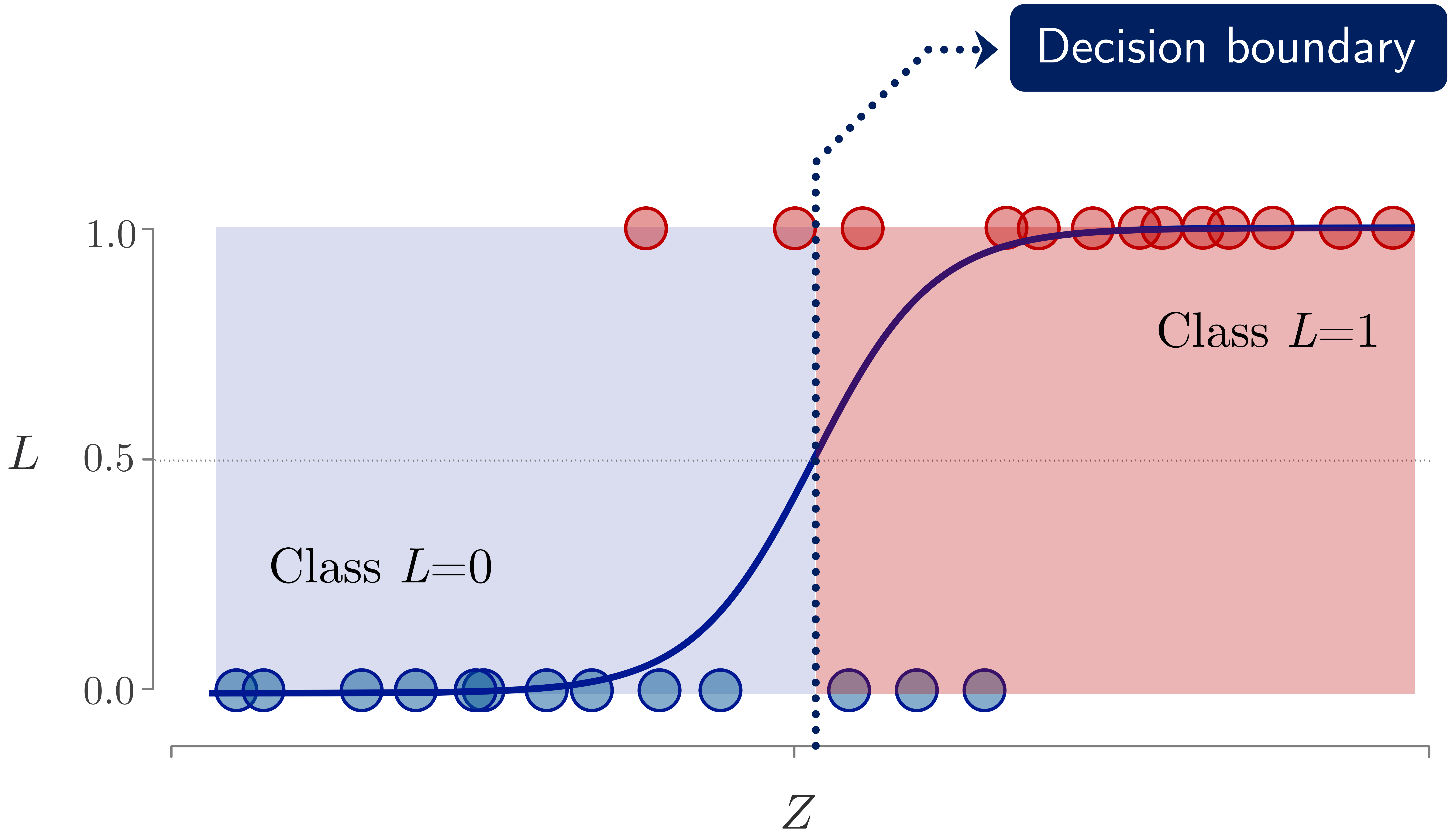
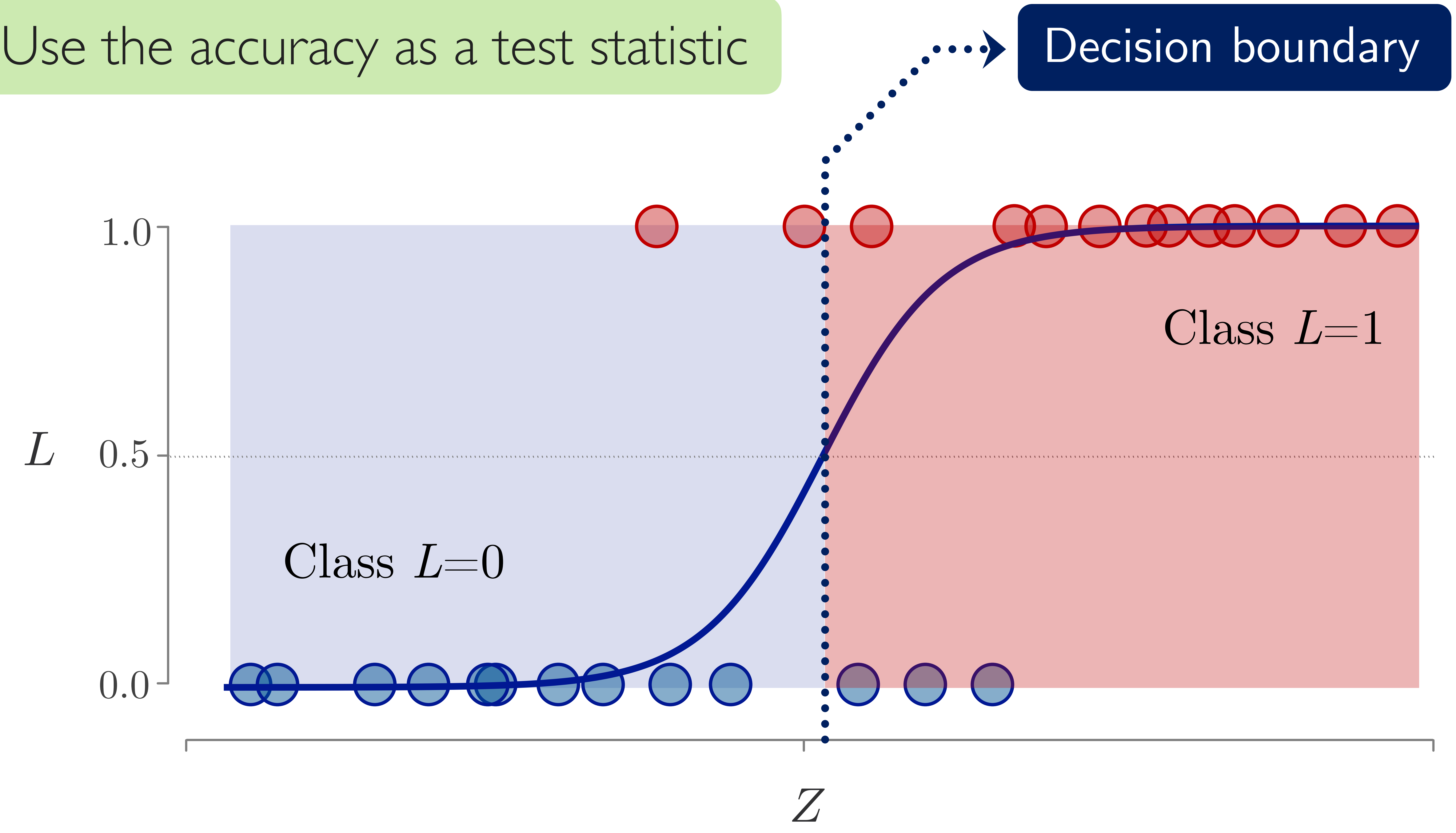


Classification accuracy-based two-sample test

Use the accuracy as a test statistic



Test statistics

$$\mathcal{D}_N := \begin{array}{c} \begin{array}{cc} Z & L \end{array} \\ \begin{bmatrix} X_1 & 0 \\ \vdots & \vdots \\ X_n & 0 \\ Y_1 & 1 \\ \vdots & \vdots \\ Y_m & 1 \end{bmatrix} \end{array}$$

$m = n$
for simplicity

Test statistics

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\mathcal{D}_N := \begin{array}{c} \begin{matrix} Z & L \end{matrix} \\ \left[\begin{matrix} X_1 & 0 \\ \vdots & \vdots \\ X_n & 0 \\ Y_1 & 1 \\ \vdots & \vdots \\ Y_m & 1 \end{matrix}\right] \end{array}
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Train a regressor

$$\widehat{R} : \mathcal{D}_N \mapsto [0, 1]$$

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$\rightarrow$ **Train a regressor** $\rightarrow$ **Mean square error**

$$\widehat{R} : \mathcal{D}_N \mapsto [0, 1]$$

$$N^{-1} \sum_{i \in [N]} \left(\widehat{R}(Z_i) - 1/2\right)^2$$

Test statistics

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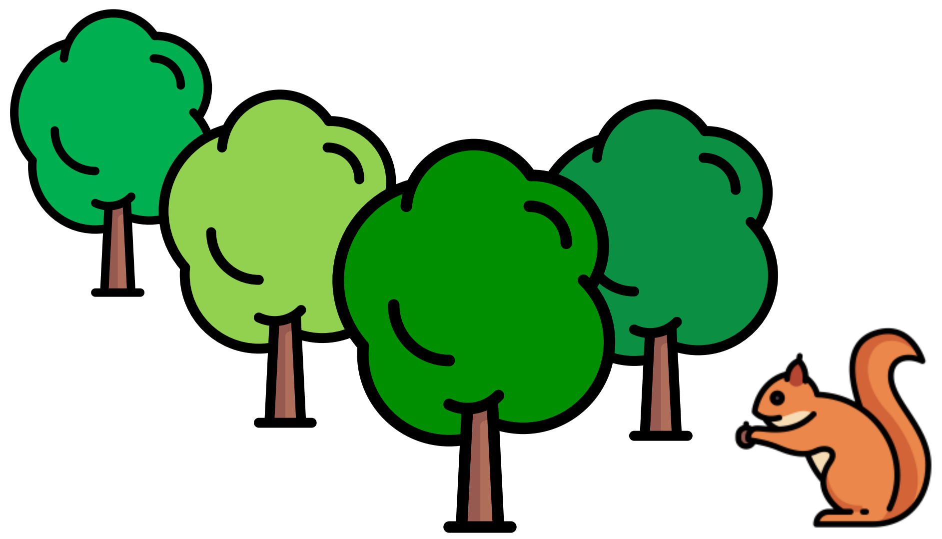
Train a classifier

$$\widehat{C} : \mathcal{D}_N \mapsto \{0, 1\}$$

Accuracy

$$N^{-1} \sum_{i \in [N]} I\left(\widehat{C}(Z) = 1\right)$$

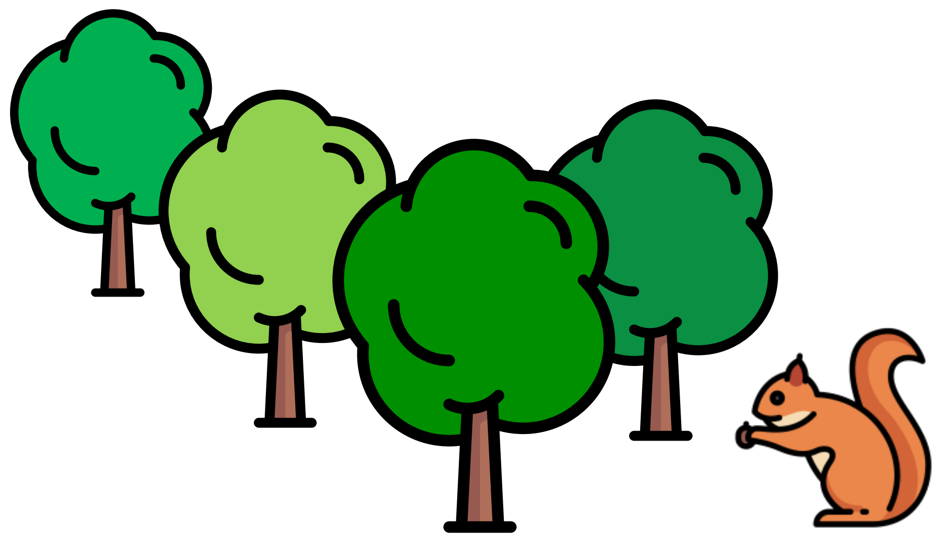
Empirical results



Random forests

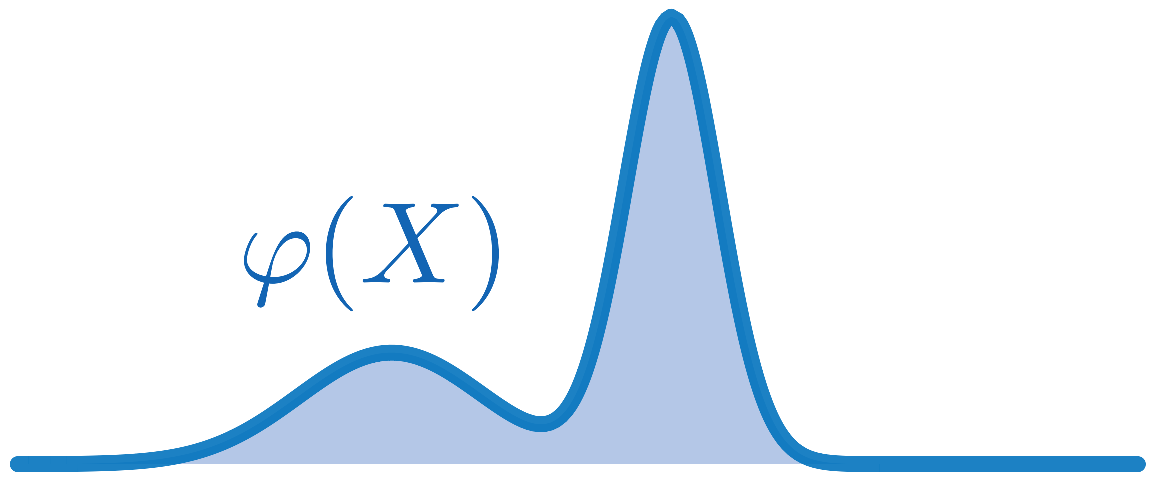
- Screen irrelevant variables
- Robust to outliers
- Handle various data types
- Empirical success

Empirical results



Random forests

versus

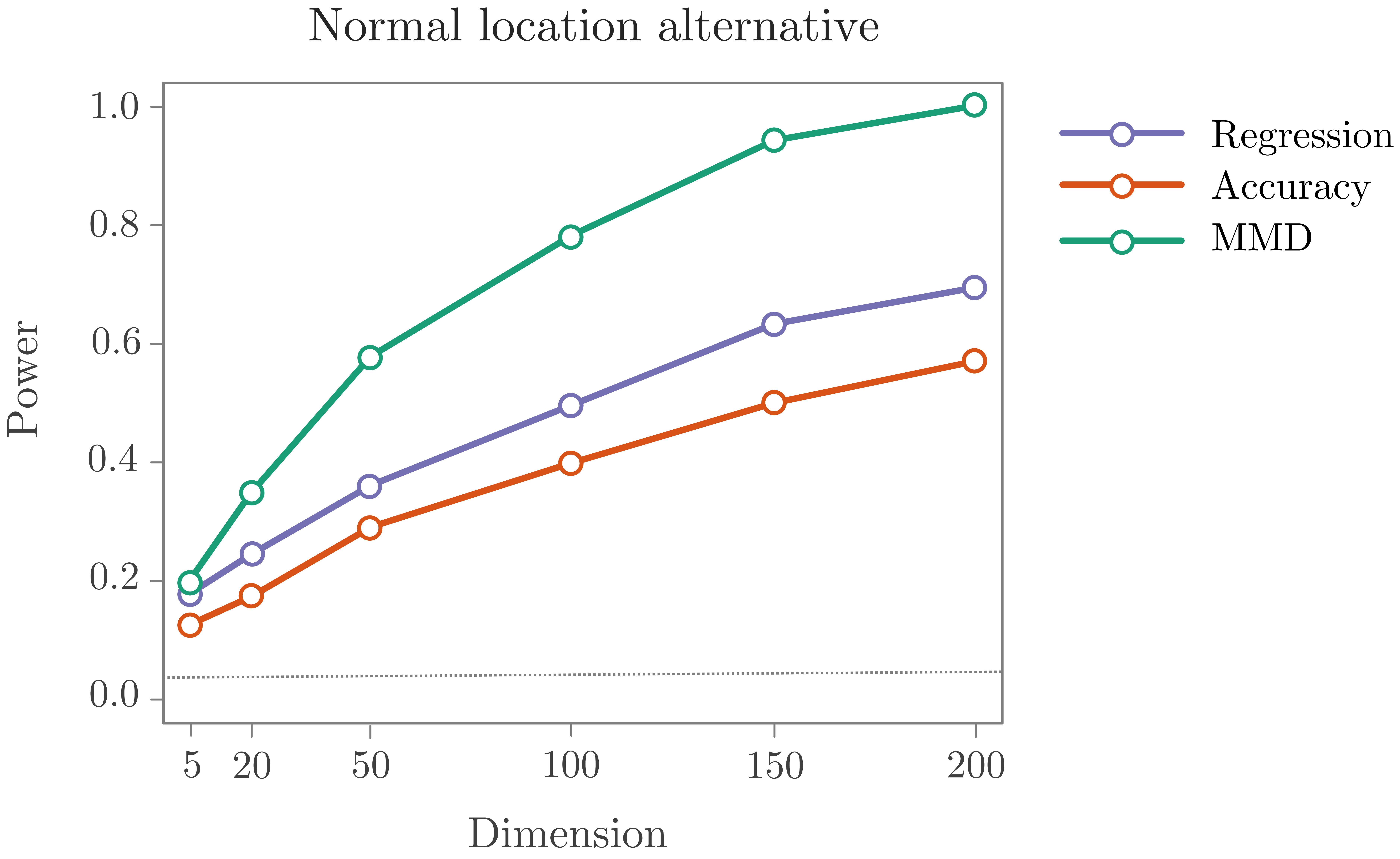


Maximum Mean Discrepancy

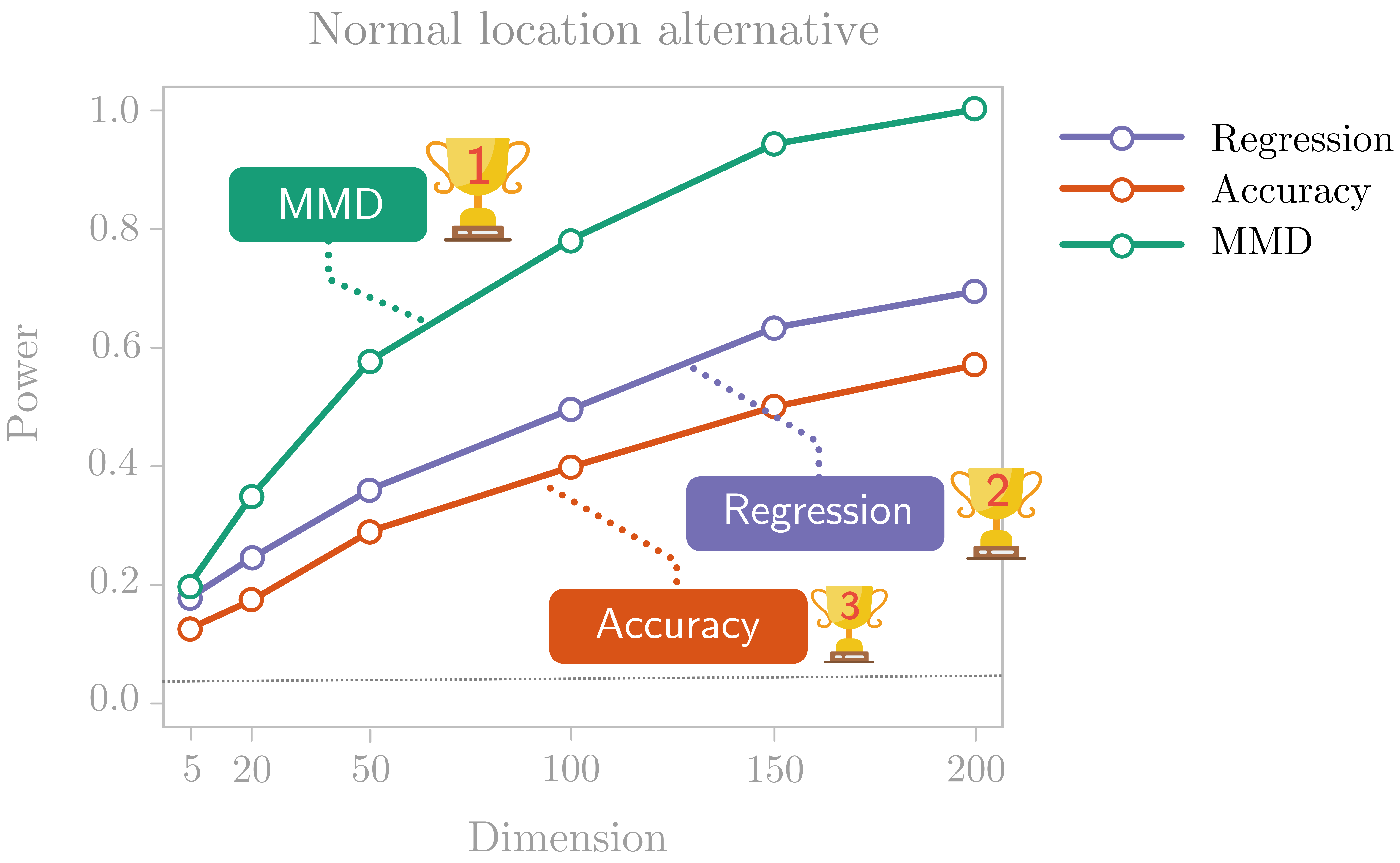
- Screen irrelevant variables
- Robust to outliers
- Handle various data types
- Empirical success

- Gretton et al. (2012)
- Popular method in ML
- Simple calculation formula
- Theoretical support

Power comparison



Power comparison



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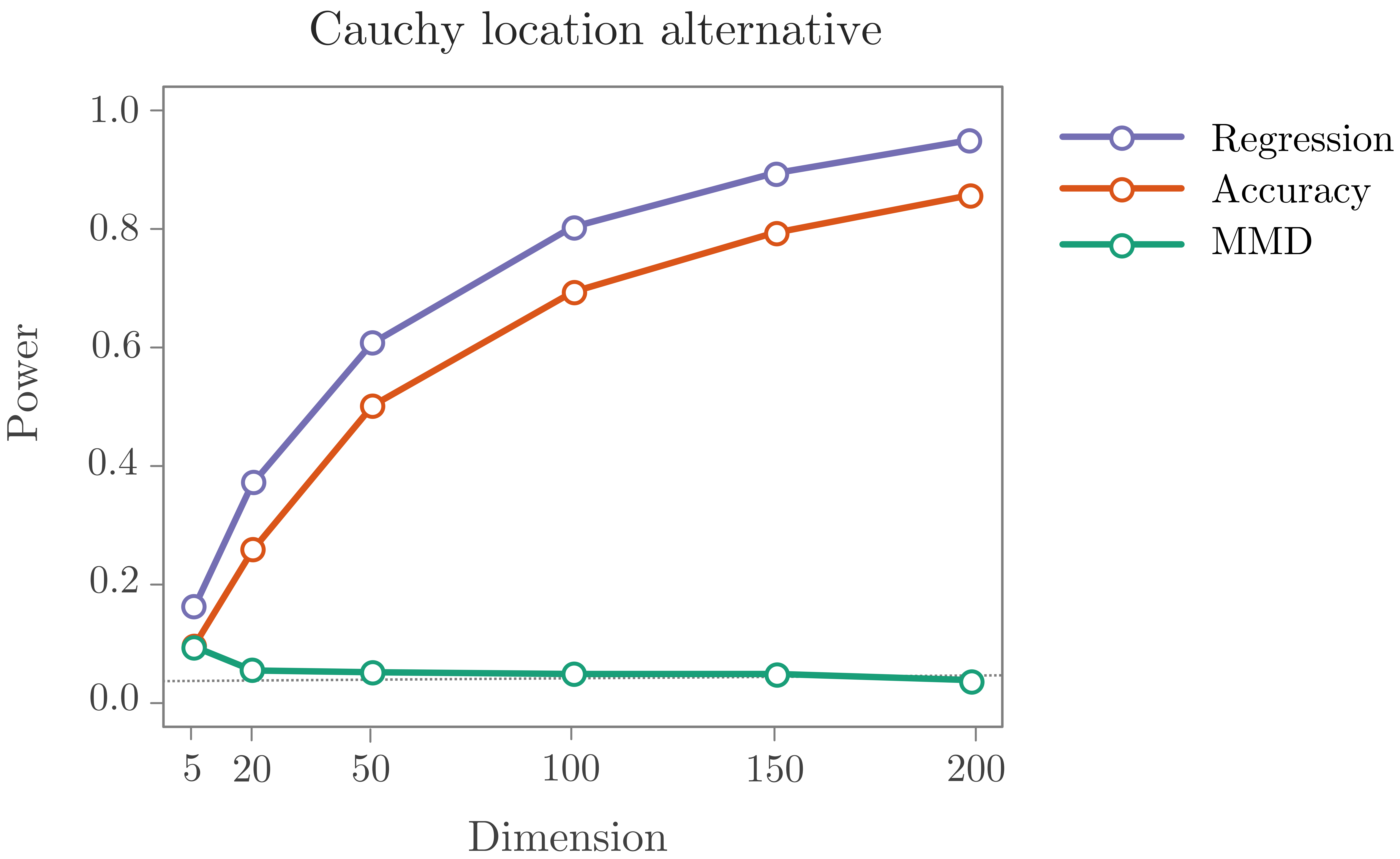

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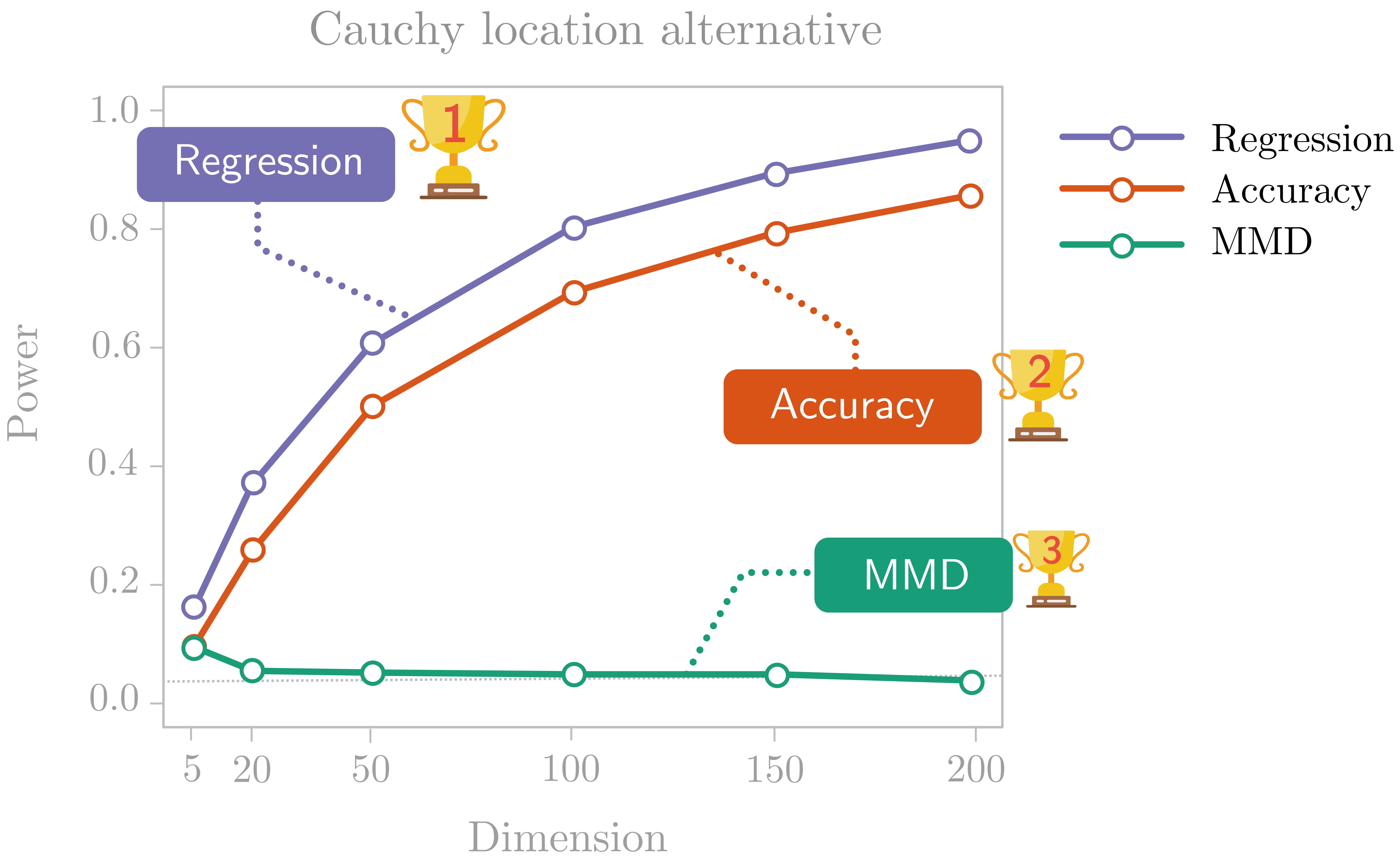


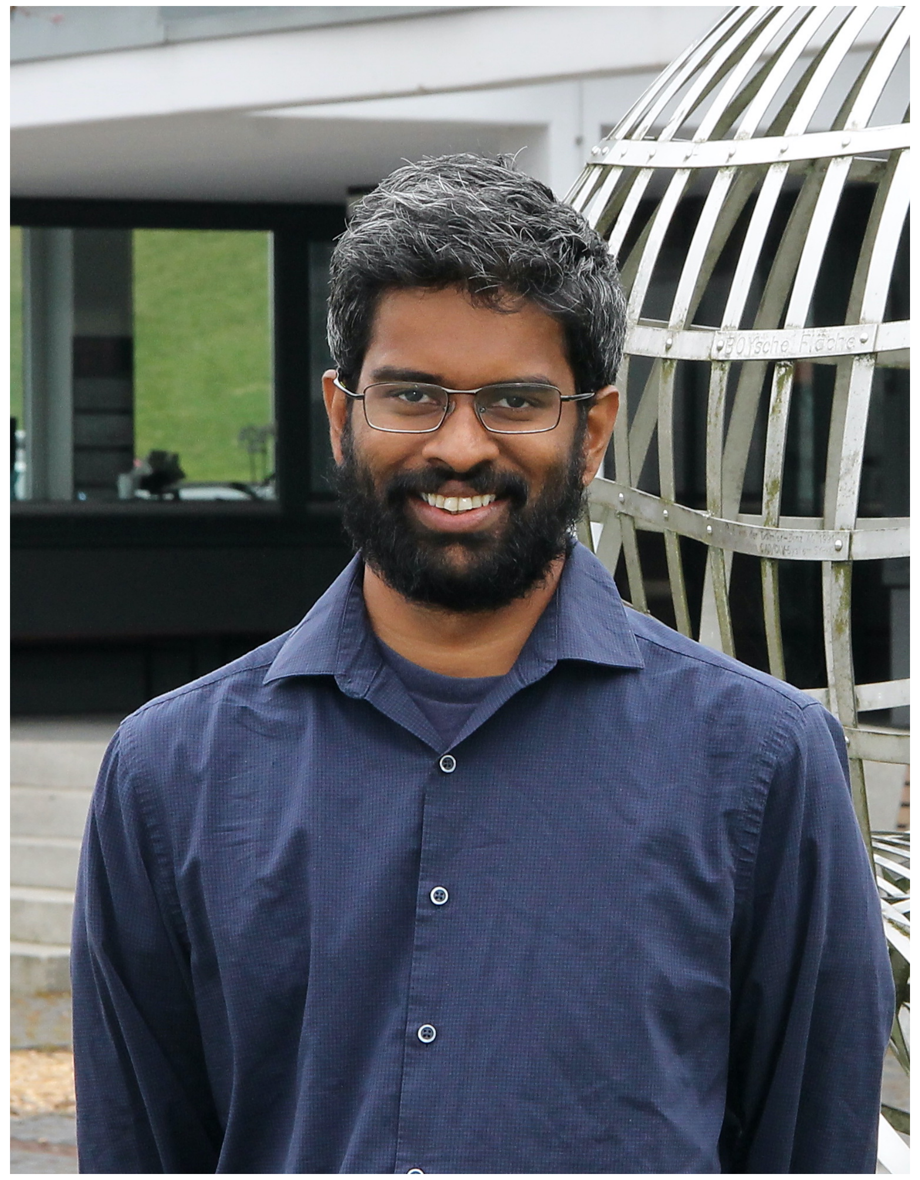
Part 1. Methodological Contributions

Part II. Theoretical Contributions

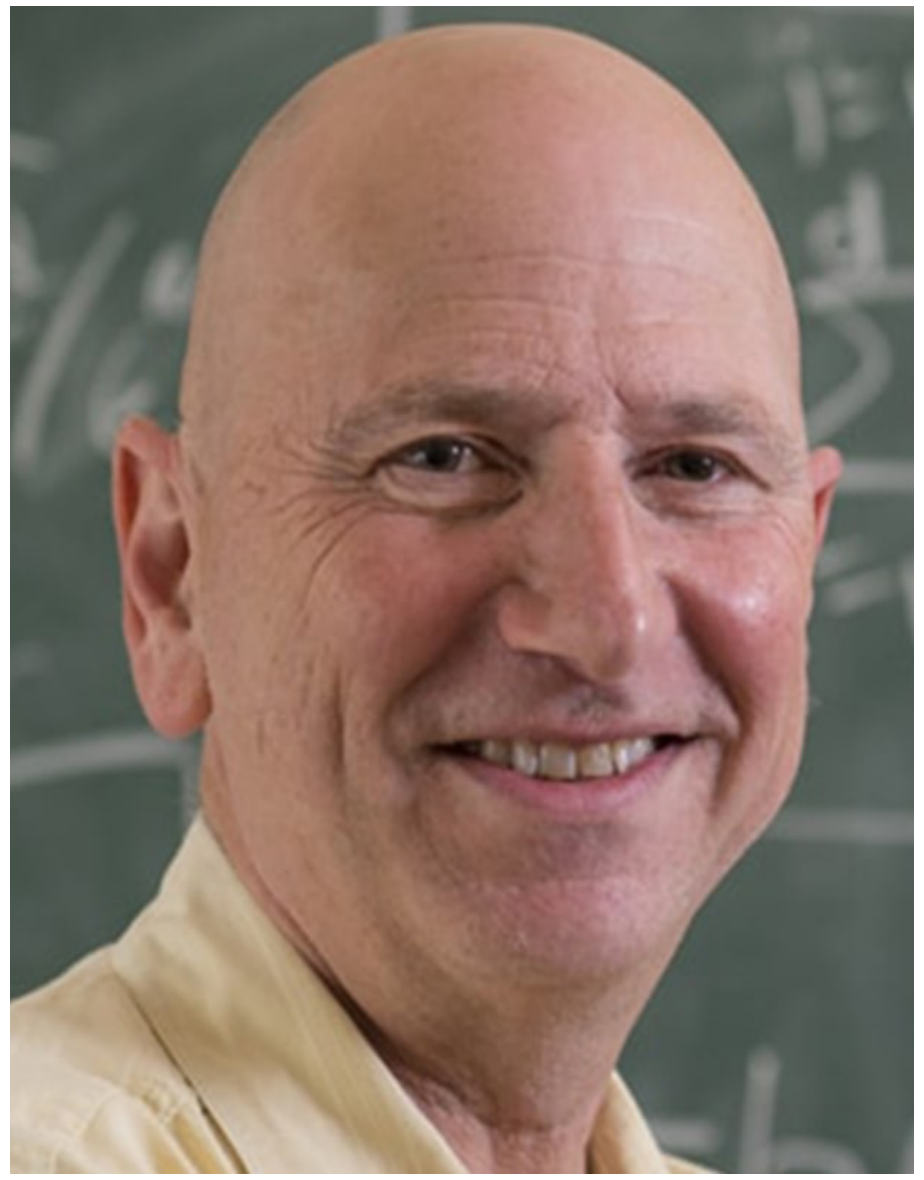
The Annals of Statistics
2022, Vol. 50, No. 1, 225–251
https://doi.org/10.1214/21-AOS2103

MINIMAX OPTIMALITY OF PERMUTATION TESTS

BY ILMUN KIM[1], SIVARAMAN BALAKRISHNAN[2,*] AND LARRY WASSERMAN[2,†]



Siva Balakrishnan
(CMU)



Larry Wasserman
(CMU)

Challenge: Random critical value

Remark the permutation test **rejects** H_0 when

$$\underbrace{T}_{\text{Test statistic}} > \underbrace{q_{1-\alpha}}_{\text{Critical value}} := \mathrm{Quantile}_{1-\alpha}(T, T_1^{\pi}, \ldots, T_B^{\pi})$$

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$$\boxed{T} > \boxed{q_{1-\alpha}} := \mathrm{Quantile}_{1-\alpha}(T, T_1^{\pi}, \ldots, T_B^{\pi})$$

Test statistic Critical value

Our **goal** is to identify **non-asymptotic conditions** under which

$$\boxed{\sup_{P \in \mathscr{P}_1} \mathbb{P}_P(T \leq q_{1-\alpha})} \leq \beta \quad \text{(Say, } \beta = 0.05\text{)}$$

Uniform Type II error over $\mathscr{P}_1$

Challenge: Random critical value

Random quantity +
Lacking independence

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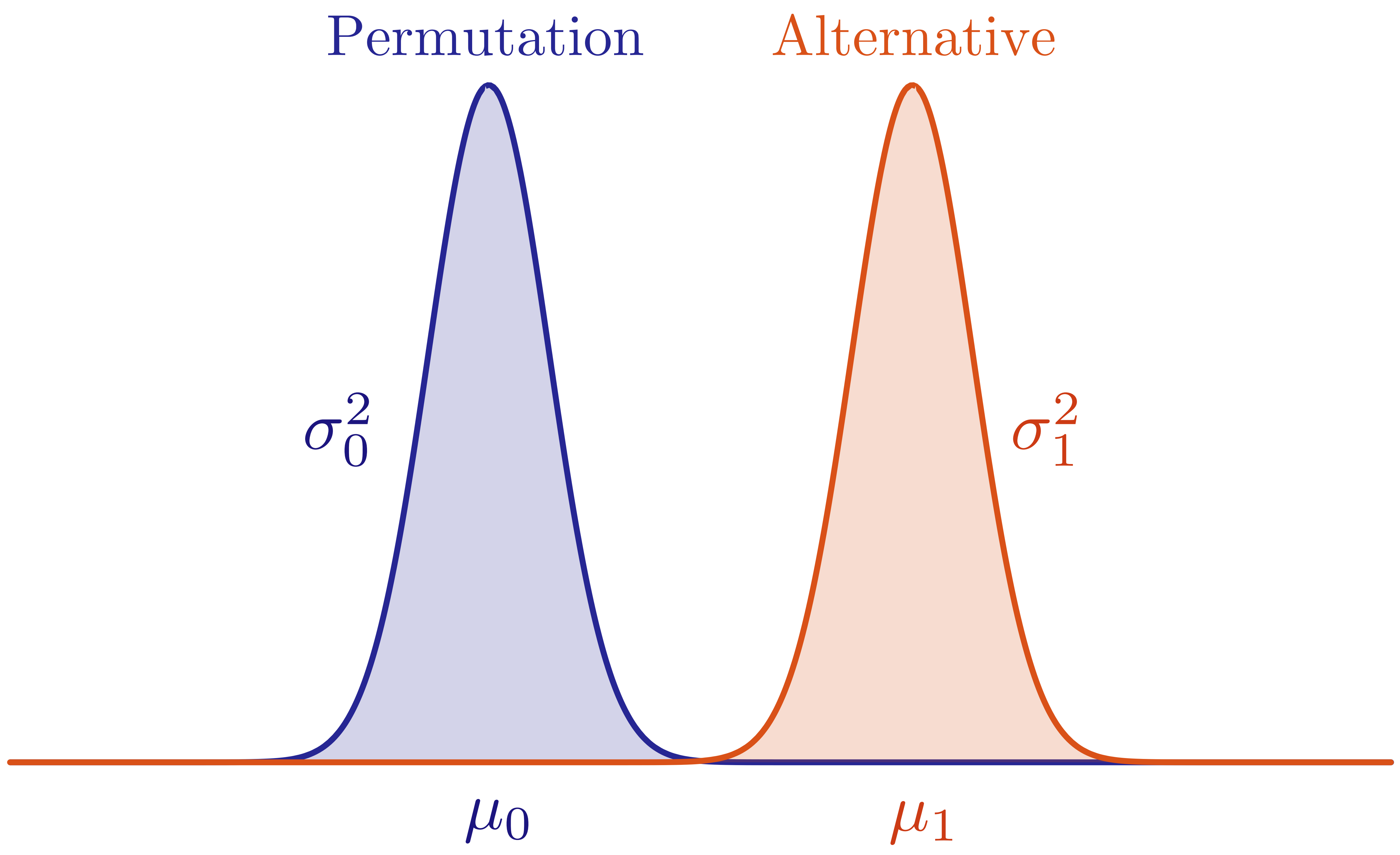
Uniform **Type II error** over $\mathscr{P}_1$

Our proposal: Two moments method

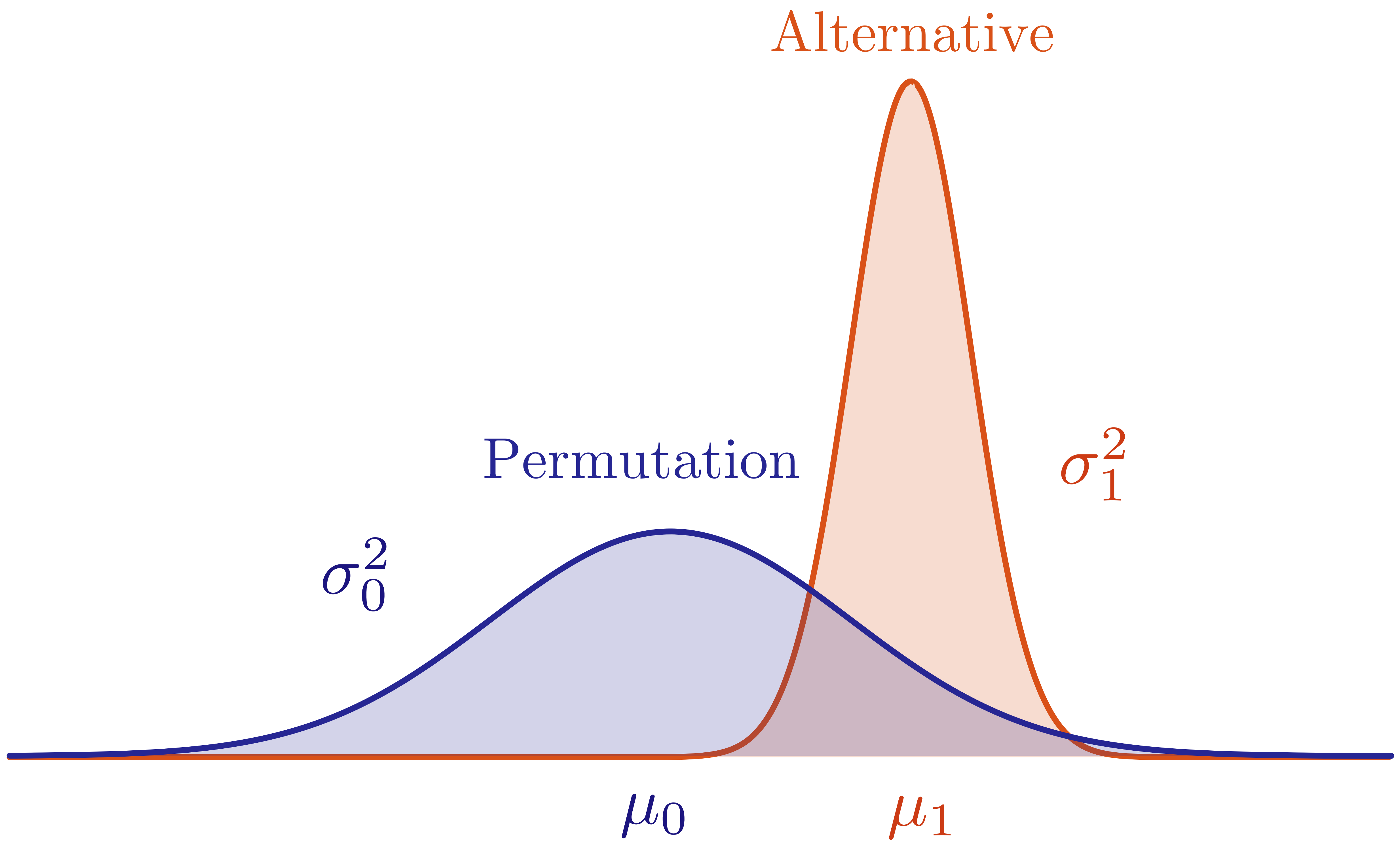
Intuition for the two moments method

- High power when signal $\mu_1 - \mu_0 \gg$ noise $\max\{\sigma_0, \sigma_1\}$



Intuition for the two moments method

- Suffer from **low power** when signal $\mu_1 - \mu_0 \ll$ noise $\max\{\sigma_0, \sigma_1\}$



Two moments method

Theorem [KBW 2022]

- The number of (random) permutations $B \gtrsim \alpha^{-2} \log(1/\beta)$

Two moments method

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Independent of the sample size!

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Signal $\gtrsim$ Noise I + Noise II

(data) (data + permutation)

Two moments method

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(data) *(data + permutation)*

Uniform Type II error: $\sup_{P \in \mathscr{P}_1} \mathbb{P}_P(T \le q_{1-\alpha}) \le \beta$

Two moments method

[Punchline] Understanding the power of the permutation test boils down to understanding the **first two moments** of T and T^{π}.

Two moments method

[Punchline] Understanding the power of the permutation test boils down to understanding the **first two moments** of T and T^{π}.

[Improvement] If we have more information about T, we can further **improve/simplify** the conditions. We will illustrate this using U-statistics.

U-statistic for two-sample testing

- Suppose that we observe $\{X_1, \ldots, X_n\} \overset{i.i.d.}{\sim} P_X$ and $\{Y_1, \ldots, Y_n\} \overset{i.i.d.}{\sim} P_Y$

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- Given a **kernel** $h(x, y)$,

$$U_n = \frac{1}{n(n-1)} \sum_{1 \le i \ne j \le n} h(X_i, X_j) + \frac{1}{n(n-1)} \sum_{1 \le i \ne j \le n} h(Y_i, Y_j) - \frac{2}{n^2} \sum_{1 \le i \le n} \sum_{1 \le j \le n} h(X_i, Y_j)$$

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$$\approx (P_X - P_Y)^2 \qquad - \underbrace{\frac{2}{n^2} \sum_{1 \le i \le n} \sum_{1 \le j \le n} h(X_i, Y_j)}_{\text{Between Similarity}}$$

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$$\approx (P_X - P_Y)^2$$

Examples

MMD (Gretton et al., 2012)
Energy (Szekely & Rizzo, 2013)

U-statistic for independence testing

- Suppose that we observe $\{(X_1, Y_1), \ldots, (X_n, Y_n)\} \overset{i.i.d.}{\sim} P_{XY}$

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$$
\begin{aligned}
U_n &= \frac{(n-2)!}{n!} \sum_{(i,j)\in I_2^n} h_X(X_i, X_j) h_Y(Y_i, Y_j) \\
&\quad + \frac{(n-4)!}{n!} \sum_{(i,j,q,r)\in I_4^n} h_X(X_i, X_j) h_Y(Y_q, Y_r) - 2\frac{(n-3)!}{n!} \sum_{(i,j,q)\in I_3^n} h_X(X_i, X_j) h_Y(Y_i, Y_q)
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$$P_X^2 P_Y^2 \qquad P_{XY} P_X P_Y$$

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Examples

HSIC (Gretton et al., 2005)
Distance Covariance (Szekely et al., 2007)

Result for U-statistics

Recall that the **permutation test** becomes **powerful** when

$$\text{“}\ \mathbb{E}_P[U_n] - \mathbb{E}_{P,\pi}[U_n^\pi] \gtrsim \sqrt{\beta^{-1}\mathbb{V}_P[U_n]} + \sqrt{\alpha^{-1}\beta^{-1}\mathbb{V}_{P,\pi}[U_n^\pi]}\ \text{”}$$

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$\mathbb{E}_{P,\pi}[U_n^\pi] = 0$ and $\mathbb{V}_{P,\pi}[U_n^\pi] \lesssim \mathbb{V}_P[U_n]$

Centered — Noise II (data + permutation) — Noise I (data)

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Simplifies to

$$\boxed{\mathbb{E}_P[U_n] \gtrsim \sqrt{\alpha^{-1}\beta^{-1}\mathbb{V}_P[U_n]}}$$

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Question. Are these **sufficient** conditions for the power guarantee also **necessary**?

Applications to minimax testing

- **Minimax analysis:** $H_0 : P = Q$ vs. H_1 : distance$(P, Q) \geq \epsilon_n$

Minimum ϵ_n for which **minimax power** is nontrivial?

$$\underbrace{\sup_{\phi \in \Phi(\alpha)}}_{\text{Over all level } \alpha \text{ tests}} \underbrace{\inf_{P \in \mathscr{P}_1(\epsilon_n)} \mathbb{E}_P[\phi]}_{\text{Worst-case power}}$$

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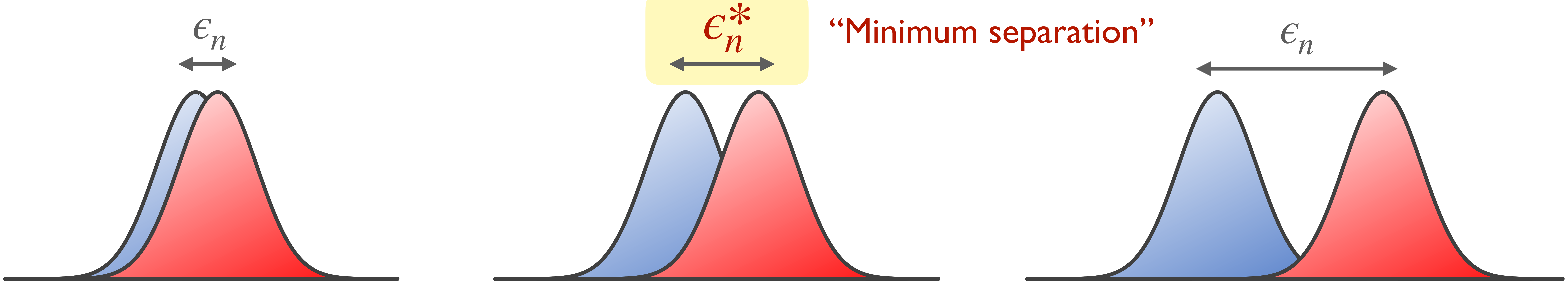
Worst-case power



Minimax power ≤ 0.05

Minimax power ≈ 0.8

Minimax power $= 1$

Applications to minimax testing

- We call ϕ is minimax rate optimal if

$$\inf_{P \in \mathscr{P}_1(\epsilon_n)} \mathbb{E}_P[\phi] \geq 1 - \beta \quad \text{whenever } \epsilon_n^* \asymp \epsilon_n$$

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- Initiated by Ingster (1987, 1994, 2000), Ingster and Suslina (2003)

I. Testing for multinomials: **(very incomplete)**

Paninski (2008), Chan et al. (2014), Bhattacharya & Valiant (2015), Diakonikolas & Kane (2016), Canonne et al. (2018), Balakrishnan & Wasserman (2019)

II. Testing for densities: **(very incomplete)**

Balasubramanian et al. (2017), Arias-Castro et al. (2018), Meynaoui et al. (2019), Li & Yuan (2019), Neykov et al. (2021), Berrett et al. (2021)

Previous tests depend on **unknown** constants

Example **Multinomial two-sample testing in ℓ_1-norm**

d: the number of bins
n: the sample size

- Chan et al. (2014) prove

$$\epsilon_n^* \asymp \max\left\{\frac{d^{1/2}}{n^{3/4}}, \frac{d^{1/4}}{n^{1/2}}\right\}$$

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- The upper bound is based on the test

$$T_{\chi^2} > C\sqrt{\min\{n,d\}} \quad \text{for some constant } C$$

Previous tests depend on **unknown** constants

Example **Density testing in ℓ_2-norm**

- Arias-Castro et al. (2018) prove

$$\epsilon_n^* \asymp n^{-\frac{2s}{4s+p}}$$

p: the dimension
s: Holder smoothness
n: the sample size

Previous tests depend on **unknown** constants

Example **Density testing in ℓ_2-norm**

- Arias-Castro et al. (2018) prove

$$\epsilon_n^* \asymp n^{-\frac{2s}{4s+p}}$$

p: the dimension
s: Holder smoothness
n: the sample size

- The upper bound is based on the test

$$T_{\text{Bin}} > 2n + Cn^{\frac{4s+3p}{4s+p}} \quad \text{for some constant } C$$

Question. Can we prove the minimax results using a test that

i) tightly controls the type I error rate

ii) does not depend on unspecified constants

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Yes! Permutation tests

Two-sample testing

Discrete ℓ_2-norm

Chi-square test statistic
(Chan et al., 2014)

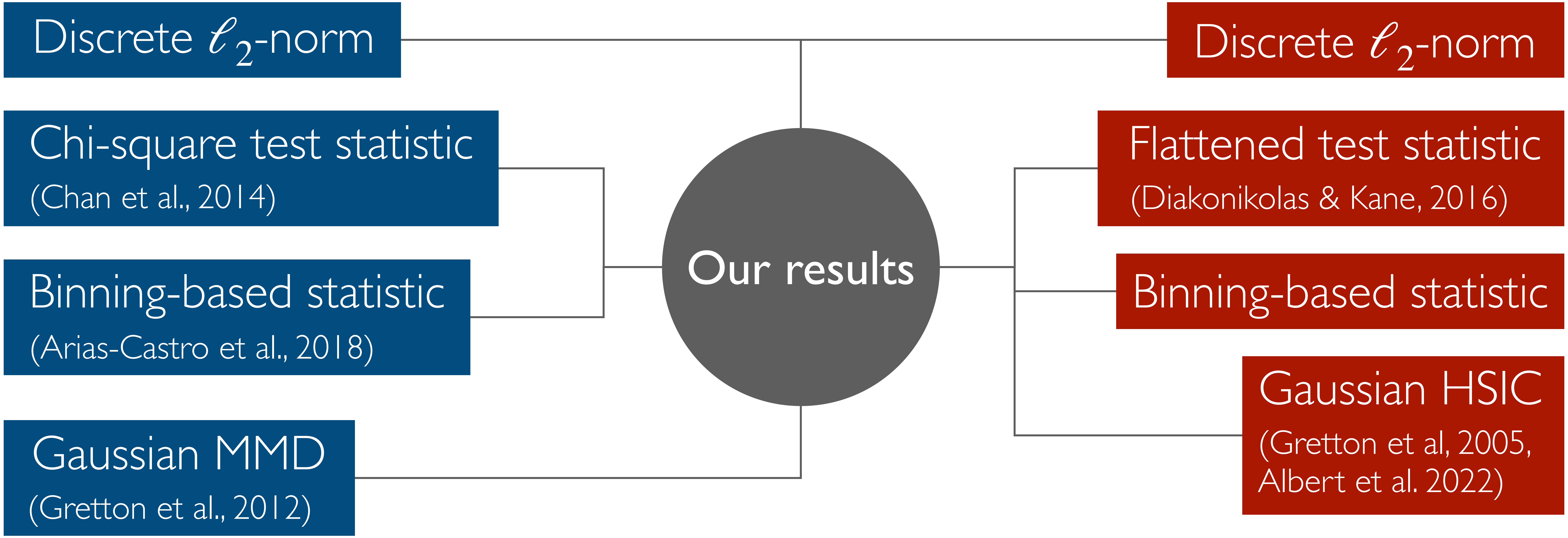
Binning-based statistic
(Arias-Castro et al., 2018)

Gaussian MMD
(Gretton et al., 2012)

Our results

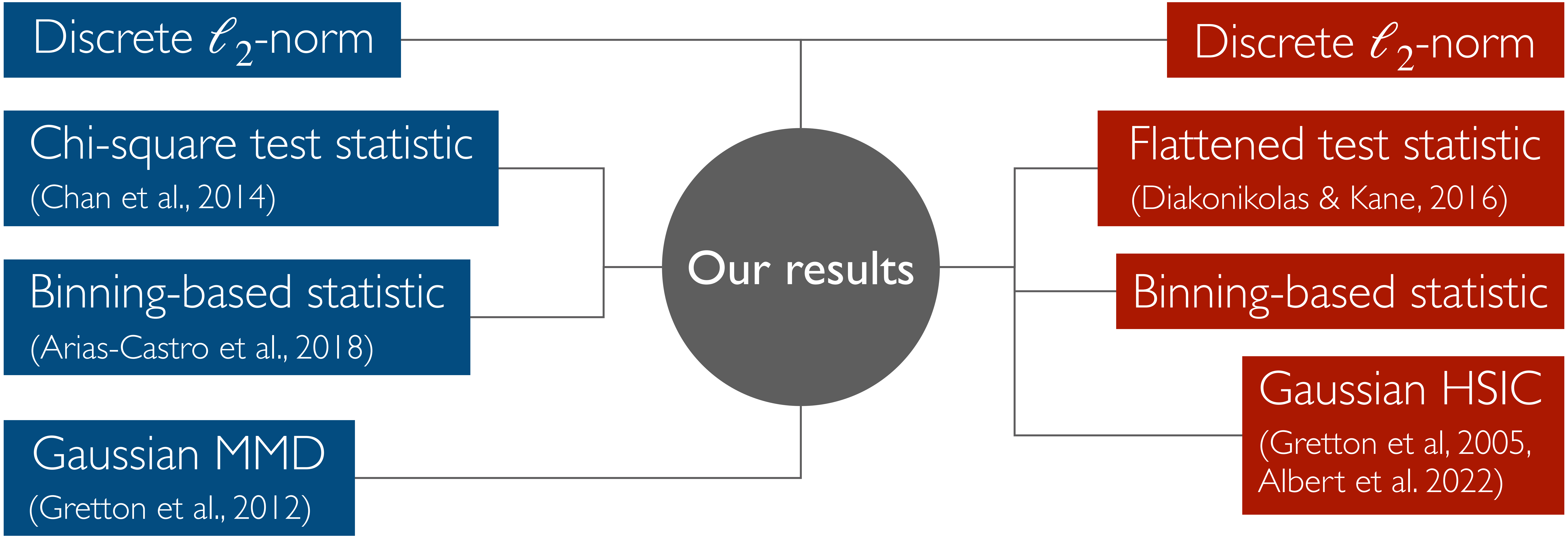
Two-sample testing

Independence testing



Two-sample testing

Independence testing



Permutation tests achieve **minimax optimality**

Follow-up

- Adaptivity
  - Schrab, Kim, Albert, Laurent, Guedj, Gretton (2023, *JMLR*)
- Computational-Power Trade-off
  - Schrab, Kim, Guedj, Gretton (2022, *NeurIPS*)
  - Choi, Kim (2024, *submitted*)
- Differential Privacy
  - Kim, Schrab (2024, *submitted*)
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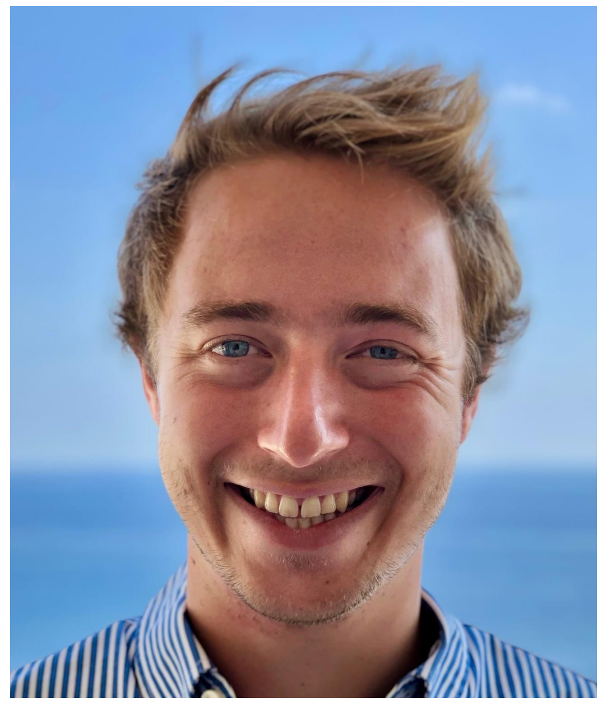
Antonin Schrab


Benjamin Guedj


Arthur Gretton


Mélisande Albert


Béatrice Laurent

Kernel two-sample test that **adapts to** unknown smoothness parameters

Follow-up

- Adaptivity
  - Schrab, Kim, Albert, Laurent, Guedj, Gretton (202

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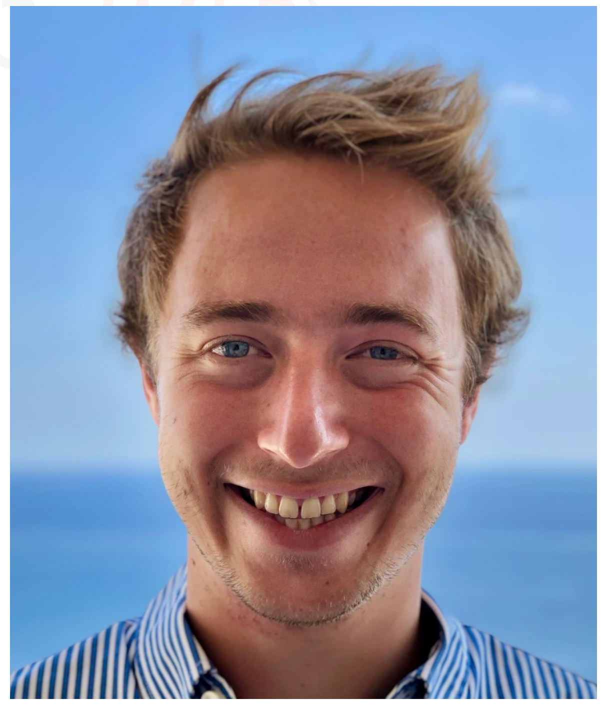

Antonin Schrab

Benjamin Guedj

Arthur Gretton

Ikjun Choi

- Computational-power trade-offs in nonparametric testing
- Implemented via incomplete U-statistics and random Fourier features

- Differential Privacy
  - Kim, Schrab (2024, *submitted*)

- Robustness
  - Schrab, Kim (2024, *submitted*)

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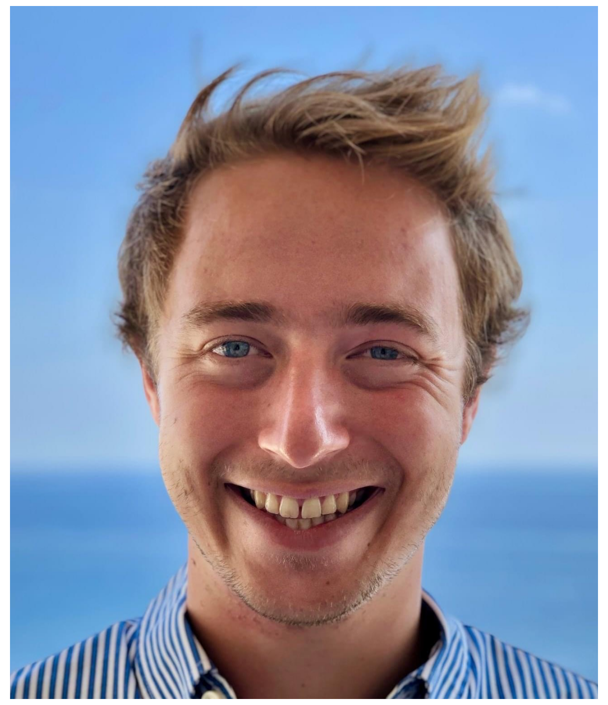

Antonin Schrab

Differentially private permutation tests applied to kernel methods

Follow-up

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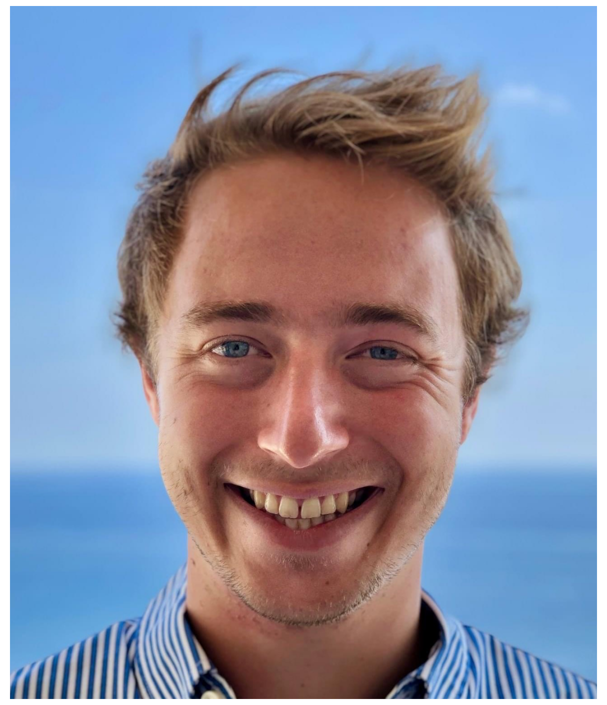

Antonin Schrab

Permutation tests that are robust to data perturbation with optimal properties

Follow-up

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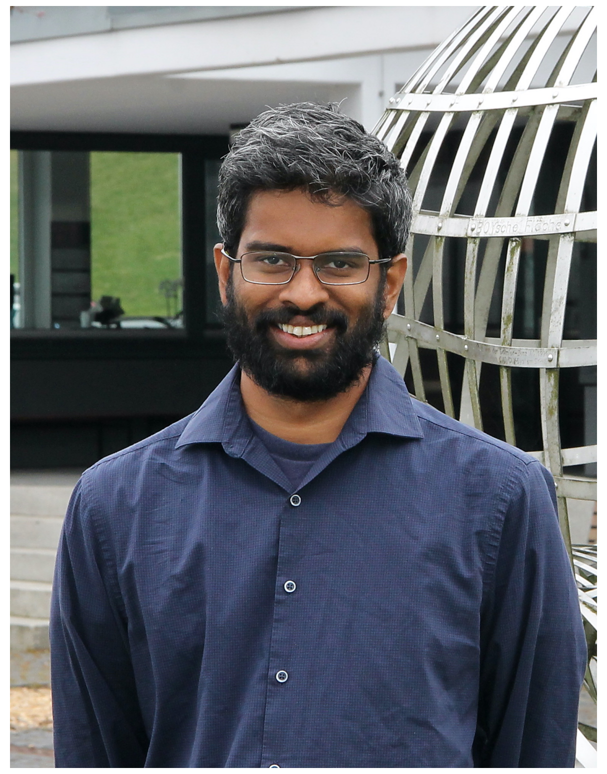
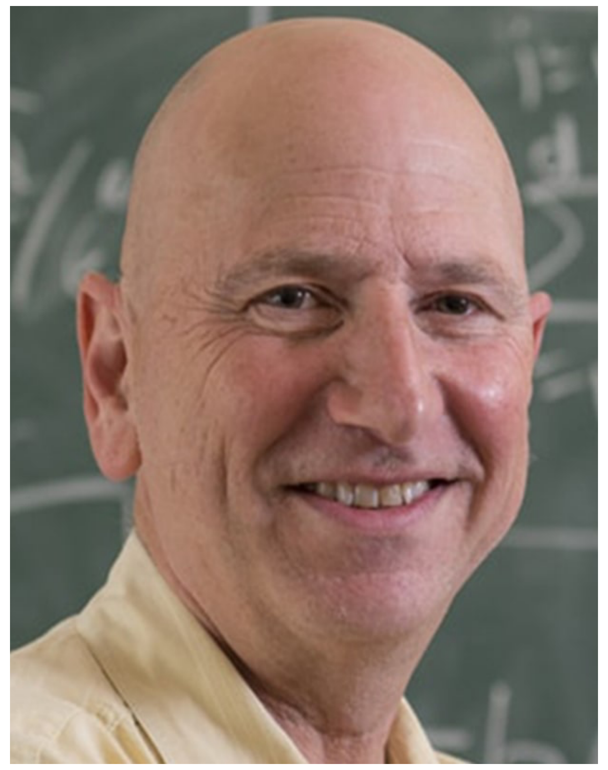
Matey Neykov



Siva Balakrishnan



Larry Wasserman

Local permutation tests for conditional independence with theoretical guarantees

Summary

- Permutation tests have **uniform, finite-sample** guarantees for any test statistic

- We have introduced a **flexible framework** for comparing distributions based on **classification and regression**

- We have provided **tools for analyzing the power** of permutation tests e.g. two moments method, exponential concentration bounds

- Permutation tests are **minimax optimal** in many problems

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Thank you!

Future Work

Theme I. Leveraging machine learning tools to tackle statistical problems

- Semi-supervised learning / transfer learning
- Conditional two-sample testing / conditional independence testing

Theme II. Understanding fundamental limits of statistical problems under different constraints and develop optimal procedures

- Optimality under privacy constraints, computational constraints etc
- Practical procedures with optimal guarantees
- Impossibility results

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