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 $\mathscr{P} = \mathscr{P}_0 \cup \mathscr{P}_1$

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

Recap: Statistical Hypothesis Testing

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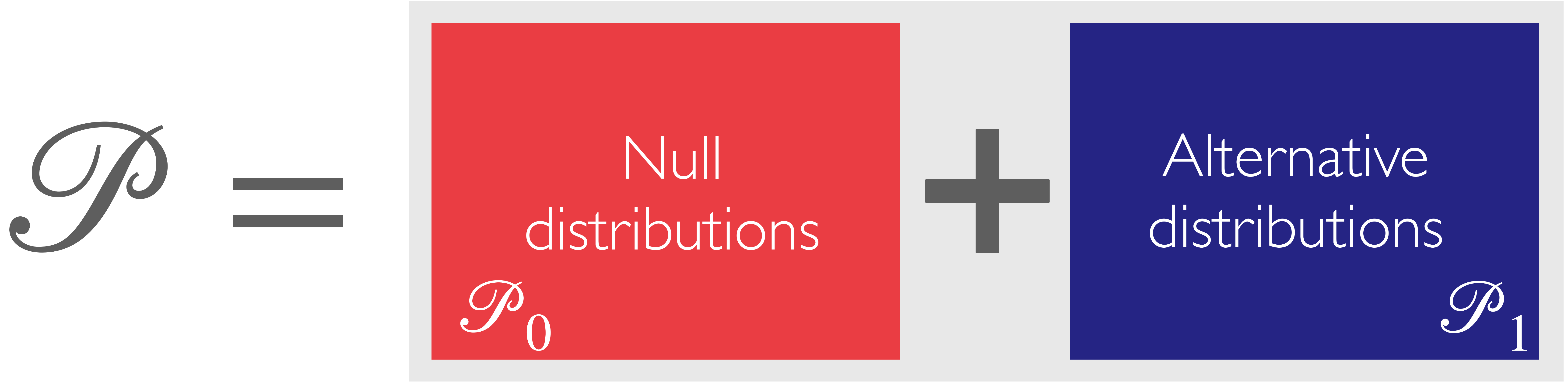


- Given $X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} P \in \mathscr{P}$, **our goal** is to determine

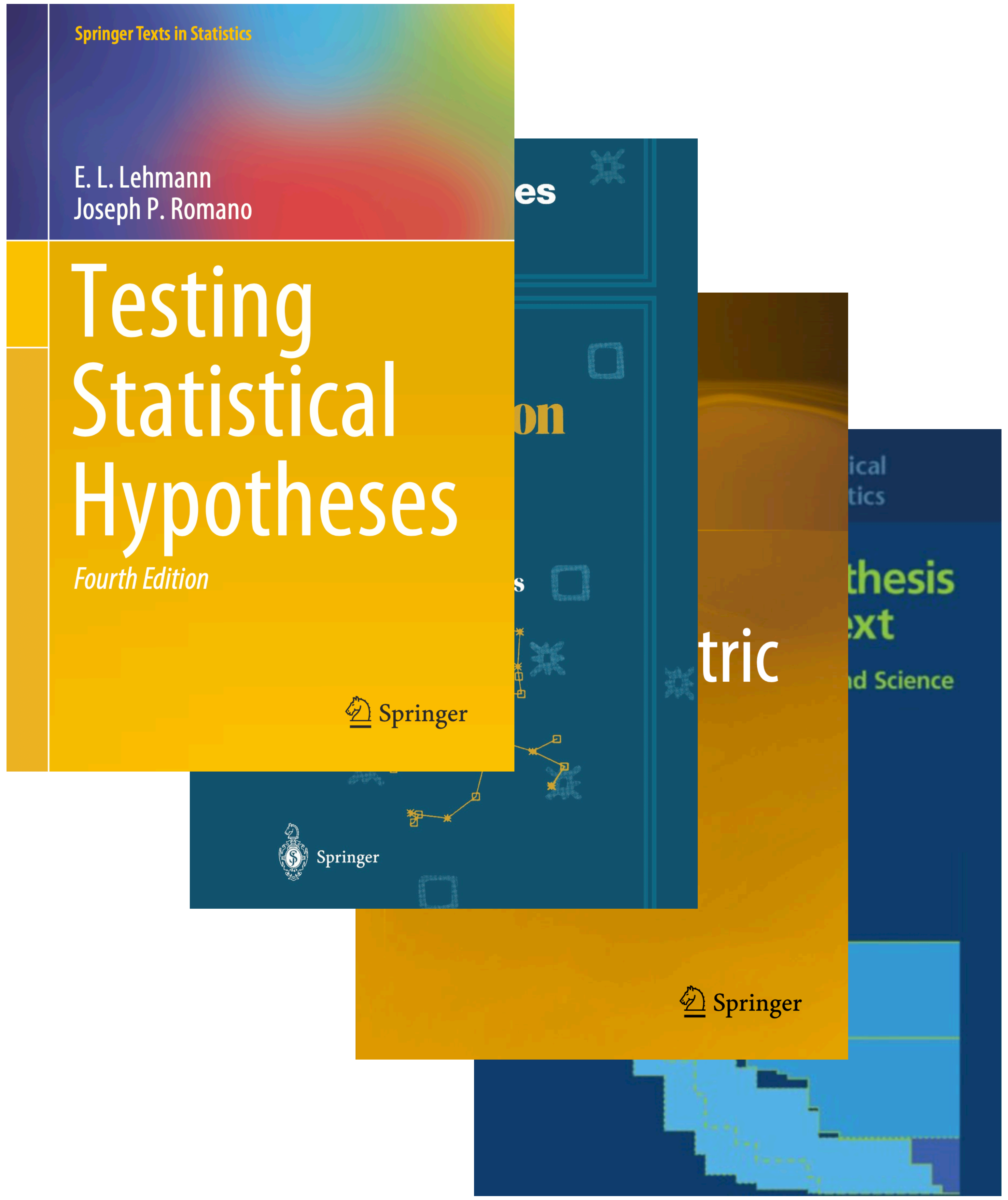
$$H_0 : P \in \mathscr{P}_0 \quad \text{versus} \quad H_1 : P \in \mathscr{P}_1$$

Recap: Statistical Hypothesis Testing

Examples include

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

⋮



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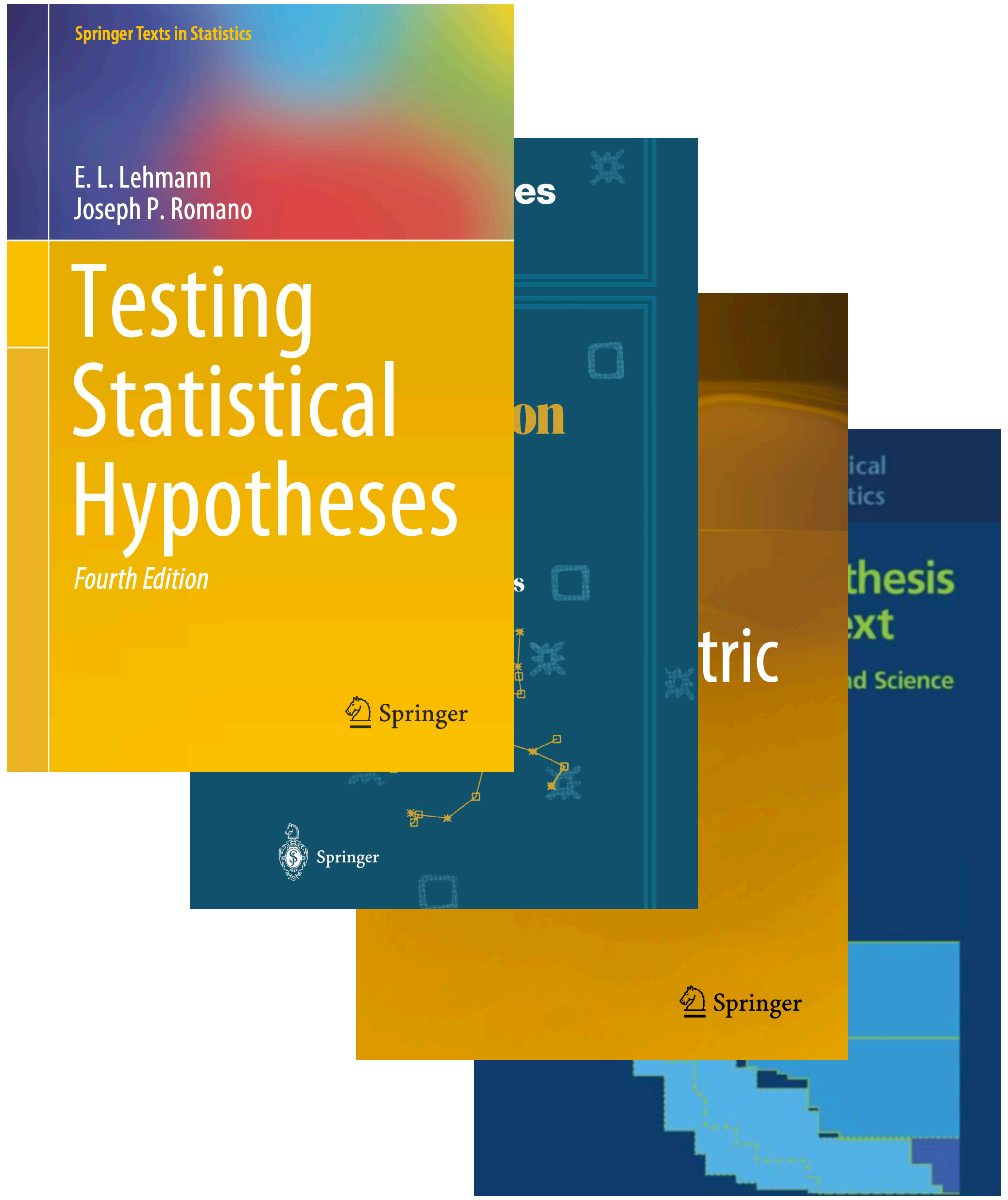
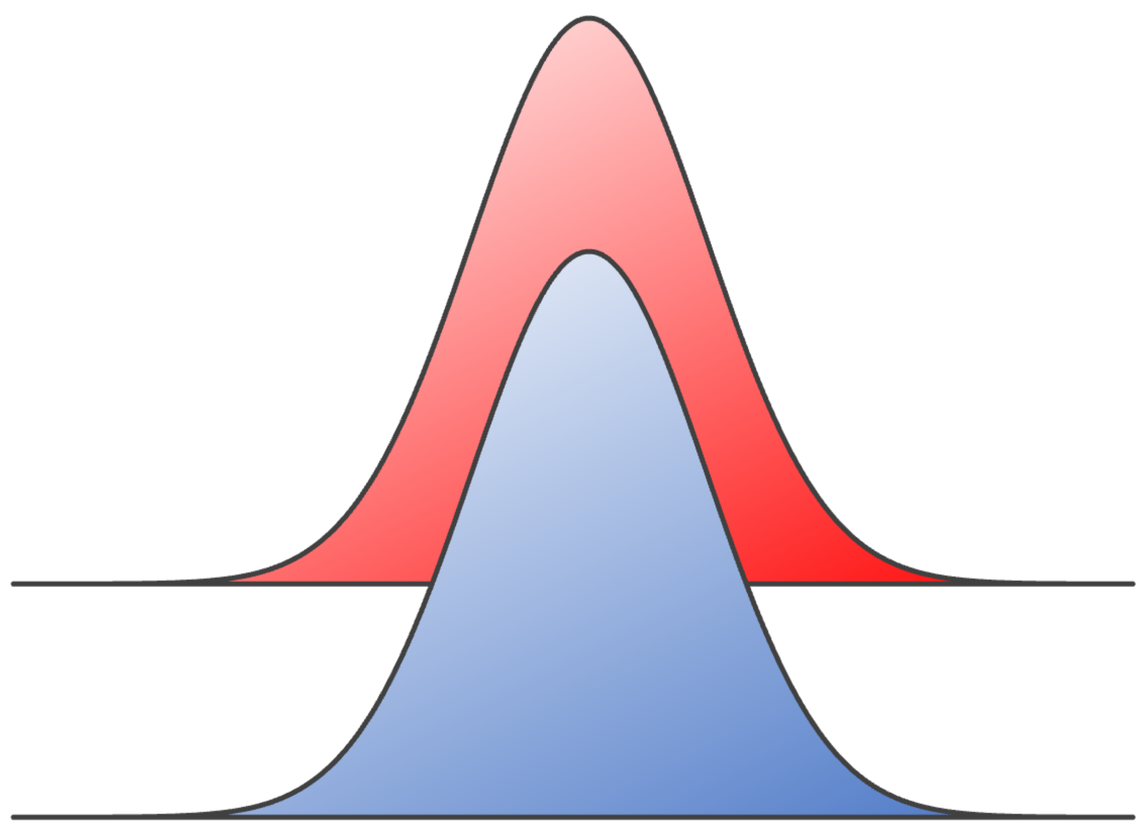


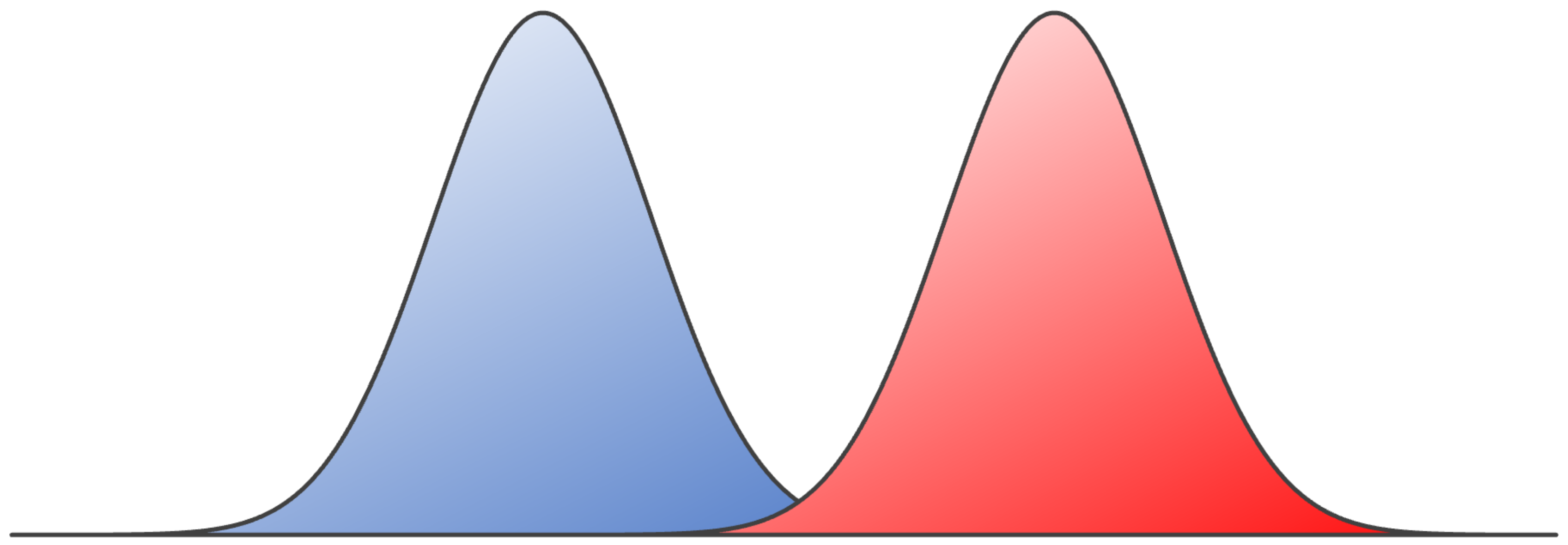
Two-Sample Problem

- 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



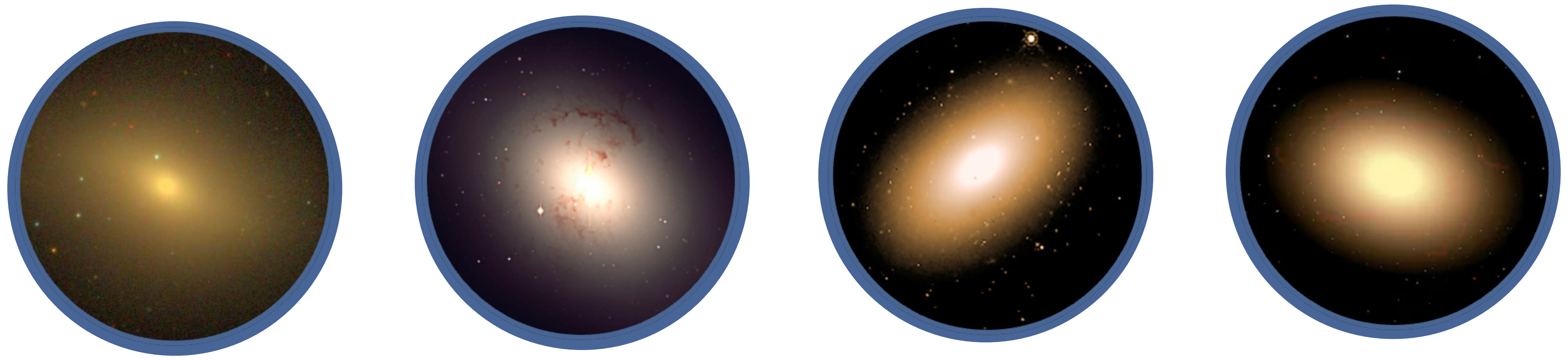
$H_0 : P_X = Q_Y$

versus



$H_1 : P_X \neq Q_Y$

Applications: Astronomy



High-mass versus Low-mass galaxies

Applications: Generative Models

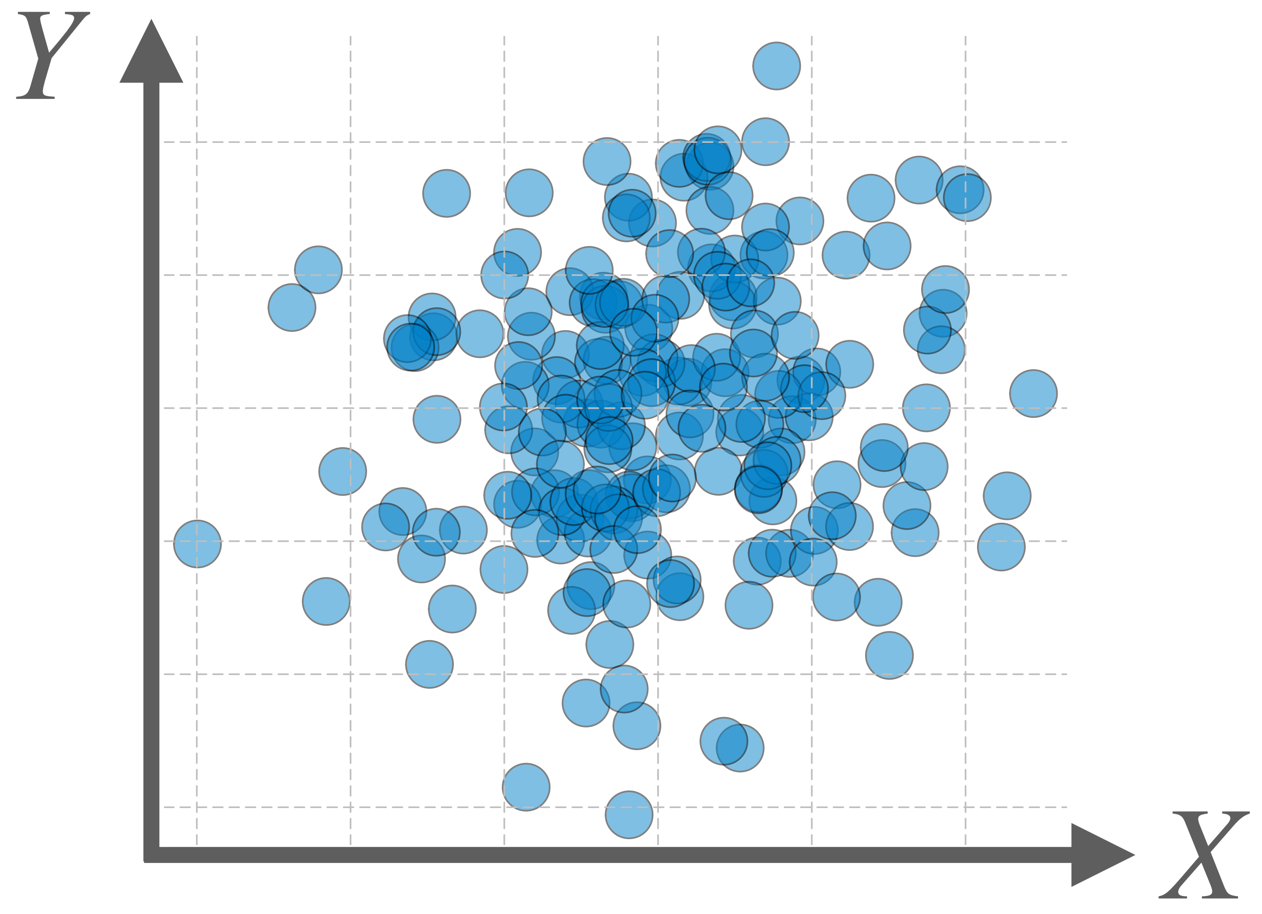
$\sim P_{\text{real}}$

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

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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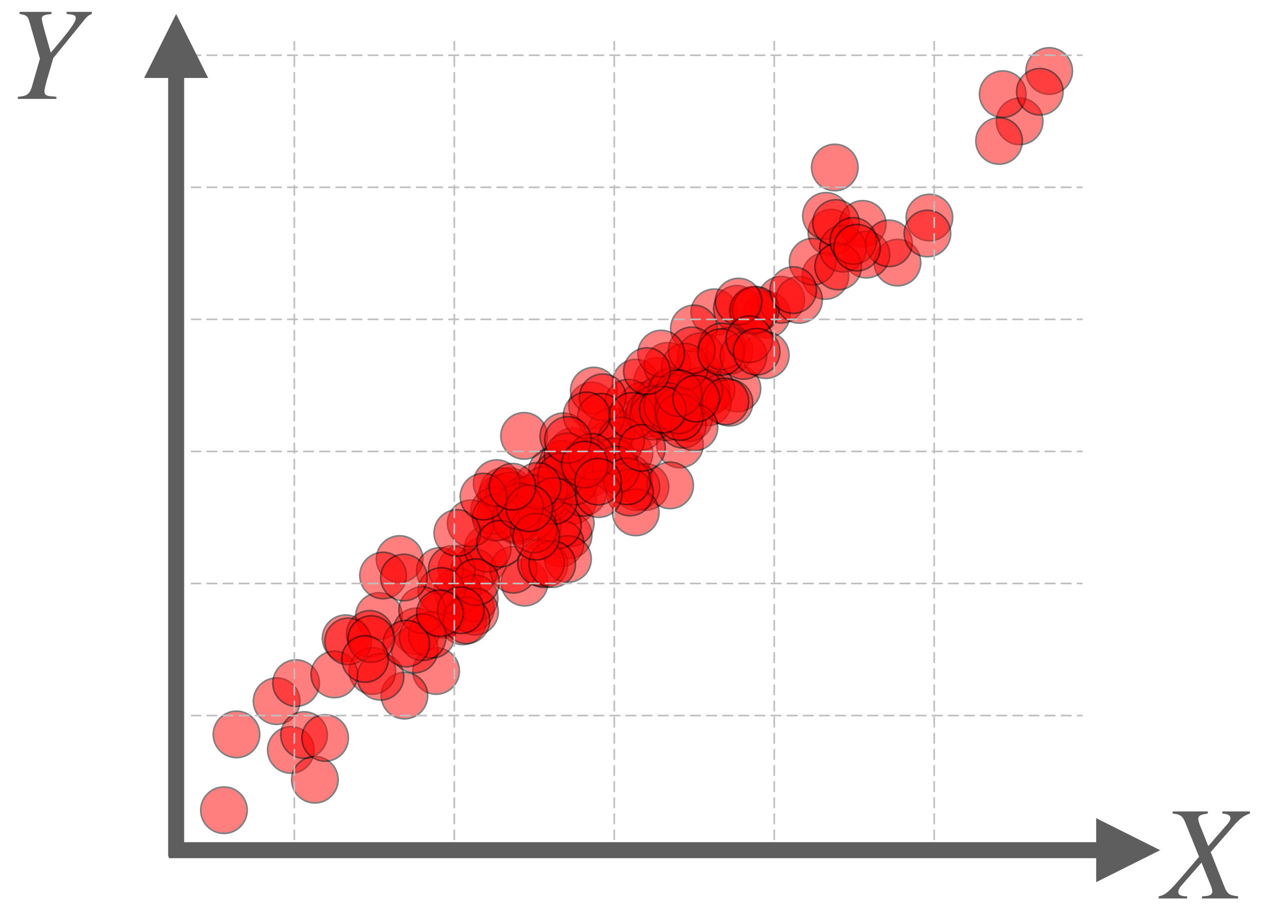

$H_0 : P_{X,Y} = P_X P_Y$

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

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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- There are two types of error we care about

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

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

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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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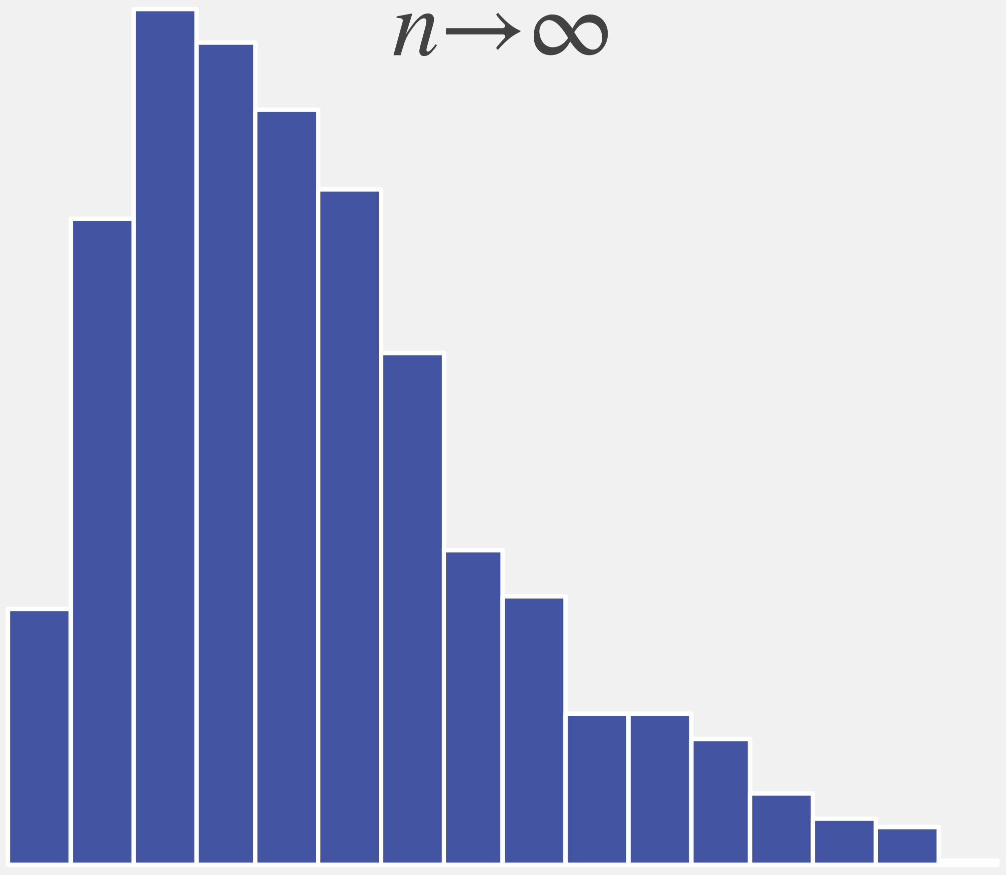
Derive the null distribution

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



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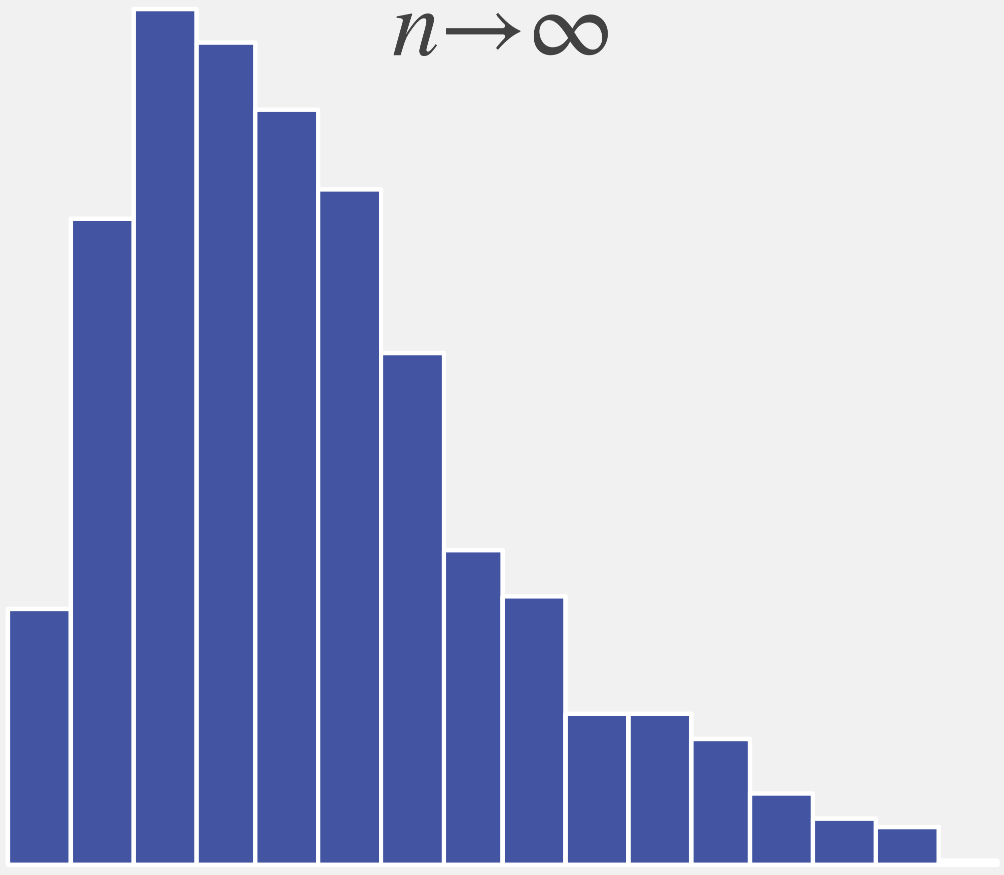
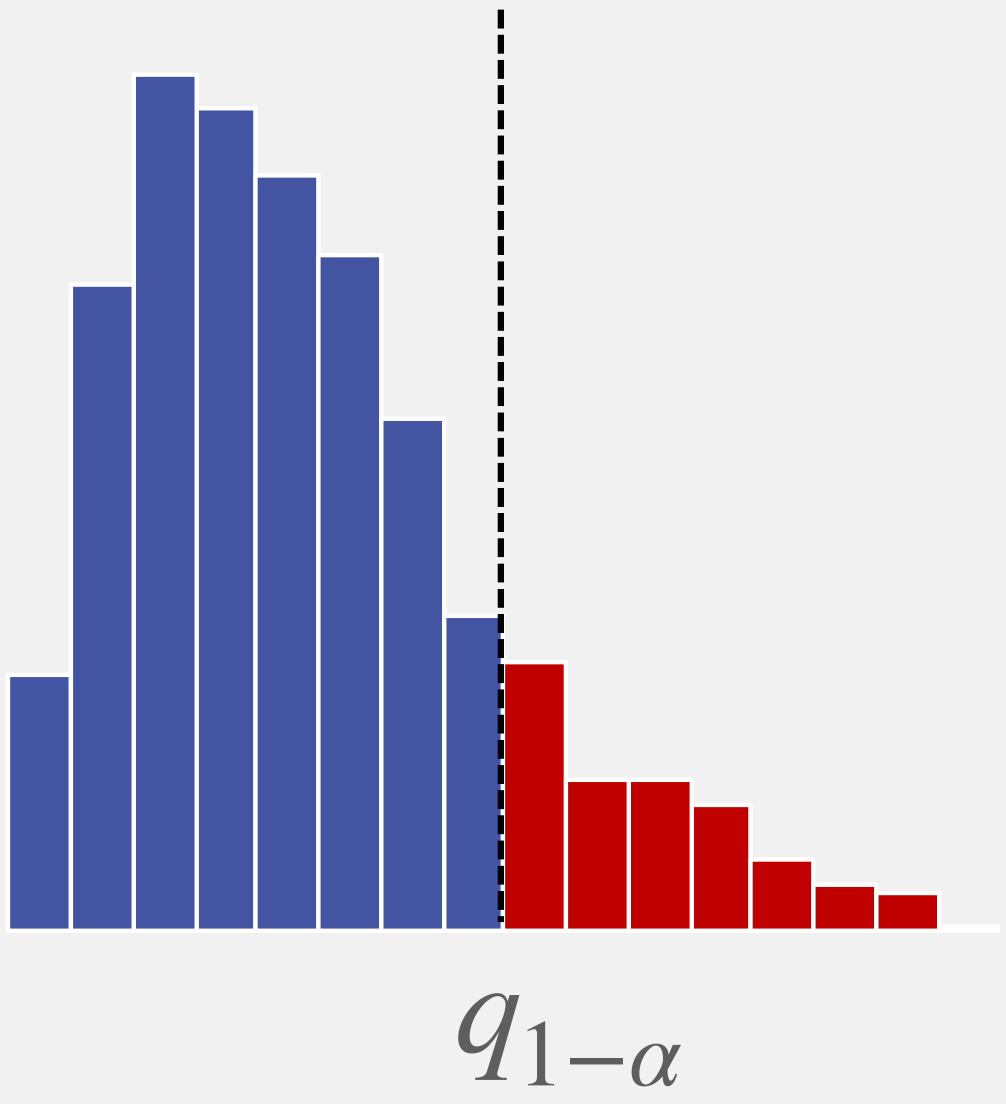


Step III

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



New Challenges

- Modern data are often **large**, **high-dimensional** and **complex**

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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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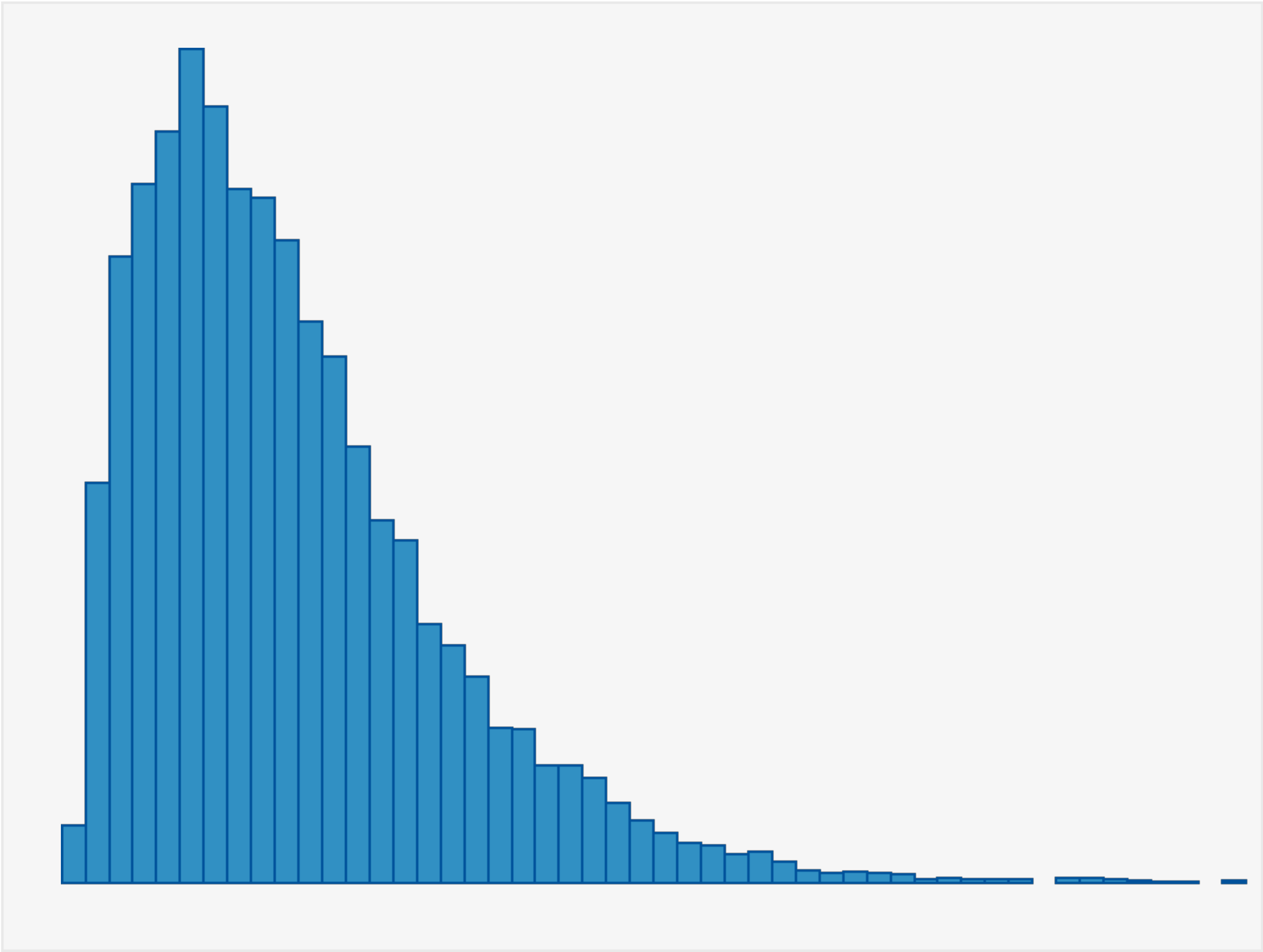
Classical asymptotic theory shows that under H_0

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

Chi-squared distribution with $(\ell_1 - 1)(\ell_2 - 1)$ d.f.

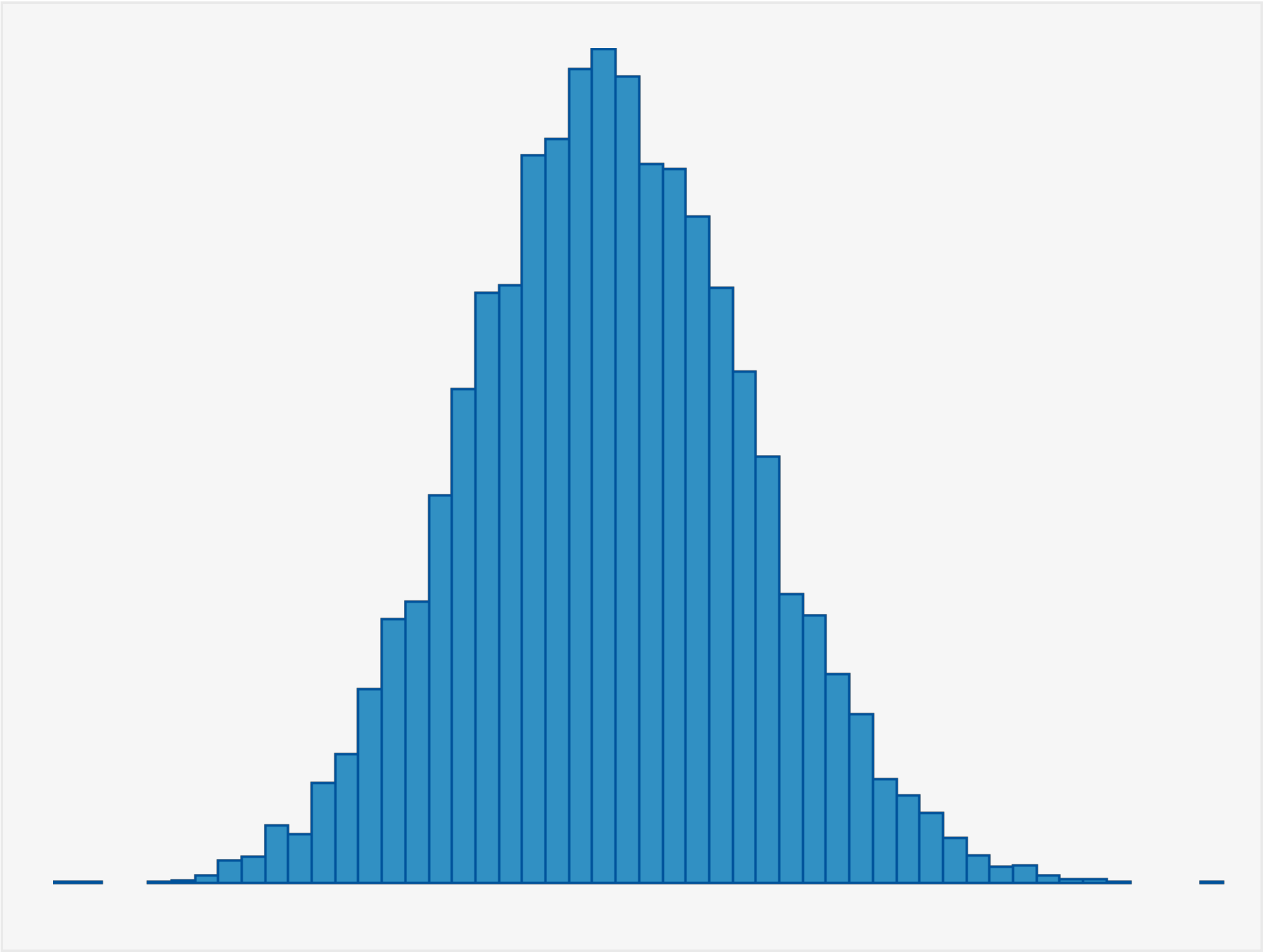
Example: χ^2-statistic in high-dimensions

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



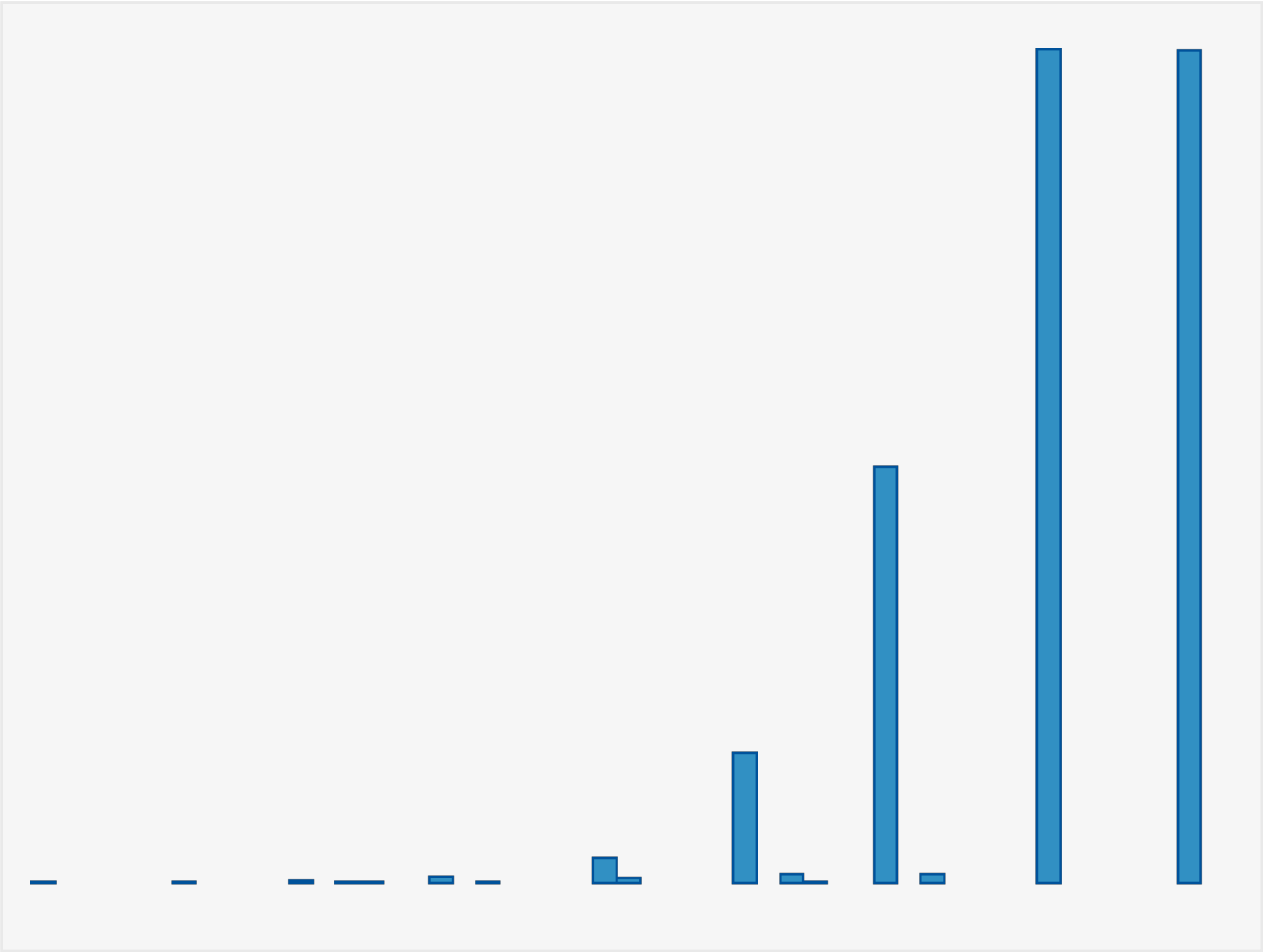
≈ Chi-square

$\ell_1 = \ell_2 = 3$



≈ Gaussian

$\ell_1 = \ell_2 = 50$



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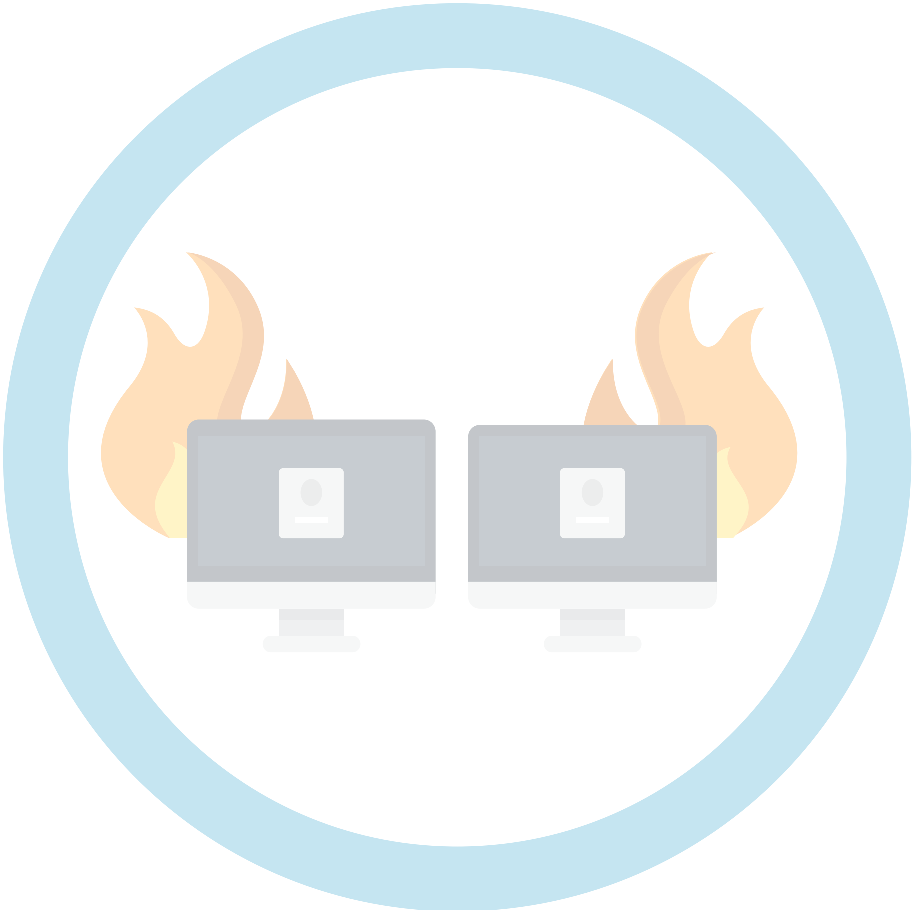
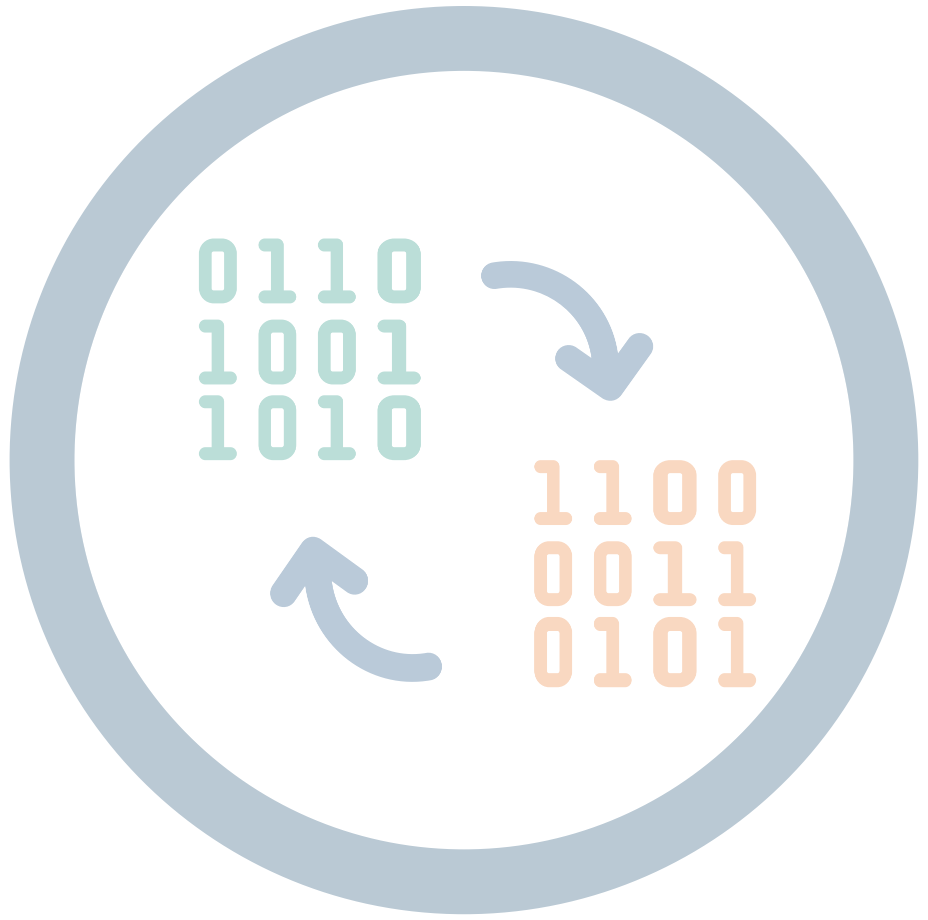
- **Uniform**, **non-asymptotic** type I error control
- **Distribution-free** for any type of test statistics
- It does not depend on **unspecified constants**
- All we need is $\{X_1, \ldots, X_n\}$ are **exchangeable** under the null

Three main challenges of the permutation approach

Power Analysis



Computational Complexity



Non-exchangeable Data

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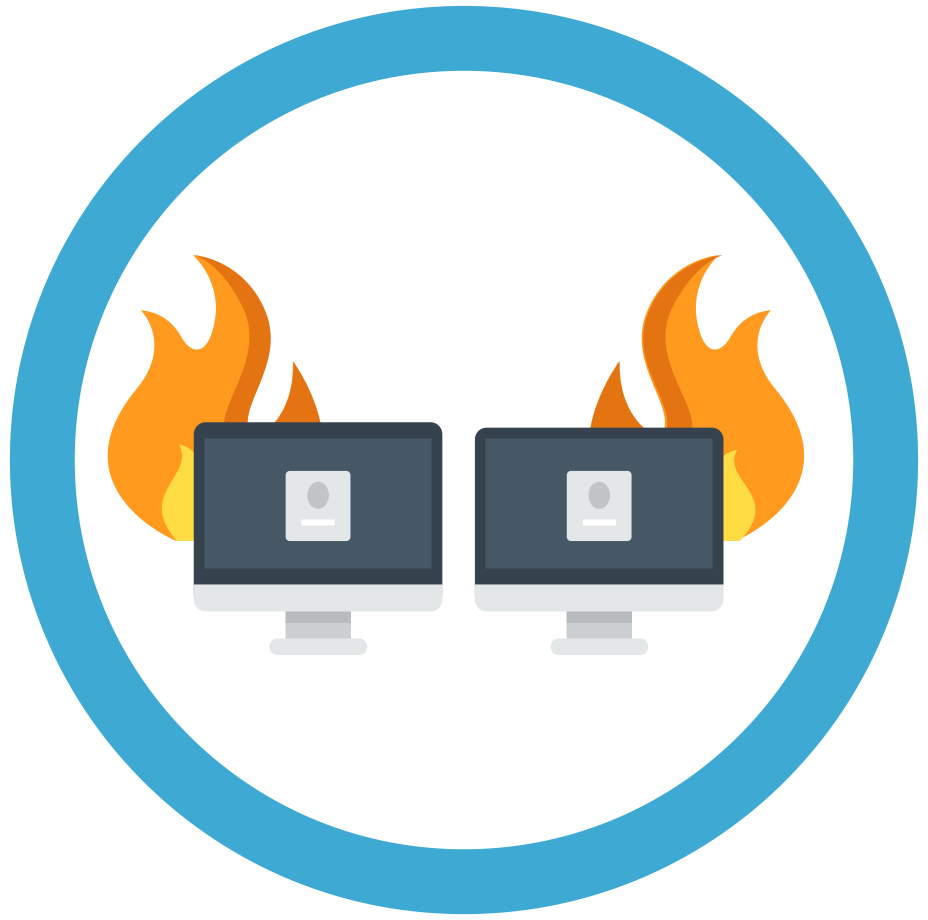

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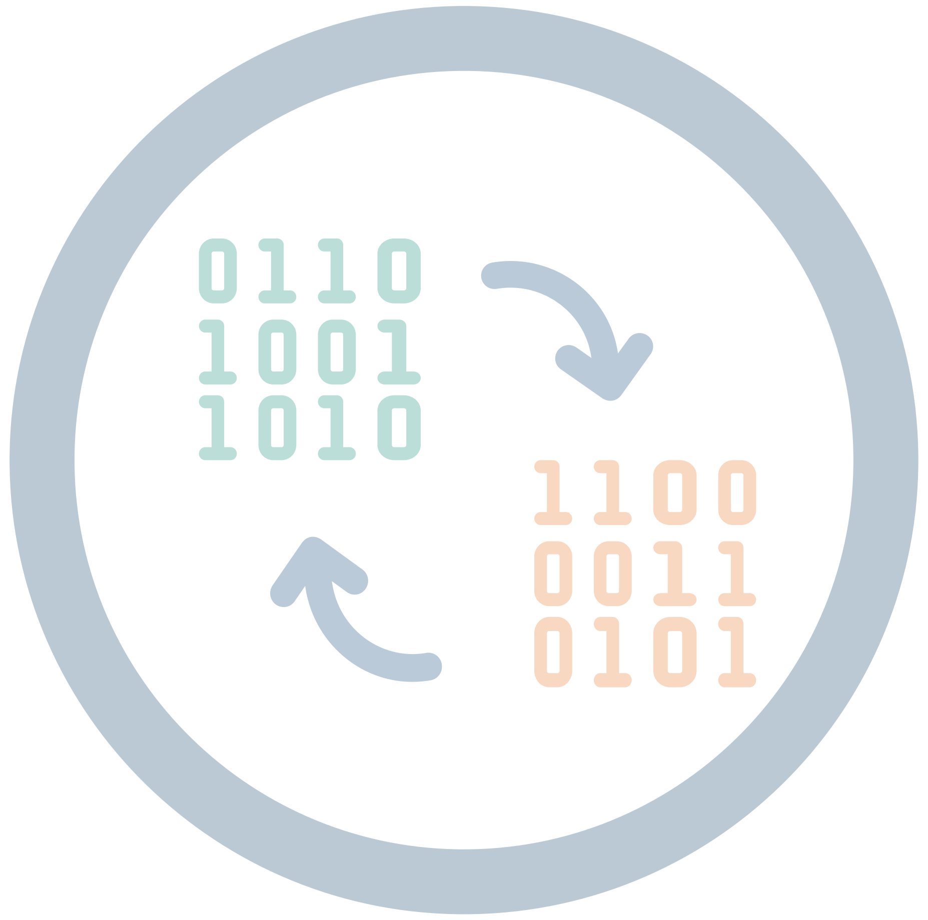

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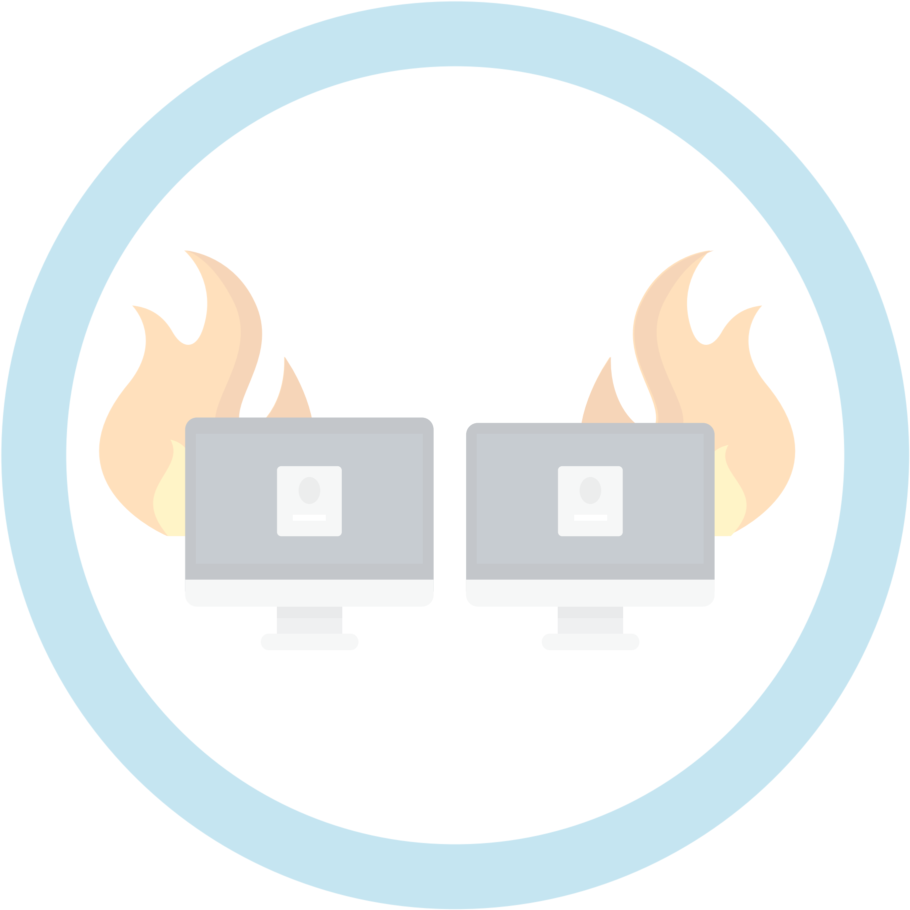

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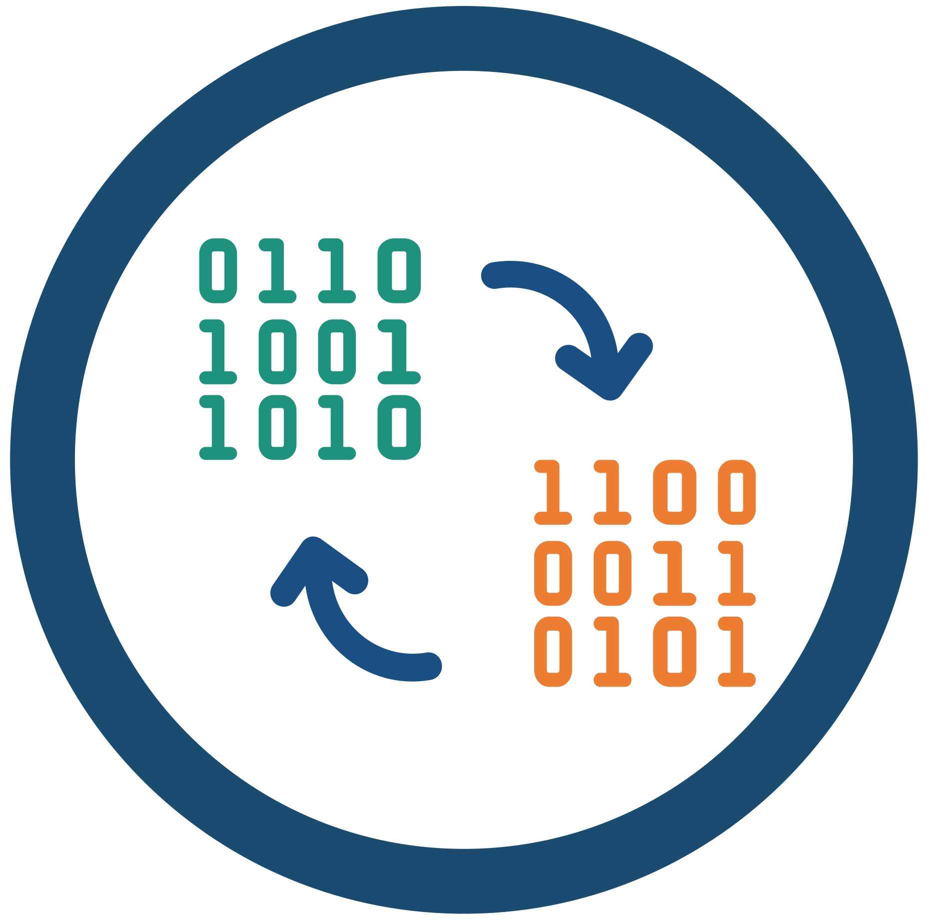


Non-exchangeable
Data

Part I. Methodological Contributions

Part II. Theoretical Contributions

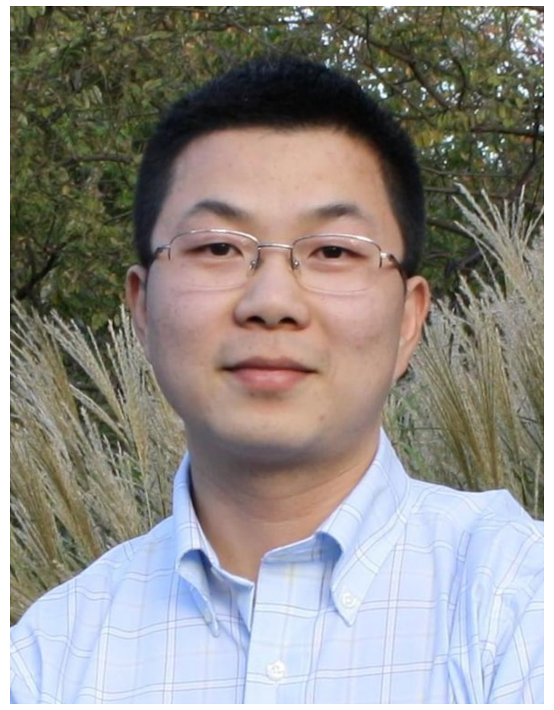
Electronic Journal of Statistics
Vol. 13 (2019) 5253–5305
ISSN: 1935-7524
https://doi.org/10.1214/19-EJS1648

Global and local two-sample tests via regression

Ilmun Kim, Ann B. Lee, and Jing Lei

Carnegie Mellon University
Department of Statistics and Data Science
5000 Forbes Avenue
Pittsburgh, PA 15213

Ann Lee
(CMU)



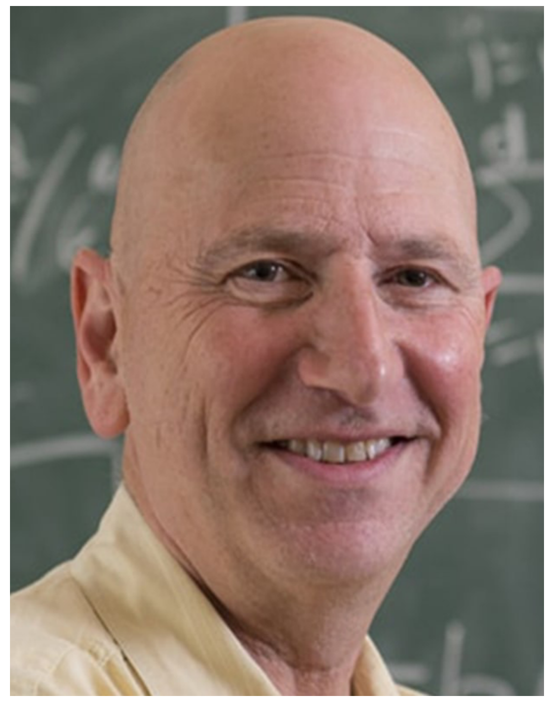
Jing Lei
(CMU)

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,§]

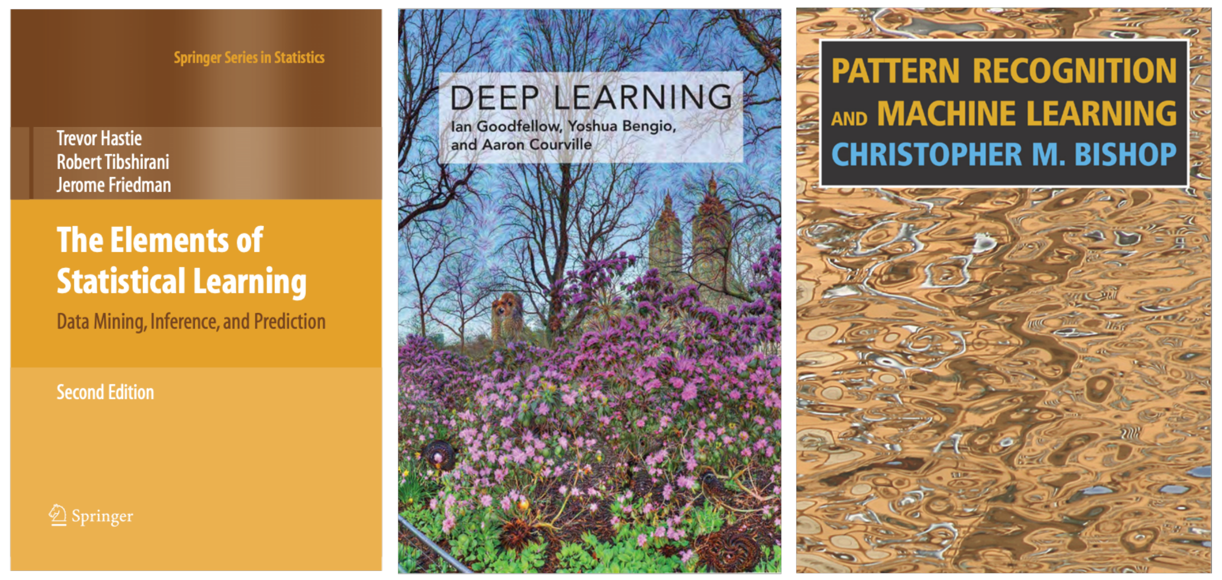
Aaditya Ramdas
(CMU)



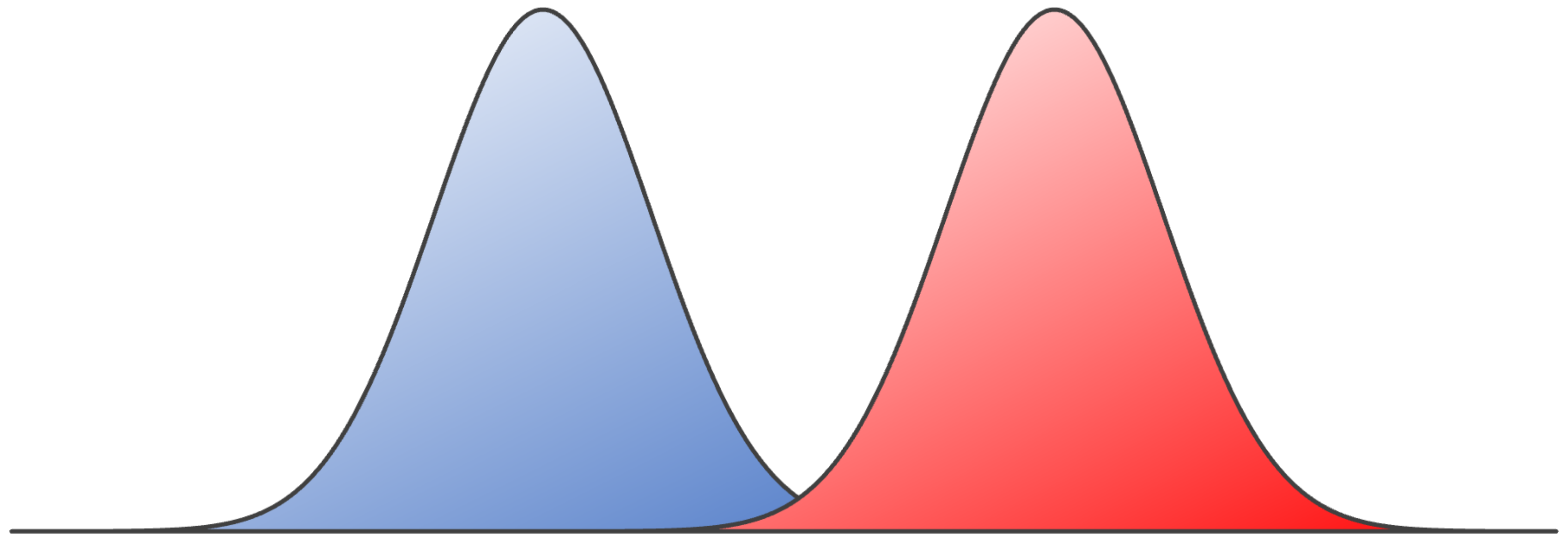
Larry Wasserman
(CMU)

Aarti Singh
(CMU)

We propose a flexible framework for two-sample testing



Classification/Regression



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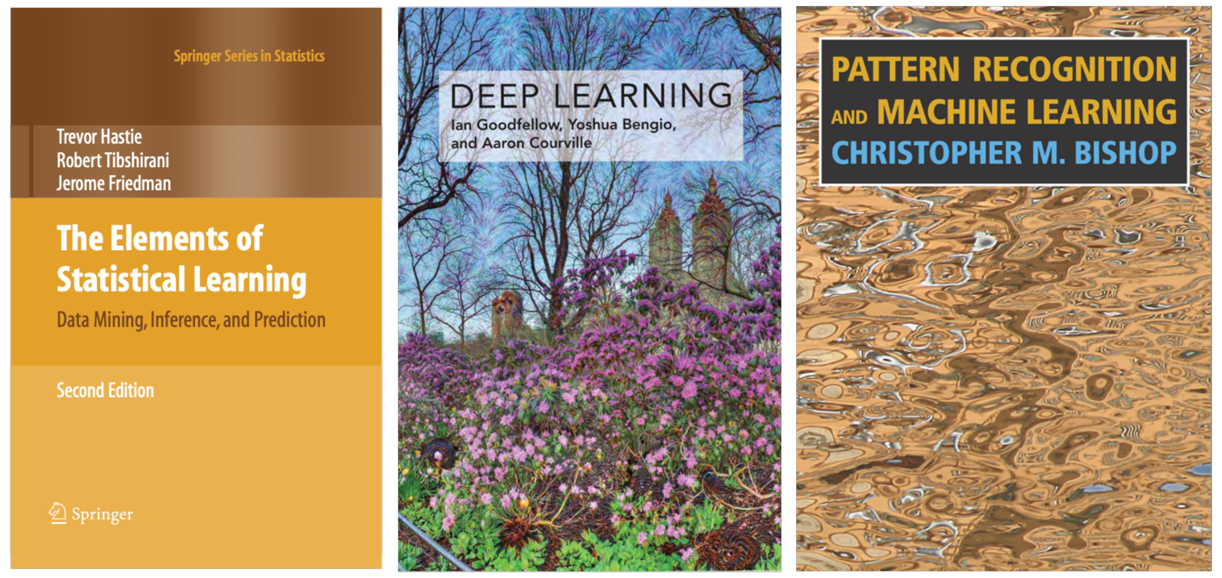

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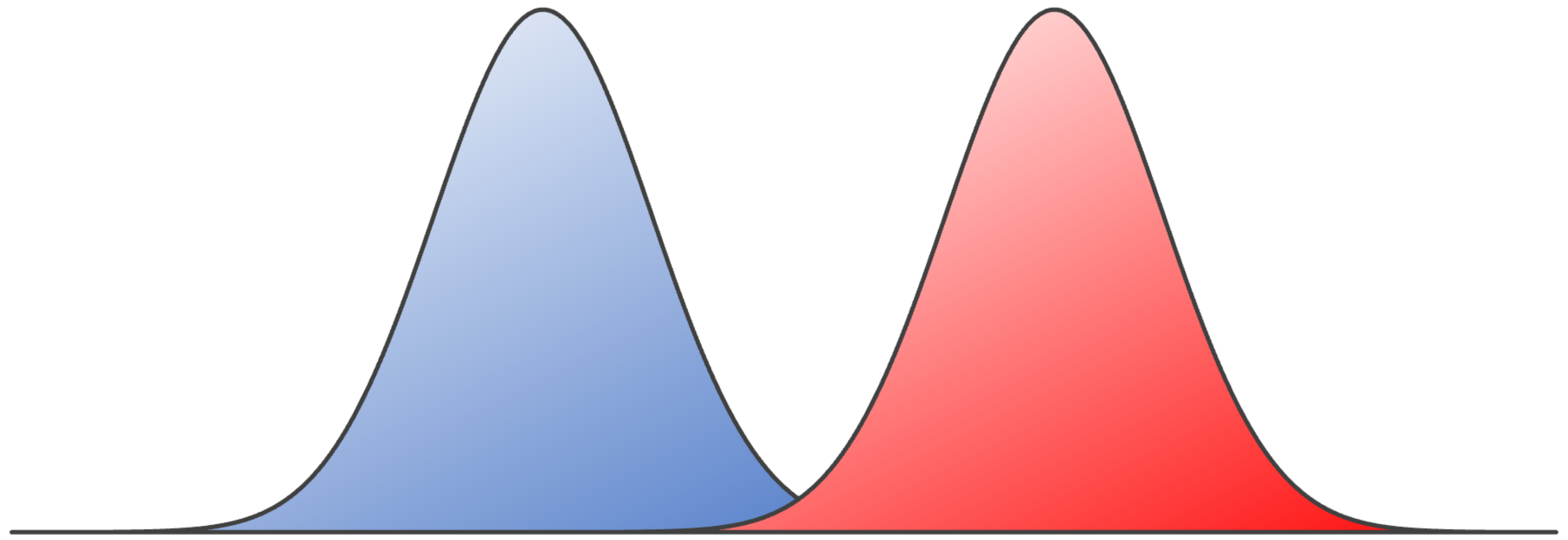

Two-sample test

Idea

- 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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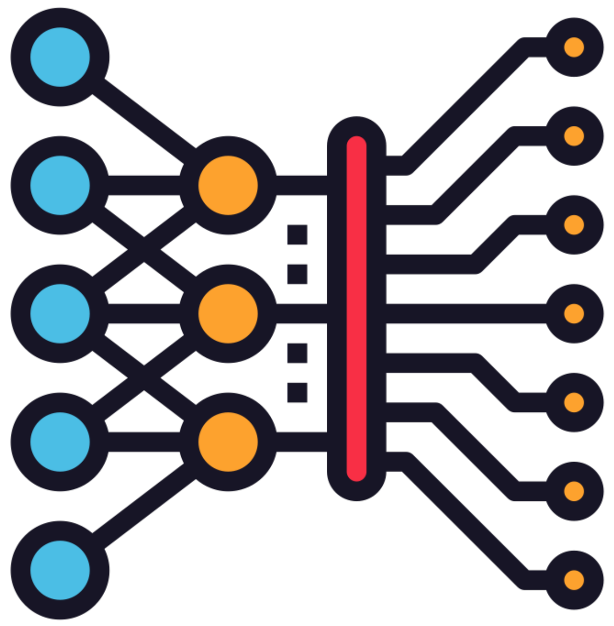
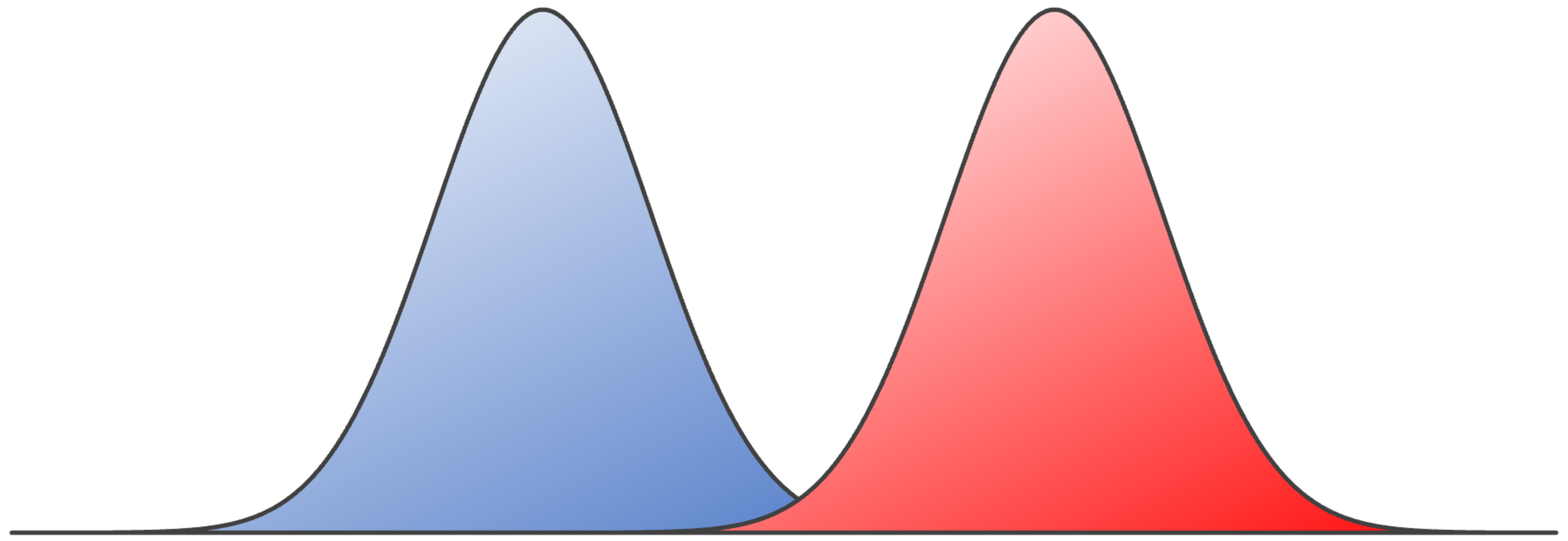


Neural networks



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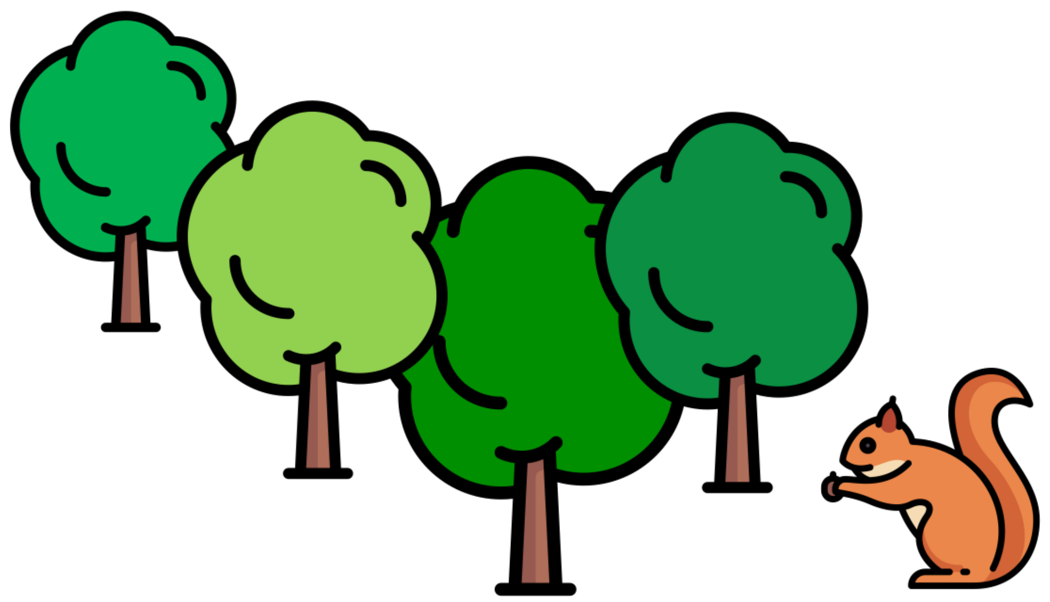
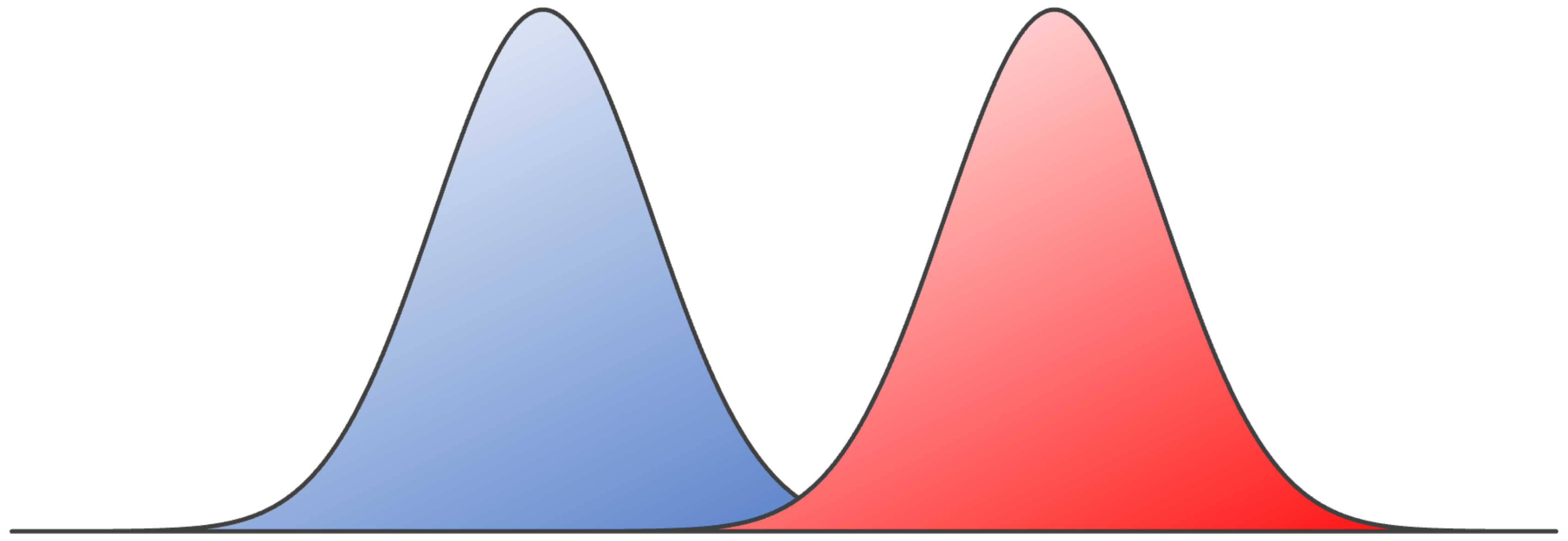


Random forests



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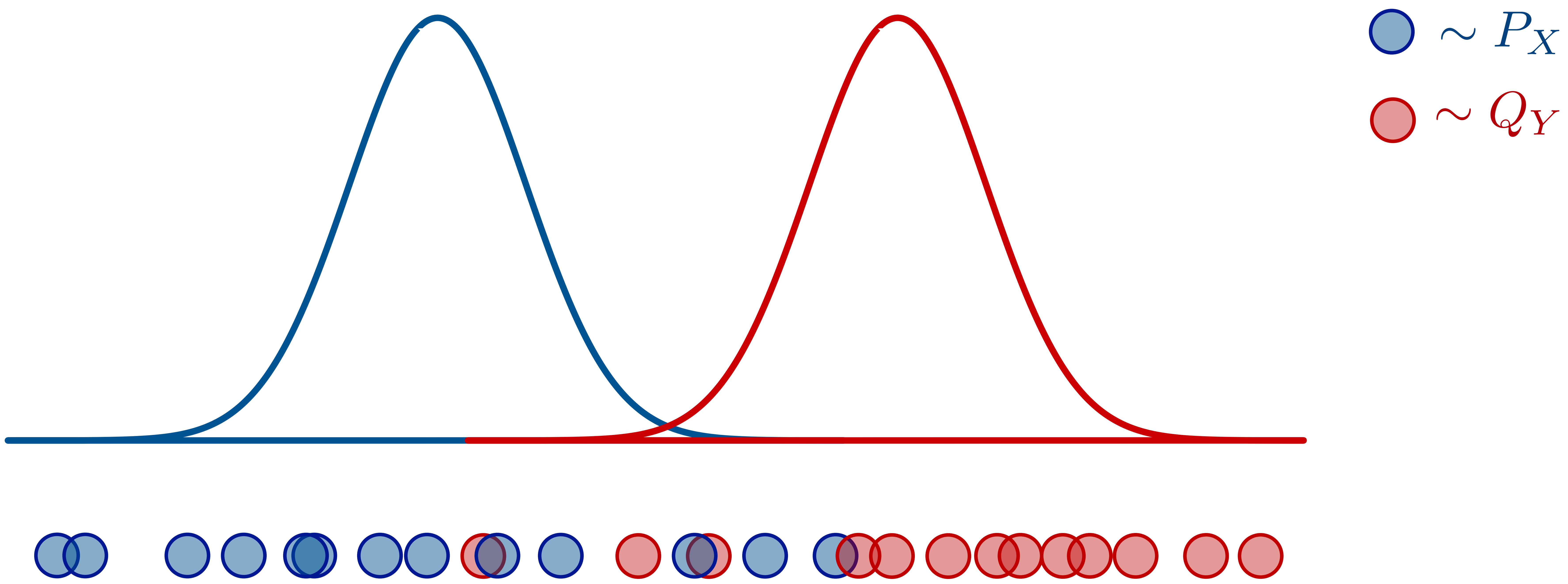
Regression-based two-sample test



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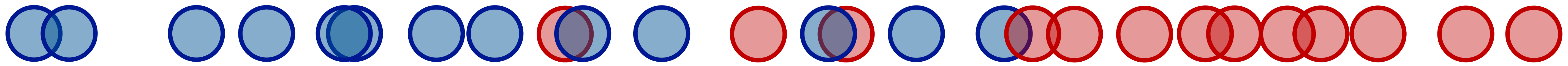

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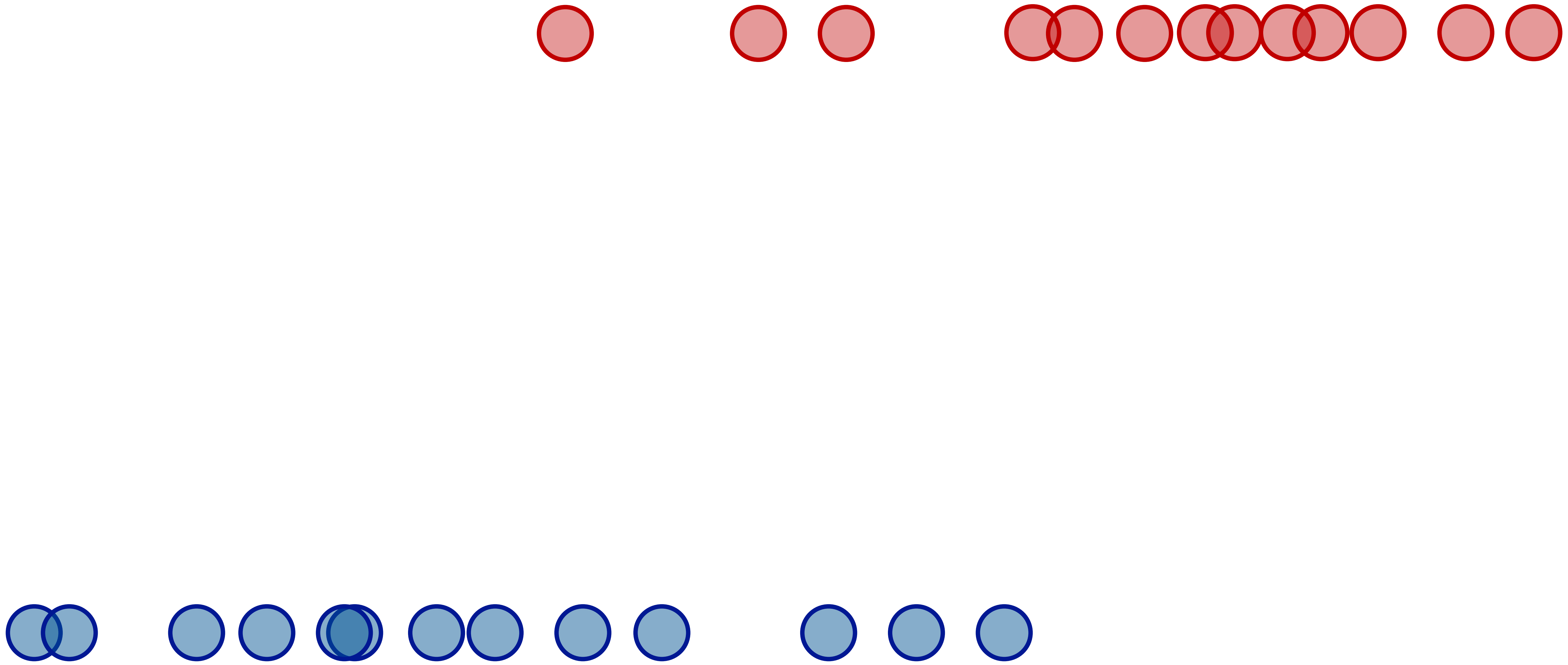

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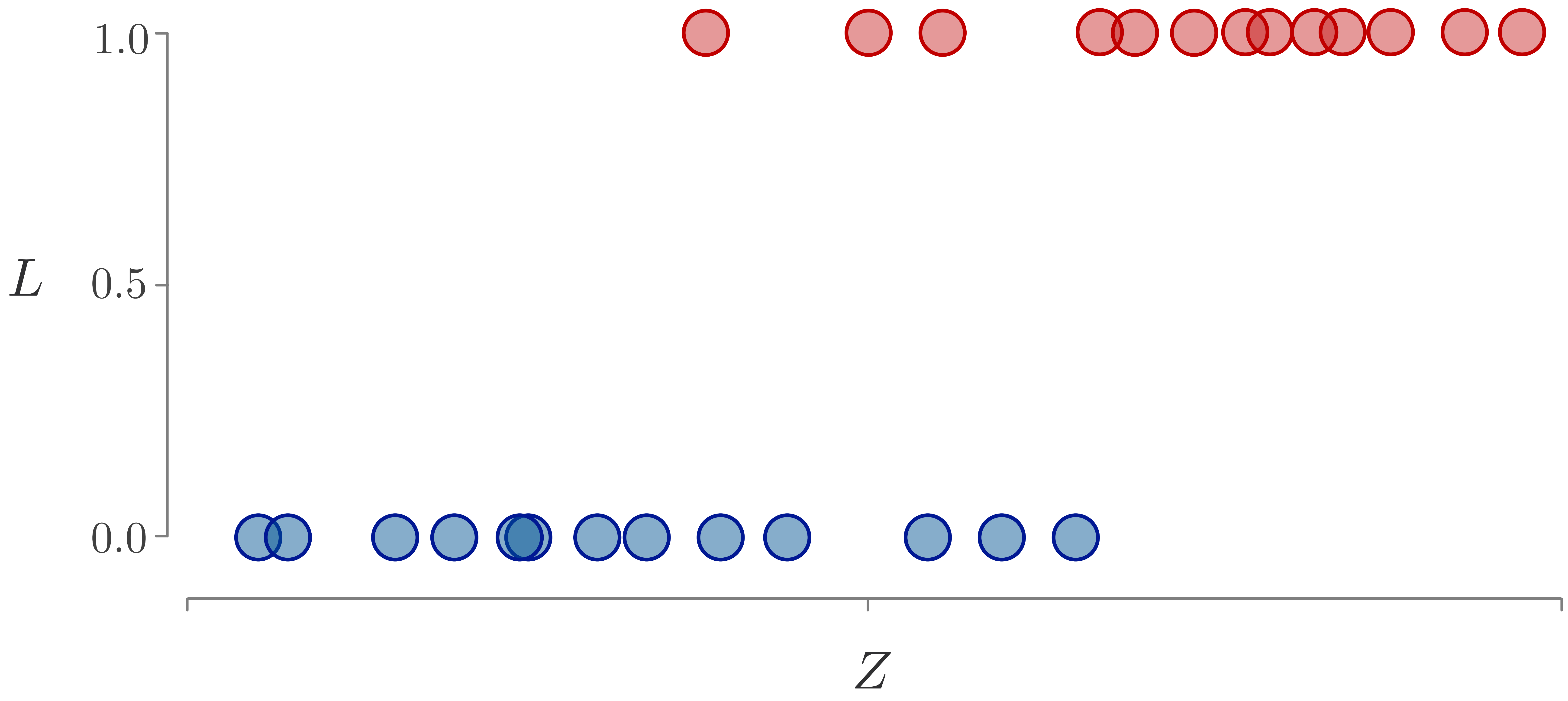

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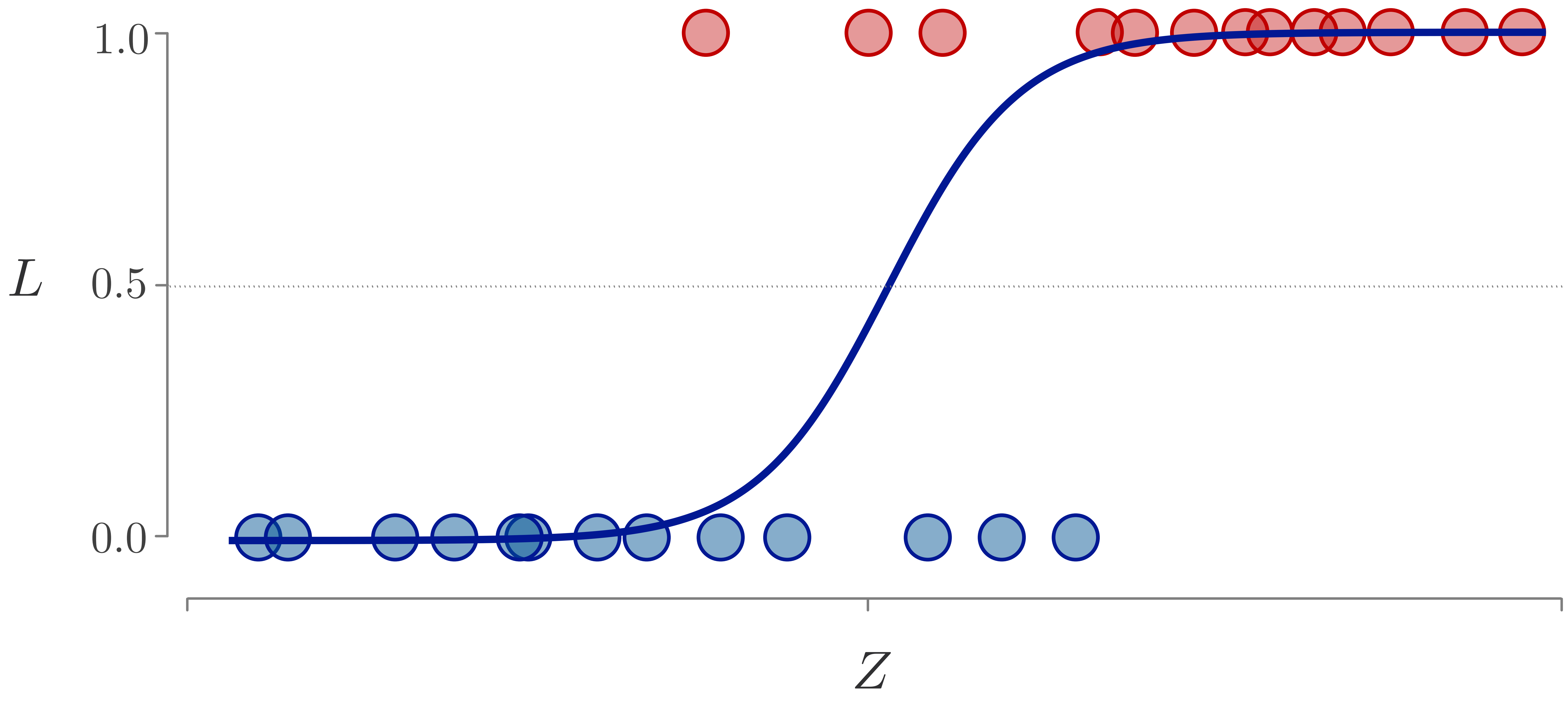
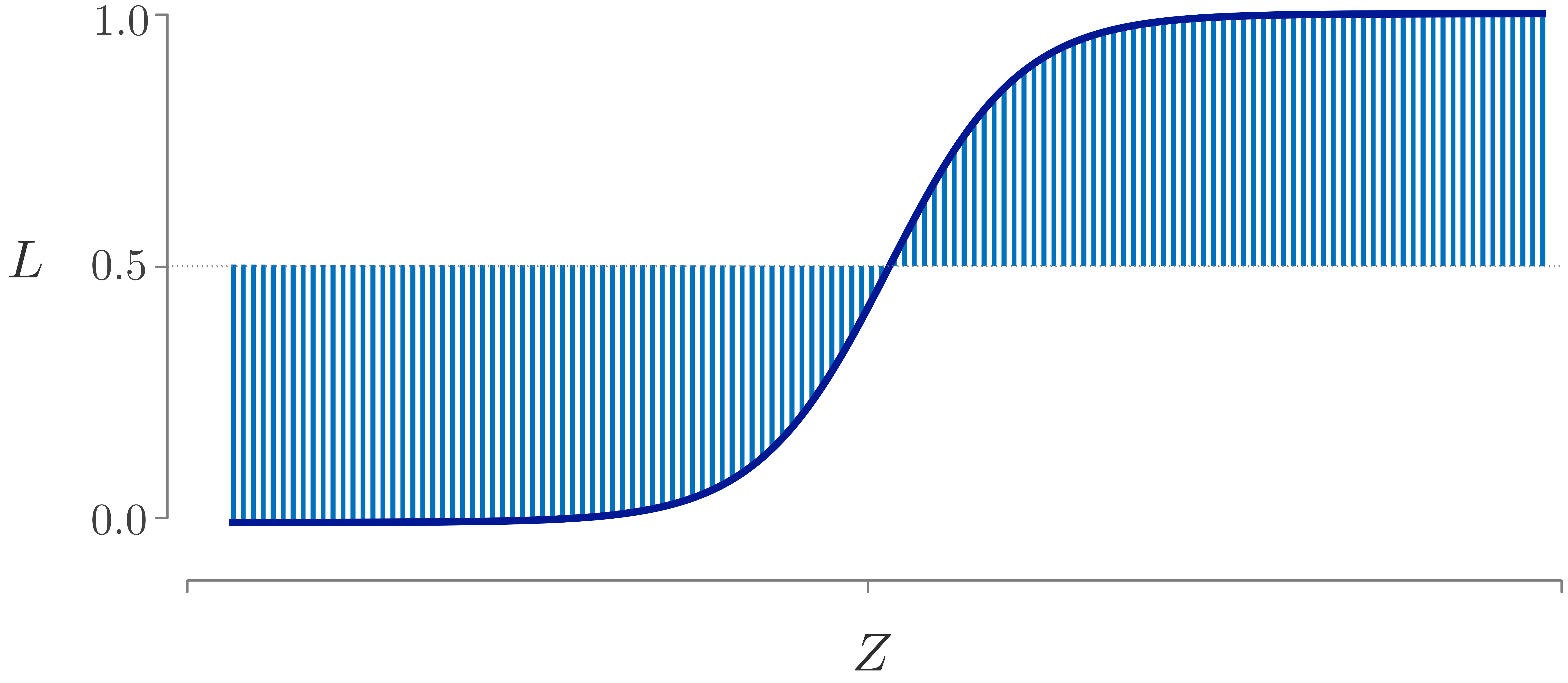


Regression-based two-sample test



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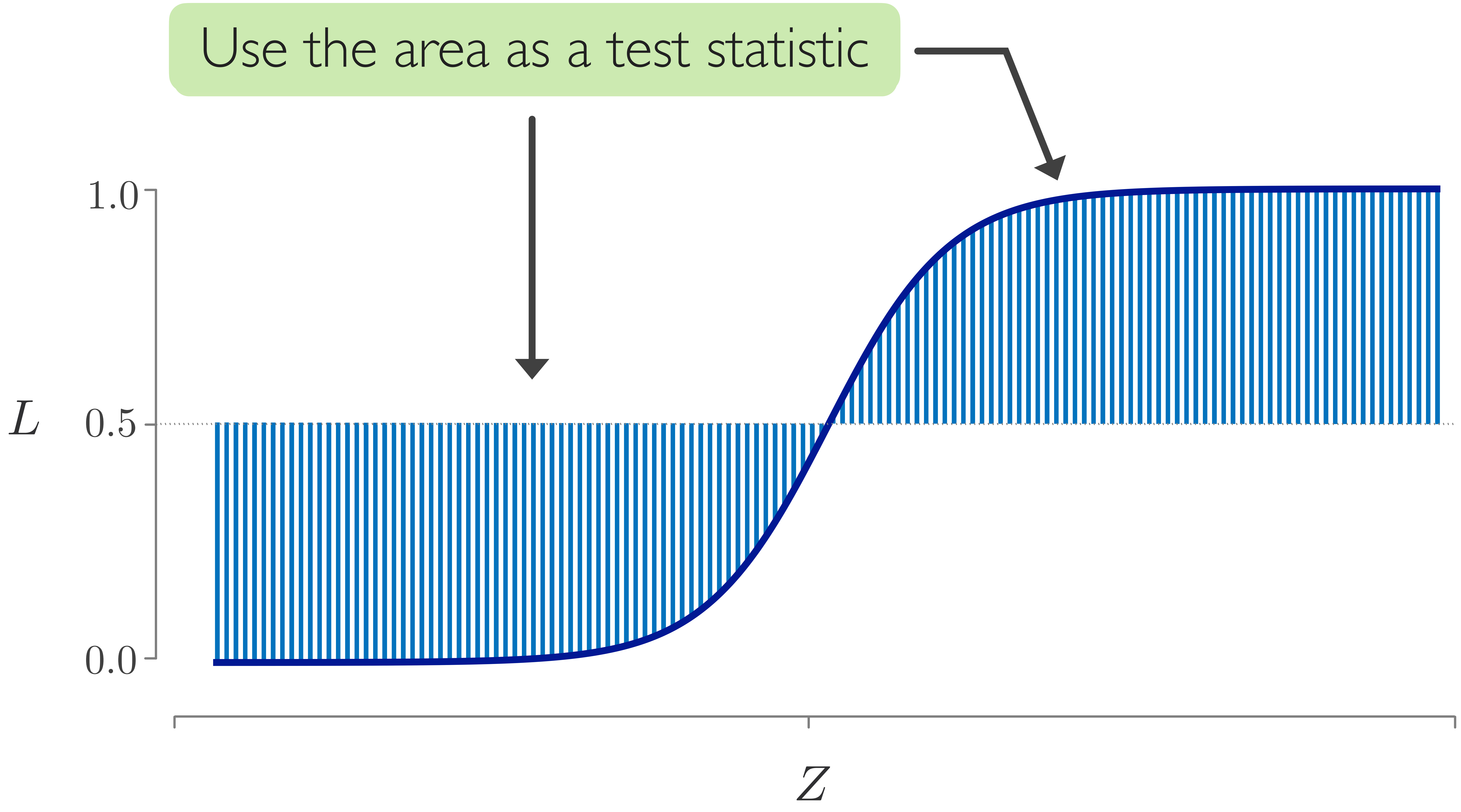
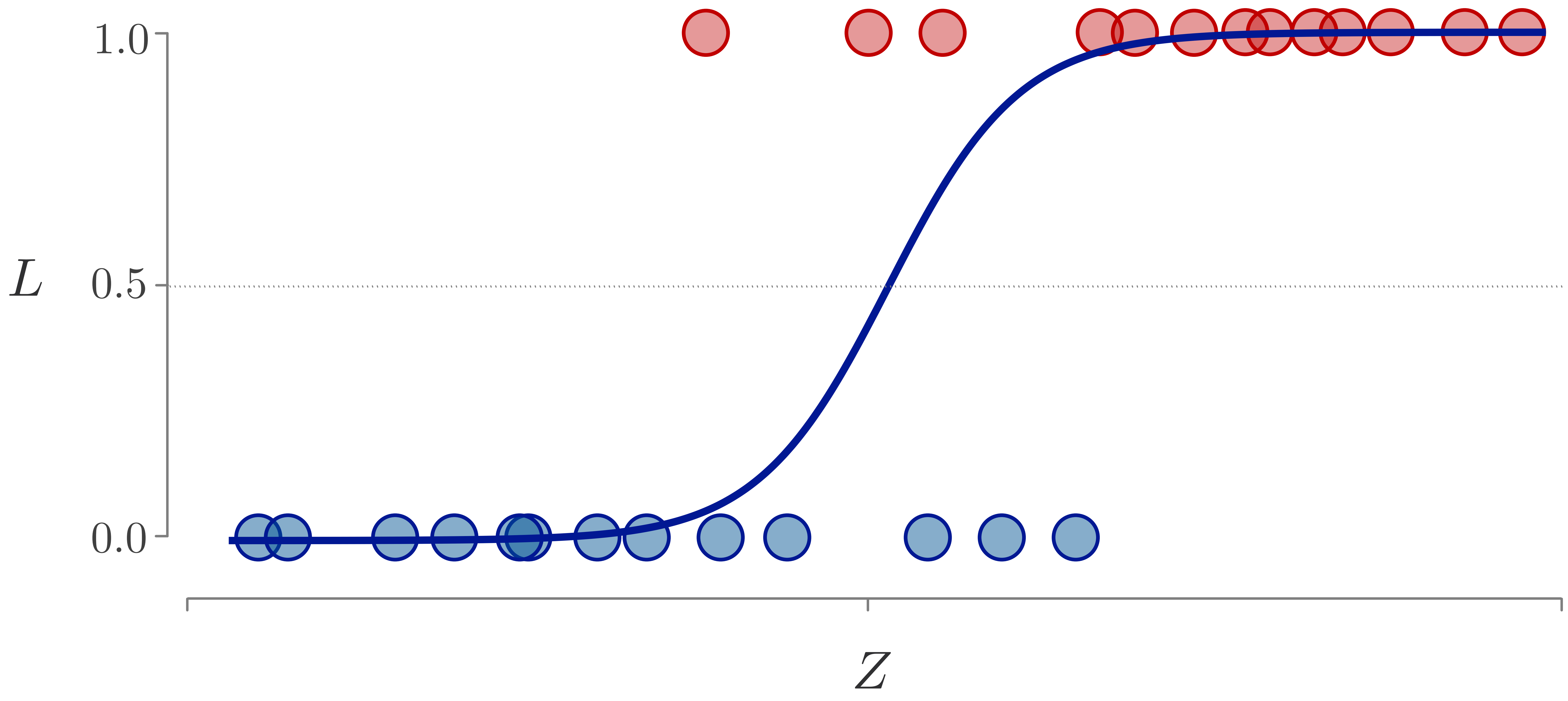


Classification accuracy-based two-sample test



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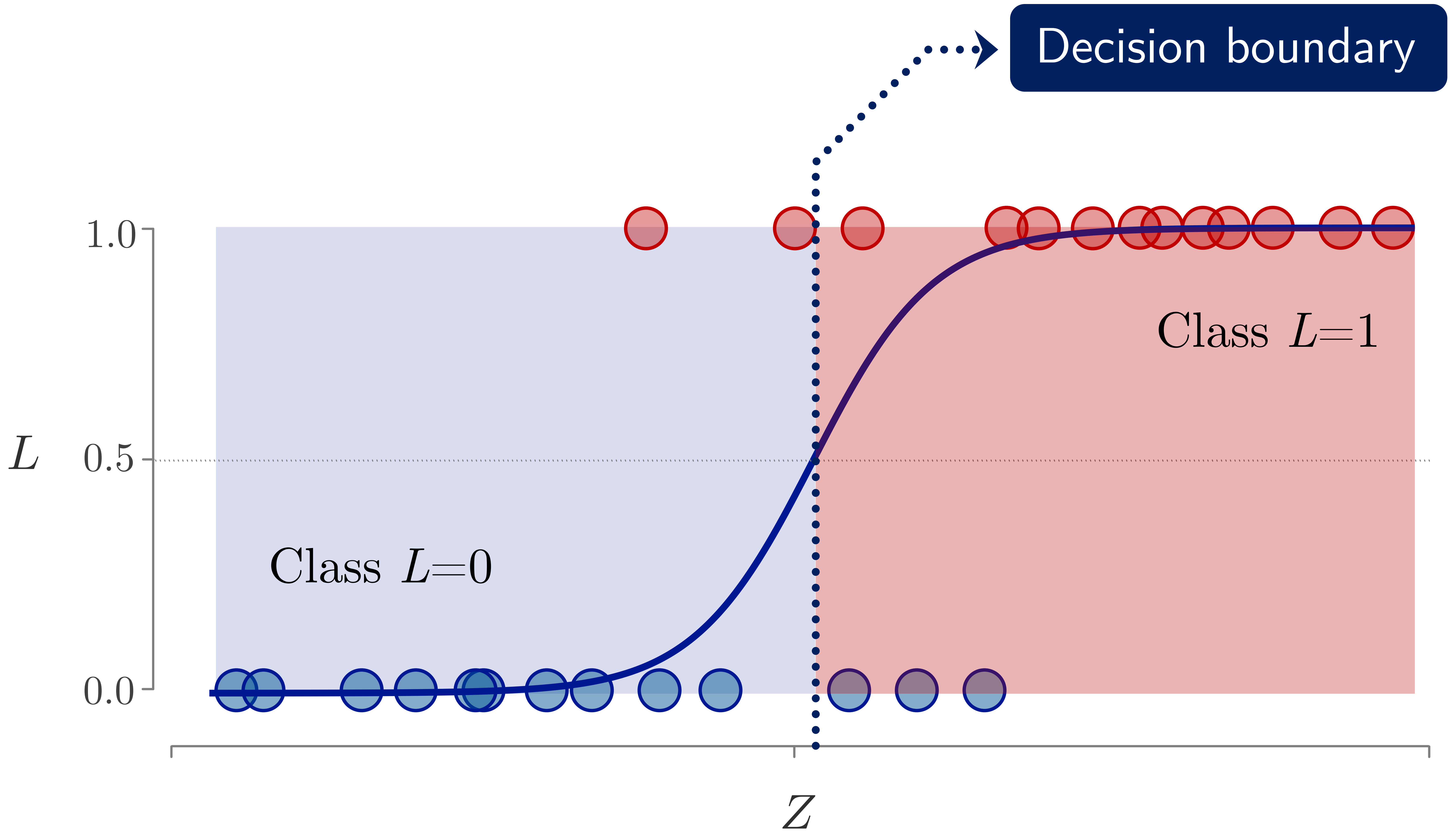
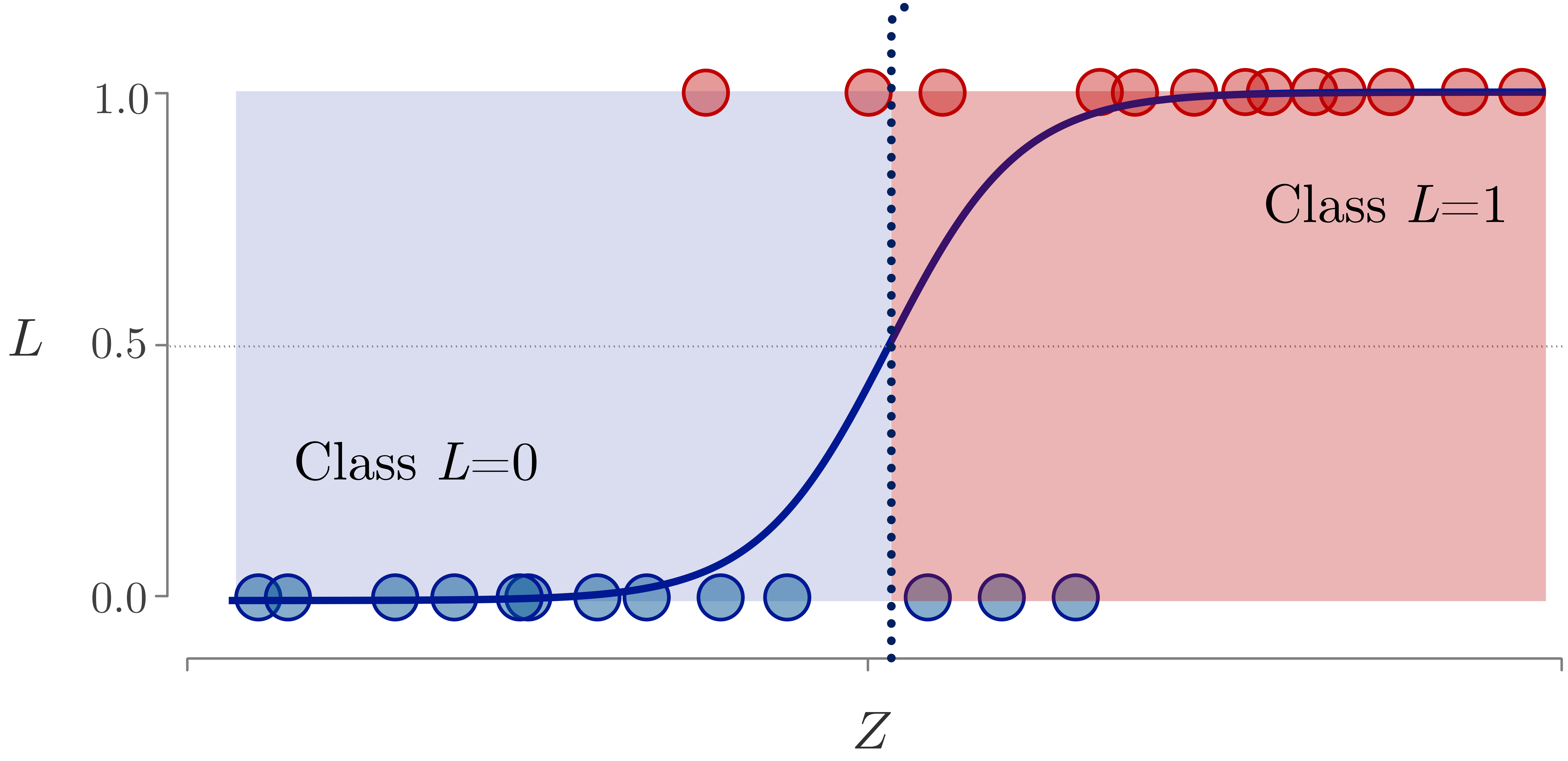


Classification accuracy-based two-sample test

Use the accuracy as a test statistic

Decision boundary



Test statistics

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

$m = n$
for simplicity

Test statistics

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Train a regressor

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

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Mean square error

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

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Train a classifier

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

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Train a regressor → **Mean square error**

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

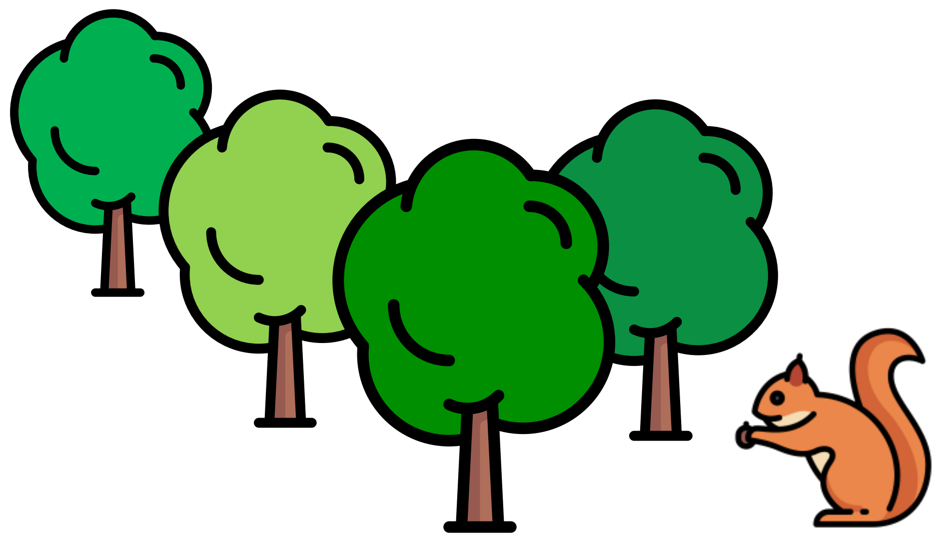
$$N^{-1} \sum_{i \in [N]} \left(\widehat{R}(Z_i) - 1/2\right)^2$$

Train a classifier → **Accuracy**

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

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

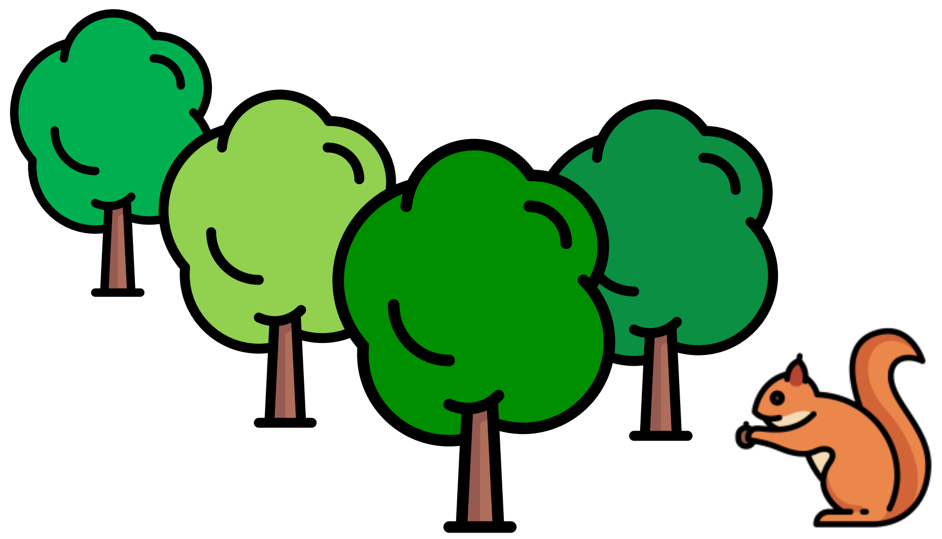
Empirical results



Random forests

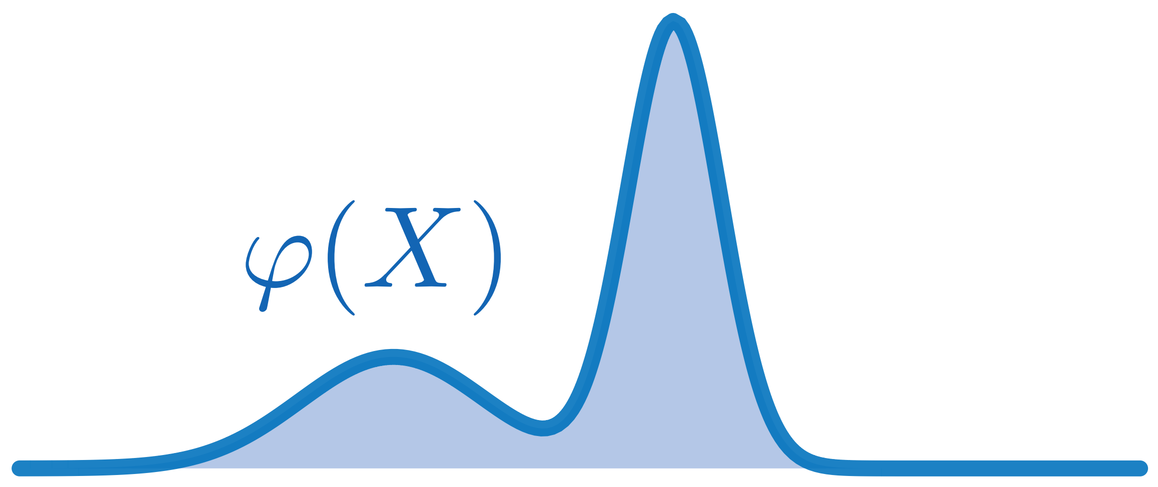
- Screen irrelevant variables
- Robust to outliers
- Handle various data types
- Empirical success

Empirical results



Random forests

versus

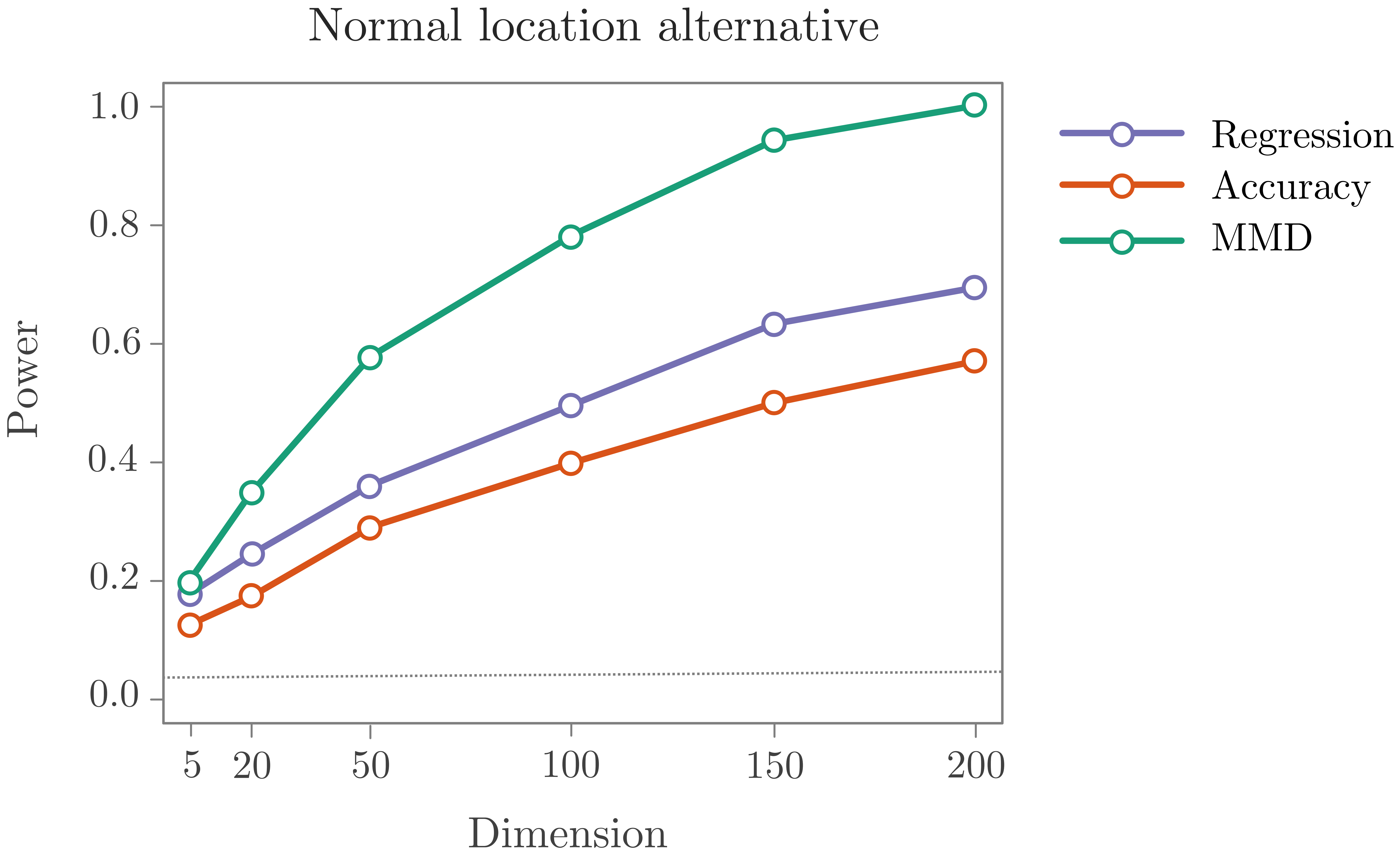


Maximum Mean Discrepancy

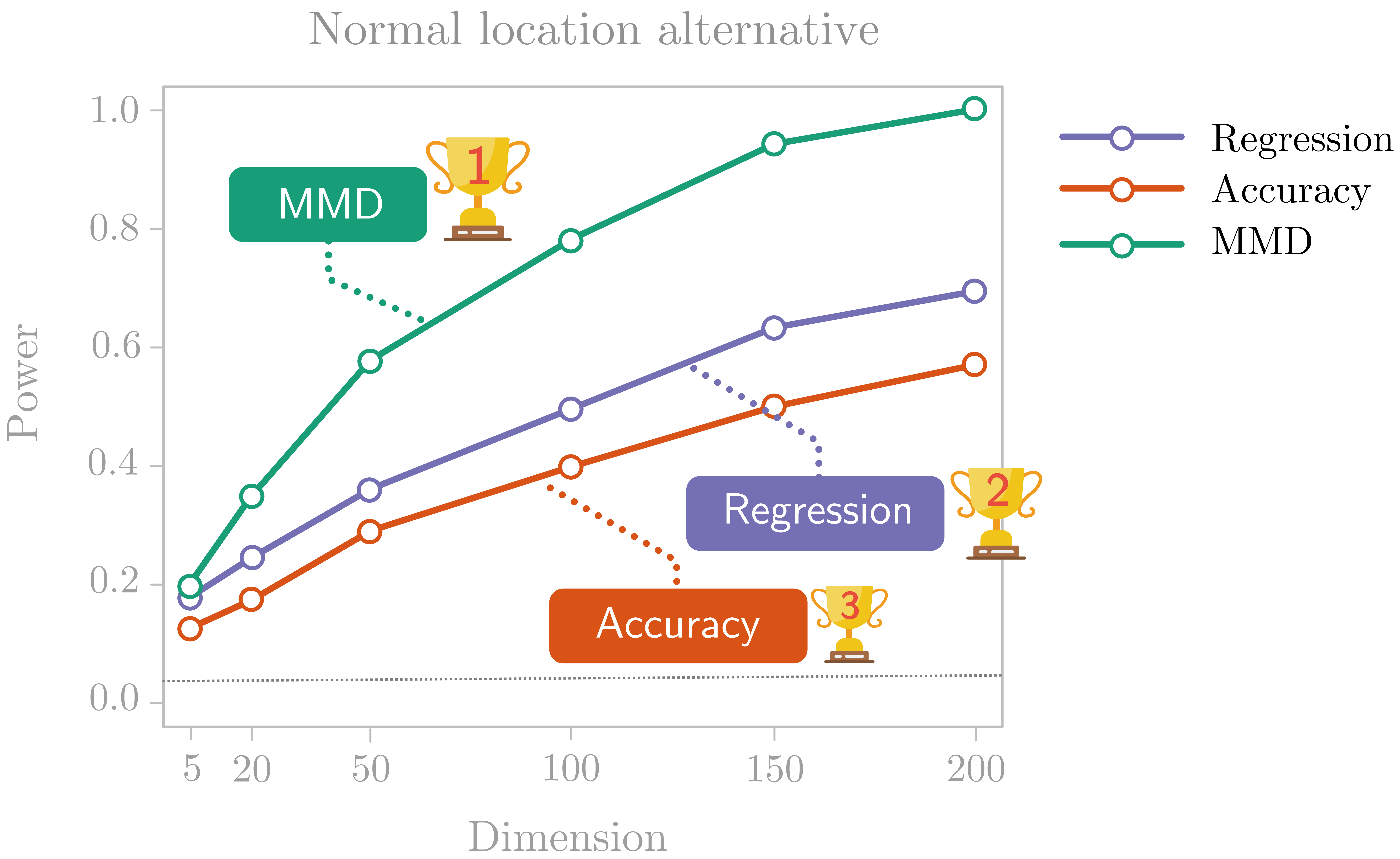
- Screen irrelevant variables
- Robust to outliers
- Handle various data types
- Empirical success

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

Power comparison



Power comparison



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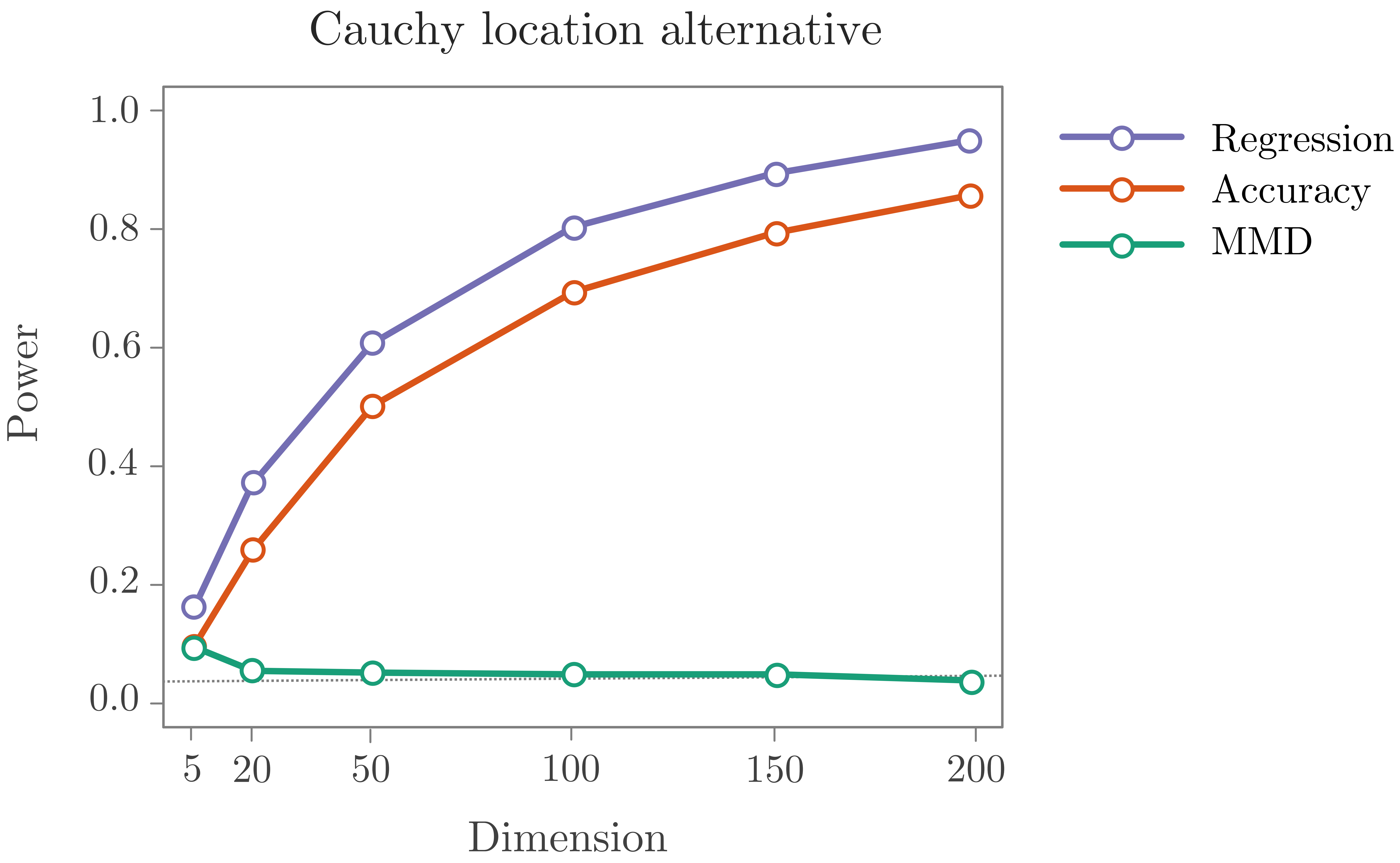
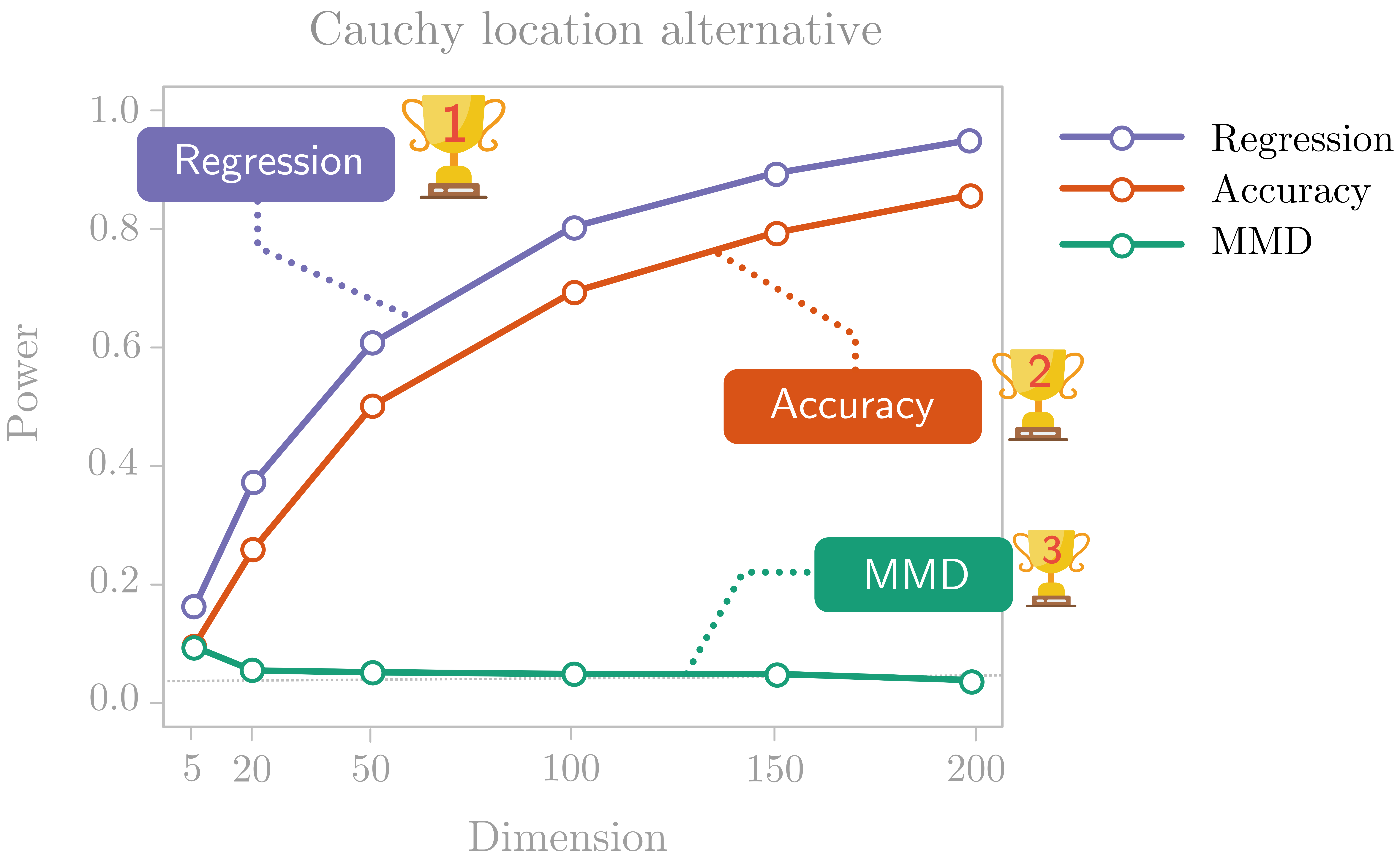


Power comparison



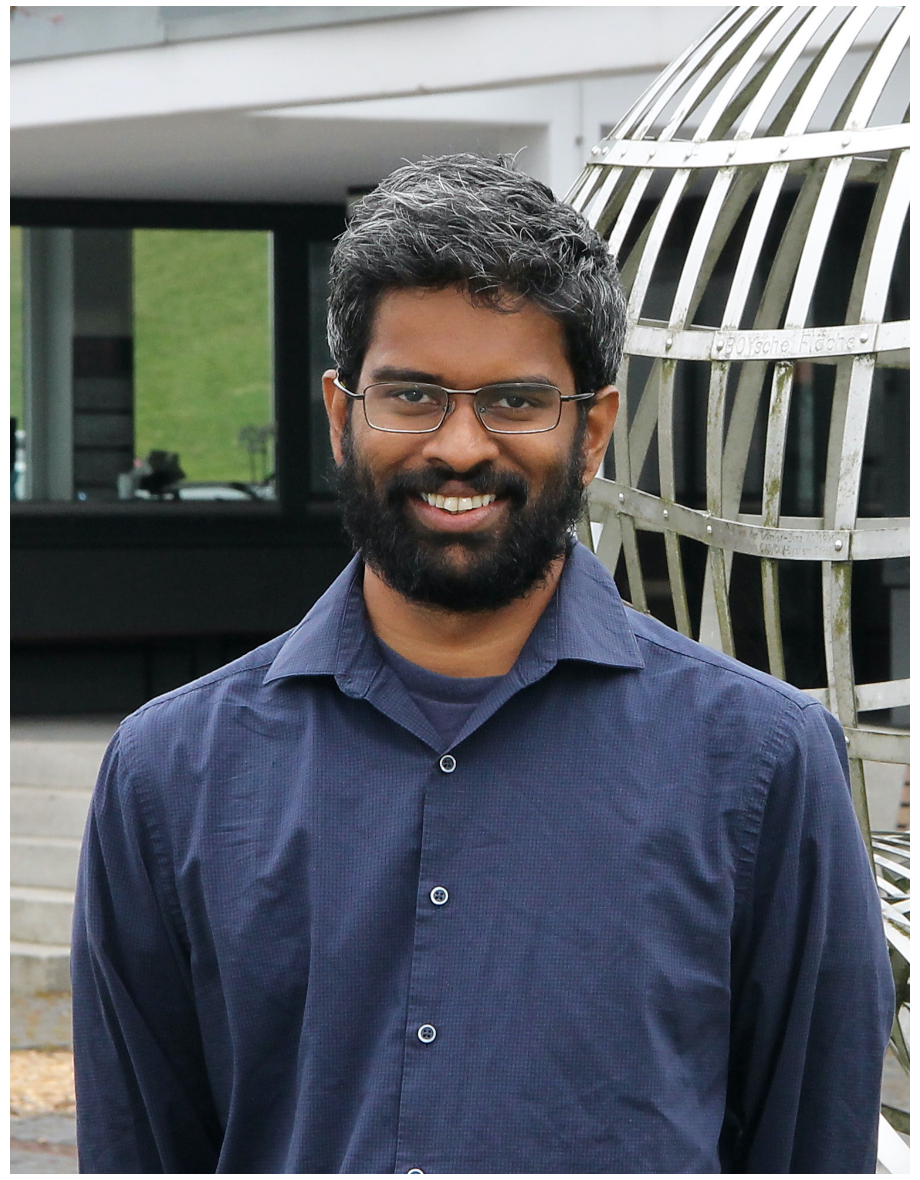
Part 1. Methodological Contributions

Part II. Theoretical Contributions

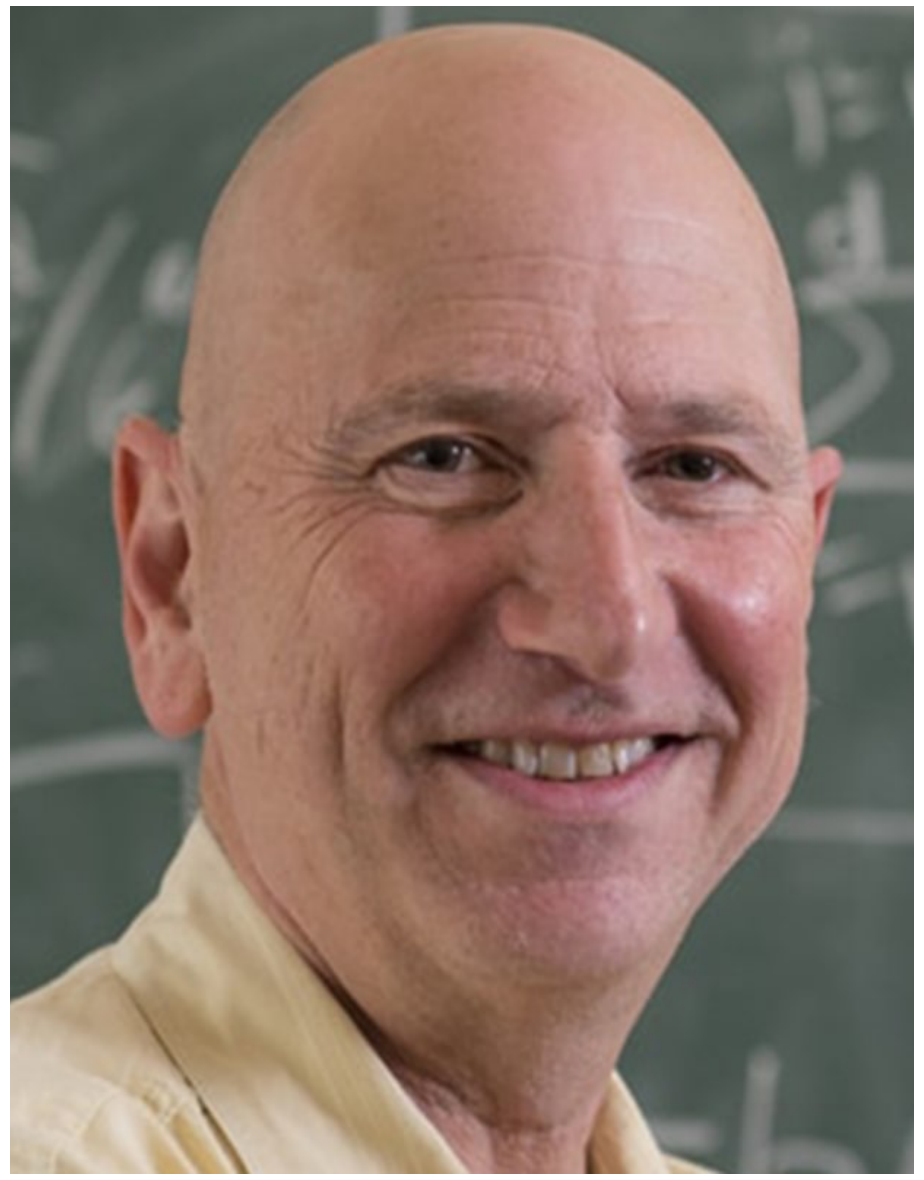
The Annals of Statistics
2022, Vol. 50, No. 1, 225–251
https://doi.org/10.1214/21-AOS2103

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

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

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

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

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

Challenge: Random critical value

Random quantity +
Lacking independence

Remark the permutation test **rejects** H_0 when

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

Test statistic Critical value

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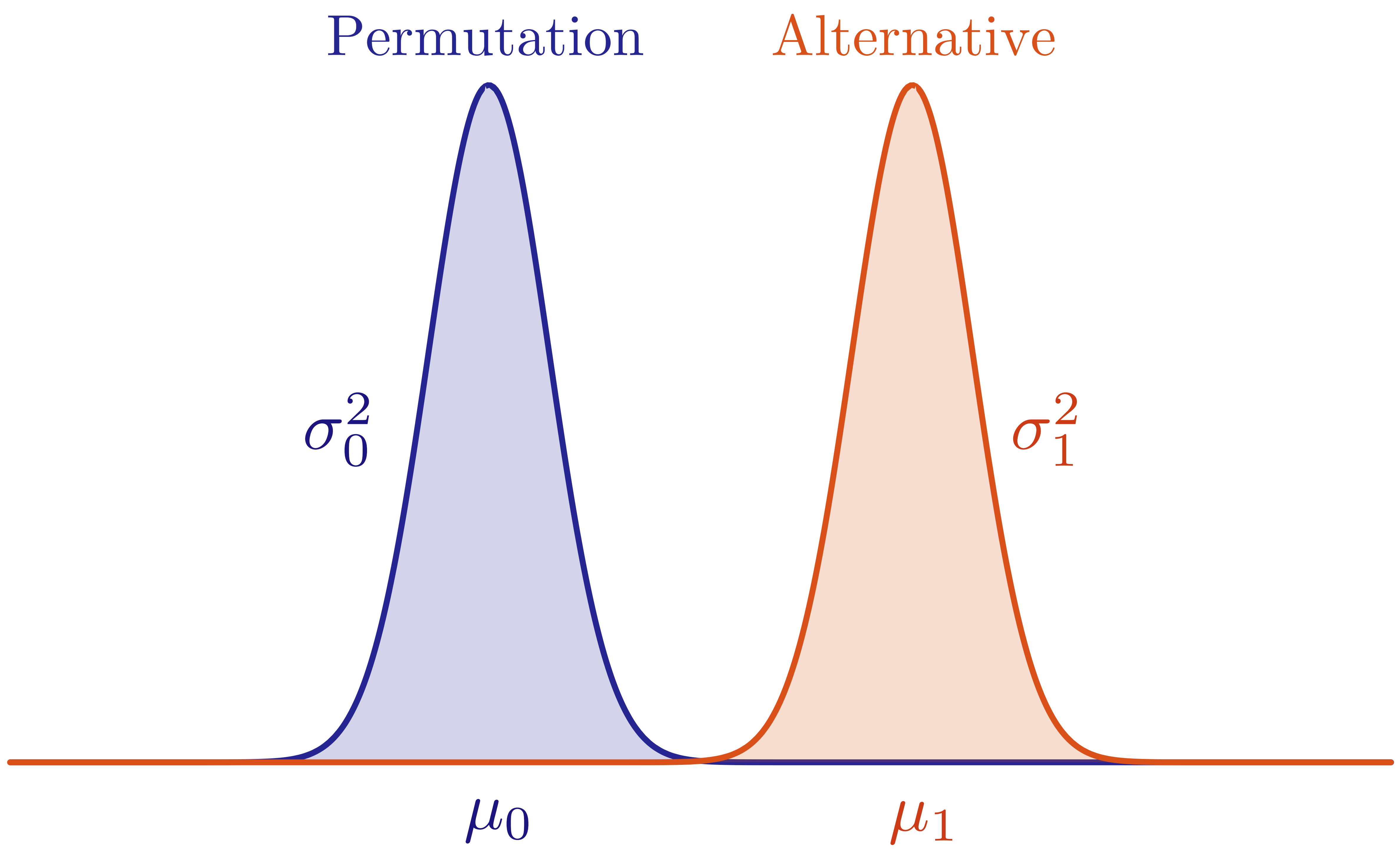
Uniform Type II error over $\mathscr{P}_1$

Our proposal: Two moments method

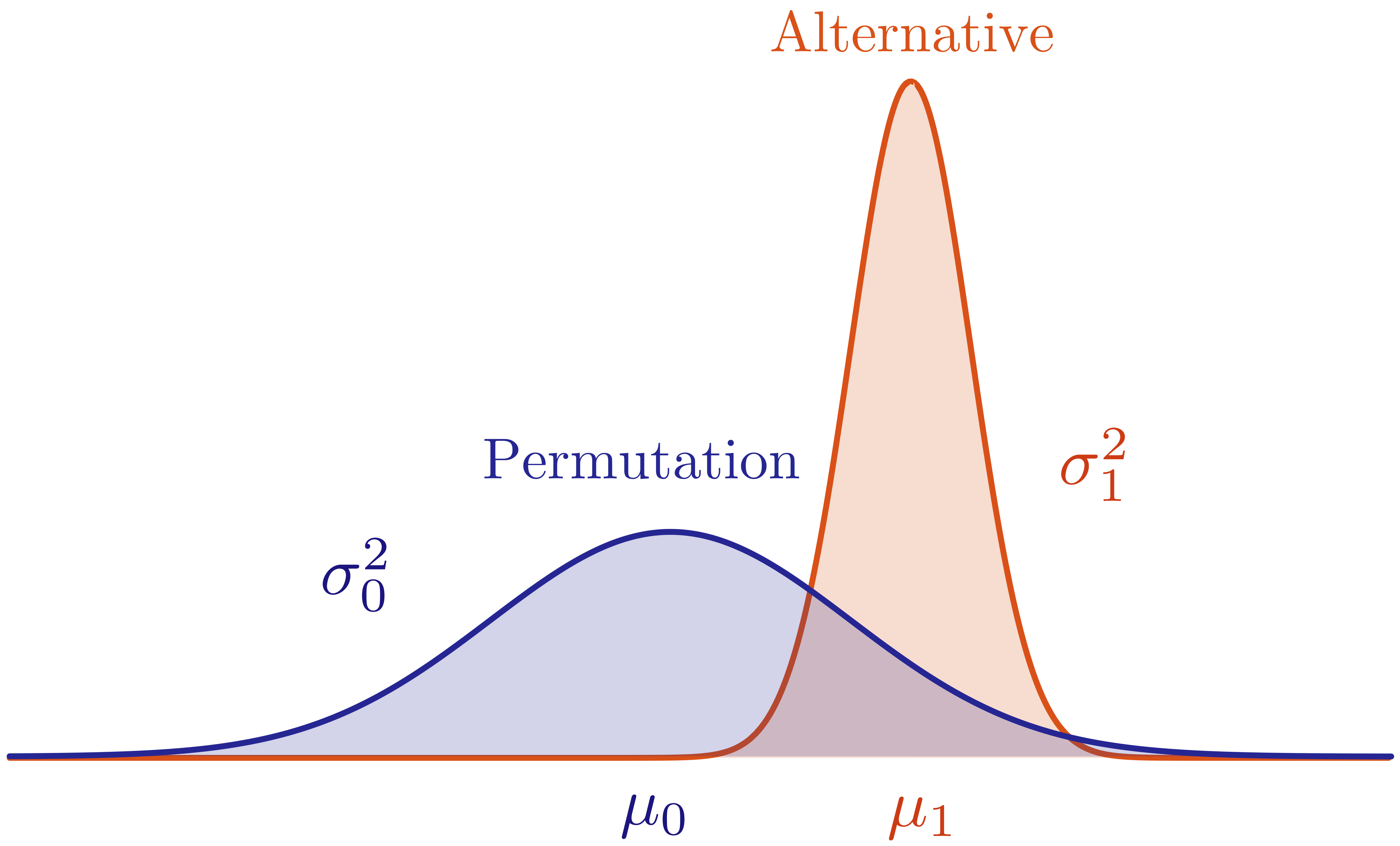
Intuition for the two moments method

- 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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- For any $P \in \mathscr{P}_1$,

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Two moments method

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Signal $\gtrsim$ Noise I + Noise II

(data) (data + permutation)

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(data) (data + permutation)

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

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 $\{Y_1, \ldots, Y_n\} \overset{i.i.d.}{\sim} P_Y$

U-statistic for two-sample testing

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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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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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$$P_X^2 P_Y^2 \qquad P_{XY} P_X P_Y$$

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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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Lemma [KBW 2022]

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

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

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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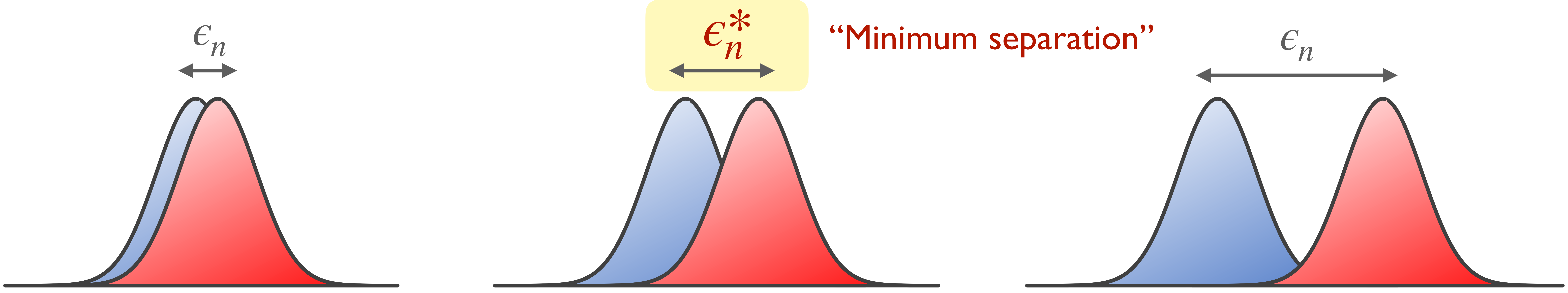

Minimax power ≤ 0.05 | Minimax power ≈ 0.8 | Minimax power $= 1$

Applications to minimax testing

- We call ϕ is minimax rate optimal if

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

- The upper bound is based on the test

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

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

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

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

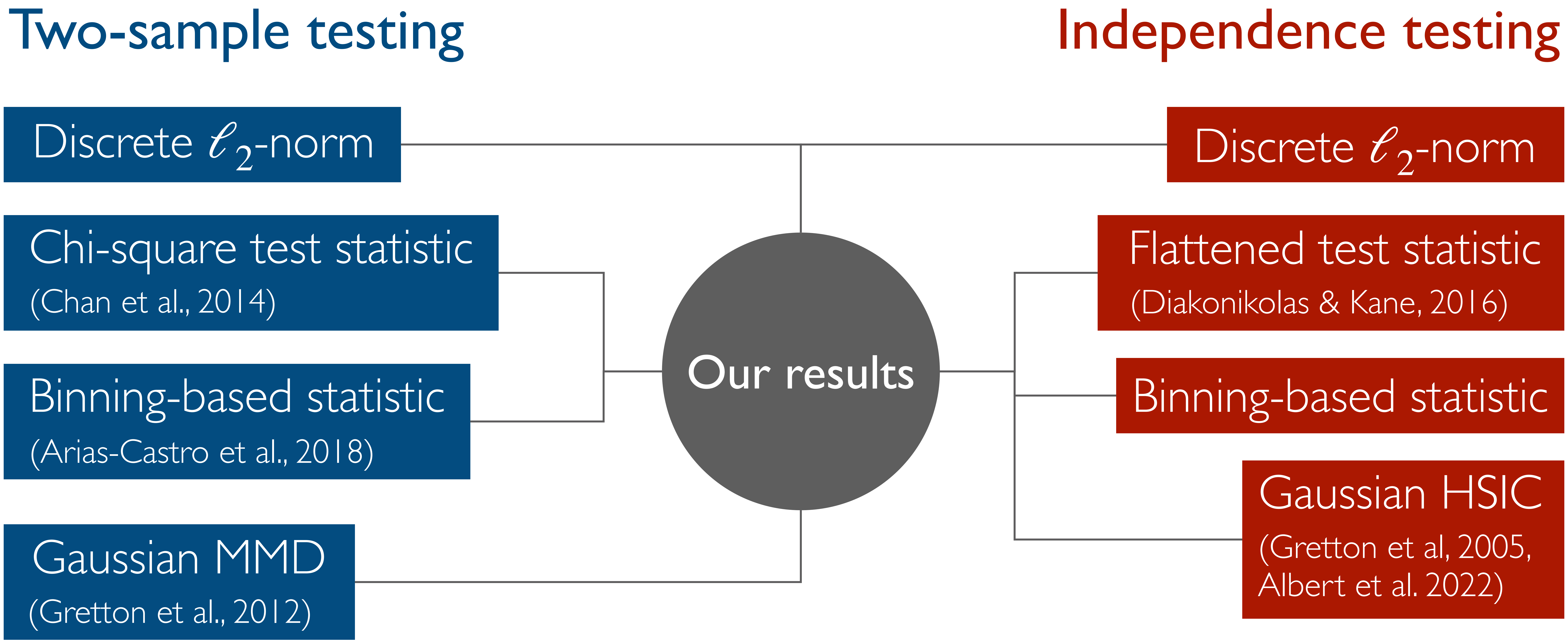
Discrete ℓ_2-norm

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

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

Gaussian MMD
(Gretton et al., 2012)

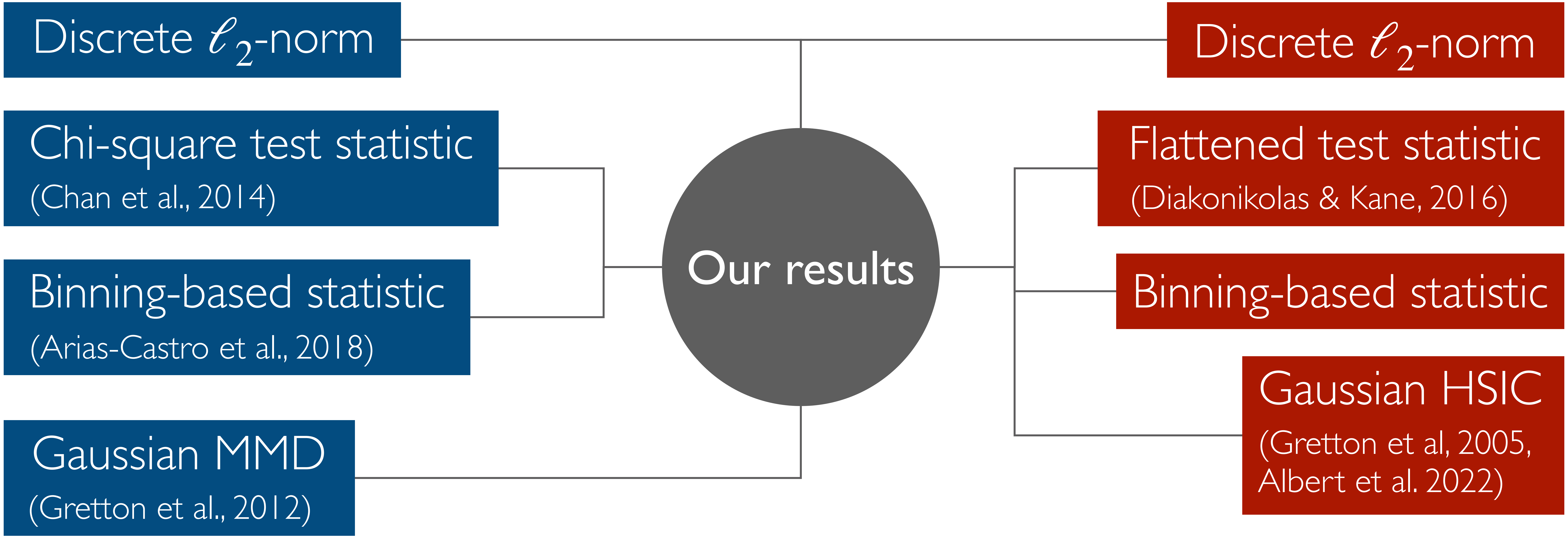
Our results



Two-sample testing
Independence testing
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
Discrete ℓ_2-norm
Flattened test statistic
(Diakonikolas & Kane, 2016)
Binning-based statistic
Gaussian HSIC
(Gretton et al, 2005,
Albert et al. 2022)

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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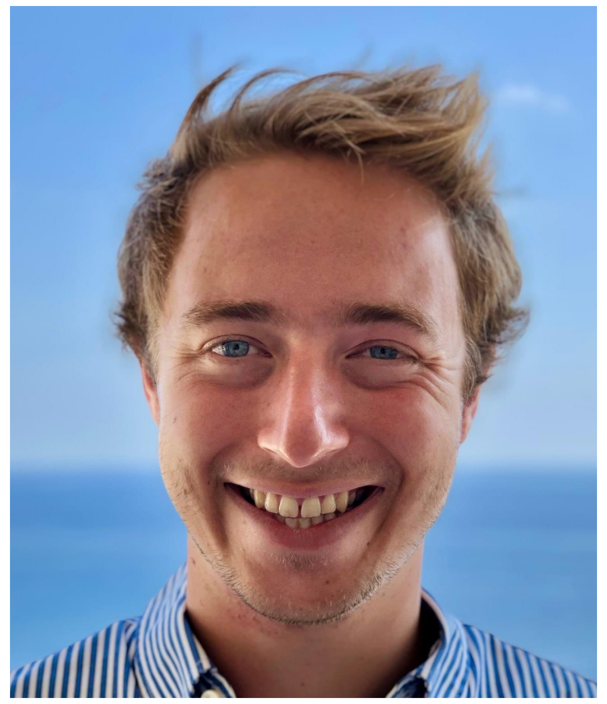
  - Kim, Neykov, Balakrishnan, Wasserman (2024+, *EJS*)



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
- Computational-Power Trade-off
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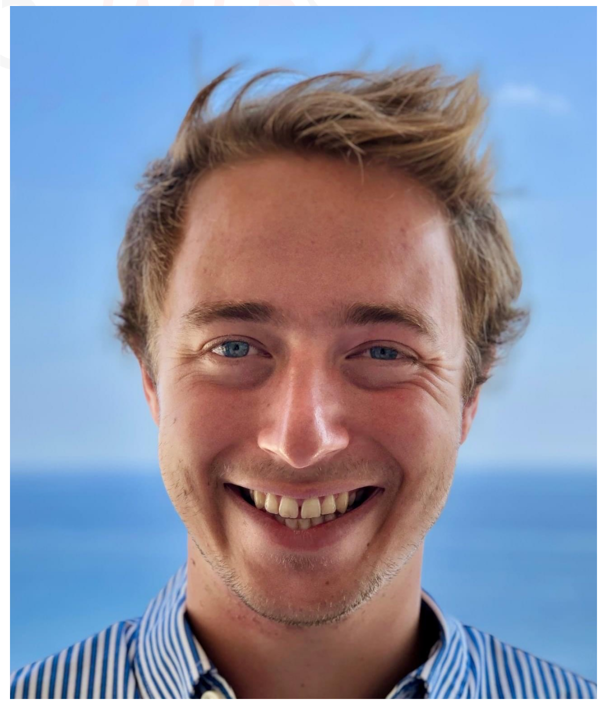
Antonin Schrab


Benjamin Guedj


Arthur Gretton


Ikjun Choi

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

Follow-up

- Adaptivity
  - Schrab, Kim, Albert, Laurent, Guedj, Gretton (2023, *JMLR*)
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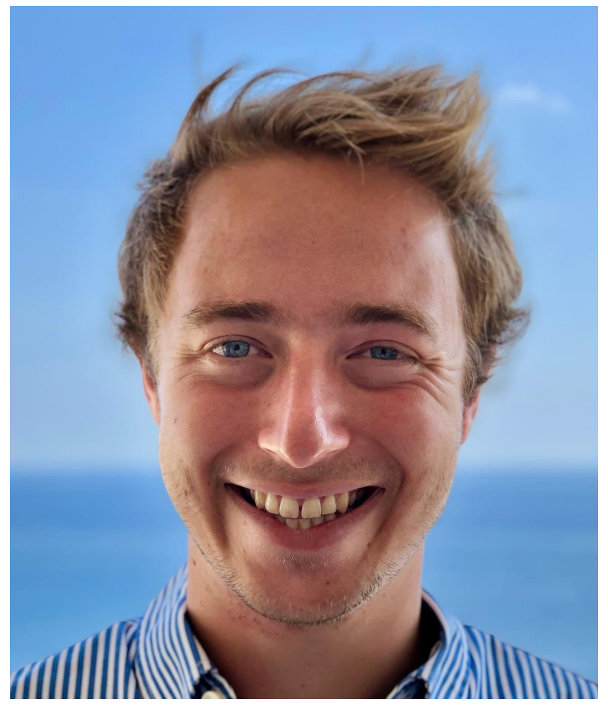

Antonin Schrab

Differentially private permutation tests applied to kernel methods

Follow-up

- Adaptivity
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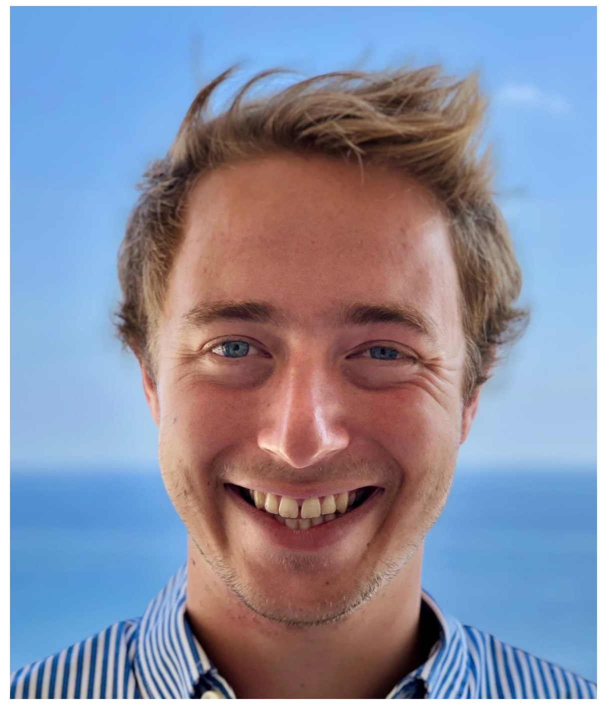

Antonin Schrab

Permutation tests that are robust to data perturbation with optimal properties

Follow-up

- Adaptivity
  - Schrab, Kim, Albert, Laurent, Guedj, Gretton (2023, *JMLR*)
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  - Schrab, Kim, Guedj, Gretton (2022, *NeurIPS*)
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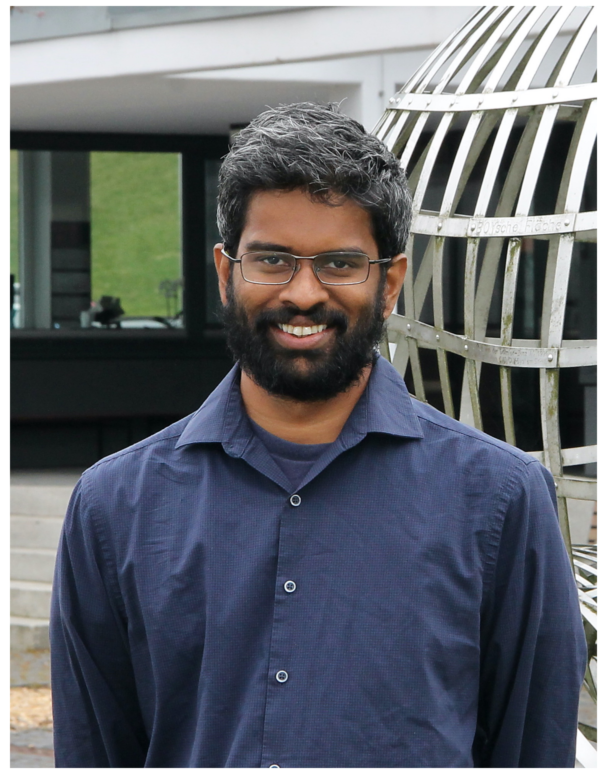
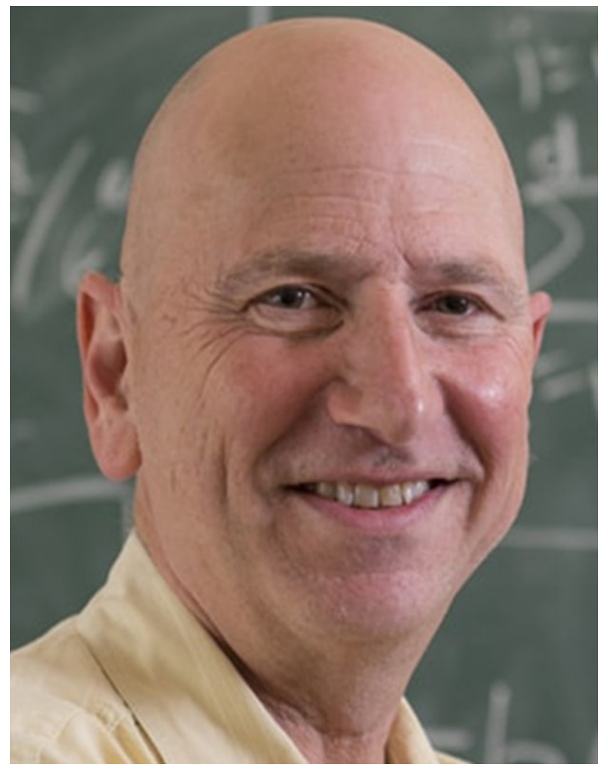
Matey Neykov


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!