

Permutation Methods for Comparing Distributions

Ilmun Kim

Department of Mathematical Sciences
KAIST

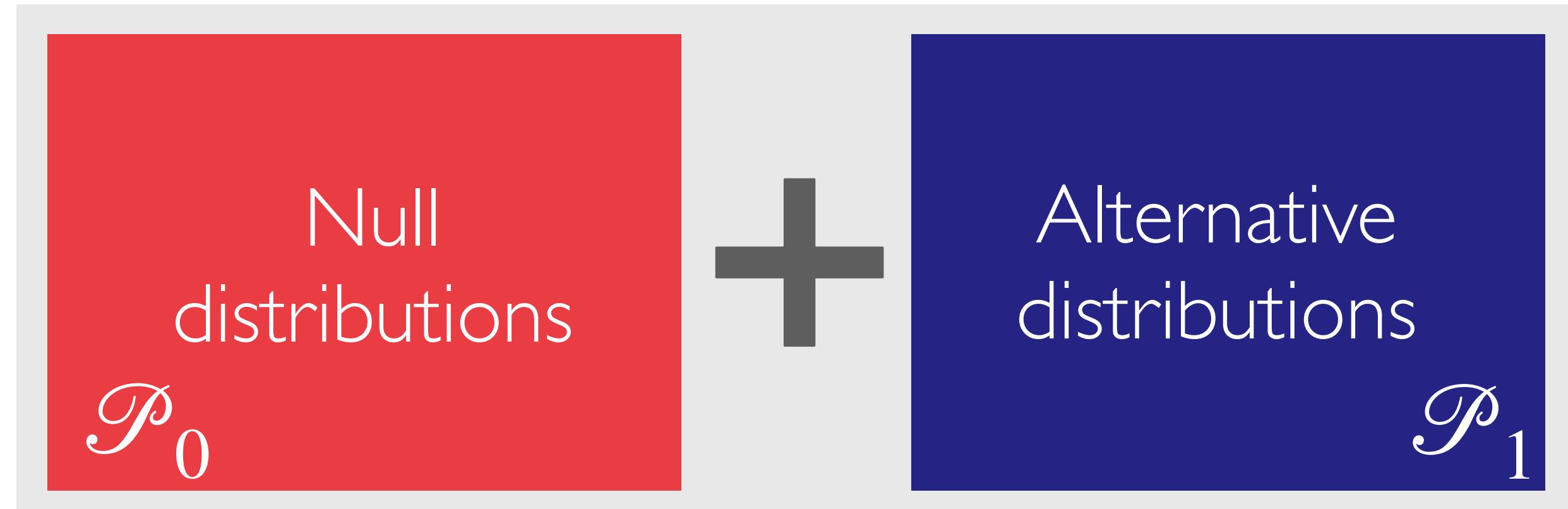


Outline of this talk

- (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 $\mathcal{P} = \mathcal{P}_0 \cup \mathcal{P}_1$

$$\mathcal{P} = \begin{matrix} \text{Null} \\ \text{distributions} \\ \mathcal{P}_0 \end{matrix} + \begin{matrix} \text{Alternative} \\ \text{distributions} \\ \mathcal{P}_1 \end{matrix}$$


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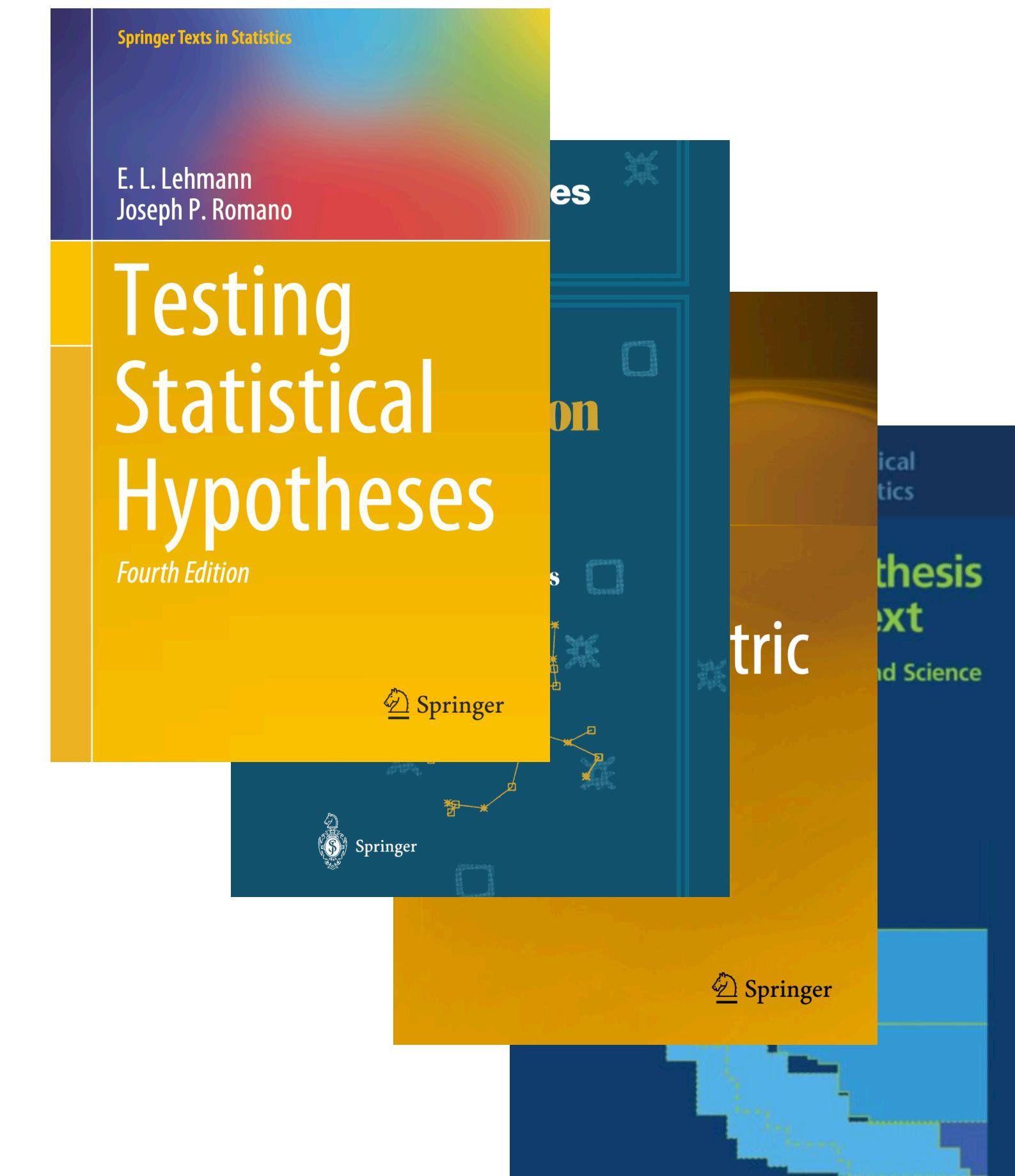
- Given $X_1, \dots, X_n \stackrel{\text{i.i.d.}}{\sim} P \in \mathcal{P}$, **our goal** is to determine

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

Recap: Statistical Hypothesis Testing

Examples include

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



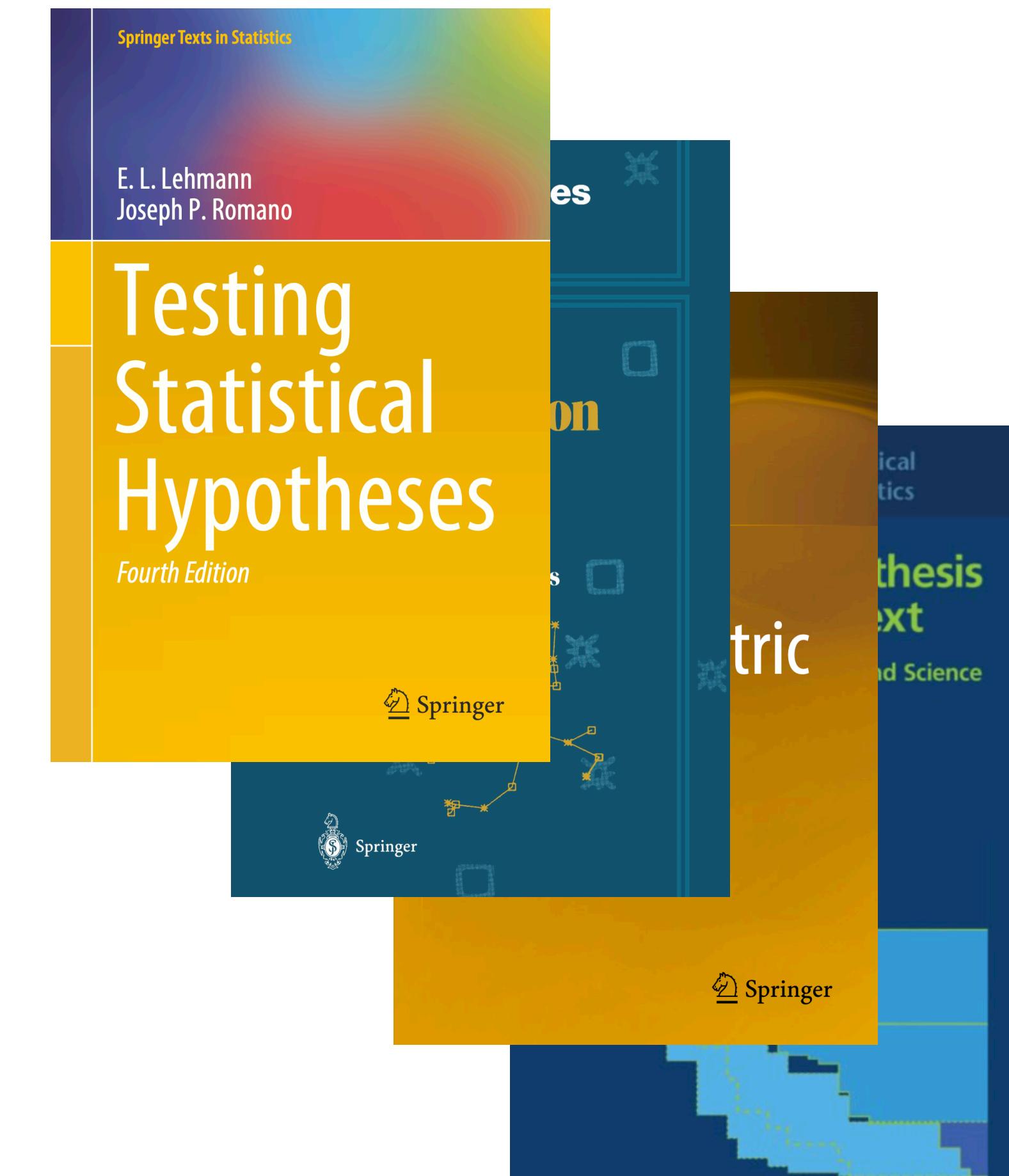
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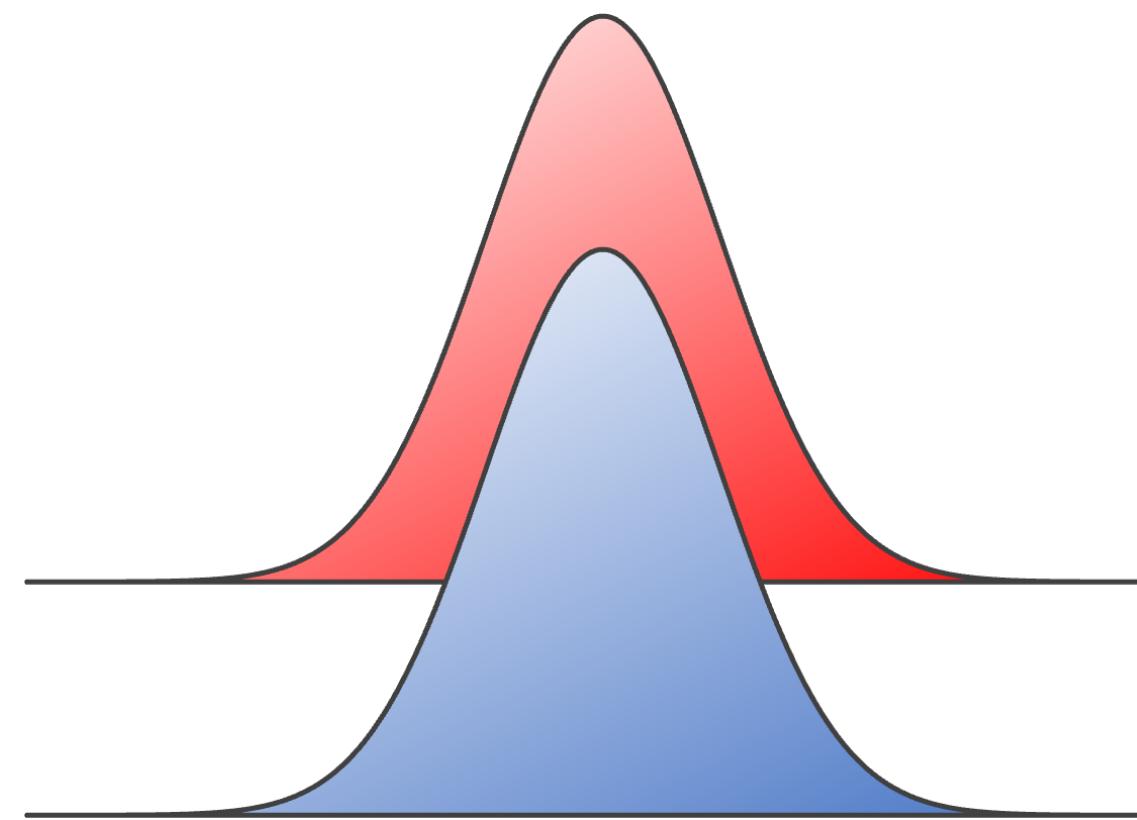
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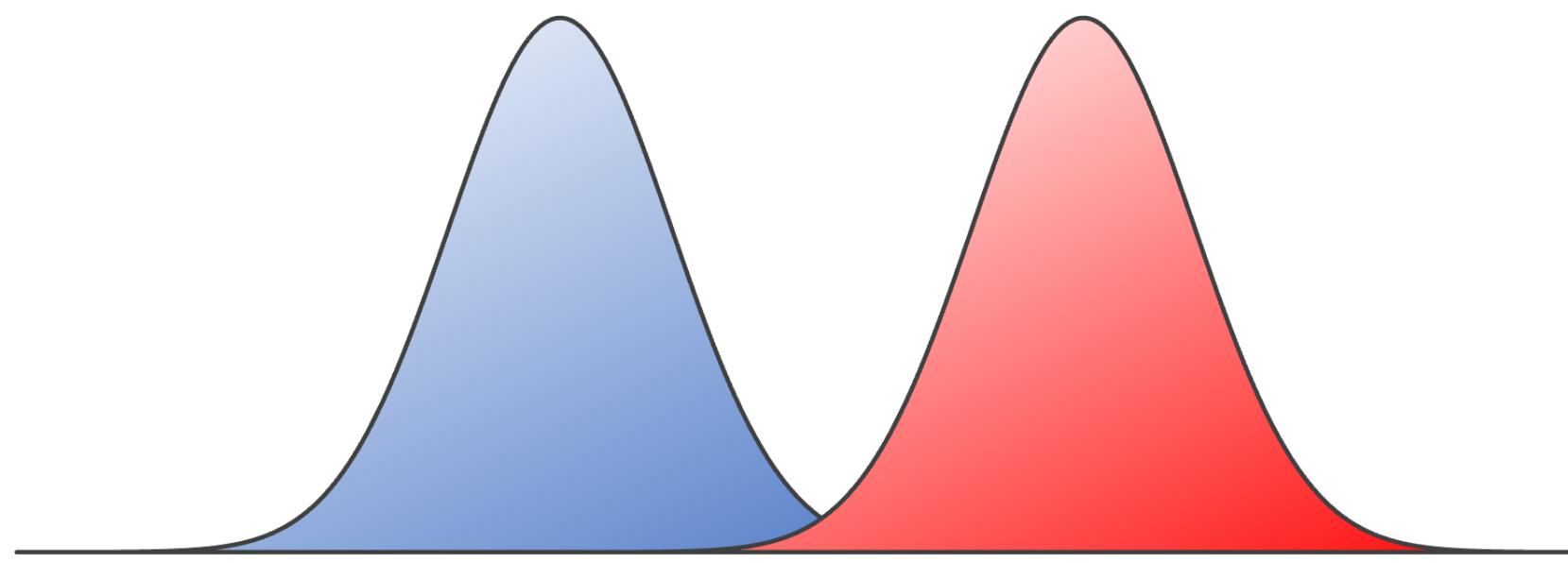
Two-Sample Problem

- Given $\{X_1, \dots, X_n\} \stackrel{\text{i.i.d.}}{\sim} P_X$ and $\{Y_1, \dots, Y_m\} \stackrel{\text{i.i.d.}}{\sim} Q_Y$

we want to test whether



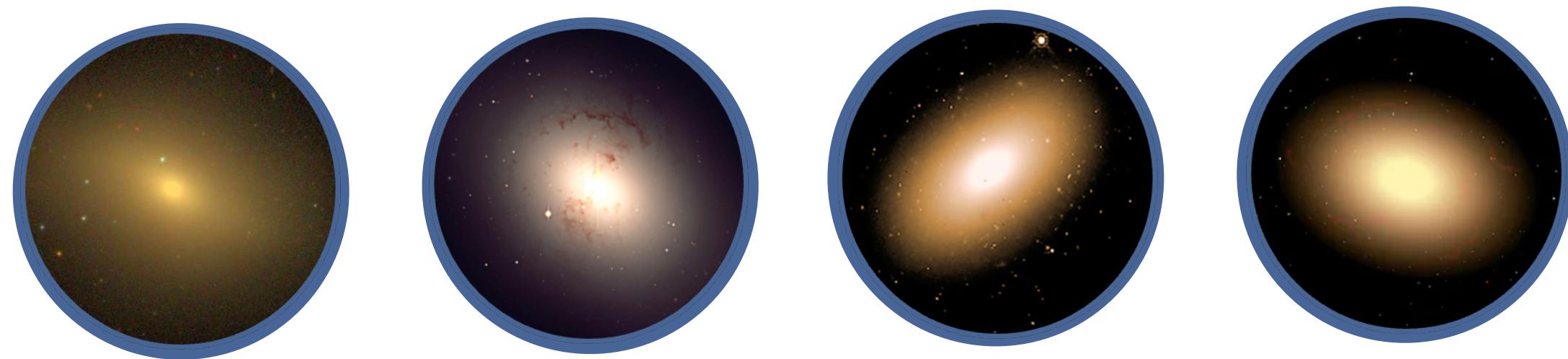
versus



$$H_0 : P_X = Q_Y$$

$$H_1 : P_X \neq Q_Y$$

Applications: Astronomy



High-mass versus Low-mass galaxies



Applications: Machine Learning



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

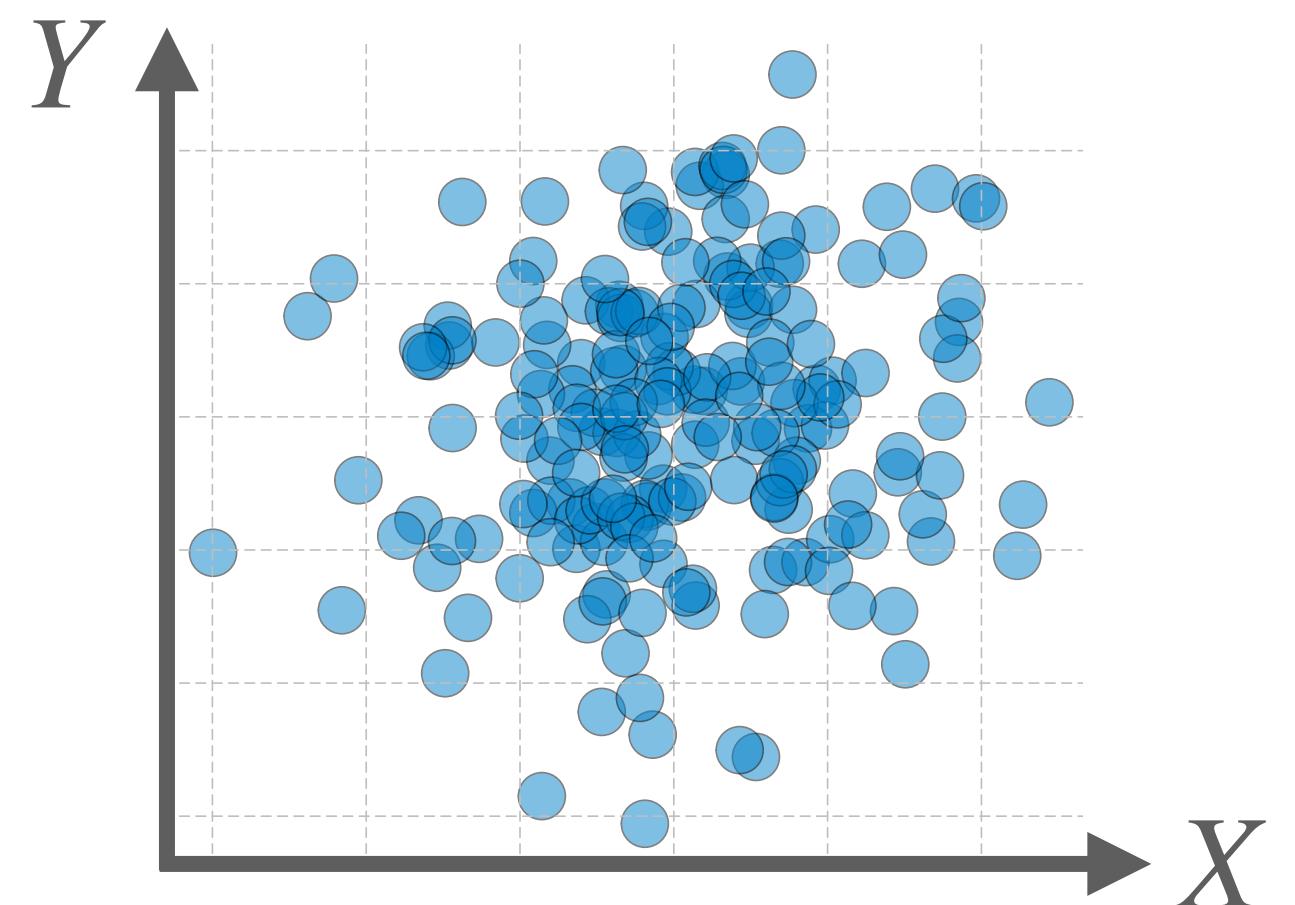


$\sim Q_{\text{artificial}}$

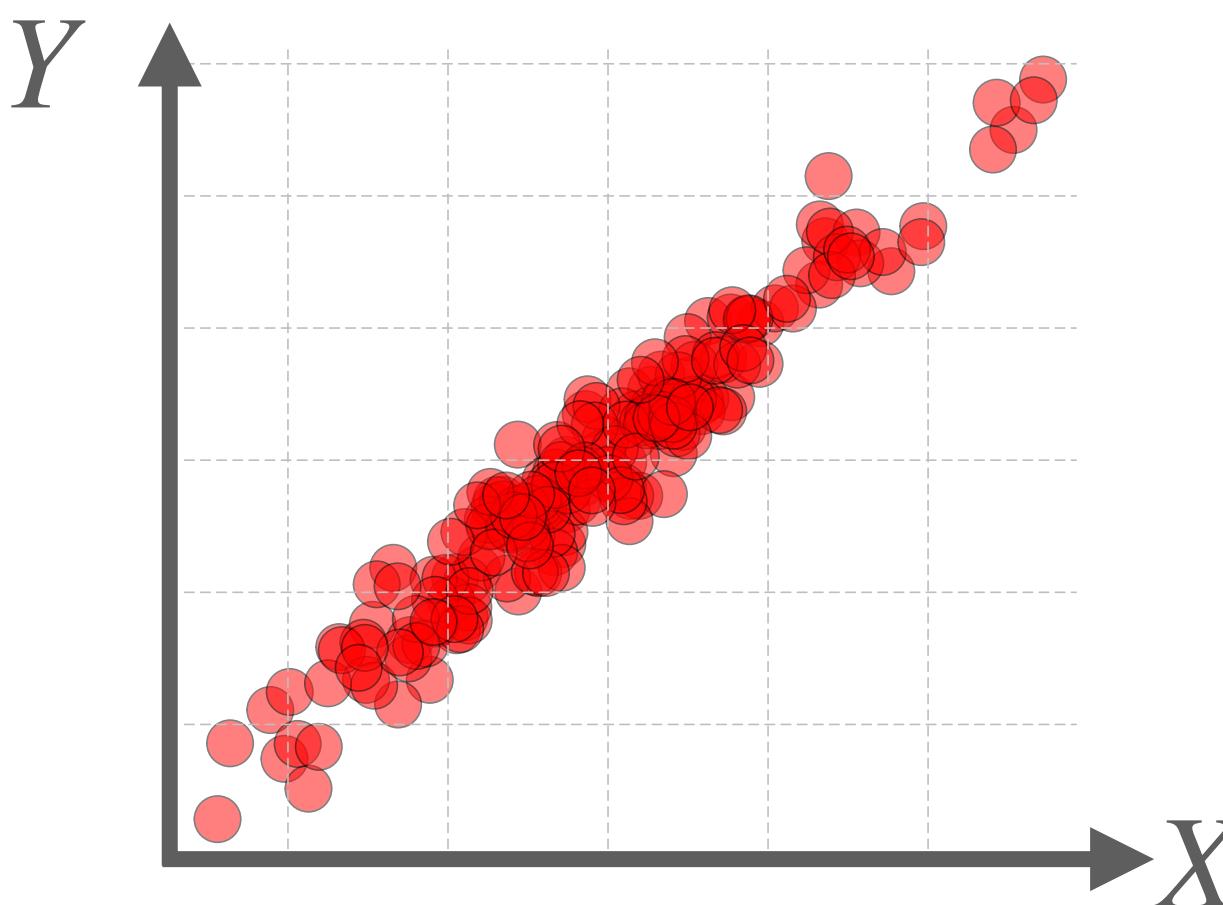
Independence Testing Problem

- Given $\{(X_1, Y_1), \dots, (X_n, Y_n)\} \stackrel{\text{i.i.d.}}{\sim} P_{X,Y}$

we want to test whether



versus



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

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

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

$$\phi : \{X_1, \dots, X_n\} \mapsto \{0,1\}$$

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Recap: Statistical Hypothesis Testing

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

$$\phi : \{X_1, \dots, X_n\} \mapsto \{0,1\}$$

- 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 I

Compute a test statistic

e.g.,

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

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

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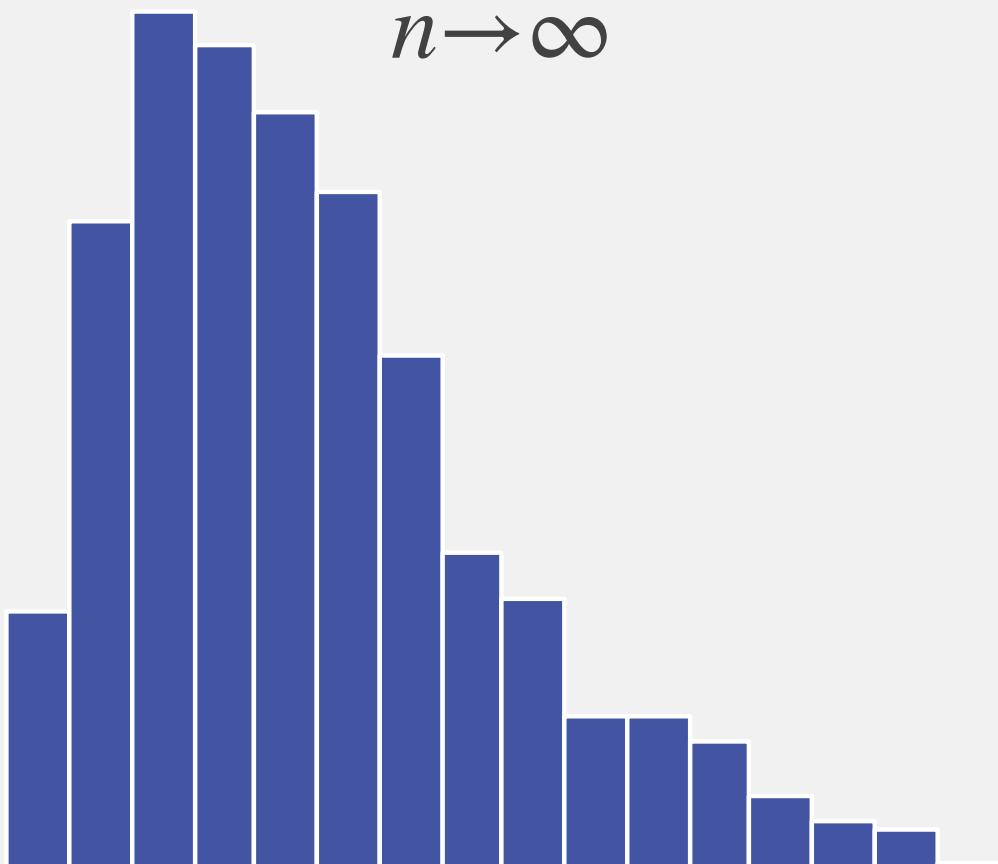
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$$\lim_{n \rightarrow \infty} \mathbb{P}(T_n \leq t)$$



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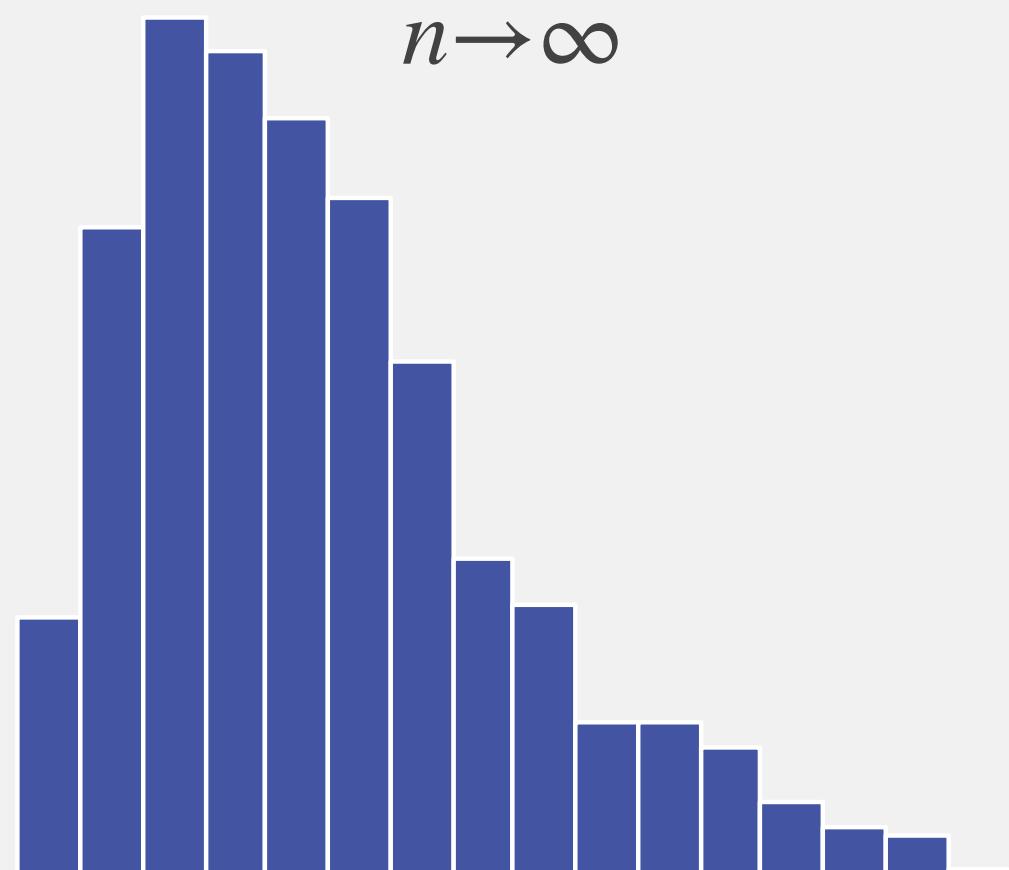
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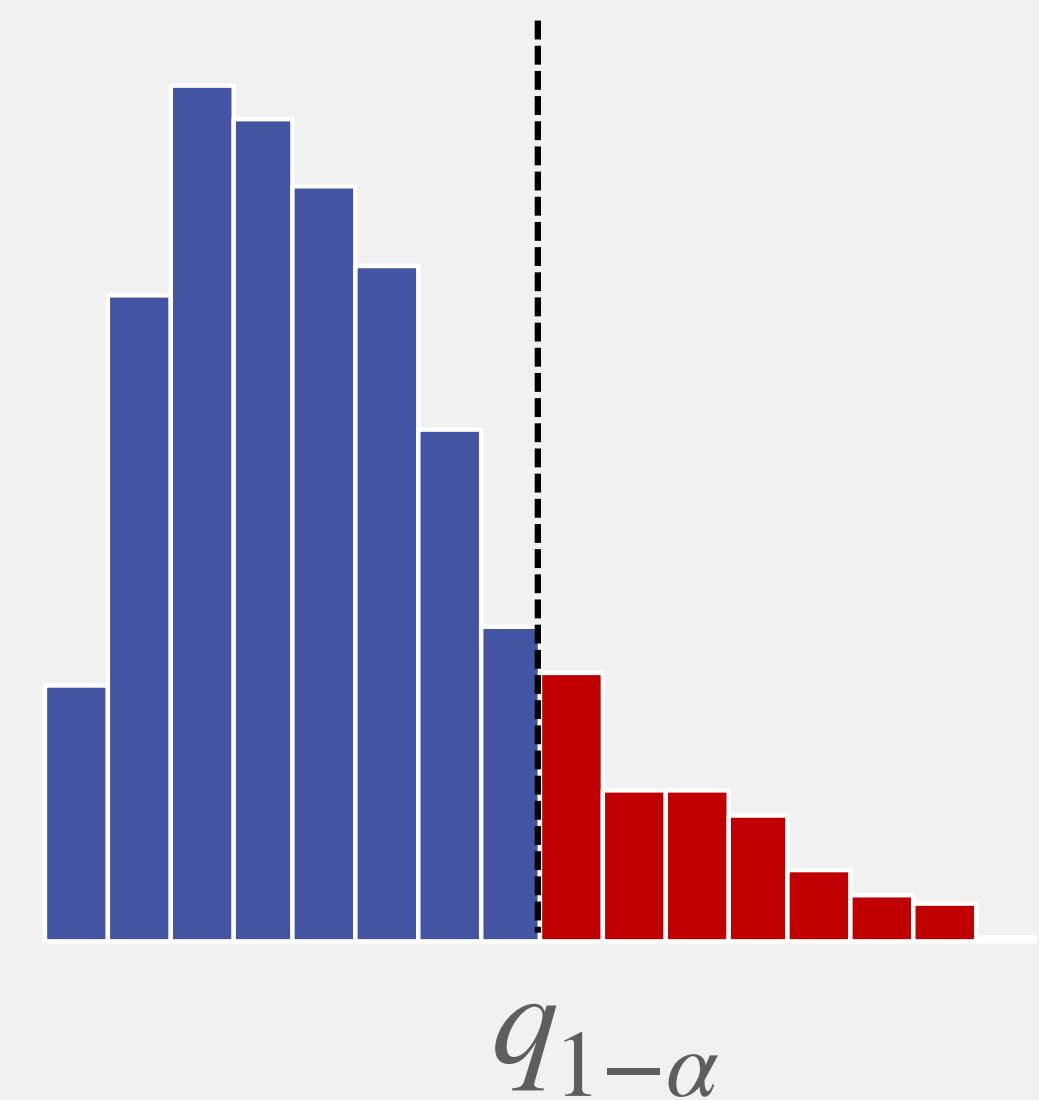
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Step III

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



New Challenges

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

New Challenges

- 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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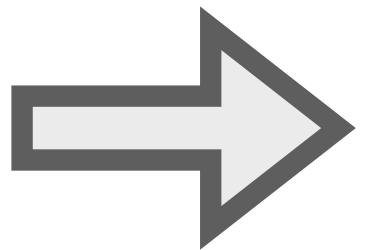
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Pearson's
chi-squared test

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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

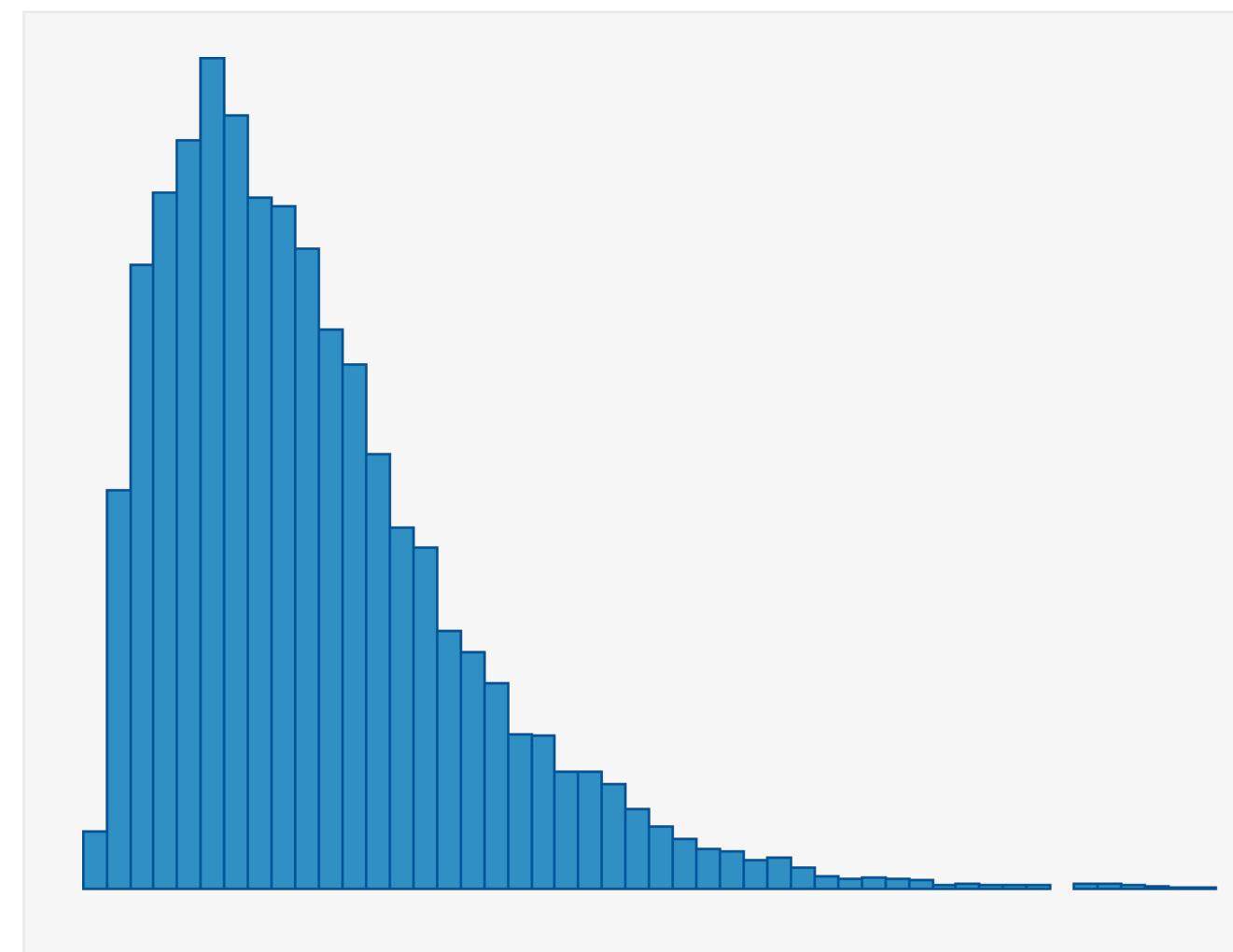
$$\chi^2 = \sum_{i=1}^{\ell_1} \sum_{j=1}^{\ell_2} \frac{(O_{ij} - E_{ij})^2}{E_{ij}}$$

approx.
~

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

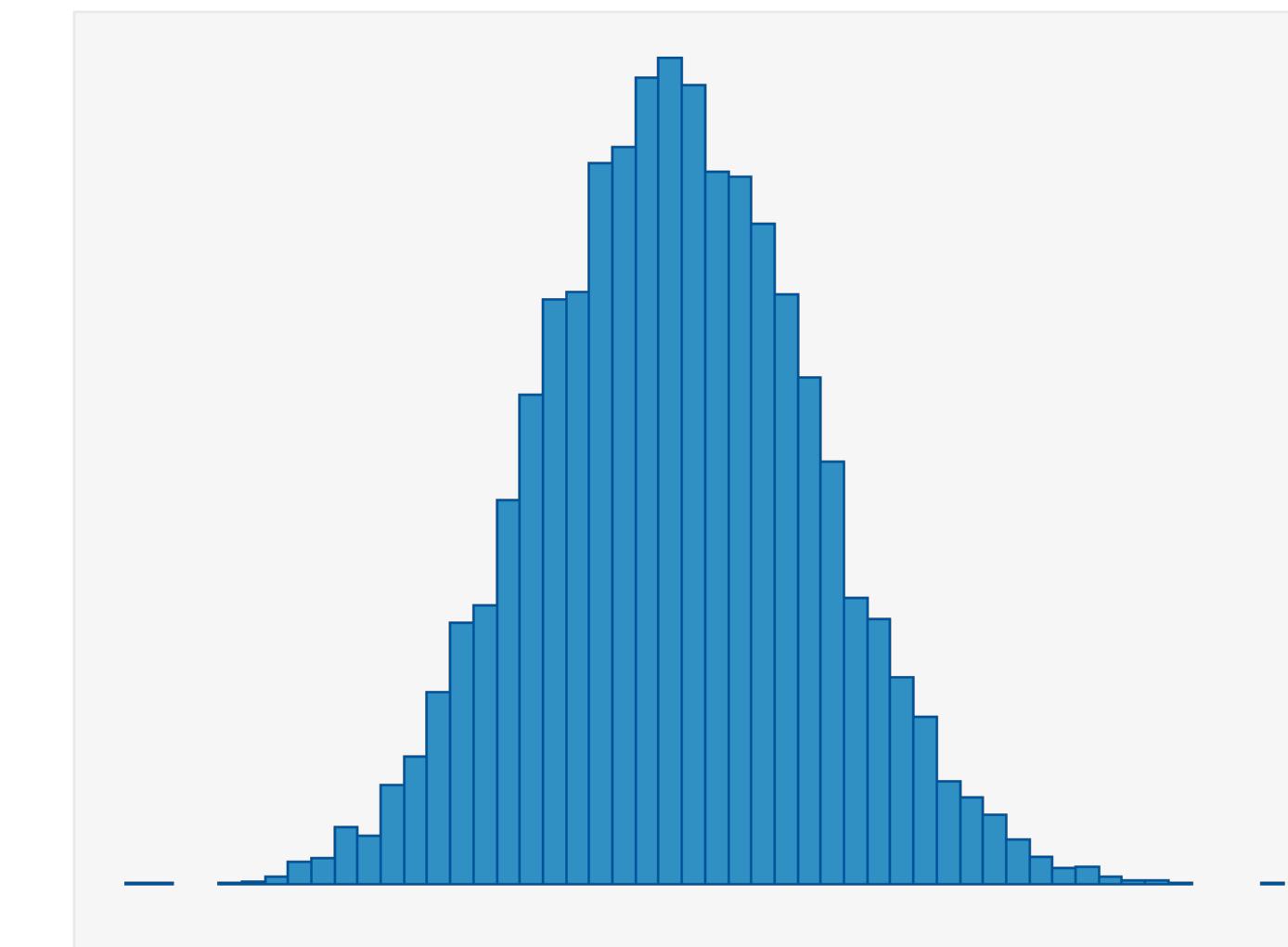
Example: χ^2 -statistic in high-dimensions

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



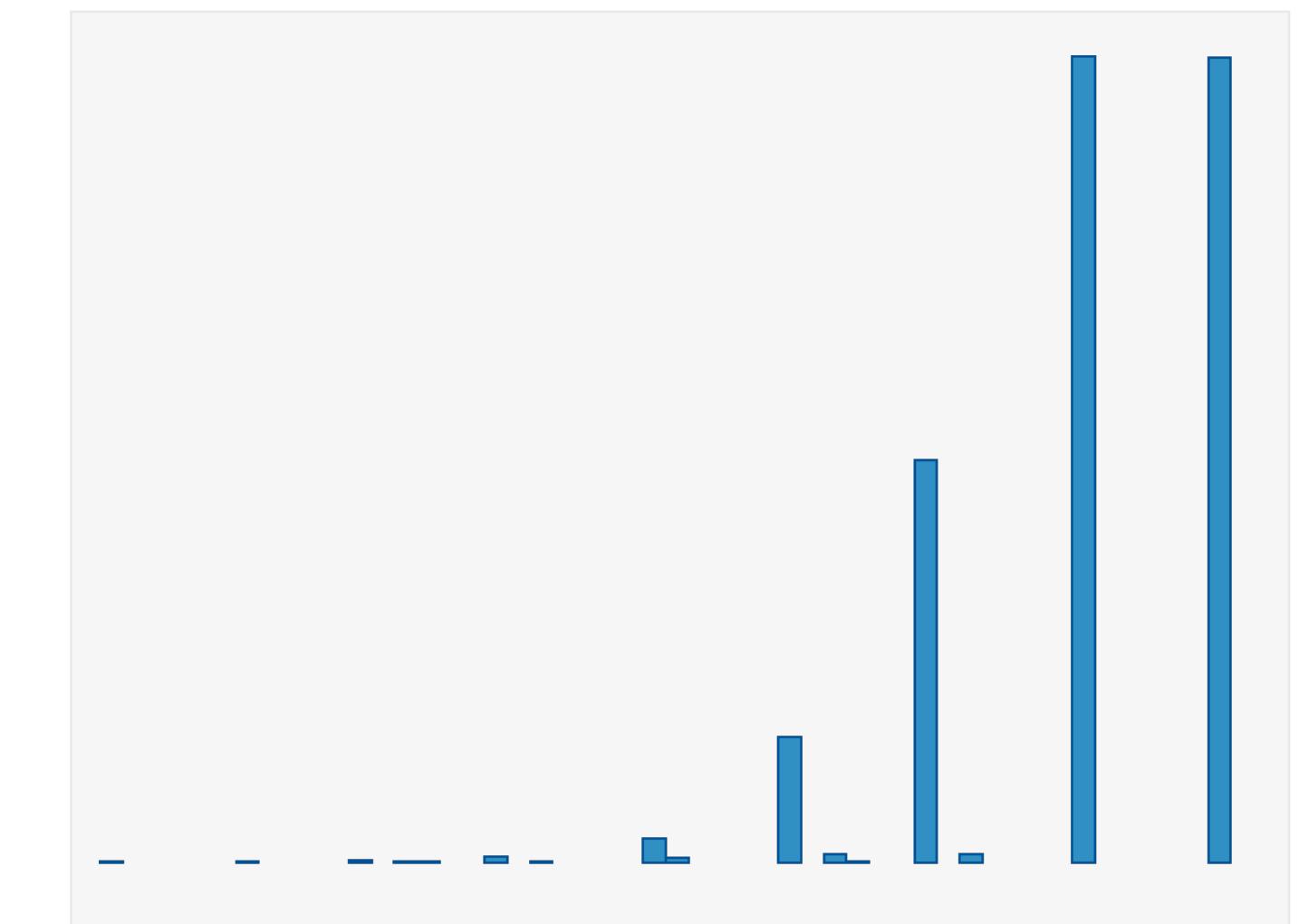
\approx Chi-square

$$\ell_1 = \ell_2 = 3$$



\approx Gaussian

$$\ell_1 = \ell_2 = 50$$



\approx Discrete

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

We aim to develop **new theory** and **methods** for hypothesis testing that improve classical approaches

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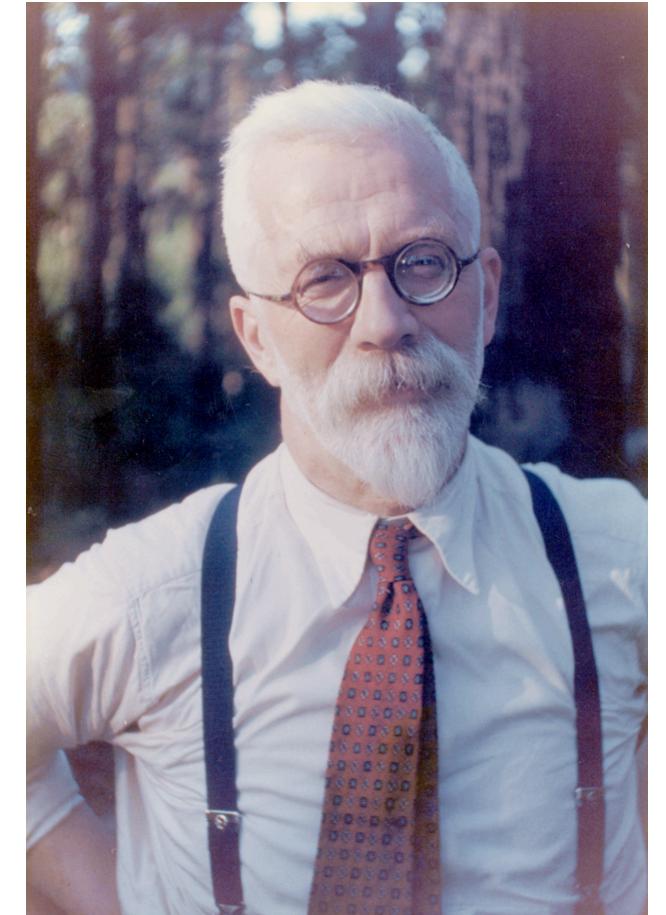
Common keyword

“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*)

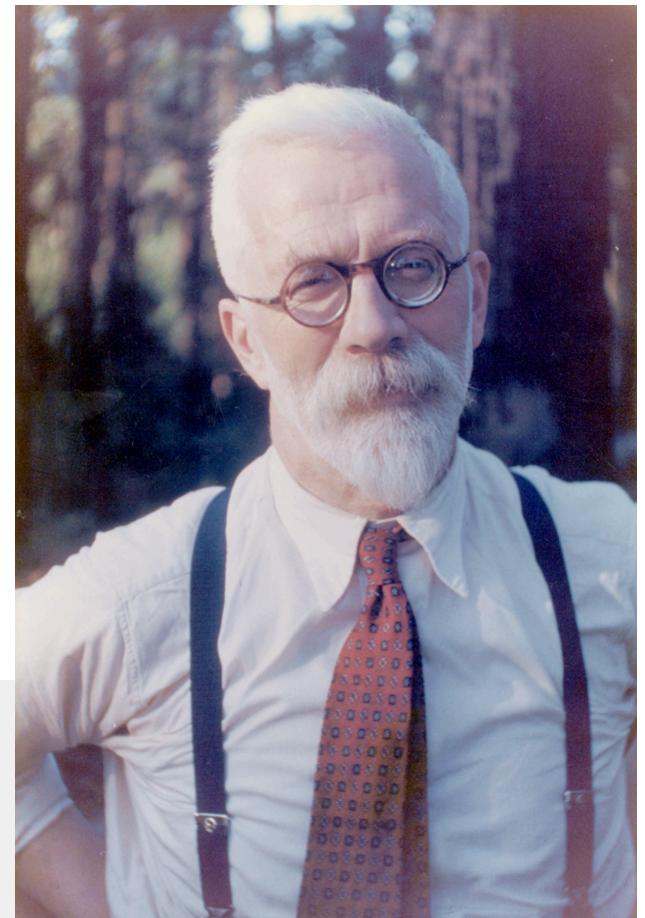
Permutation tests

- The use of permutation methods dates back to Fisher in 1935



Permutation tests

- The use of permutation methods dates back to Fisher in 1935



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

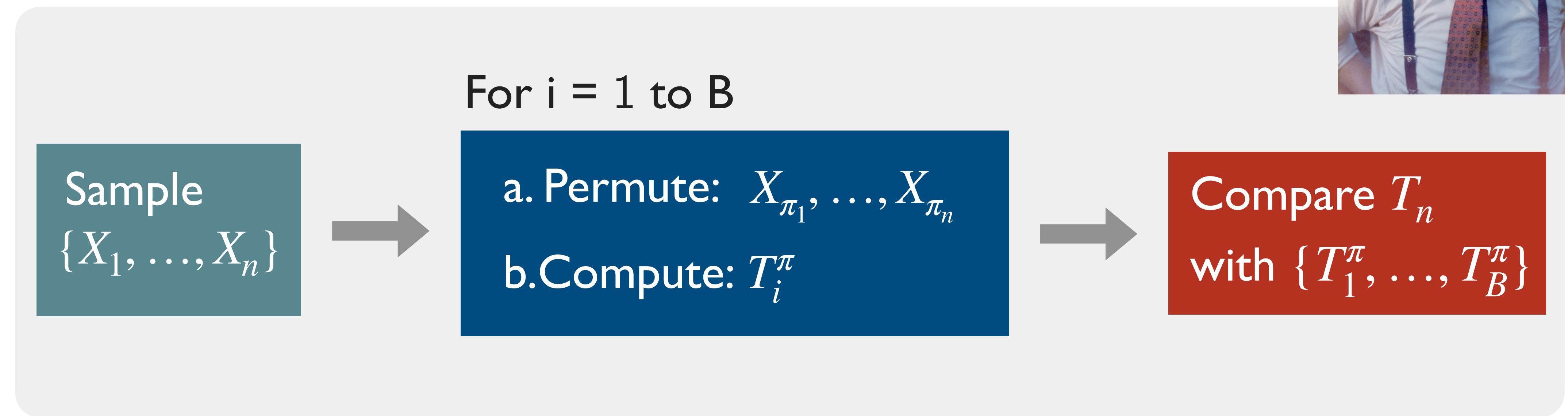
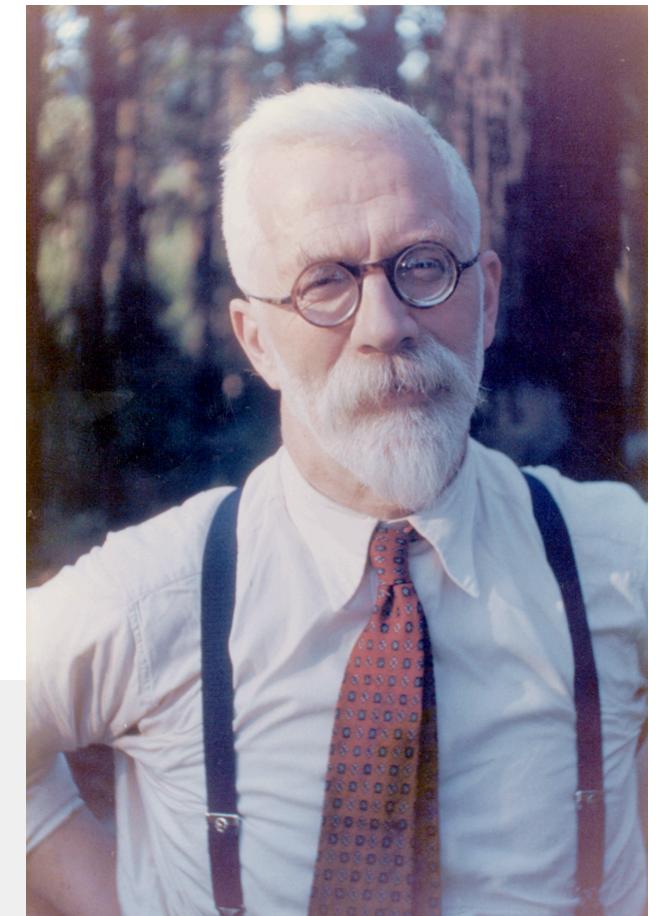
For i = 1 to B

a. Permute: $X_{\pi_1}, \dots, X_{\pi_n}$
b. Compute: T_i^π

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

Permutation tests

- The use of permutation methods dates back to Fisher in 1935



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

Key features of permutation tests

$$\sup_{P \in \mathcal{P}_0} \mathbb{P}_{\textcolor{red}{P}}(p_{\text{perm}} \leq \alpha) \leq \alpha \quad \left\{ \begin{array}{l} \text{for any } \alpha \in (0,1) \\ \text{for any } n \geq 1 \end{array} \right.$$

Class of all null distributions

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

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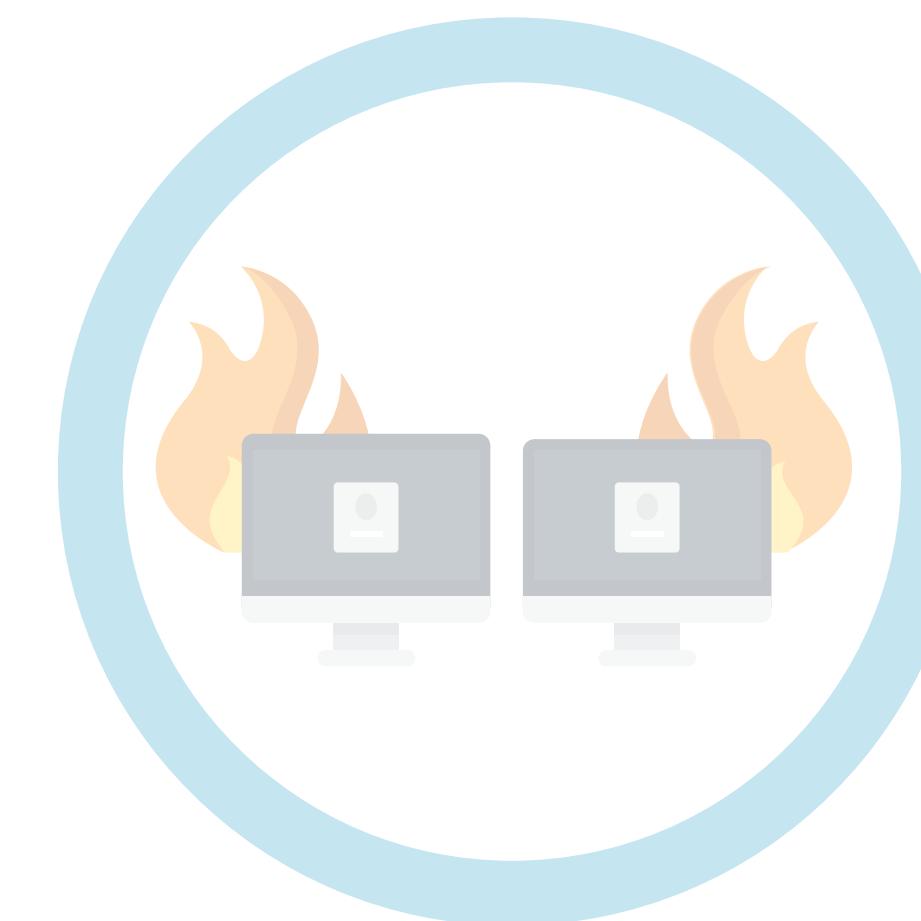
Class of all null distributions

- **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 $\{X_1, \dots, X_n\}$ are **exchangeable** under the null

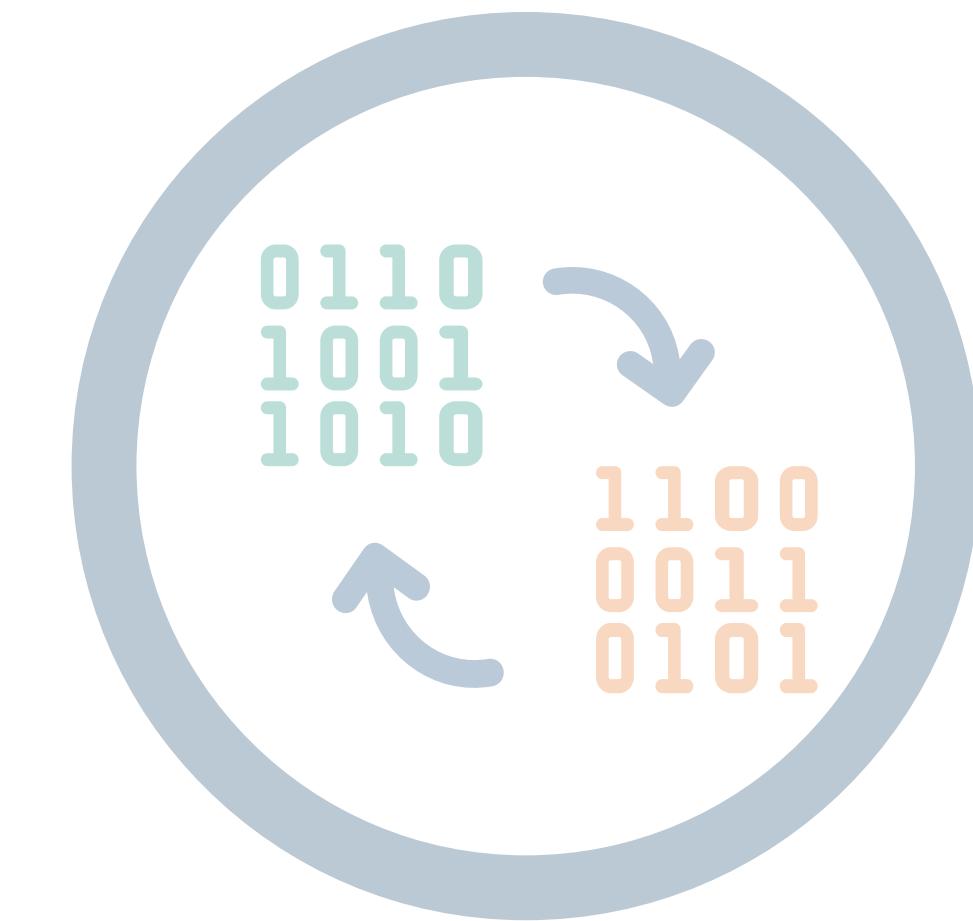
Three main challenges of the permutation approach



Power Analysis



Computational
Complexity

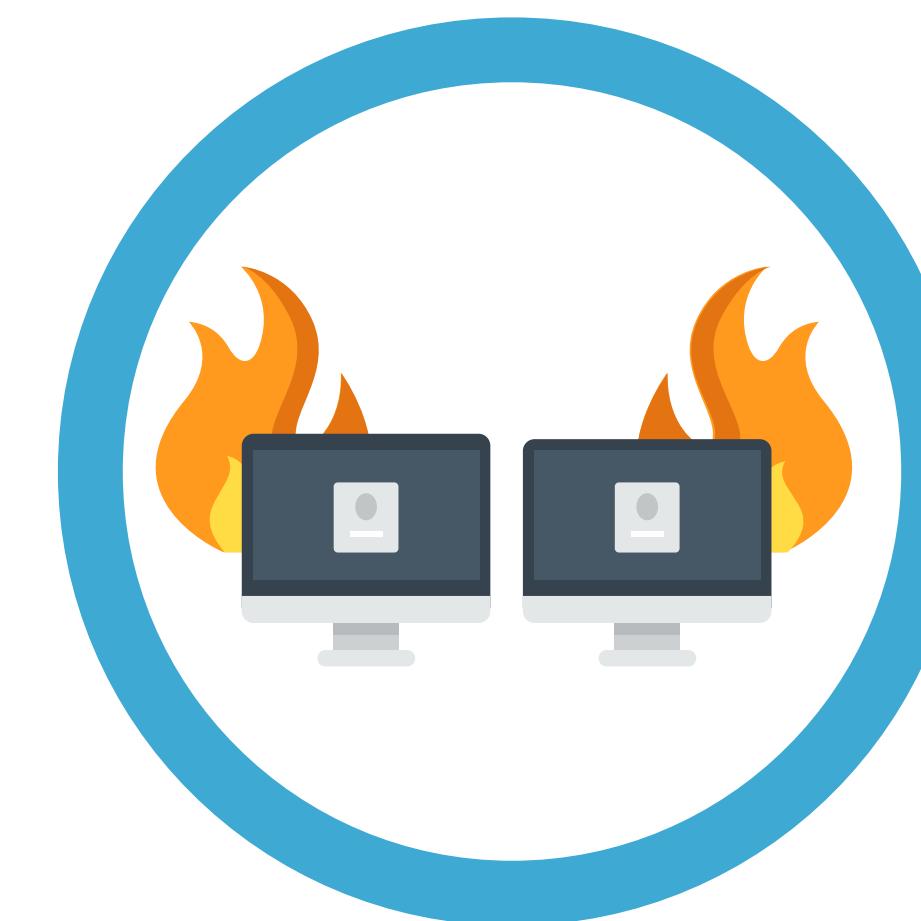


Non-exchangeable
Data

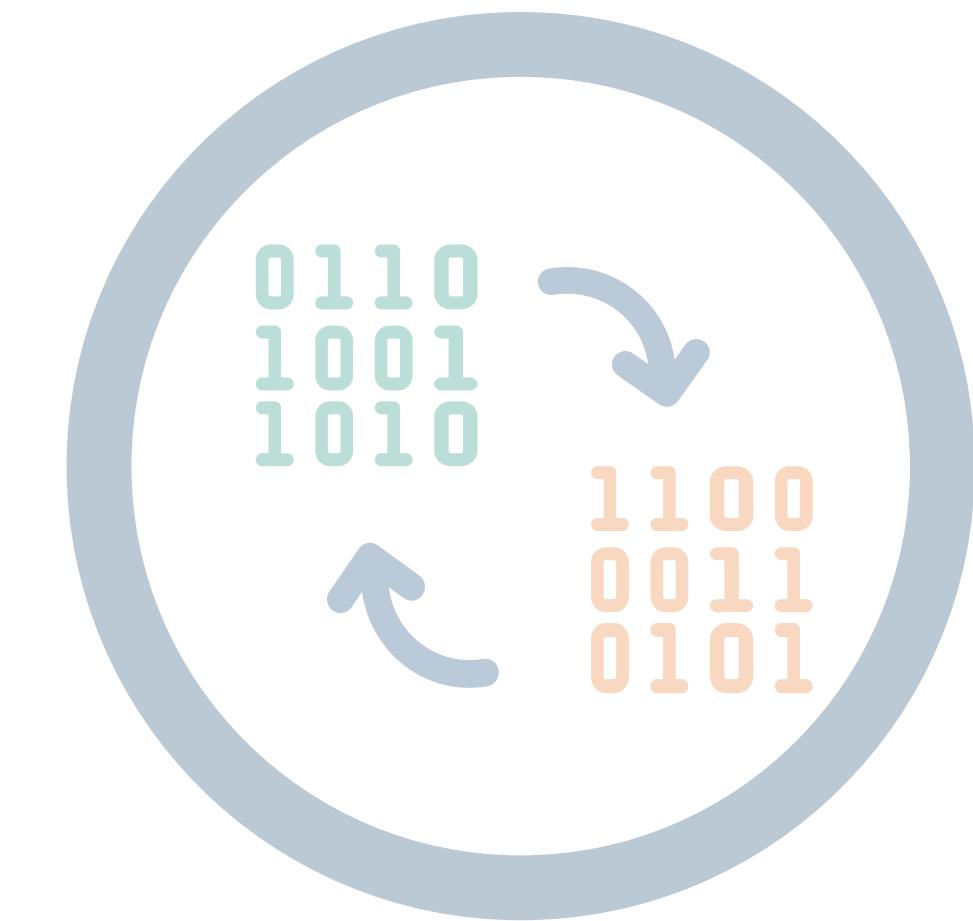
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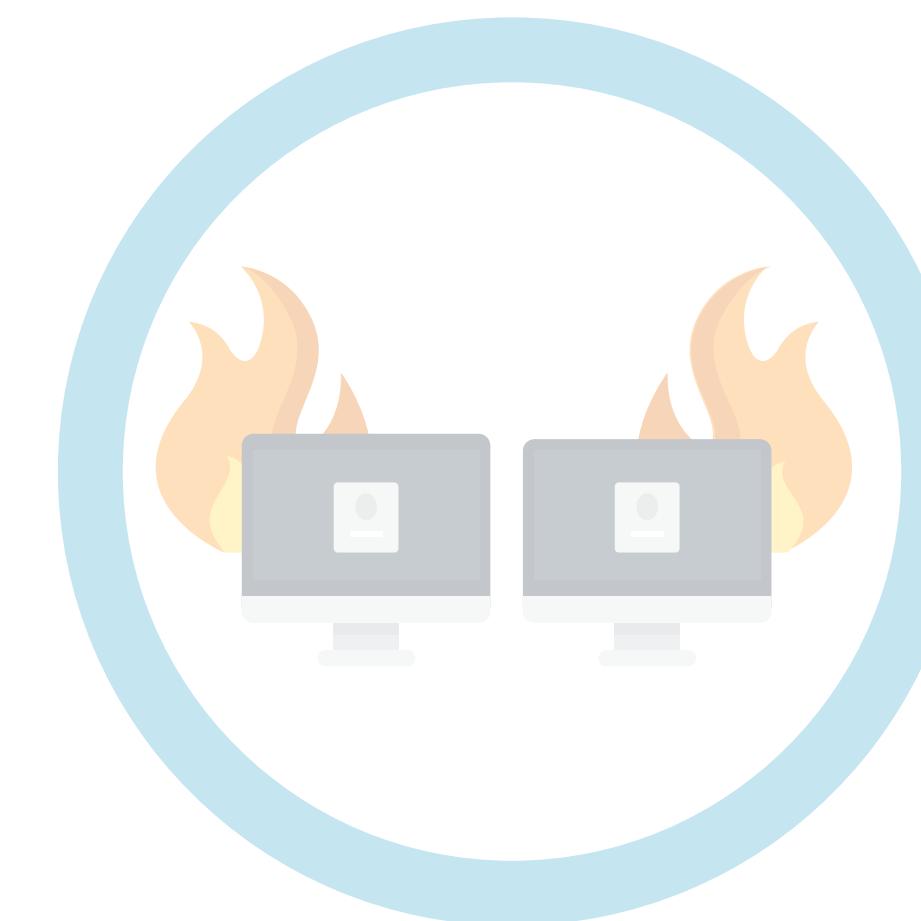


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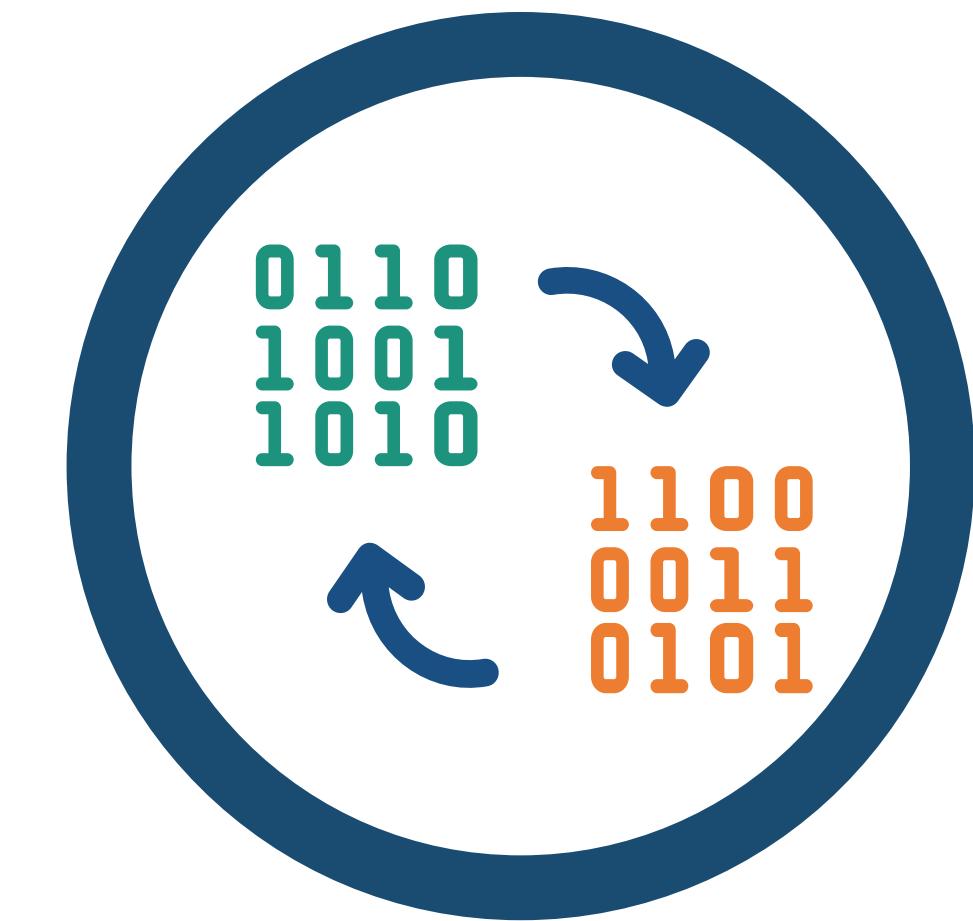
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Part I. Methodological Contributions

Part II. Theoretical Contributions

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<https://doi.org/10.1214/19-EJS1648>

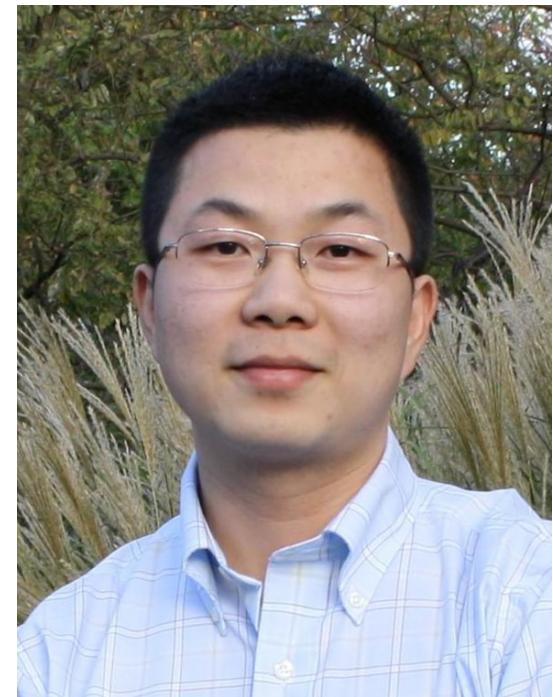
Global and local two-sample tests via regression

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Carnegie Mellon University
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Pittsburgh, PA 15213



Ann Lee
(CMU)



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

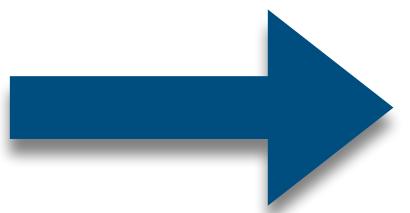
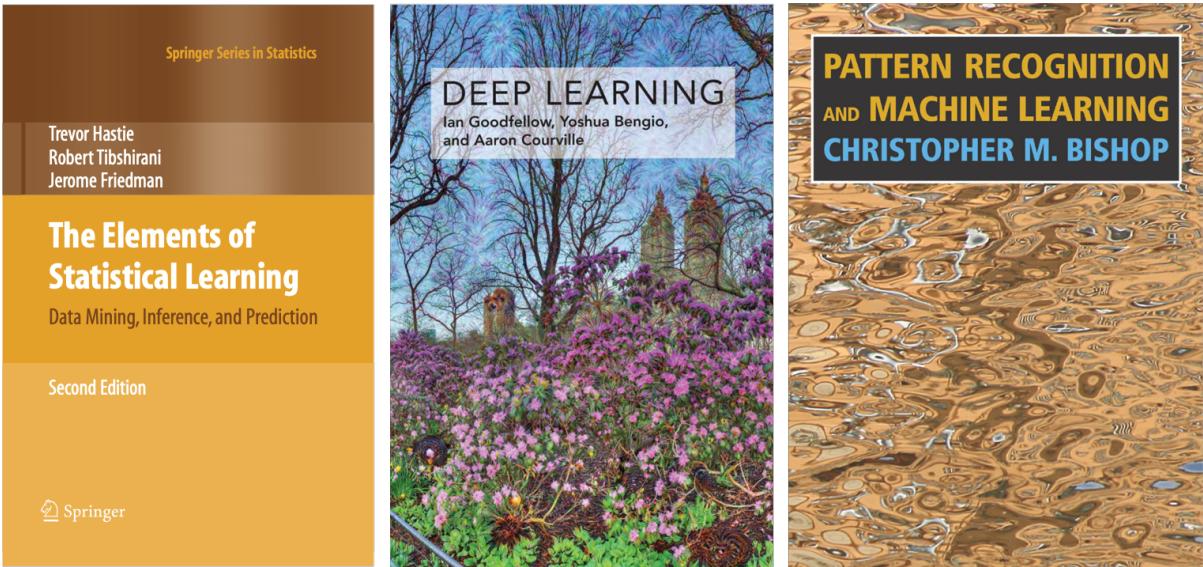


Larry Wasserman
(CMU)

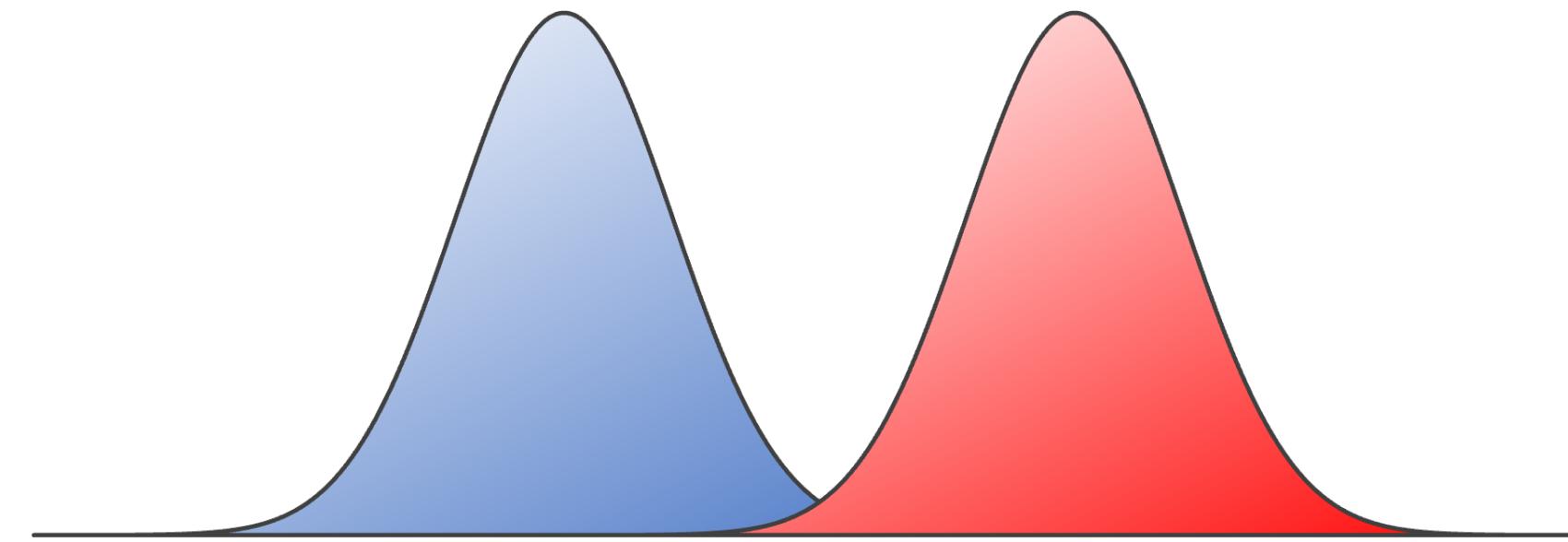


Aarti Singh
(CMU)

We propose a flexible framework for two-sample testing

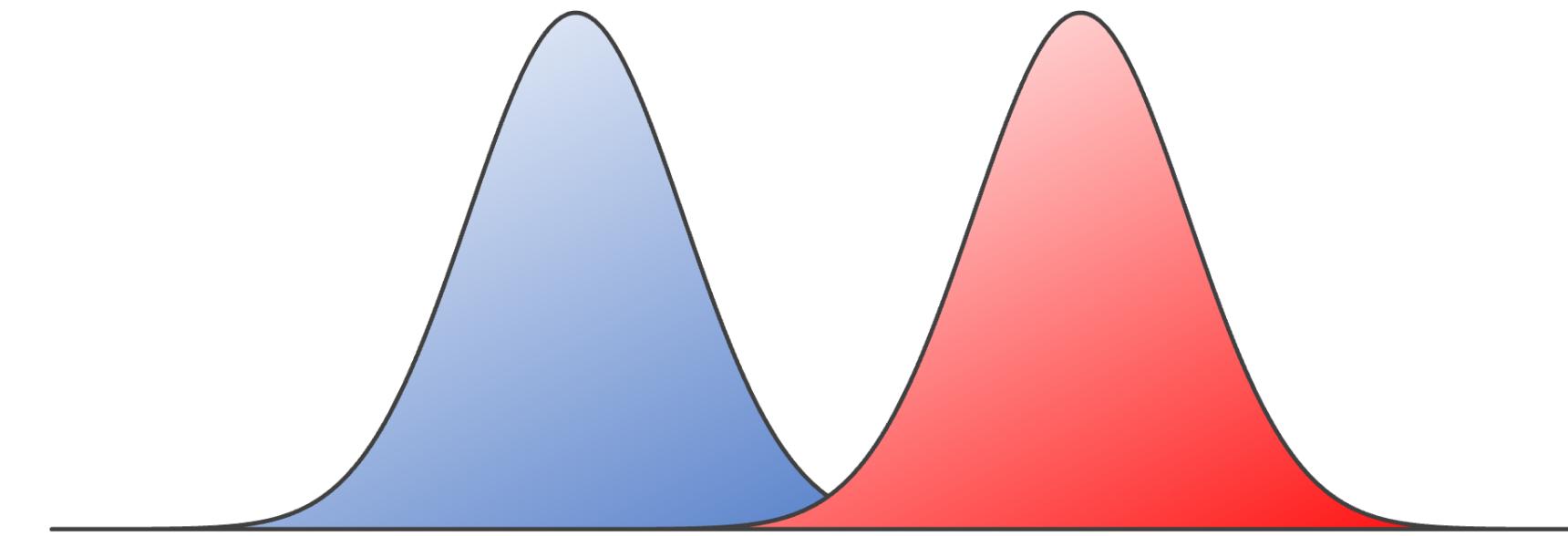
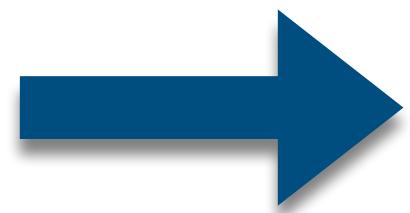
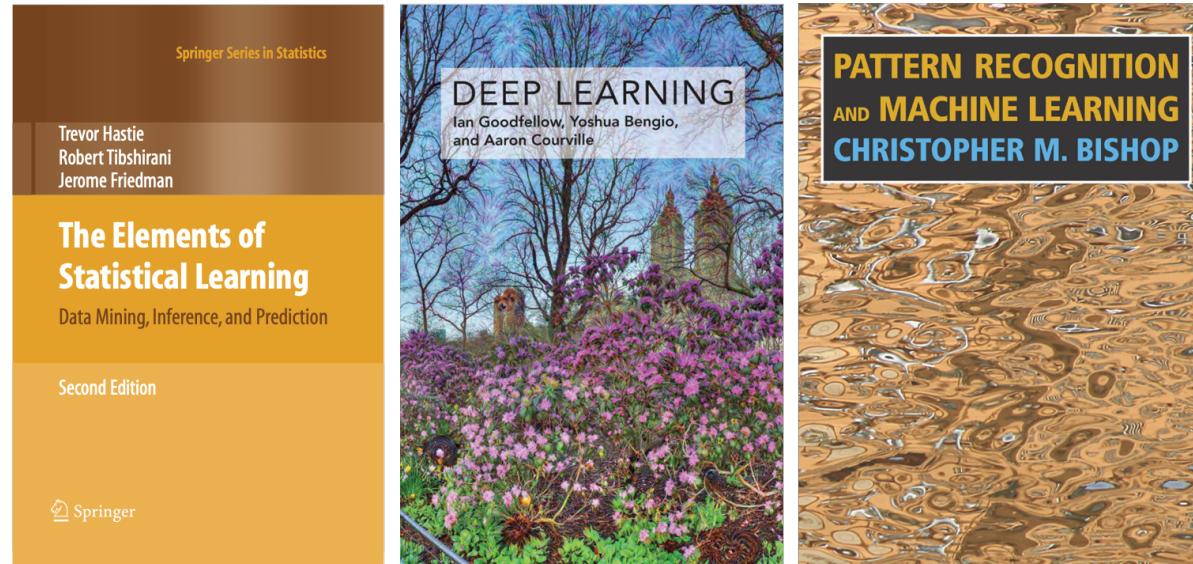


Classification/Regression



Two-sample test

We propose a flexible framework for two-sample testing



Classification/Regression

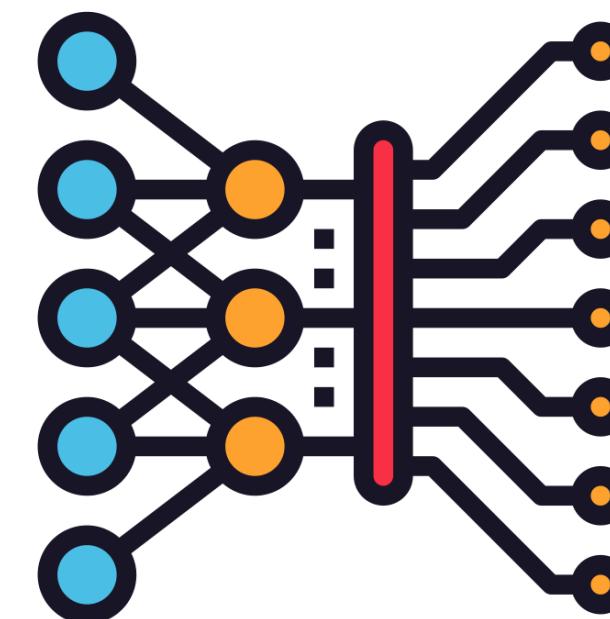
Two-sample test



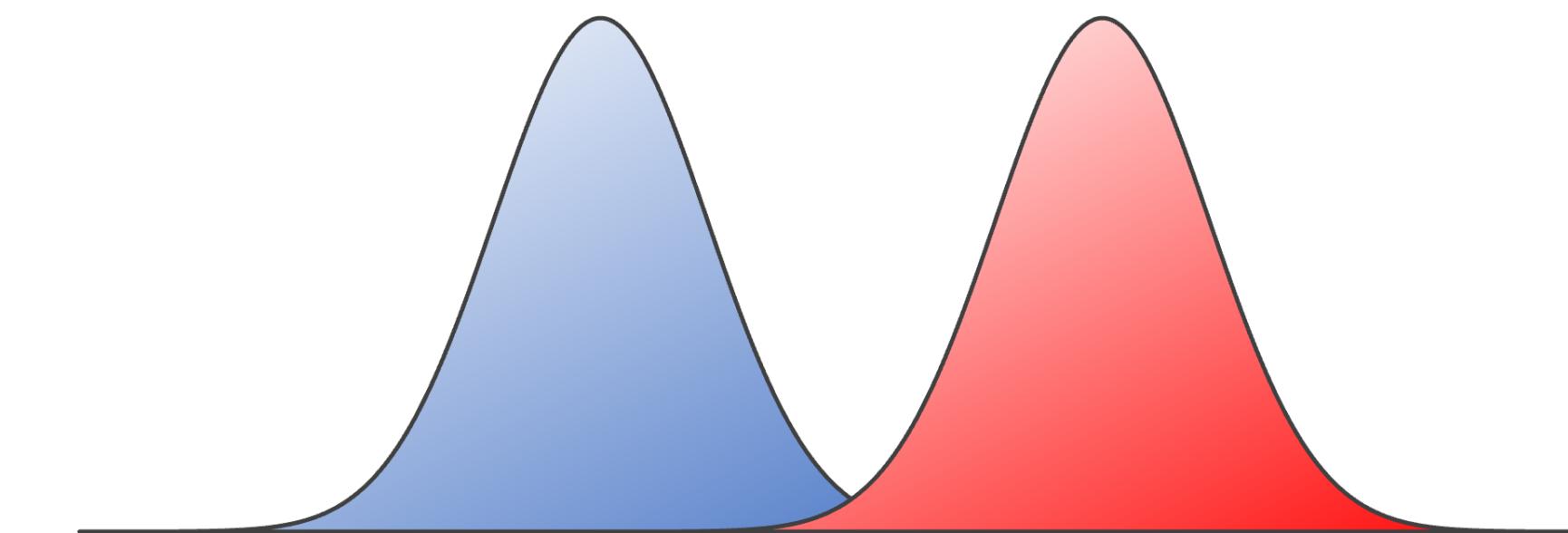
Idea

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

We propose a **flexible** framework for two-sample testing



Neural networks



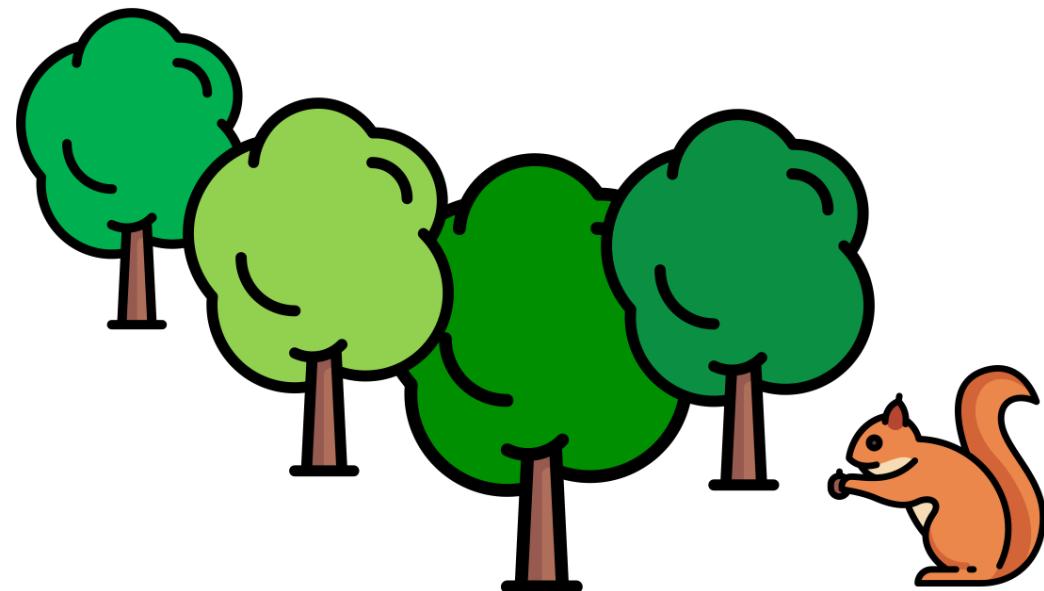
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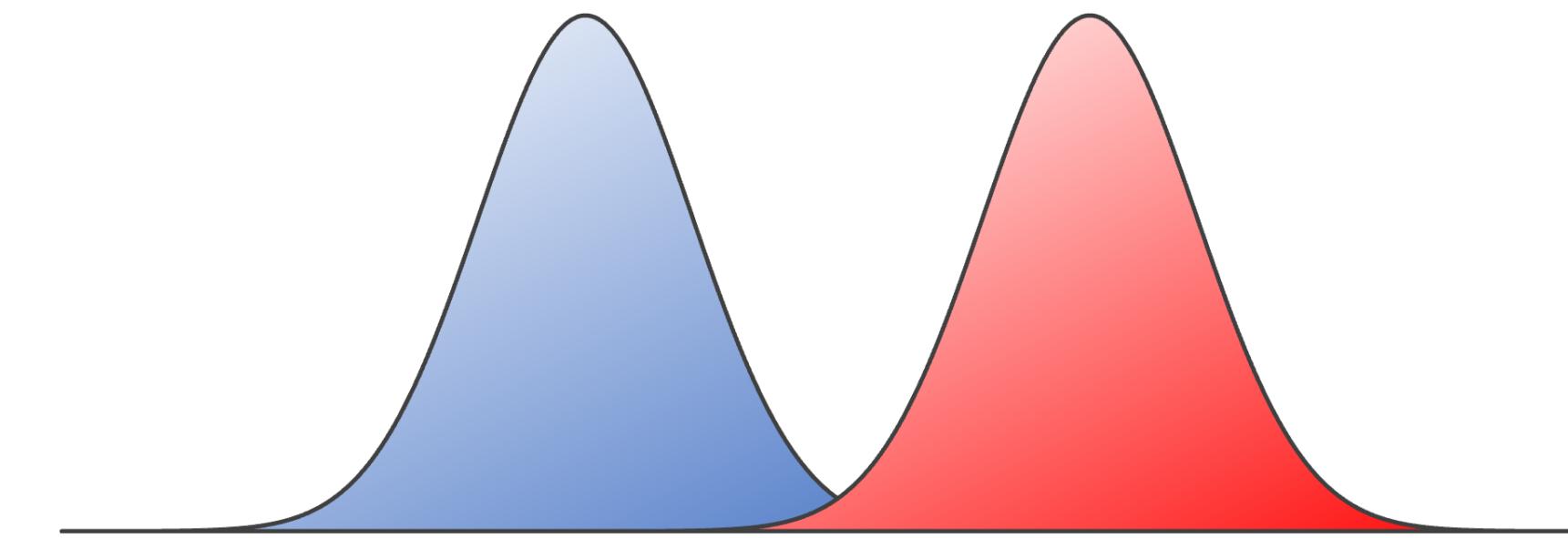
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Random forests



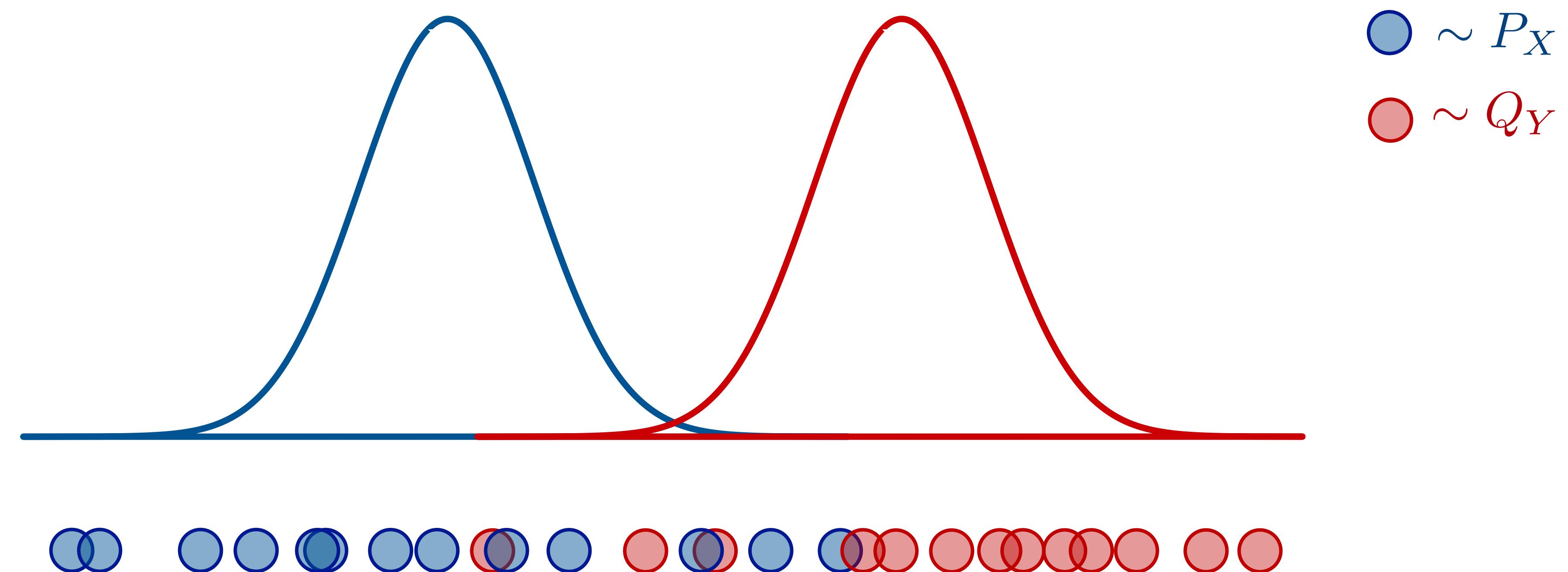
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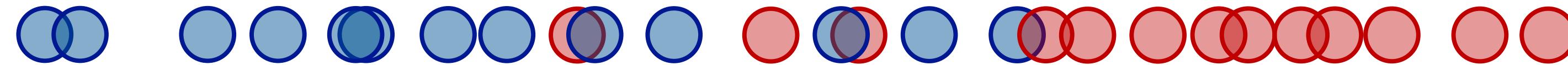
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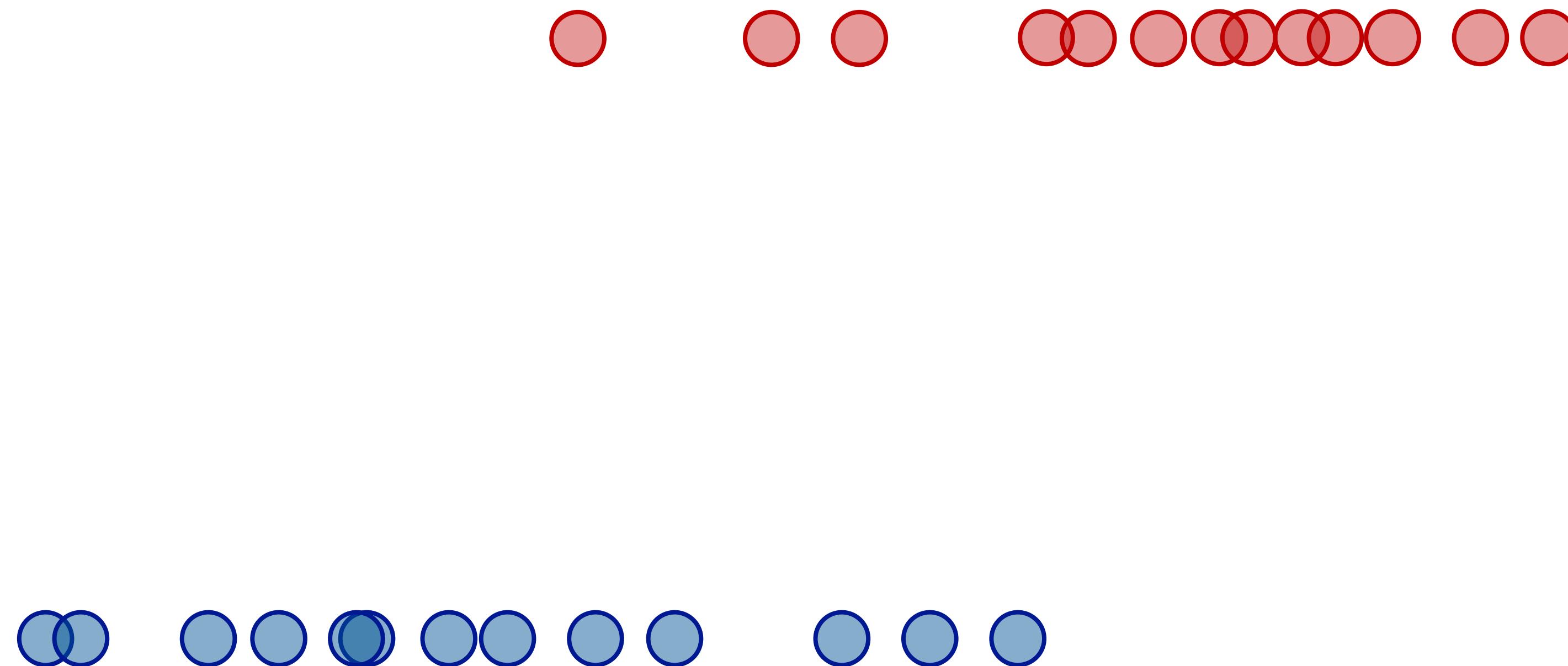
Regression-based two-sample test



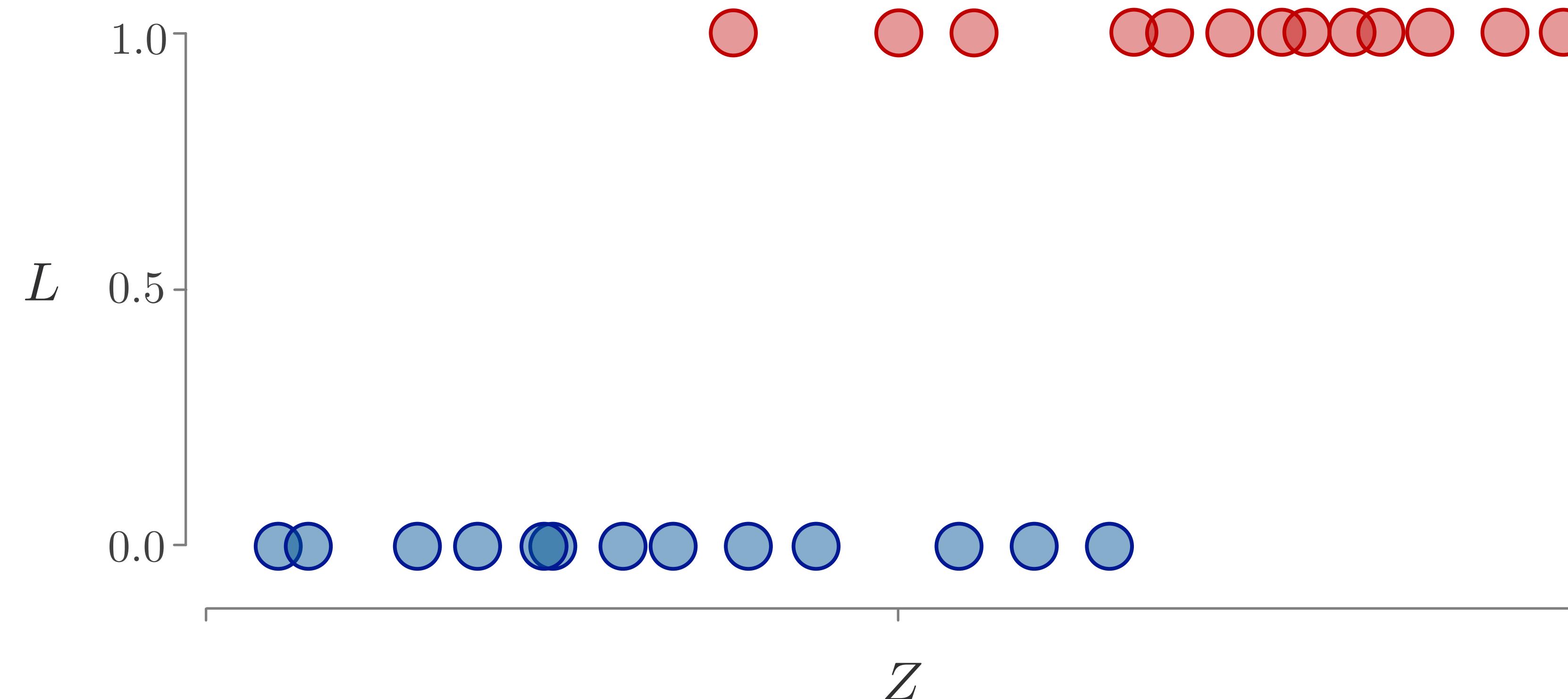
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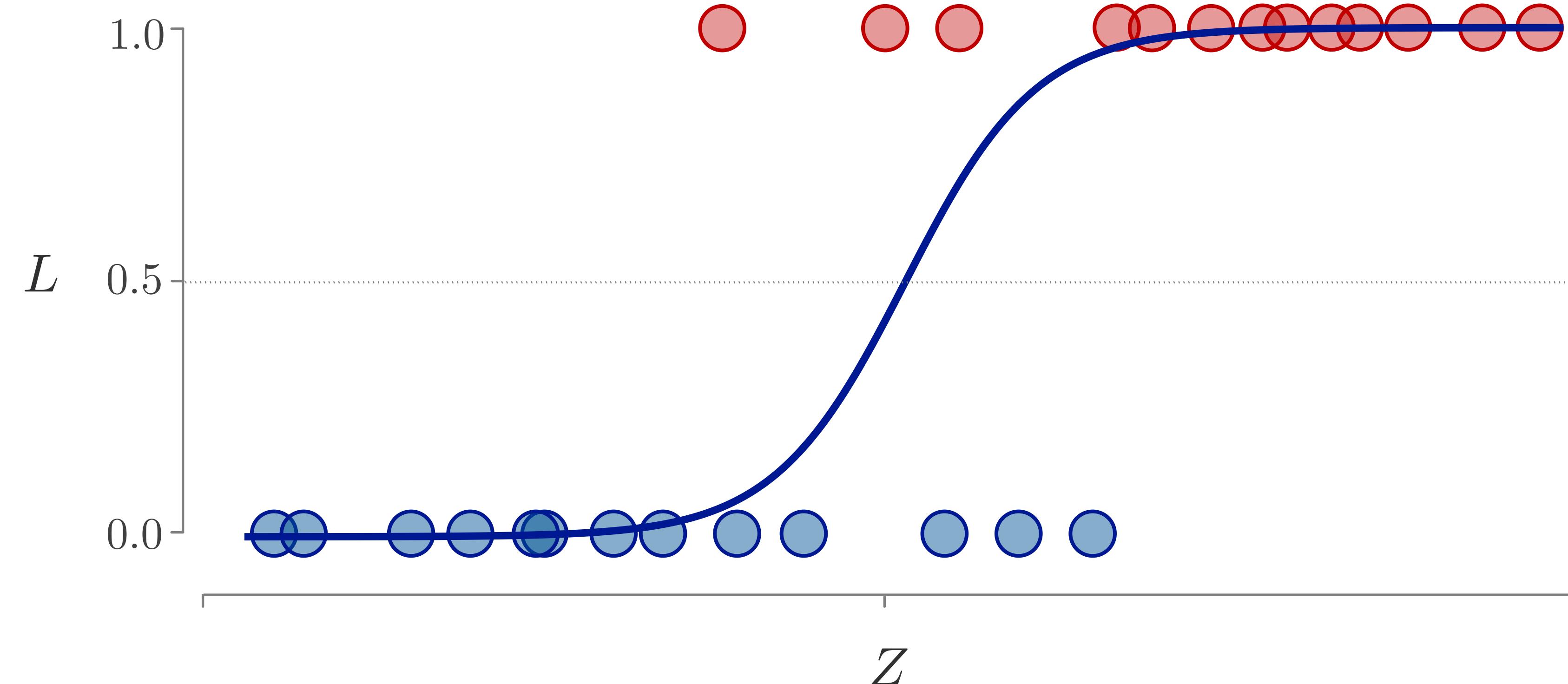
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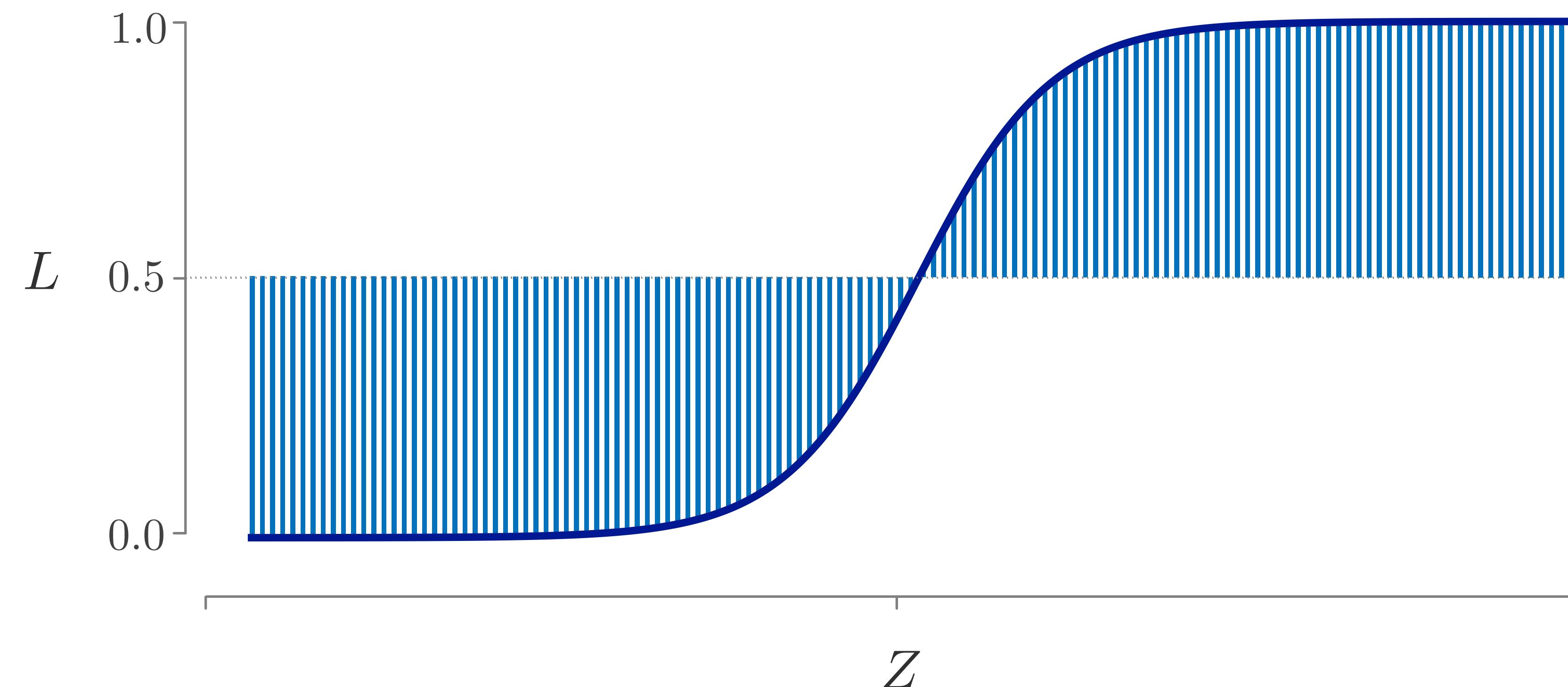
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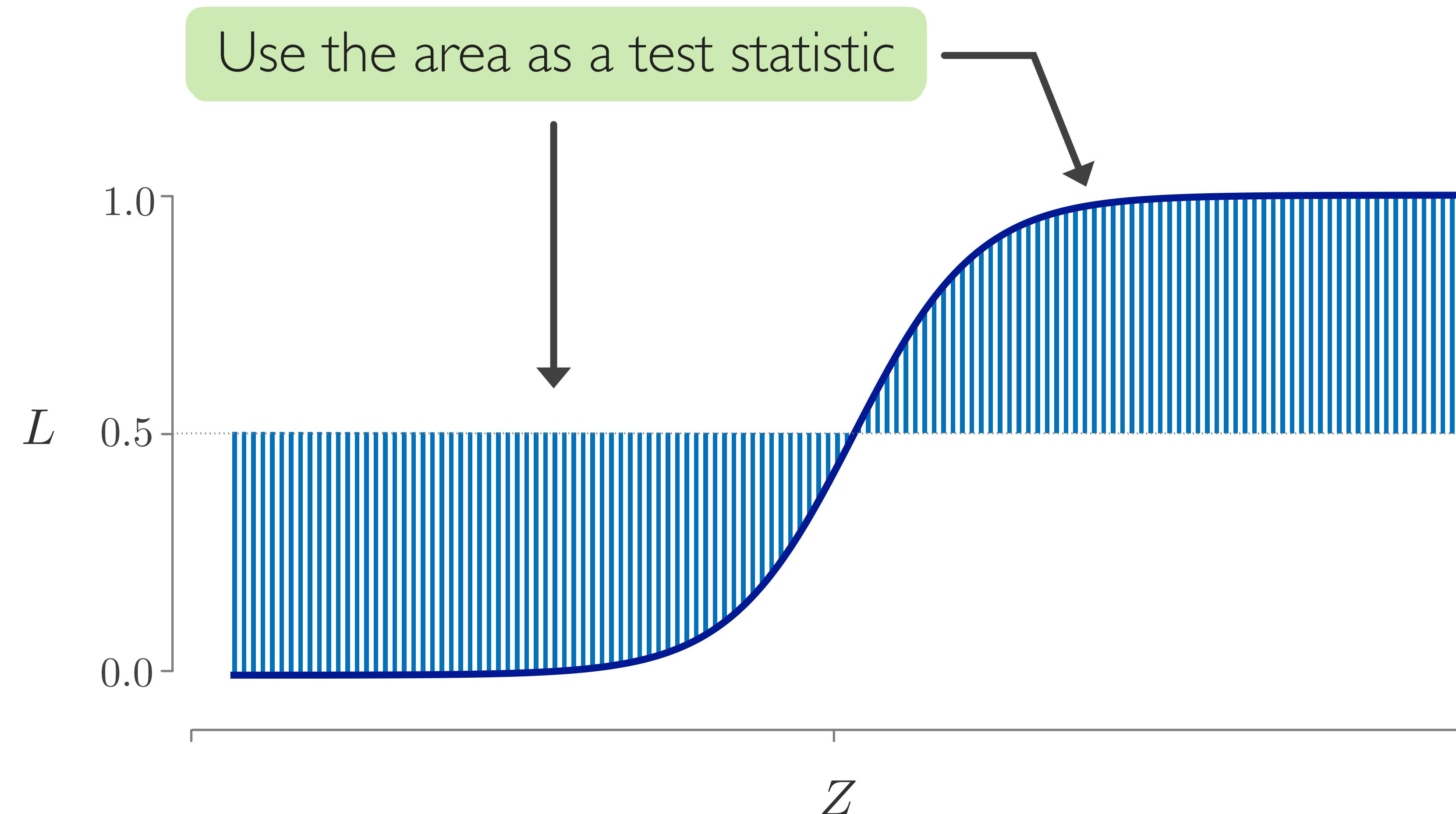
Regression-based two-sample test



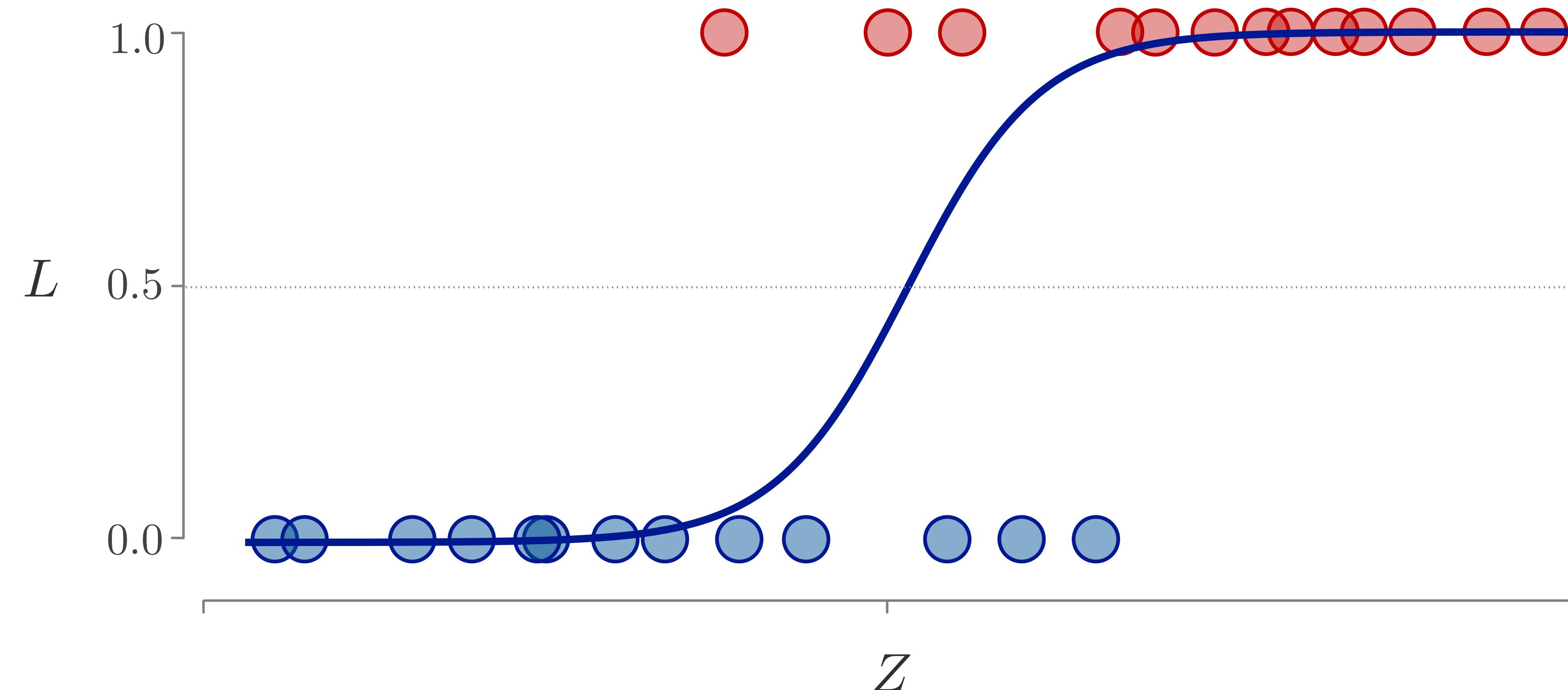
Regression-based two-sample test



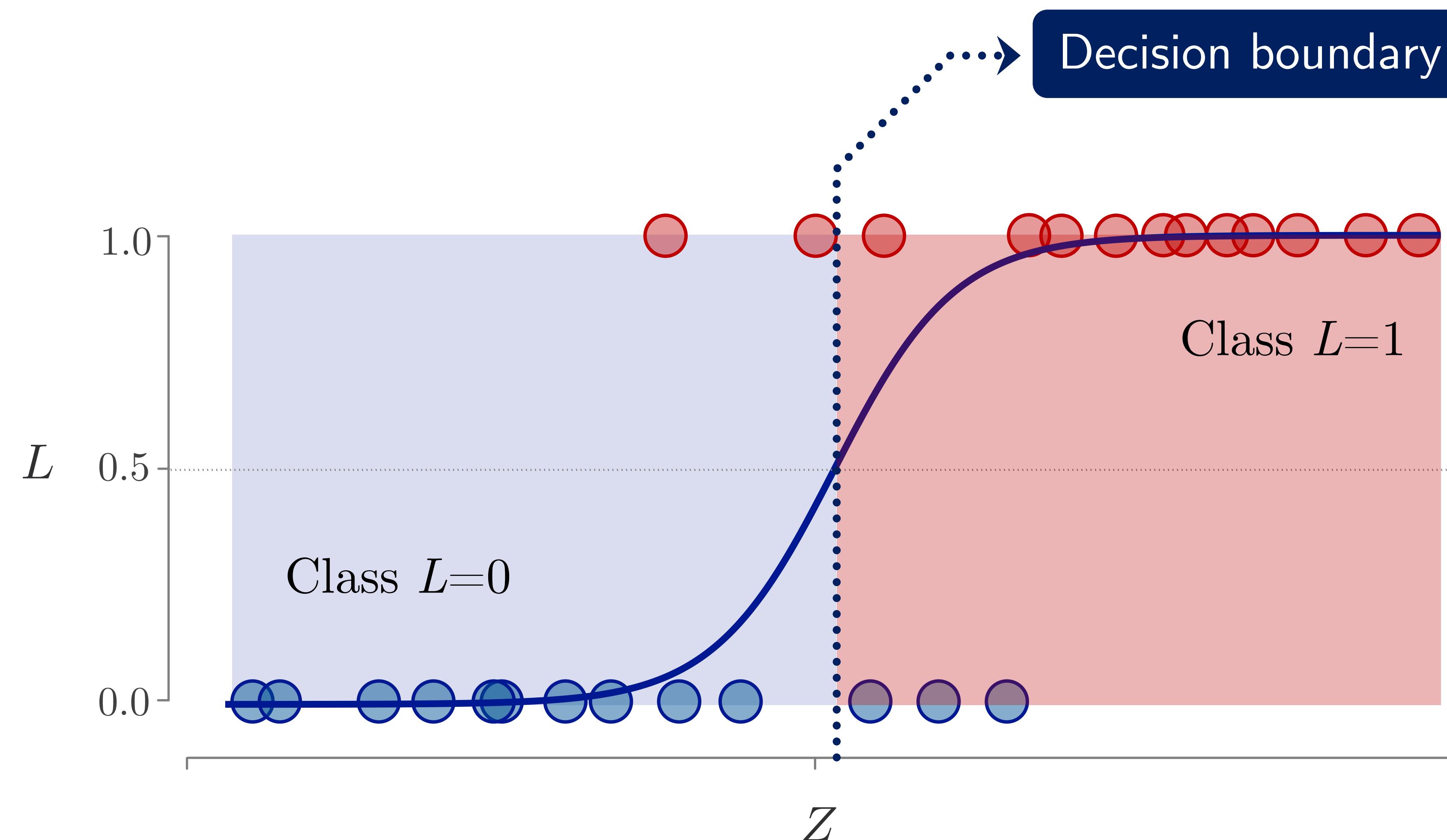
Regression-based two-sample test



Classification accuracy-based two-sample test



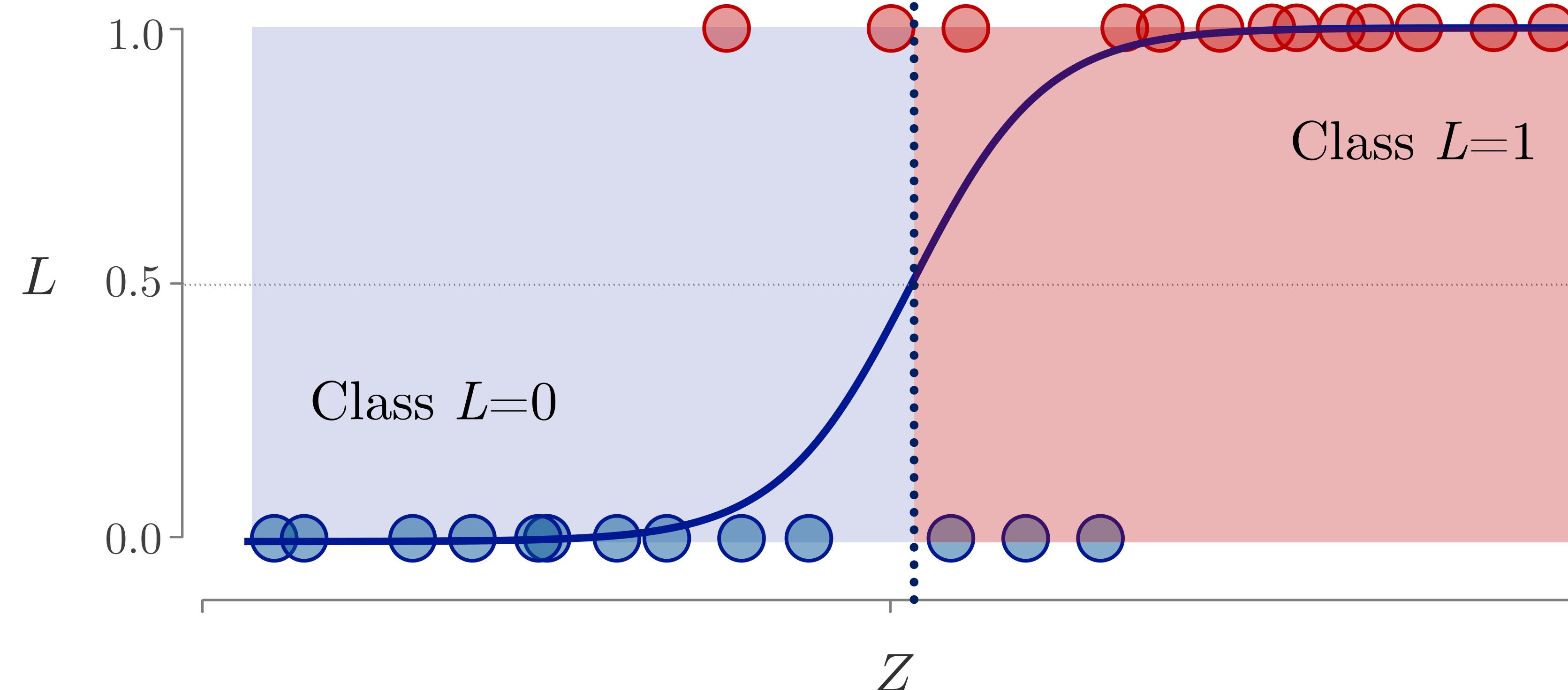
Classification accuracy-based two-sample test



Classification accuracy-based two-sample test

Use the accuracy as a test statistic

Decision boundary



Test statistics

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

$m = n$
for simplicity

Test statistics

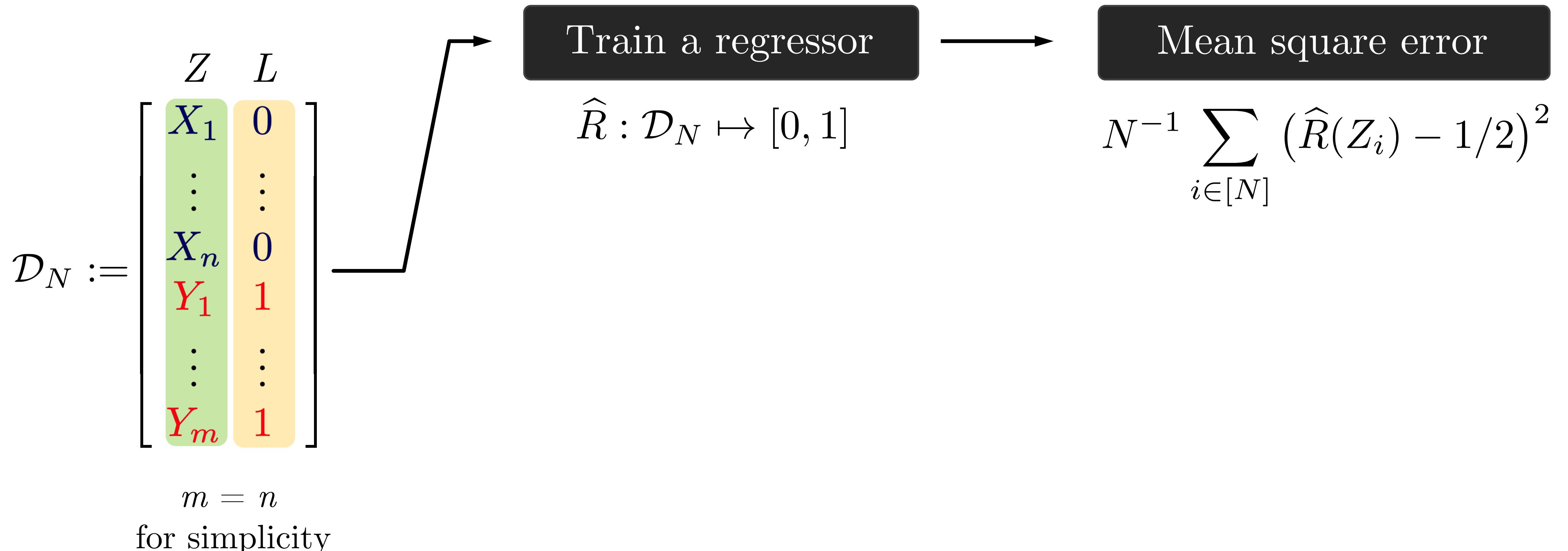
$$\mathcal{D}_N := \begin{bmatrix} Z & L \\ X_1 & 0 \\ \vdots & \vdots \\ X_n & 0 \\ Y_1 & 1 \\ \vdots & \vdots \\ Y_m & 1 \end{bmatrix}$$

Train a regressor

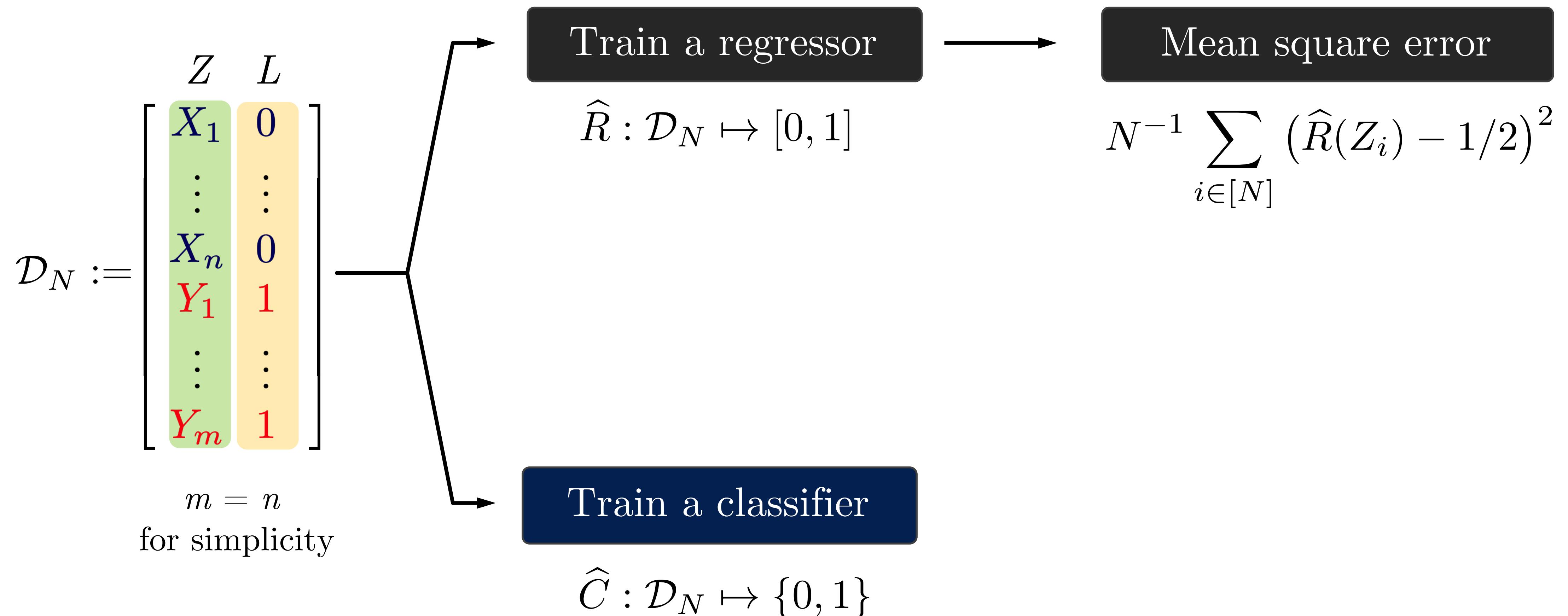
$$\hat{R} : \mathcal{D}_N \mapsto [0, 1]$$

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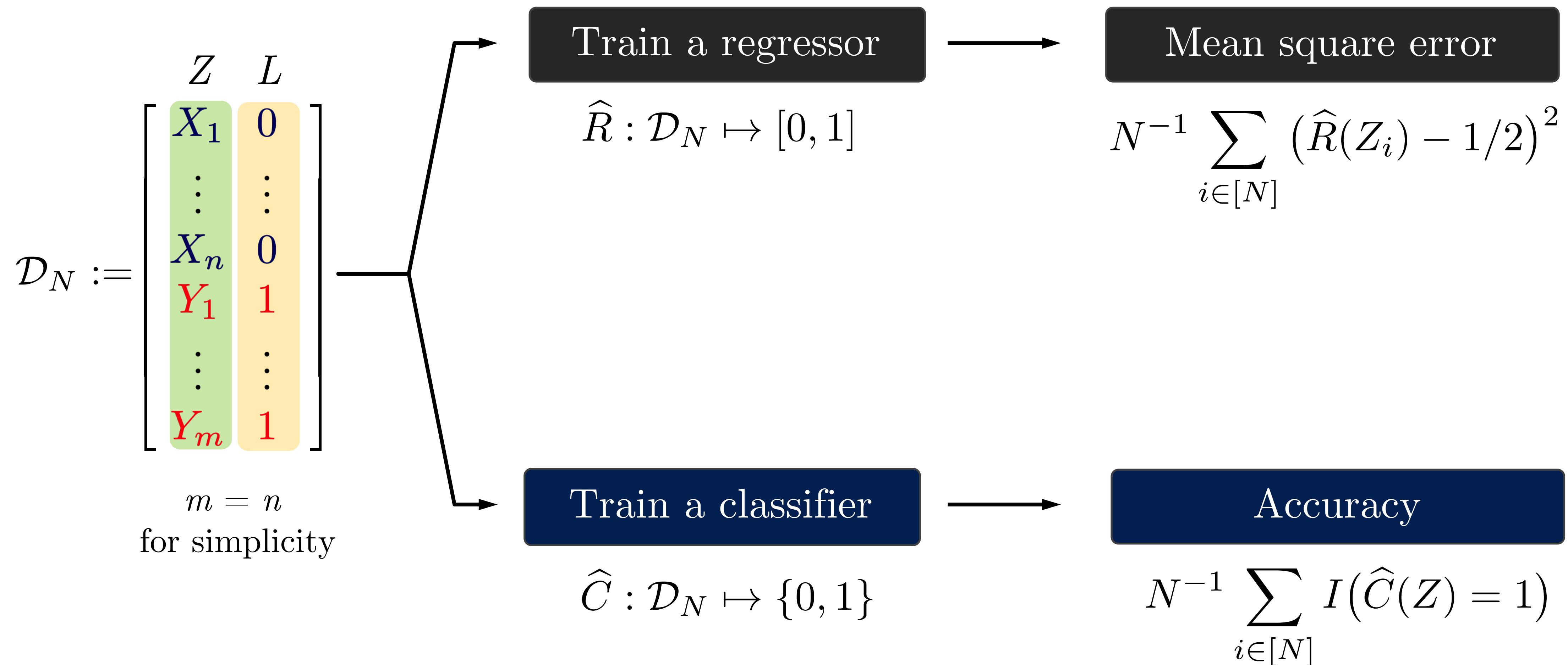
Test statistics



Test statistics



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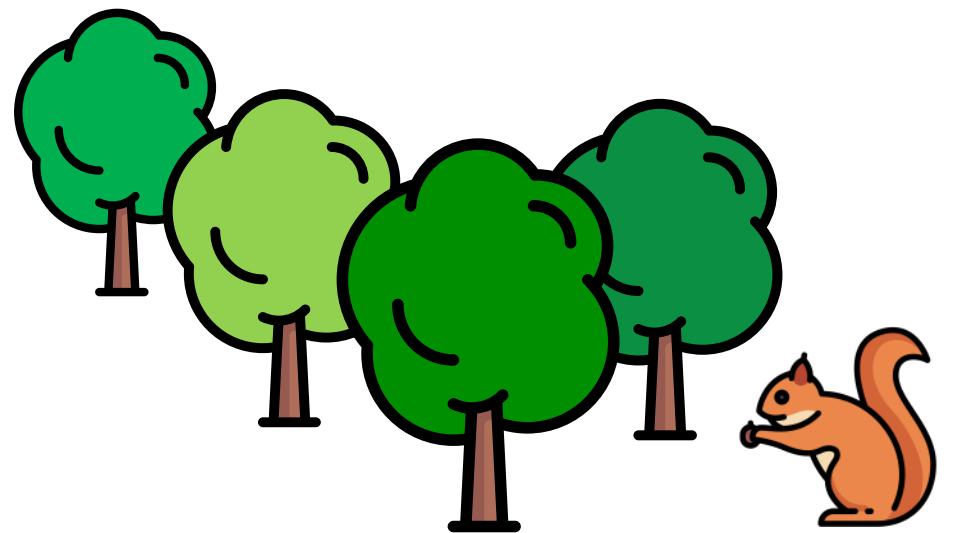
Empirical results



Random forests

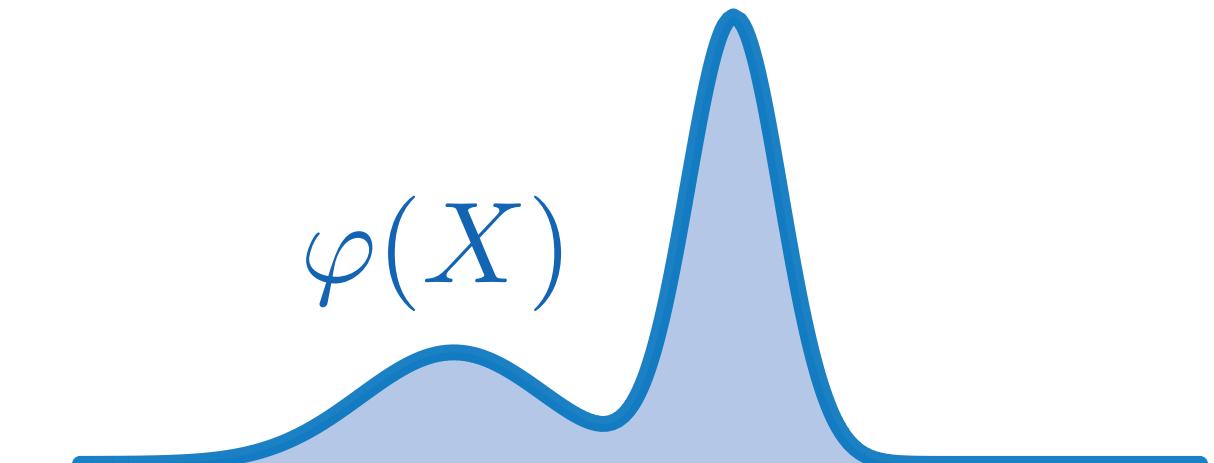
- Screen irrelevant variables
- Robust to outliers
- Handle various data types
- Empirical success

Empirical results



Random forests

versus



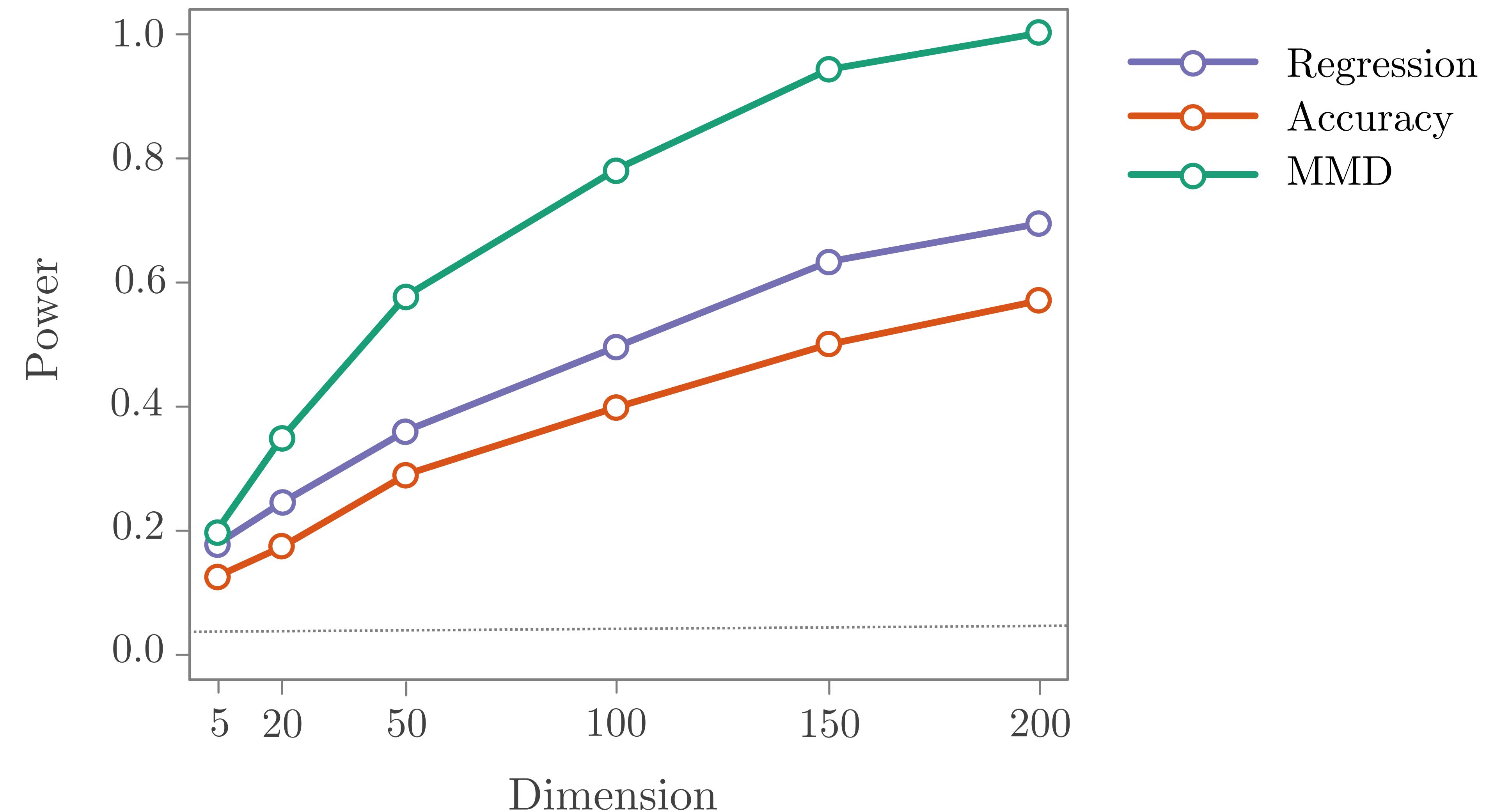
Maximum Mean Discrepancy

- 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

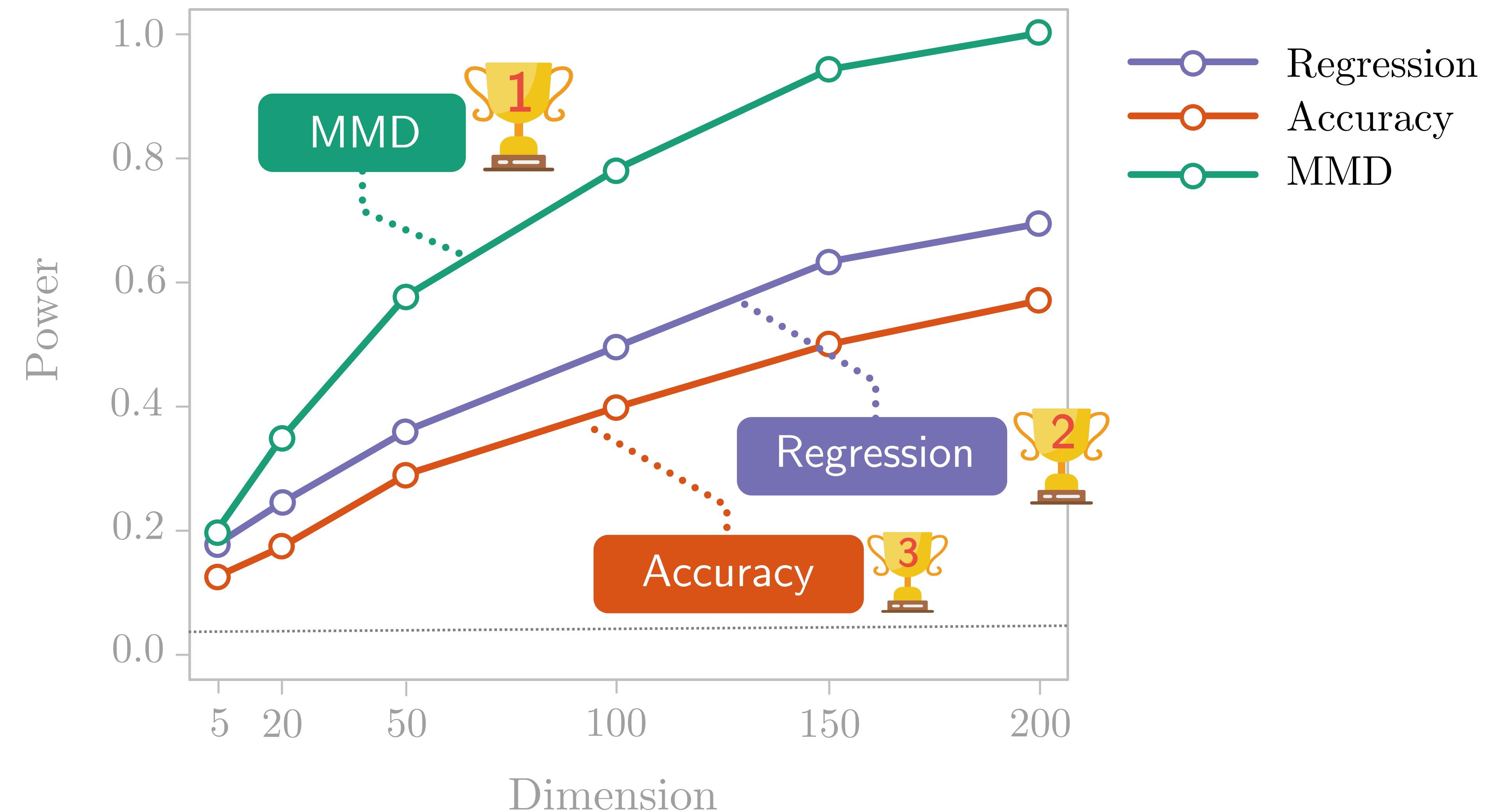
Power comparison

Normal location alternative



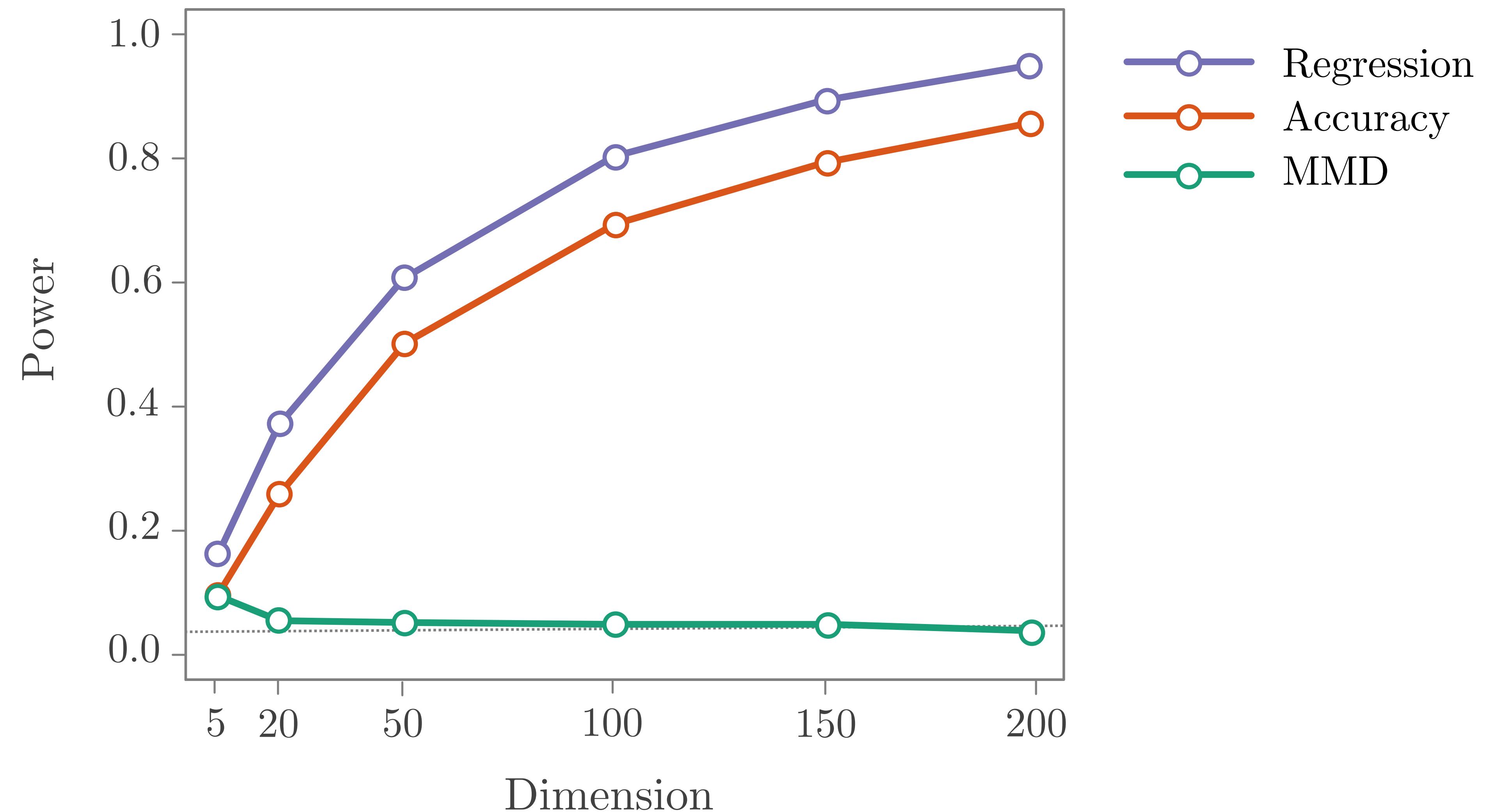
Power comparison

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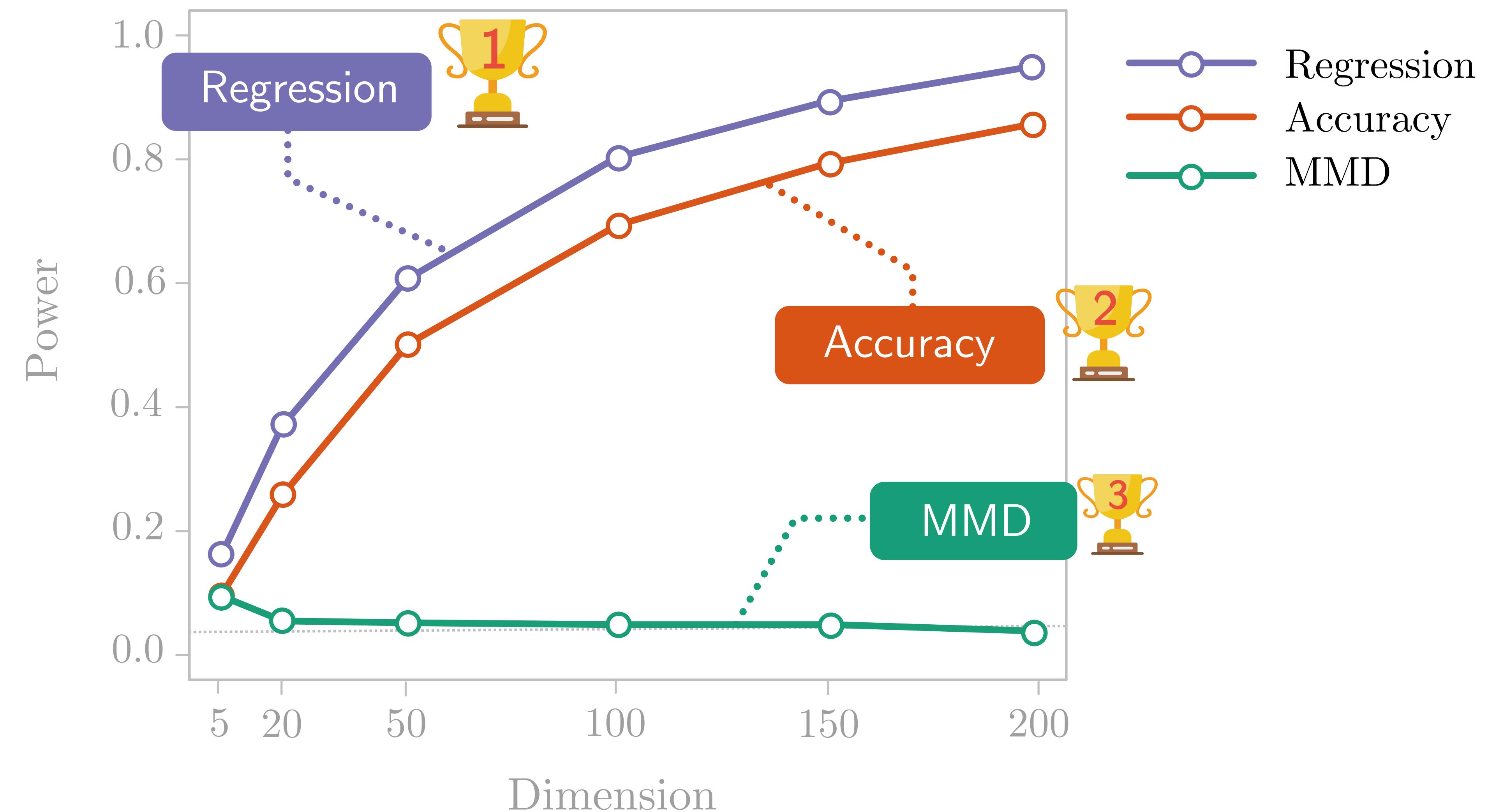
Power comparison

Cauchy location alternative



Power comparison

Cauchy location alternative

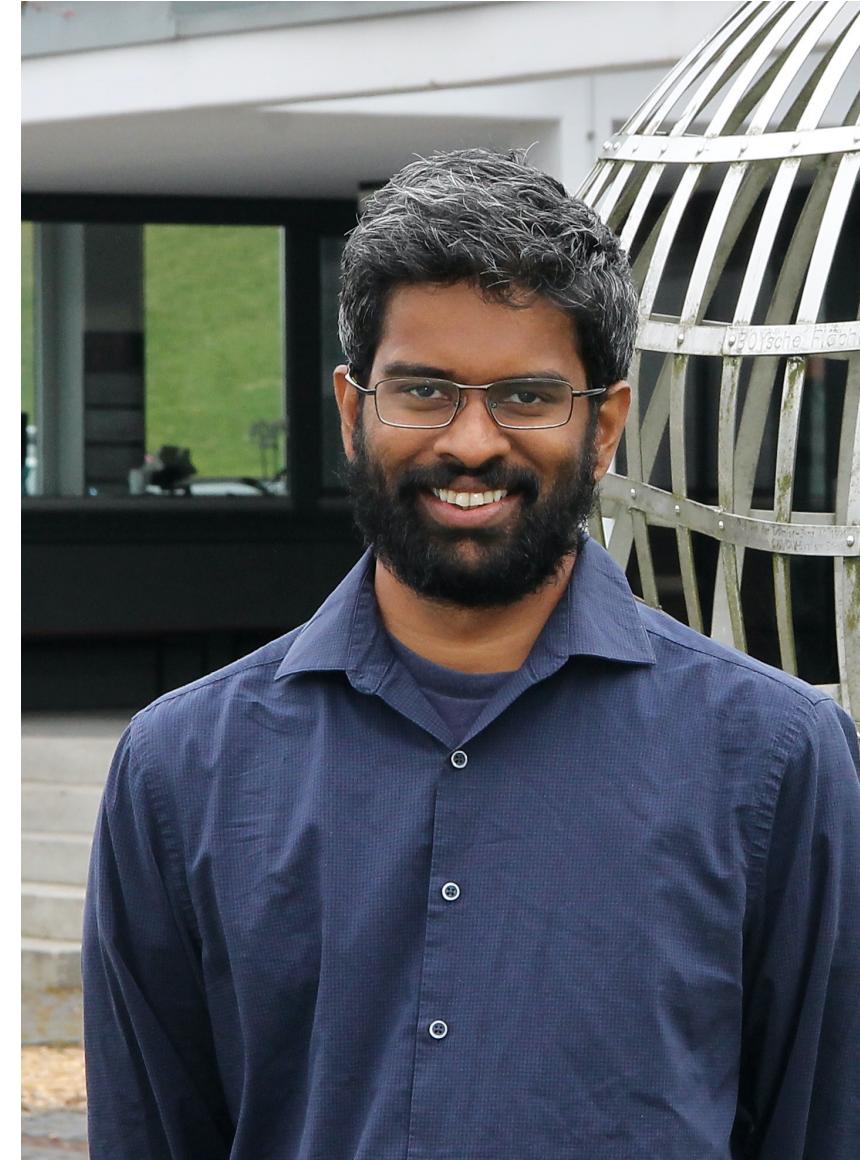


Part I. Methodological Contributions

Part II. Theoretical Contributions

MINIMAX OPTIMALITY OF PERMUTATION TESTS

BY ILMUN KIM¹, 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

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

Test statistic

Critical value

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Test statisticCritical value

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

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

Uniform Type II error over \mathcal{P}_1

Challenge: Random critical value

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Random quantity +
Lacking independence

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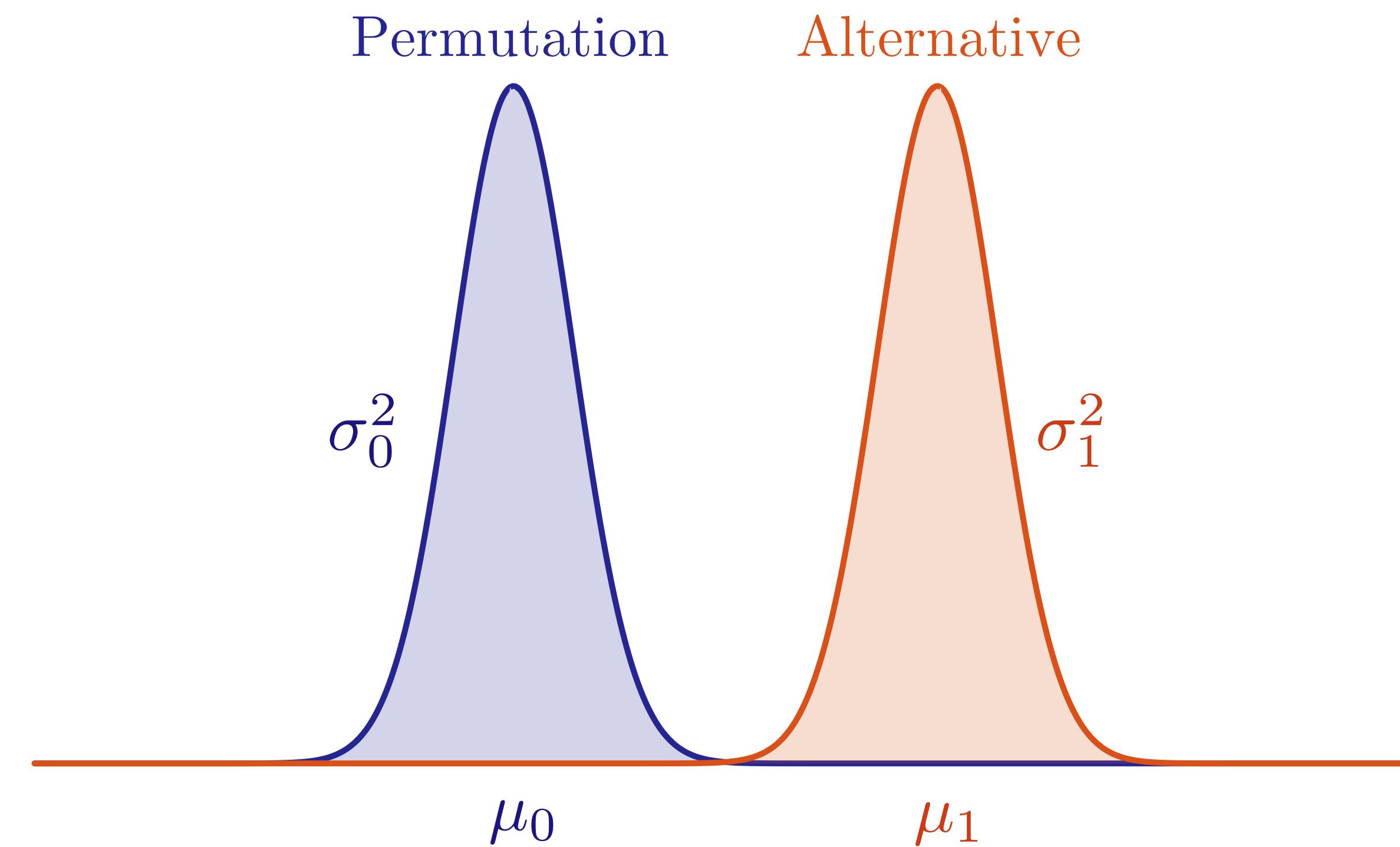
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Uniform **Type II error** over \mathcal{P}_1

Our proposal: Two moments method

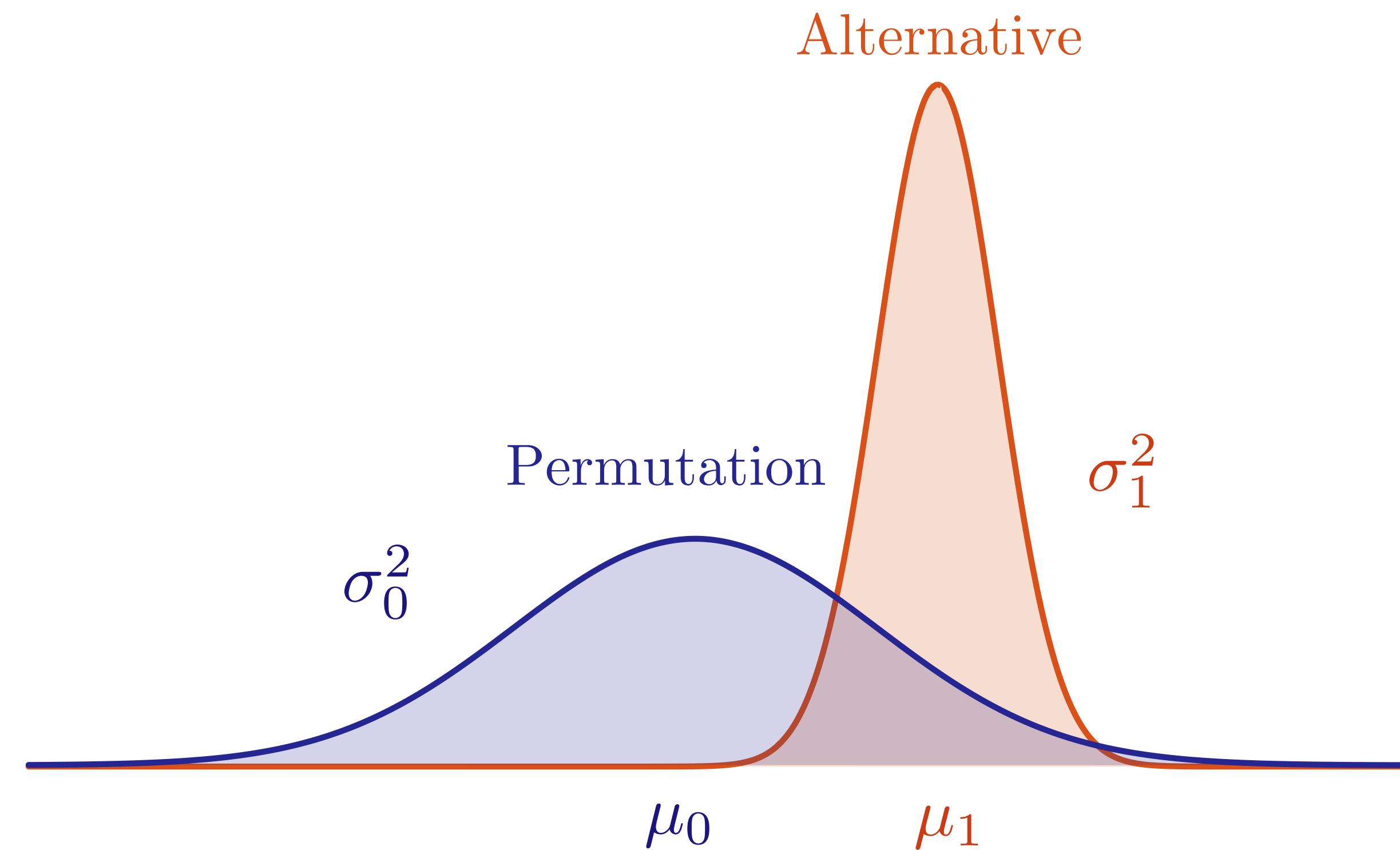
Intuition for the two moments method

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

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 $\{X_1, \dots, X_n\} \stackrel{i.i.d.}{\sim} P_X$ and $\{Y_1, \dots, Y_n\} \stackrel{i.i.d.}{\sim} P_Y$

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

$$\begin{aligned} U_n = & \frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} h(X_i, X_j) + \frac{1}{n(n-1)} \sum_{1 \leq i \neq j \leq n} h(Y_i, Y_j) \\ & - \frac{2}{n^2} \sum_{1 \leq i \leq n} \sum_{1 \leq j \leq n} h(X_i, Y_j) \end{aligned}$$

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Between Similarity

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Within Similarity **Within Similarity**
Between Similarity

Examples

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

U-statistic for independence testing

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$$+ \frac{(n-4)!}{n!} \sum_{(i,j,q,r) \in I_4^n} h_X(X_i, X_j) h_Y(Y_q, Y_r) - 2 \frac{(n-3)!}{n!} \sum_{(i,j,q) \in I_3^n} h_X(X_i, X_j) h_Y(Y_i, Y_q)$$

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$P_X^2 P_Y^2$

$P_{XY} P_X P_Y$

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Examples

HSIC (Gretton et al., 2005)

Distance Covariance (Szekely et al., 2007)

$P_X^2 P_Y^2$

$P_{XY} P_X P_Y$

Result for U-statistics

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

$$\left| \mathbb{E}_P[U_n] - \mathbb{E}_{P,\pi}[U_n^\pi] \right| \gtrsim \sqrt{\beta^{-1} \mathbb{V}_P[U_n]} + \sqrt{\alpha^{-1} \beta^{-1} \mathbb{V}_{P,\pi}[U_n^\pi]}$$

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Question: Can we further simplify **these two moments** involving π ?

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Lemma [KBW 2022]

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

Centered

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

Noise II
(data + permutation)

Noise I
(data)

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Simplifies to



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(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. $H_1 : \text{distance}(P, Q) \geq \epsilon_n$

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

$$\sup_{\phi \in \Phi(\alpha)} \inf_{P \in \mathcal{P}_1(\epsilon_n)} \mathbb{E}_P[\phi]$$

Over all level α tests

Worst-case power

Applications to minimax testing

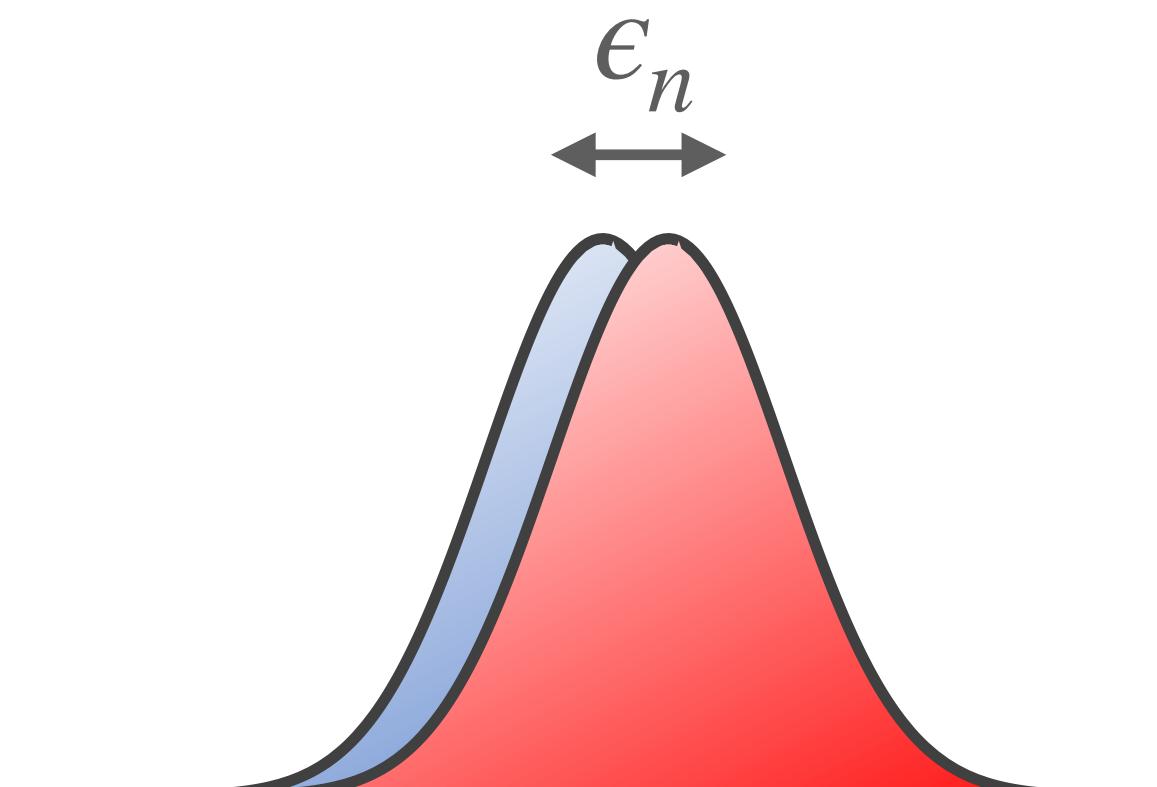
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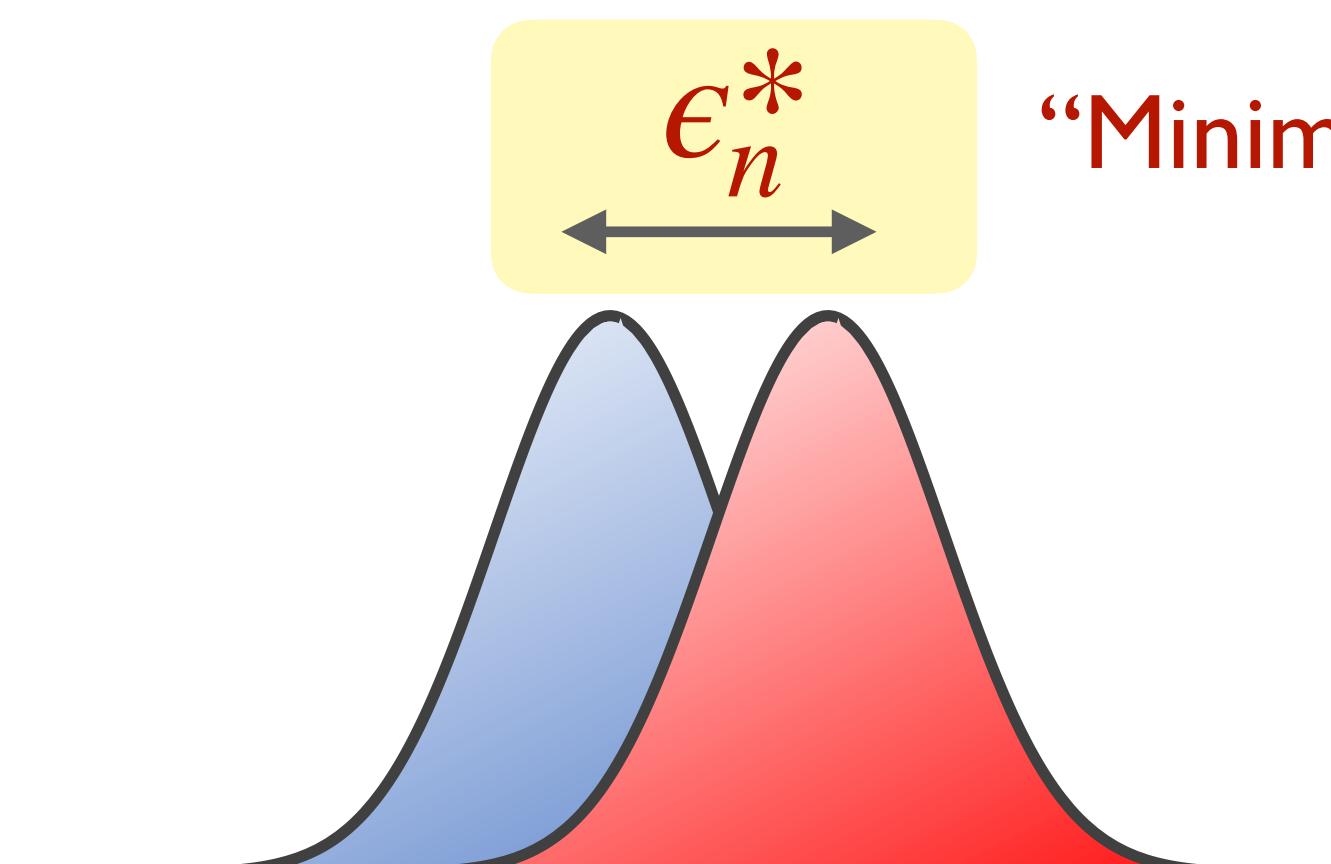
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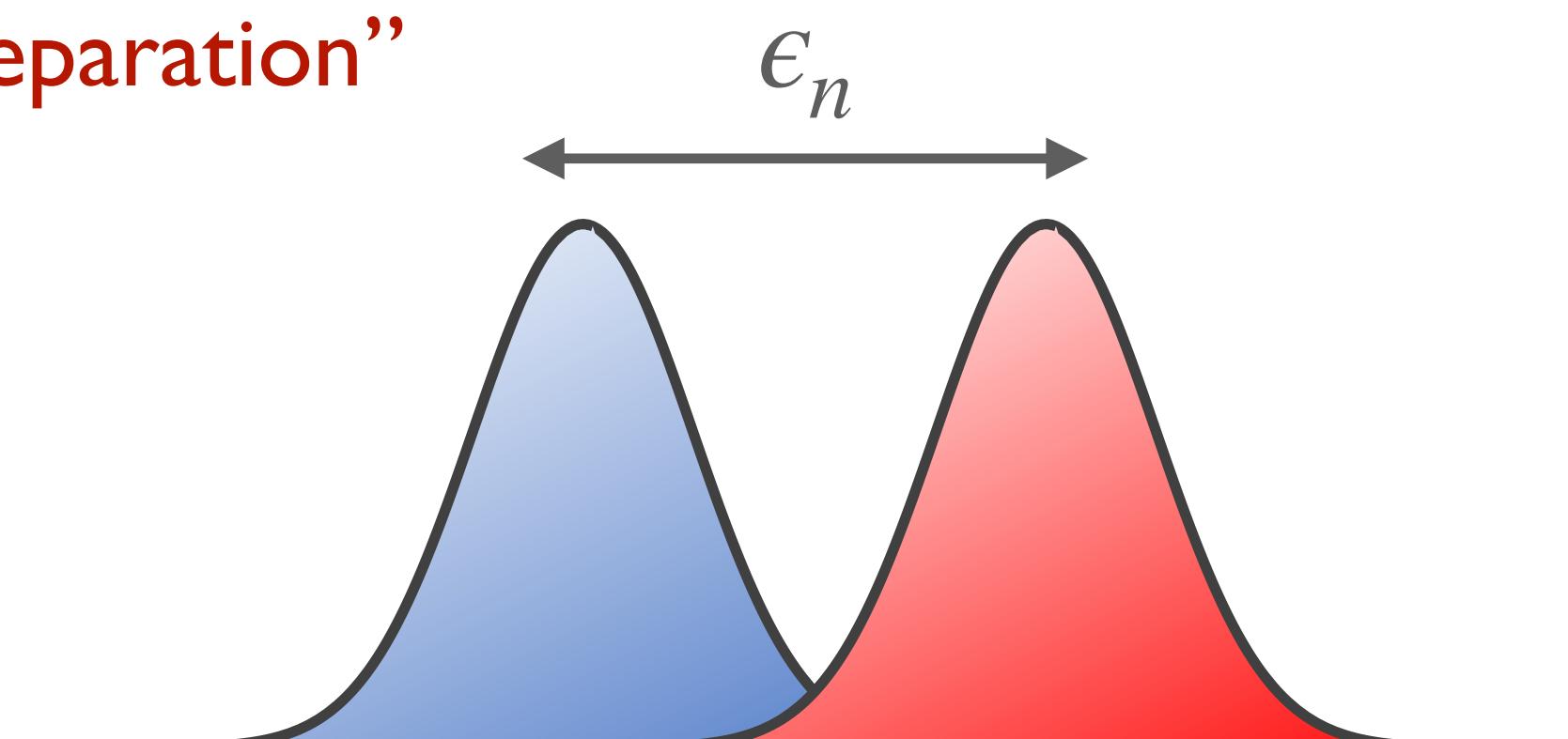
Worst-case power



Minimax power ≤ 0.05



Minimax power ≈ 0.8



Minimax power = 1

Applications to minimax testing

- We call ϕ is **minimax rate optimal** if

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

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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

- Chan et al. (2014) prove

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

d : the number of bins
 n : the sample size

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- The upper bound is based on the test

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

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Example Density testing in ℓ_2 -norm

- Arias-Castro et al. (2018) prove

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

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

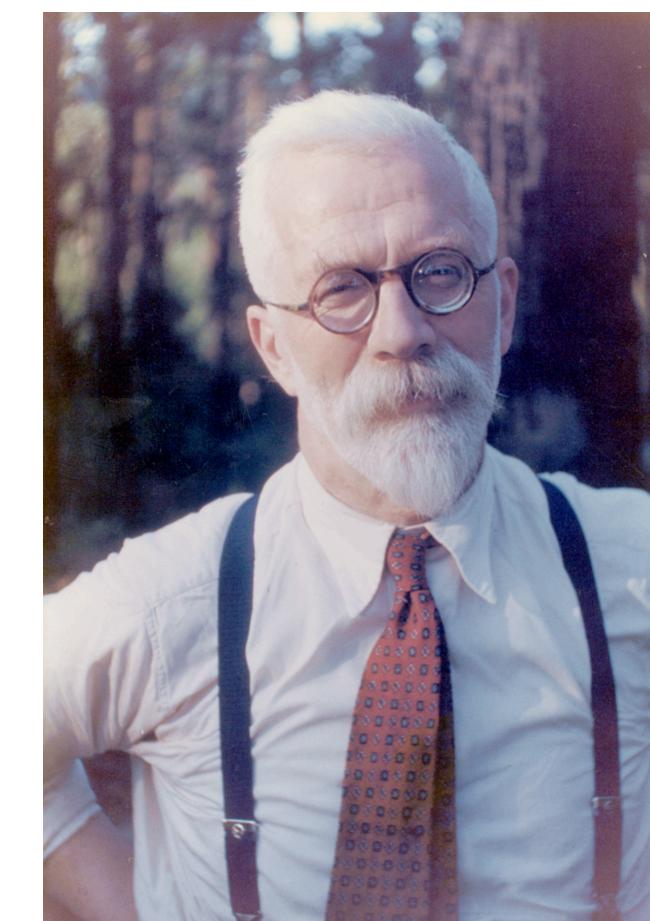
Question. Can we prove the minimax results using a test that

- i) *tightly* controls the type I error rate
- ii) does not depend on *unspecified* constants

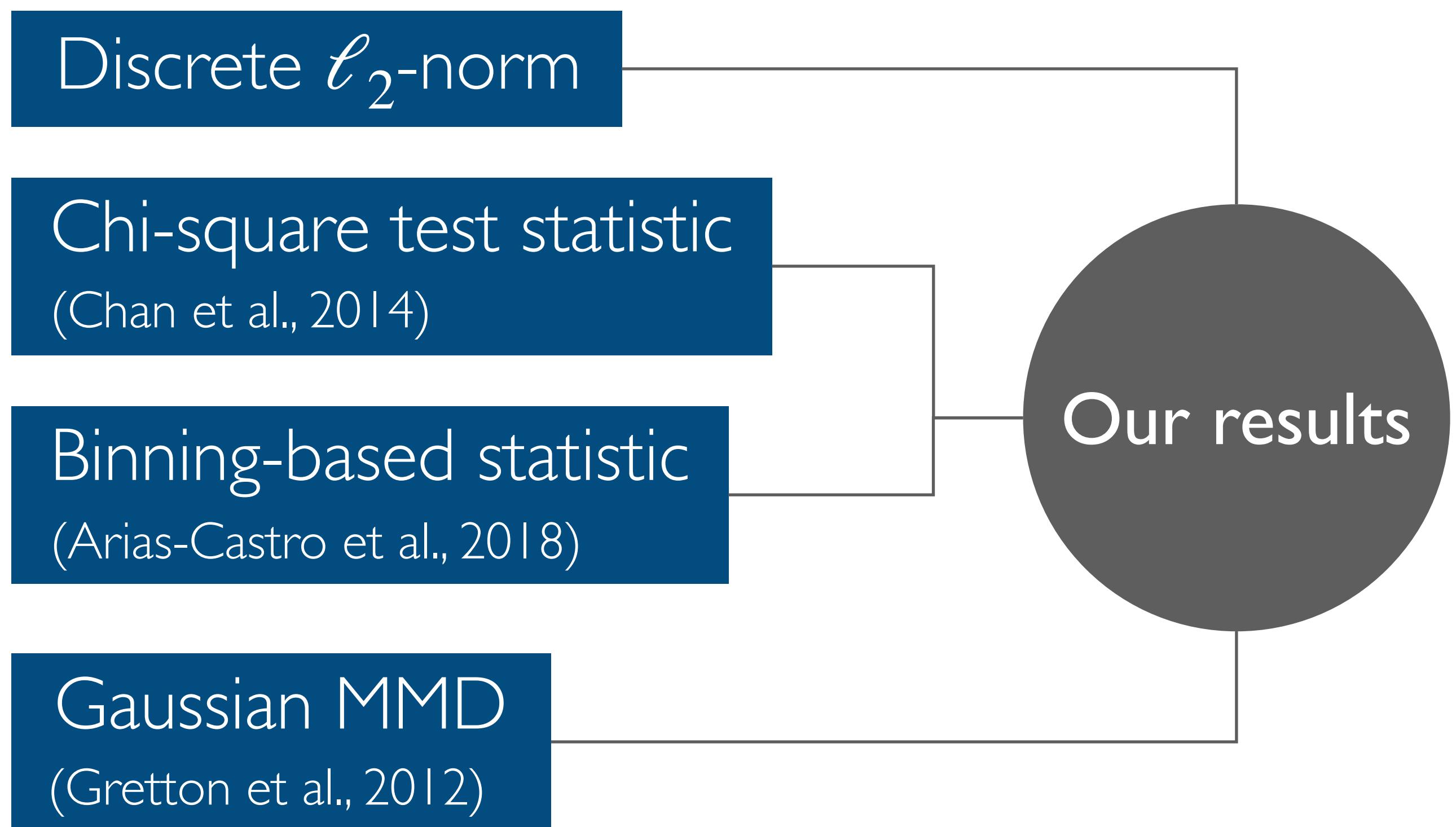
Question. Can we prove the minimax results using a test that

- i) *tightly* controls the type I error rate
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Yes! Permutation tests



Two-sample testing



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)

Independence testing

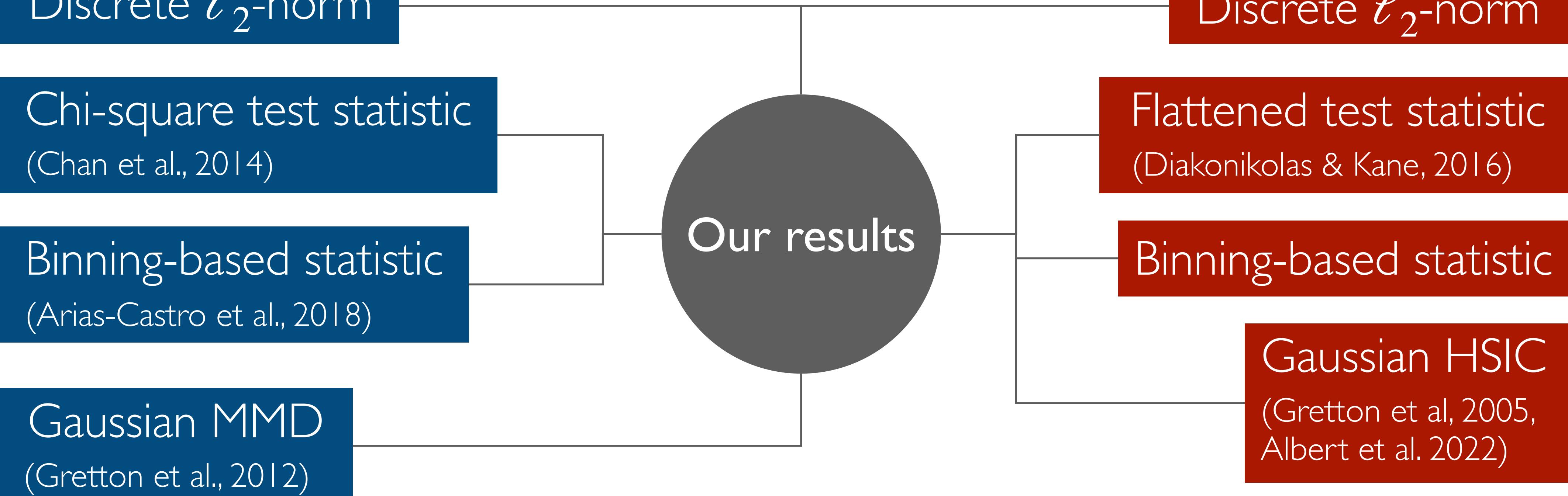
Discrete ℓ_2 -norm

Flattened test statistic
(Diakonikolas & Kane, 2016)

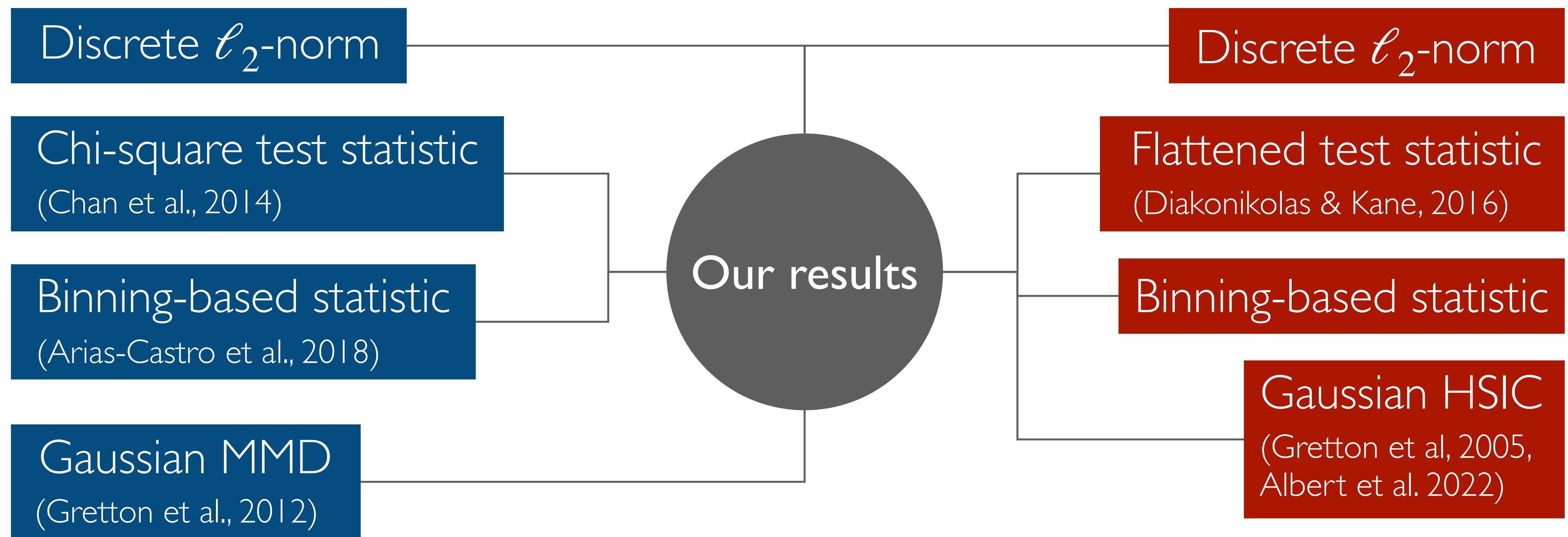
Binning-based statistic

Gaussian HSIC
(Gretton et al, 2005,
Albert et al. 2022)

Our results



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)

- Robustness

- Schrab, Kim (2024, submitted)

- Conditional Independence

- Kim, Neykov, Balakrishnan, Wasserman (2022, *AoS*)
- 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

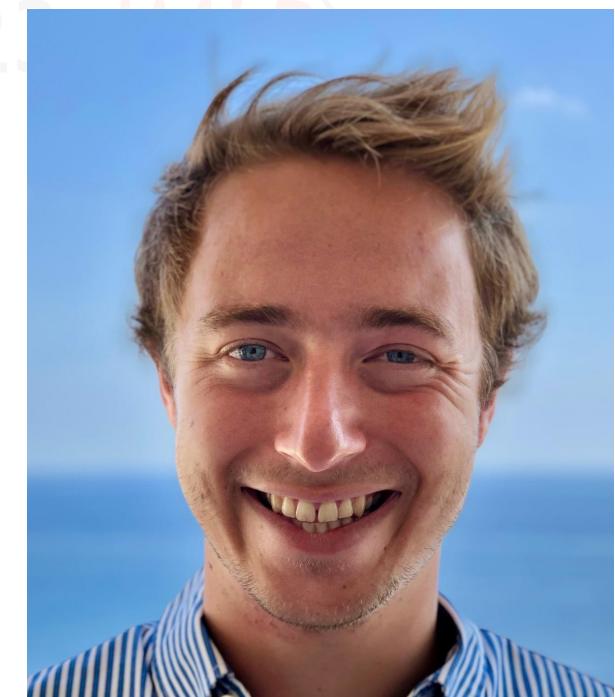
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- Schrab, Kim, Albert, Laurent, Guedj, Gretton (2022, *AoS*)

- **Computational-Power Trade-off**

- Schrab, **Kim**, Guedj, Gretton (2022, *NeurIPS*)
- Choi, **Kim** (2024, submitted)



Antonin Schrab



Benjamin Guedj



Arthur Gretton



Ikjun Choi

- **Differential Privacy**

- Kim, Schrab (2024, submitted)

- **Robustness**

- Schrab, Kim (2024, submitted)

- **Conditional Independence**

- Kim, Neykov, Balakrishnan, Wasserman (2022, *AoS*)
- Kim, Neykov, Balakrishnan, Wasserman (2024+, *EJS*)

- 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*)

- **Computational-Power Trade-off**

- Schrab, Kim, Guedj, Gretton (2022, *NeurIPS*)
- Choi, Kim (2024, *submitted*)

- **Differential Privacy**

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Differentially private permutation tests
applied to kernel methods

Follow-up

- **Adaptivity**

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

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- Schrab, Kim, Guedj, Gretton (2022, *NeurIPS*)
 - Choi, Kim (2024, *submitted*)

- **Differential Privacy**

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



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Permutation tests that are robust to data perturbation with optimal properties

Follow-up

- **Adaptivity**

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

- **Computational-Power Trade-off**

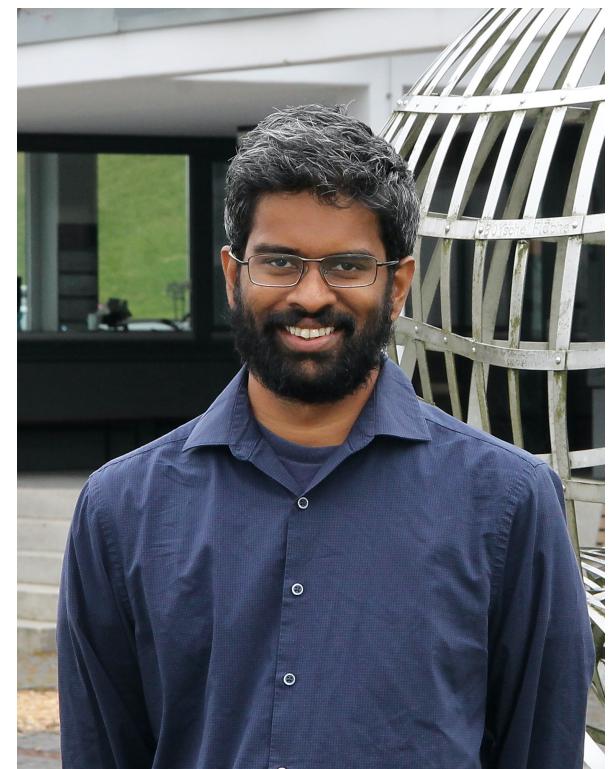
- Schrab, Kim, Guedj, Gretton (2022, *NeurIPS*)
- Choi, Kim (2024, submitted)

- **Differential Privacy**

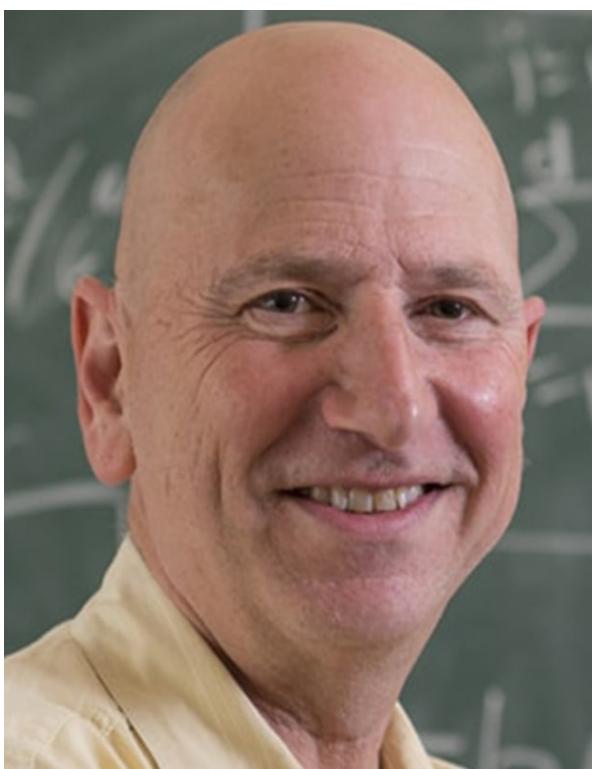
- Kim, Schrab (2024, submitted)



Matey Neykov



Siva Balakrishnan



Larry Wasserman

- **Robustness**

- Schrab, Kim (2024, submitted)

- **Conditional Independence**

- Kim, Neykov, Balakrishnan, Wasserman (2022, *AoS*)
- Kim, Neykov, Balakrishnan, Wasserman (2024+, *EJS*)

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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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

Thank you!