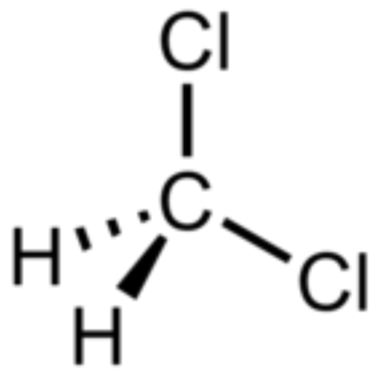
Harnessing Extra Randomness

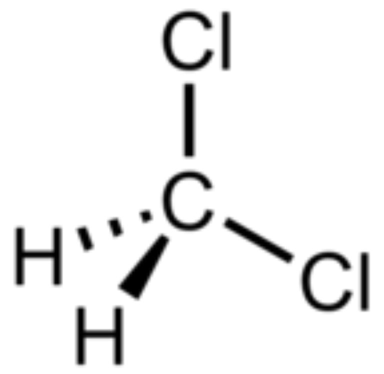
Replicability, Flexibility & Causality

F. Richard Guo
Statistical Laboratory, University of Cambridge

Feb, 2023
Based on joint work w/ Rajen Shah

Organic solvents such as  are widely used in the food industry.

Methylene Chloride

Organic solvents such as  are widely used in the food industry.

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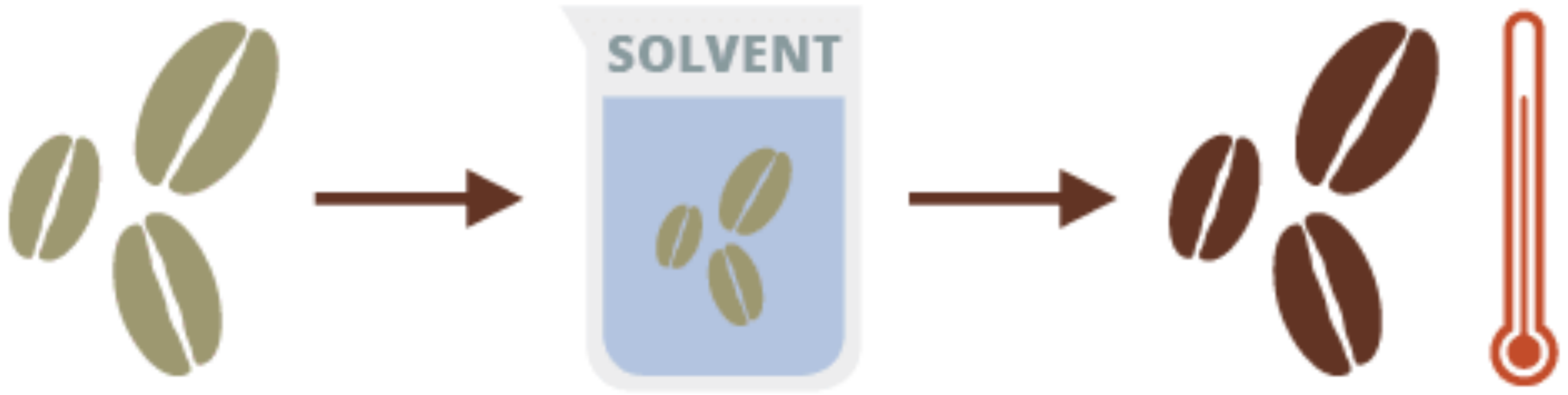

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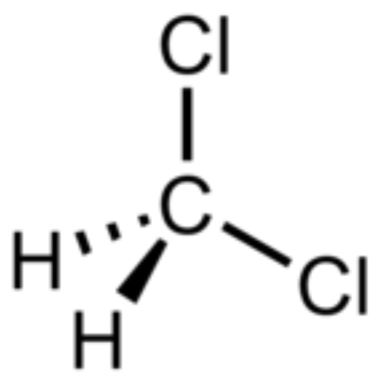
Organic solvents such as  are widely used in the food industry.

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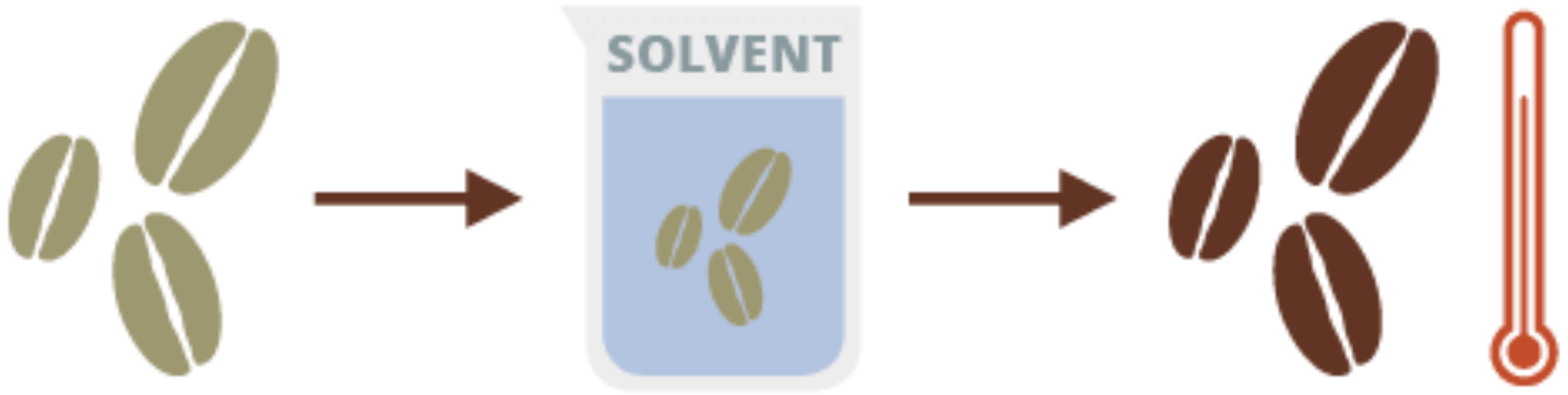

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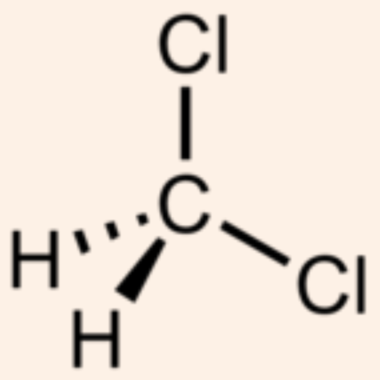

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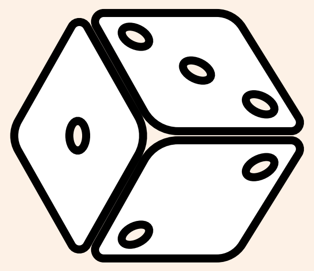

Extra Randomness

Randomized procedures

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👉 Output of the procedure is a random function of data.

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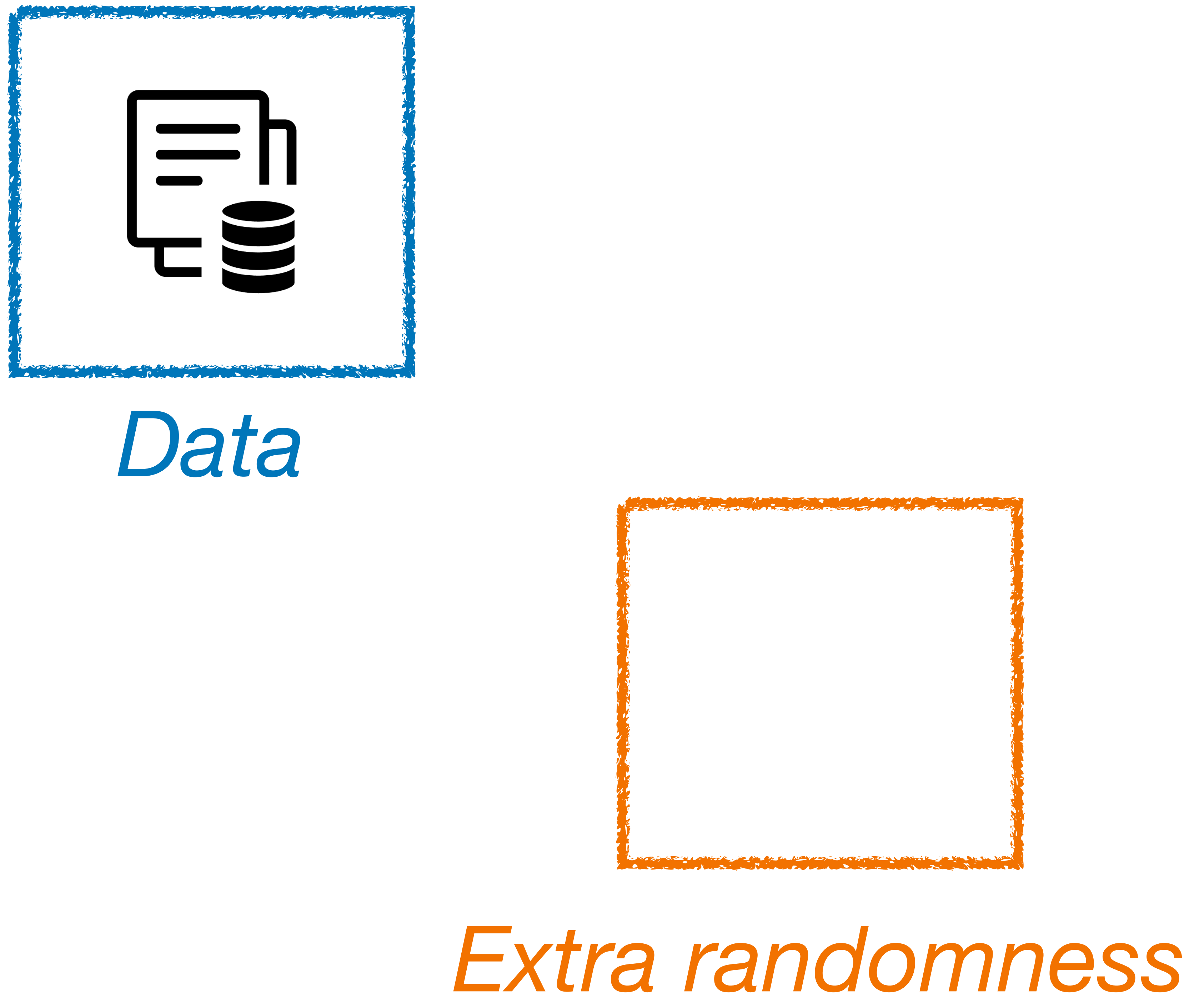

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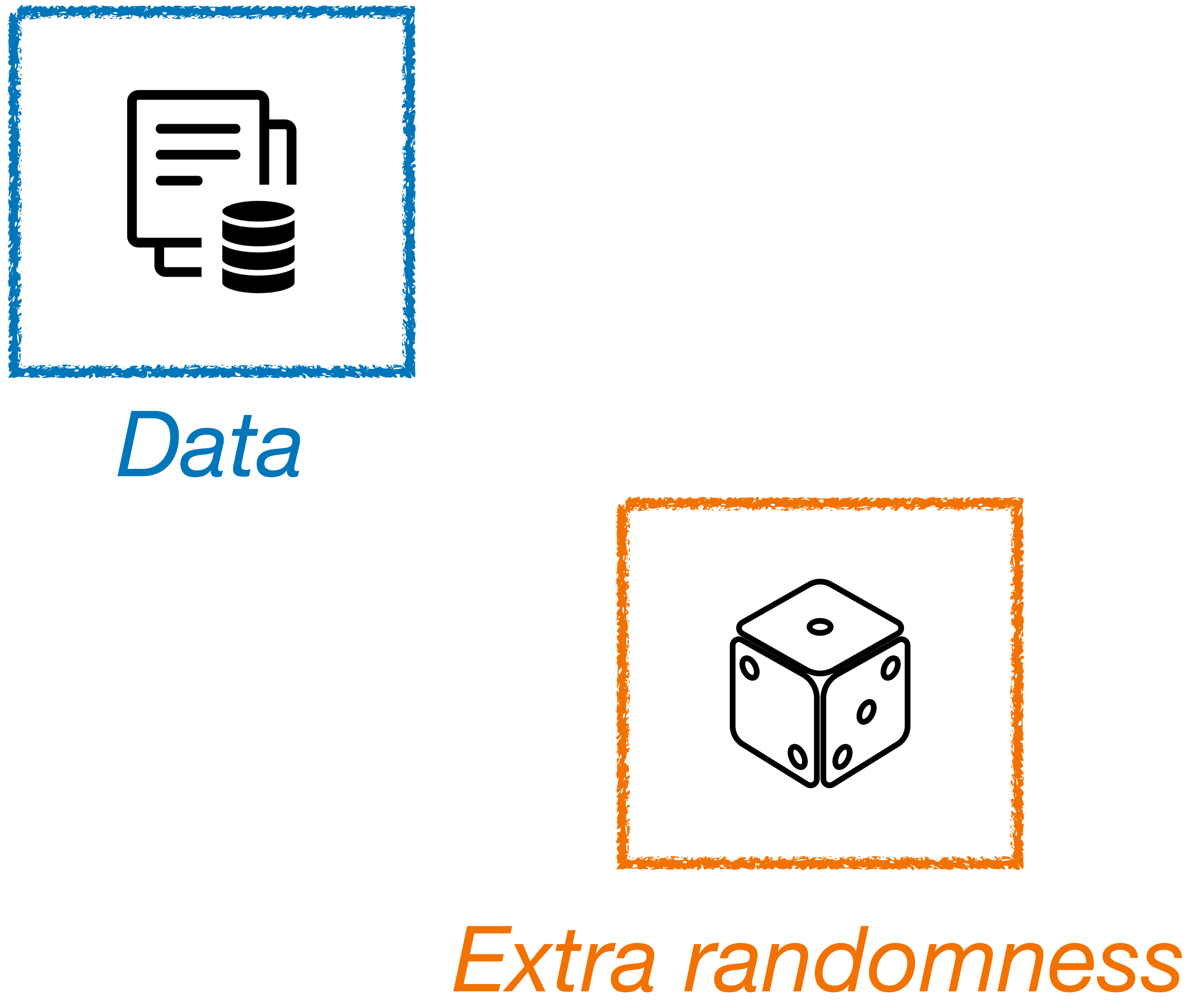

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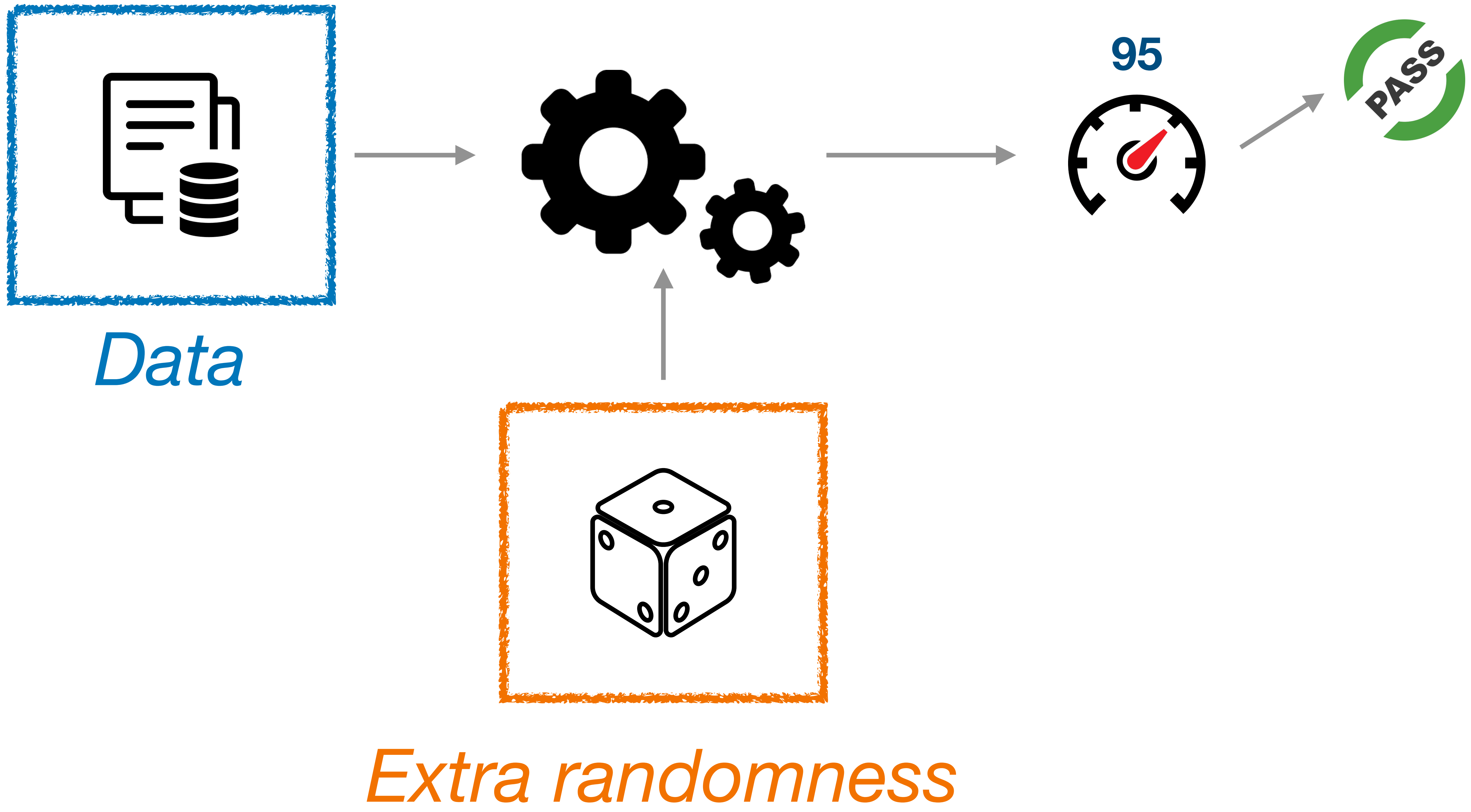

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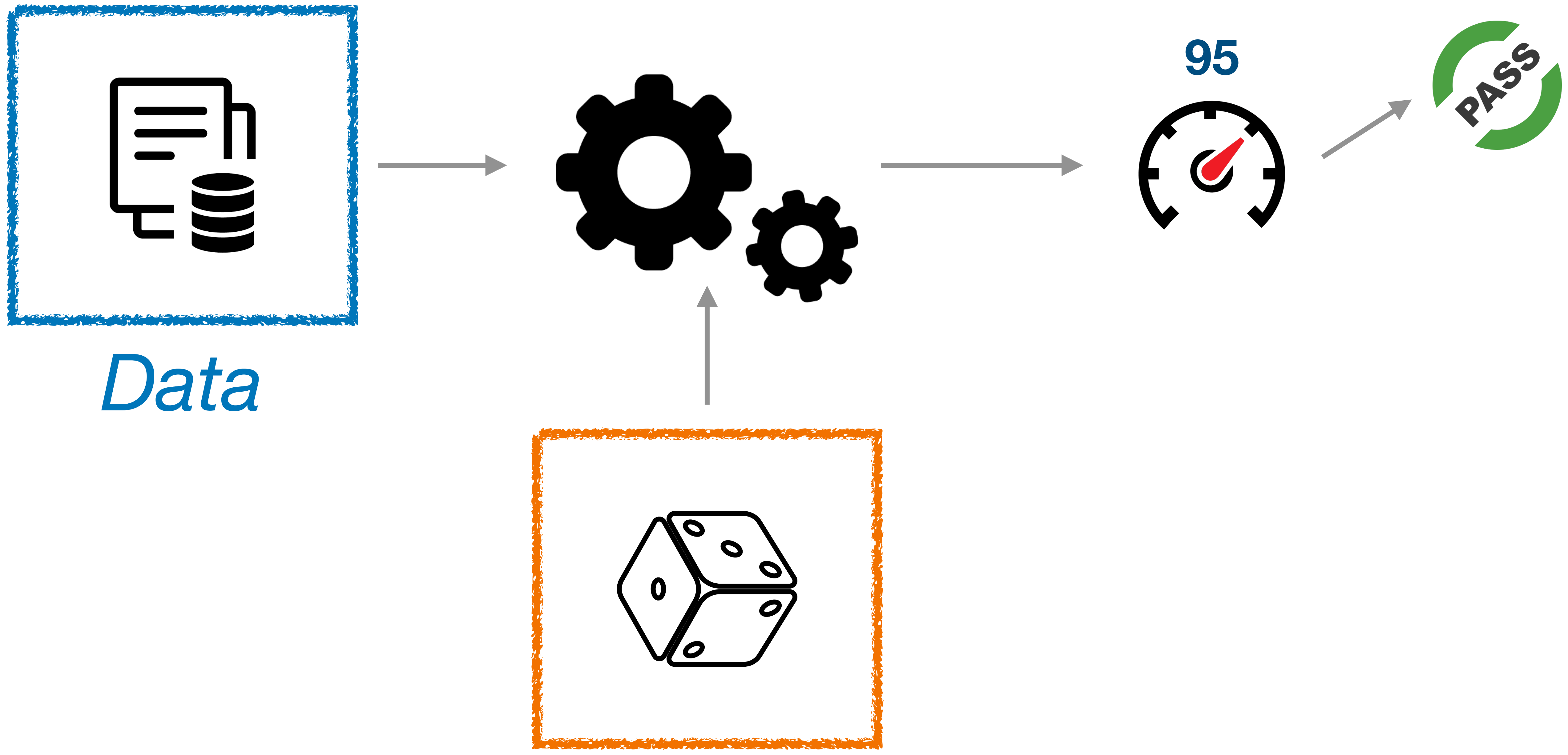

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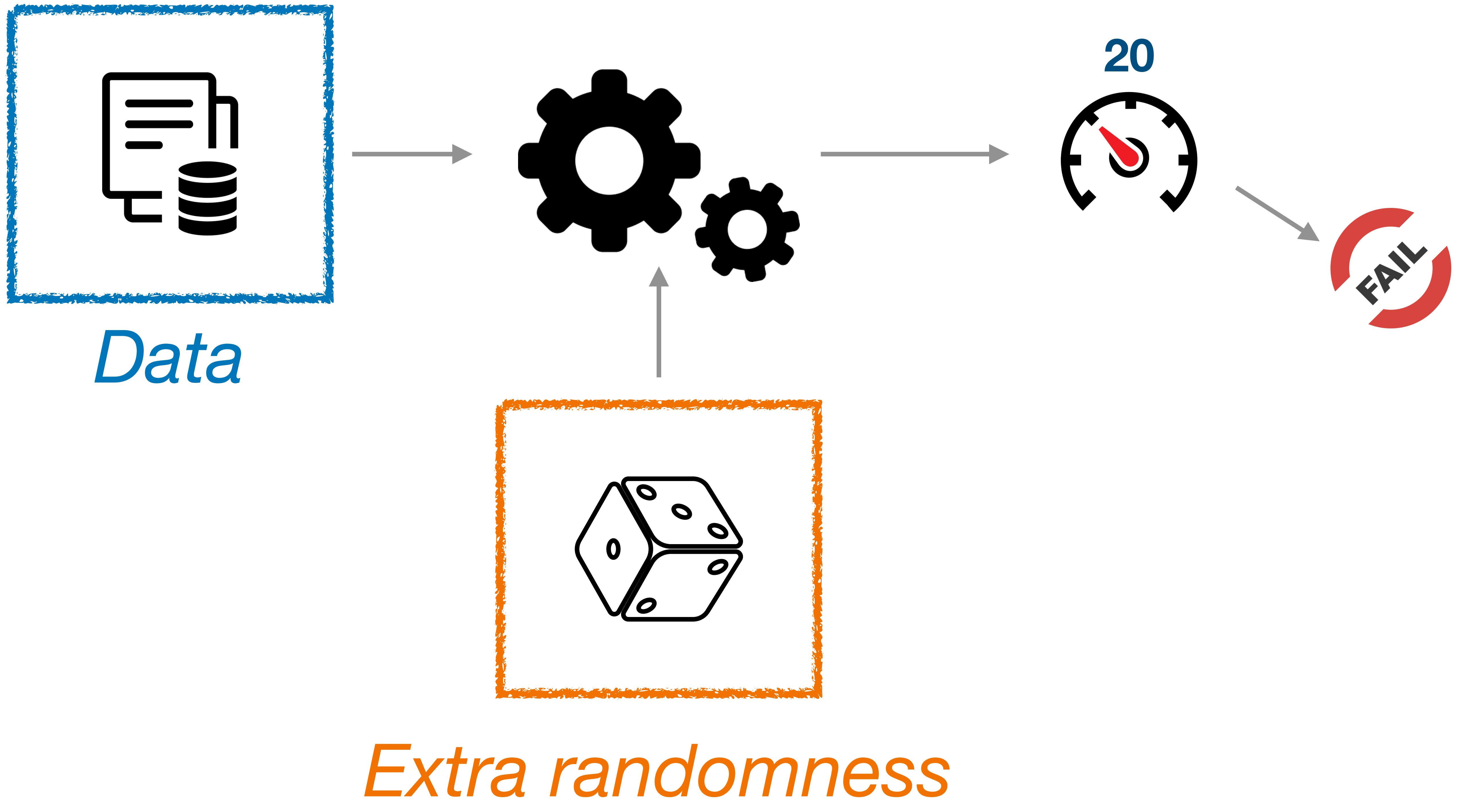

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  Randomly divide iid data into several parts for different purposes.

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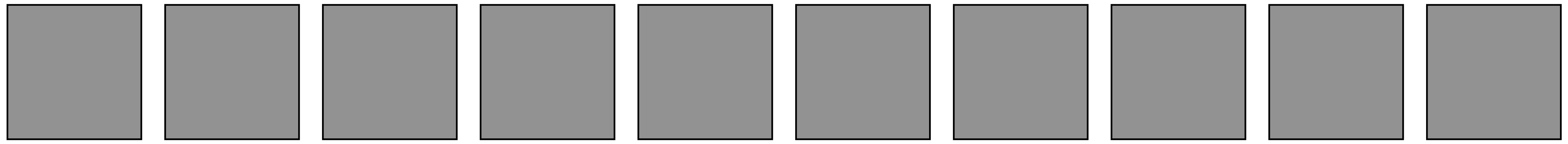

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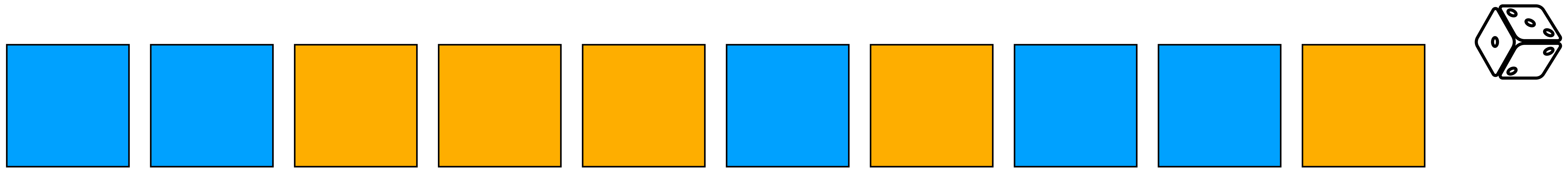

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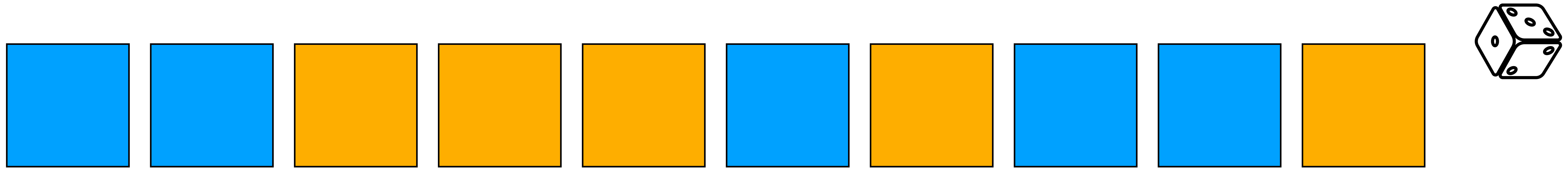

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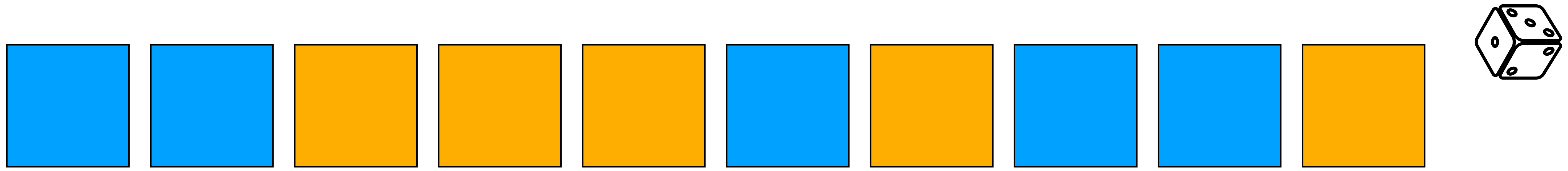

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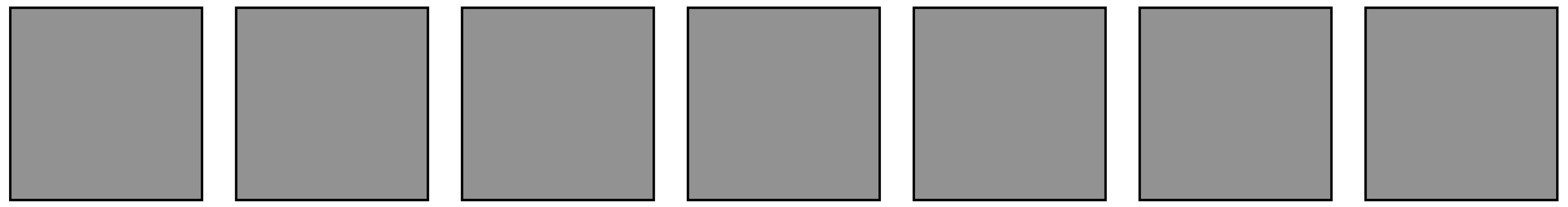

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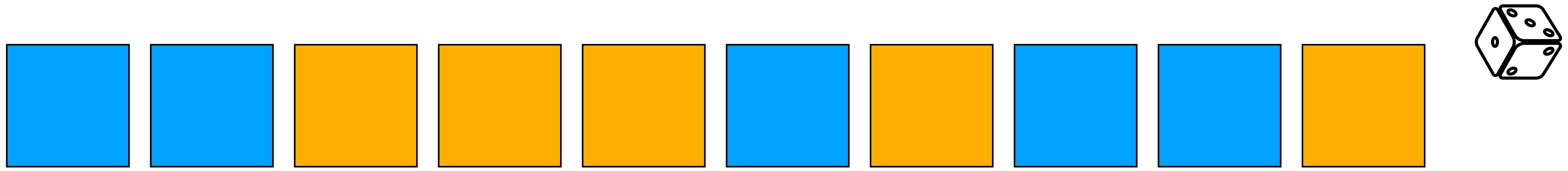

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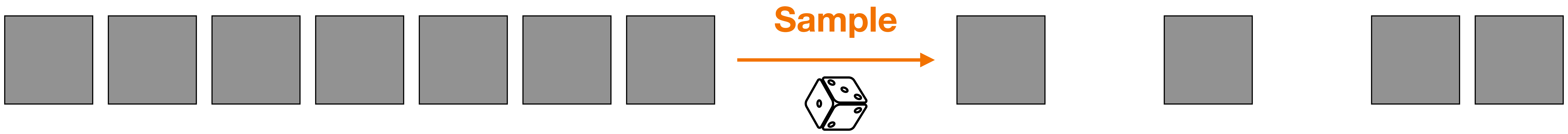

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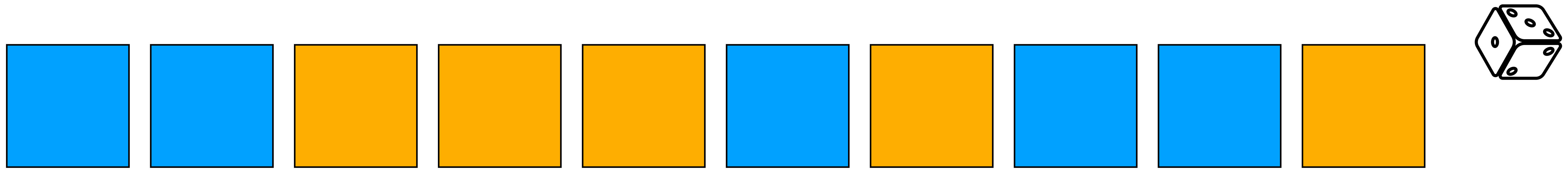

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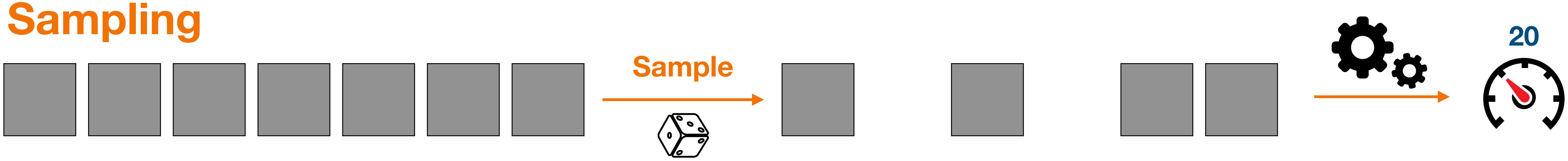

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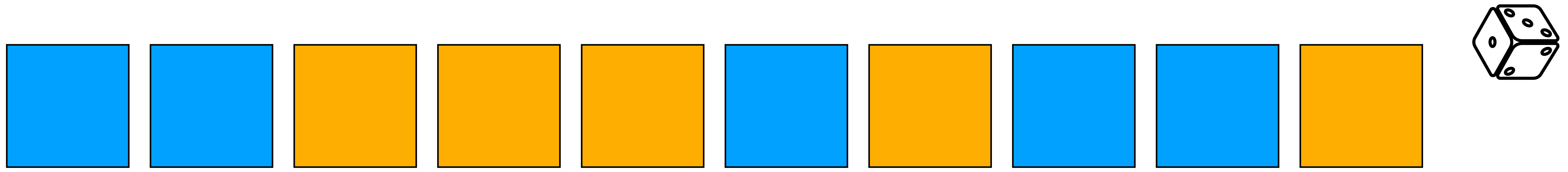

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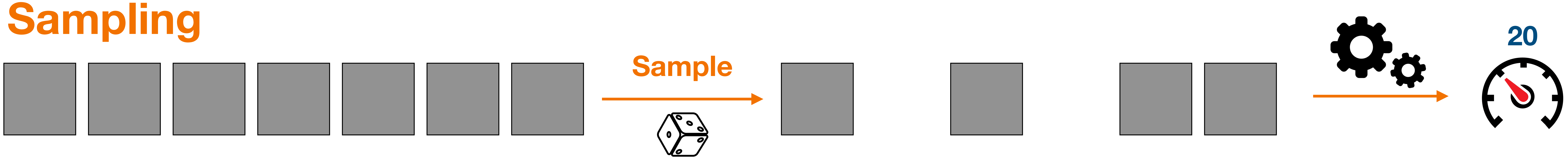

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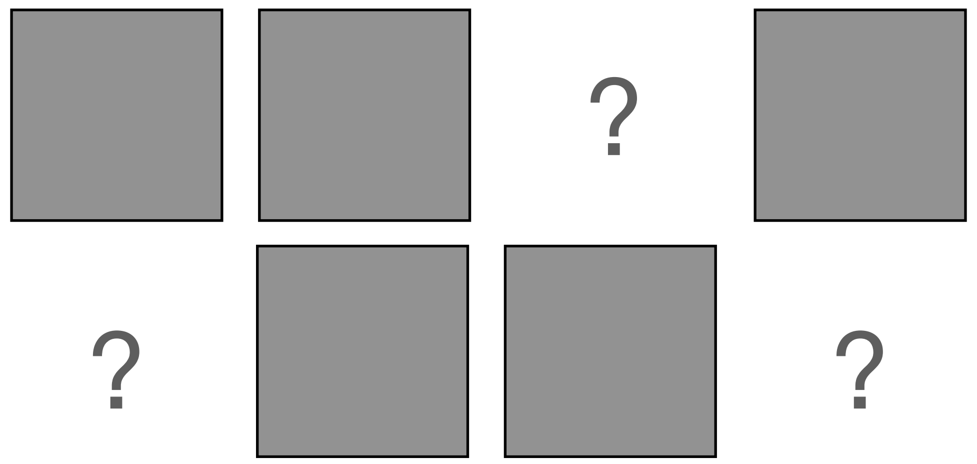

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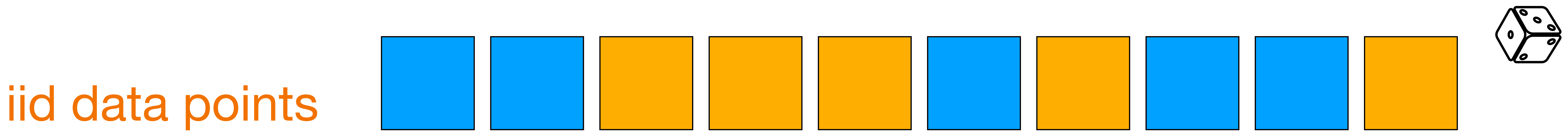

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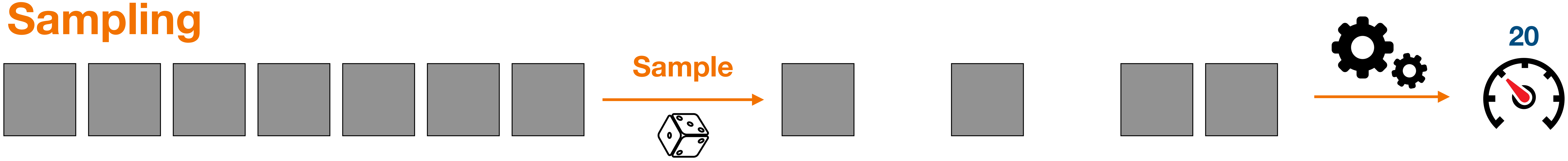

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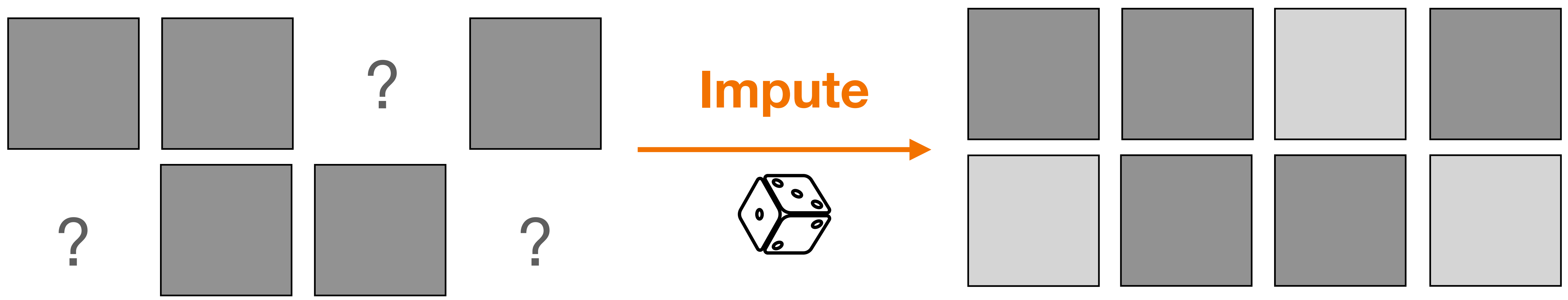

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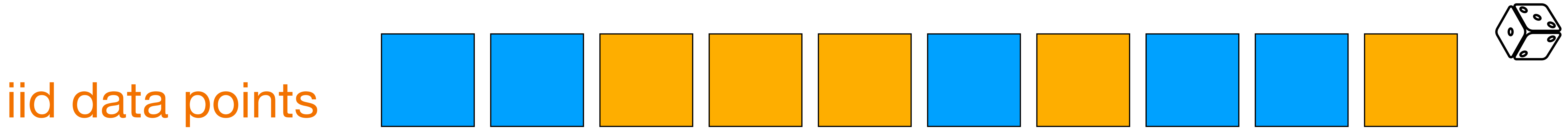

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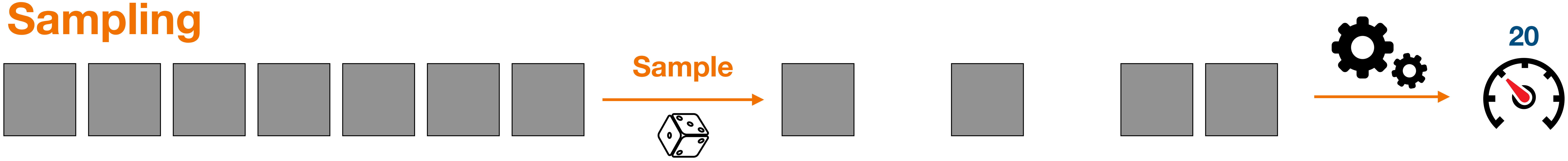

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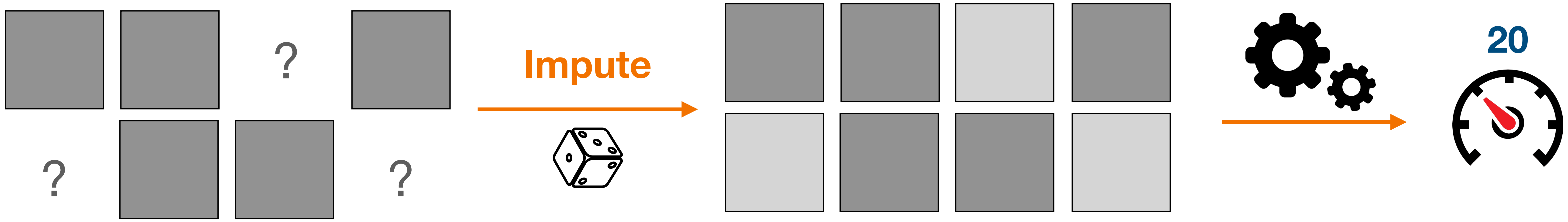

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3. Harness extra randomness for many great applications!

Dilemma of data splitting

Bill, PhD, an economist

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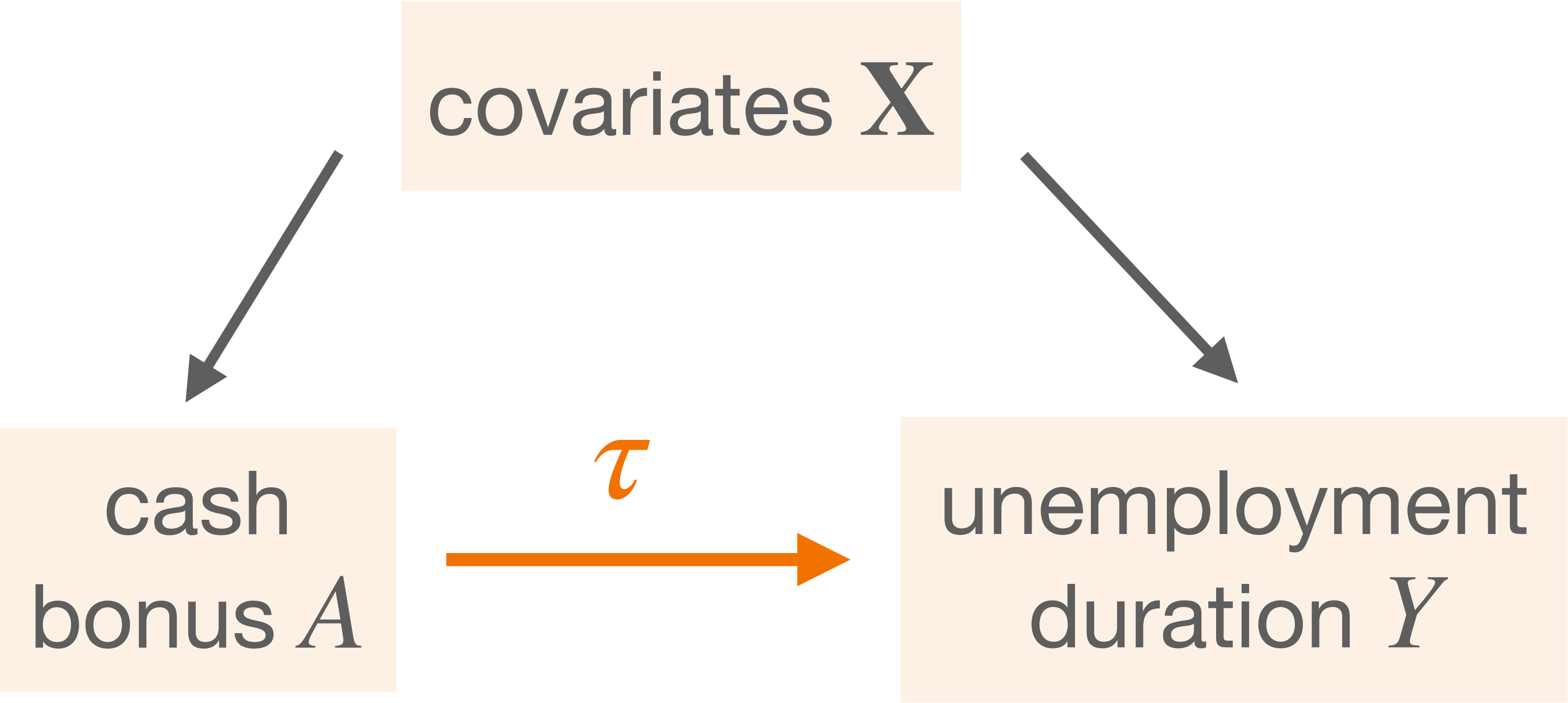

covariates $\boldsymbol{X}$

cash bonus A

τ

unemployment duration Y

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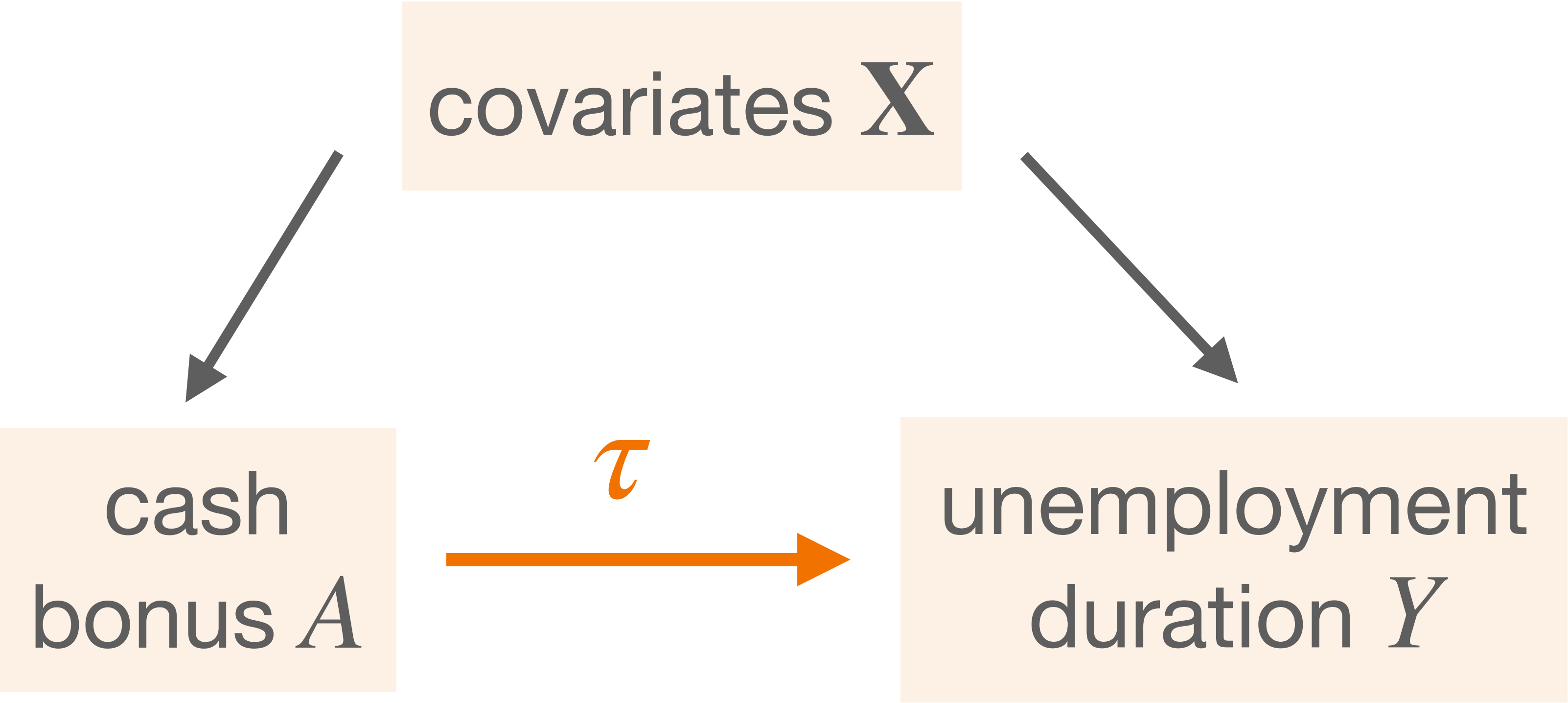

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$$\eta_1 = \mathbb{P}(A \,|\, \mathbf{X})$$

$$\eta_2 = \mathbb{E}[Y | A, \mathbf{X}]$$

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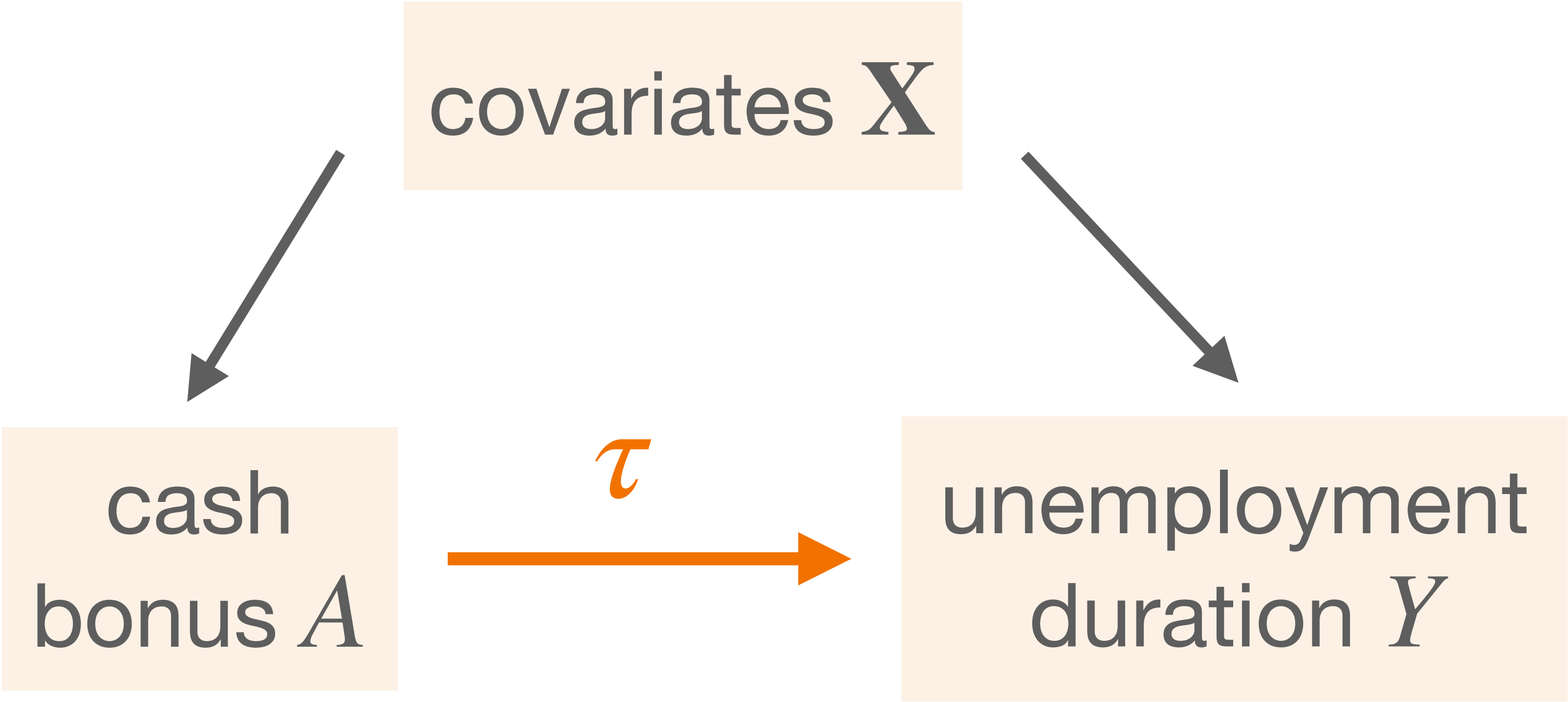

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Targeted / Double ML: permit using flexible ML tools to estimate η_1, η_2.

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(van der Laan & Rose, 2011; Newey and Robins, 2018; Chernozhukov et al., 2018; Díaz, 2020; Kennedy, 2022)

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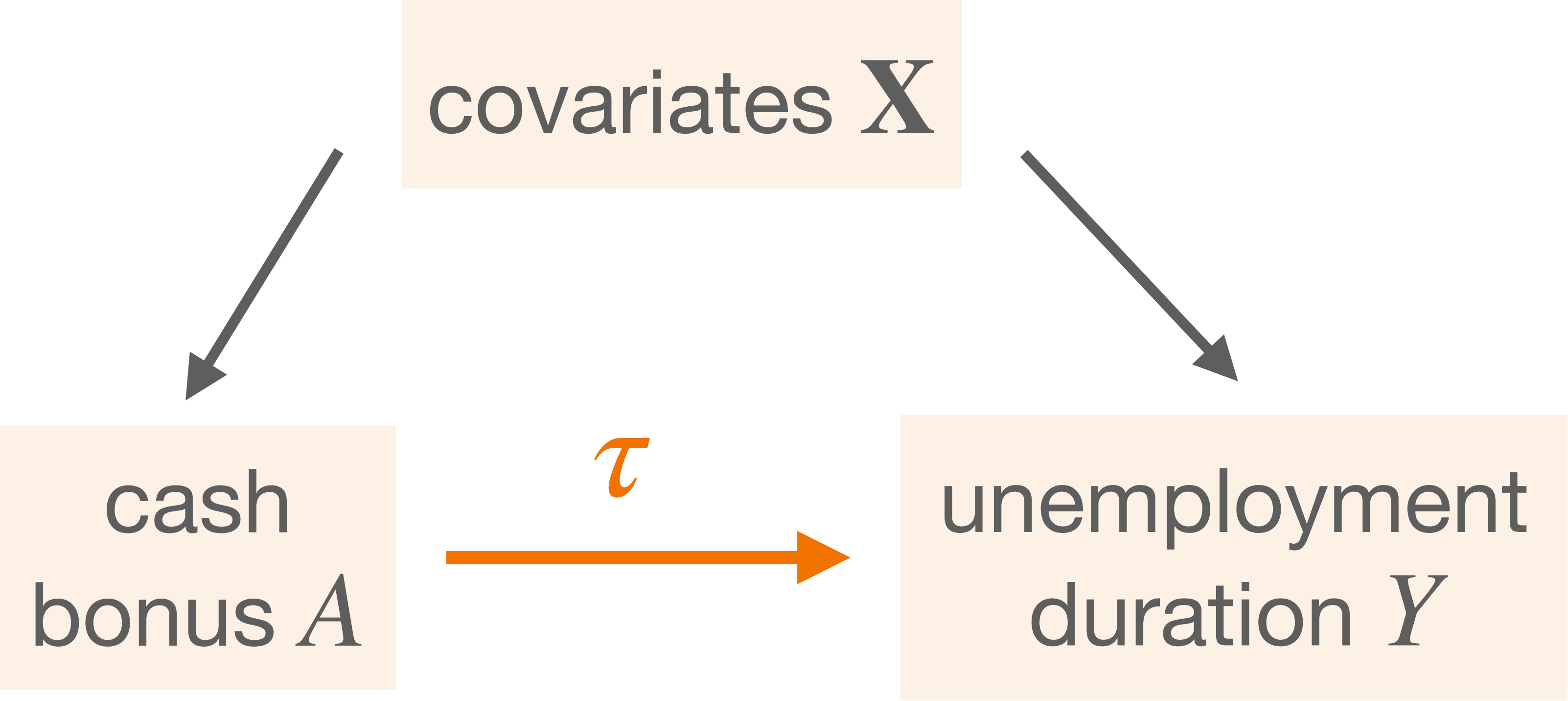

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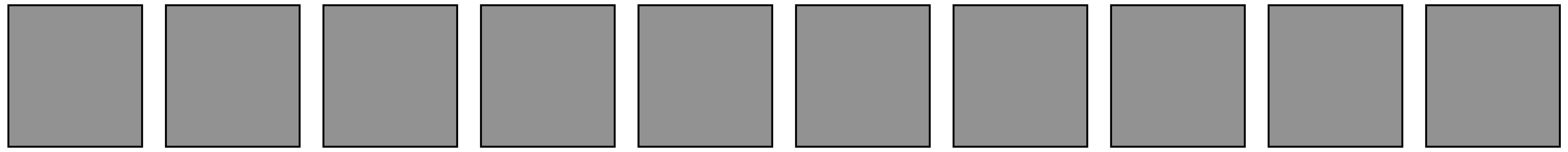

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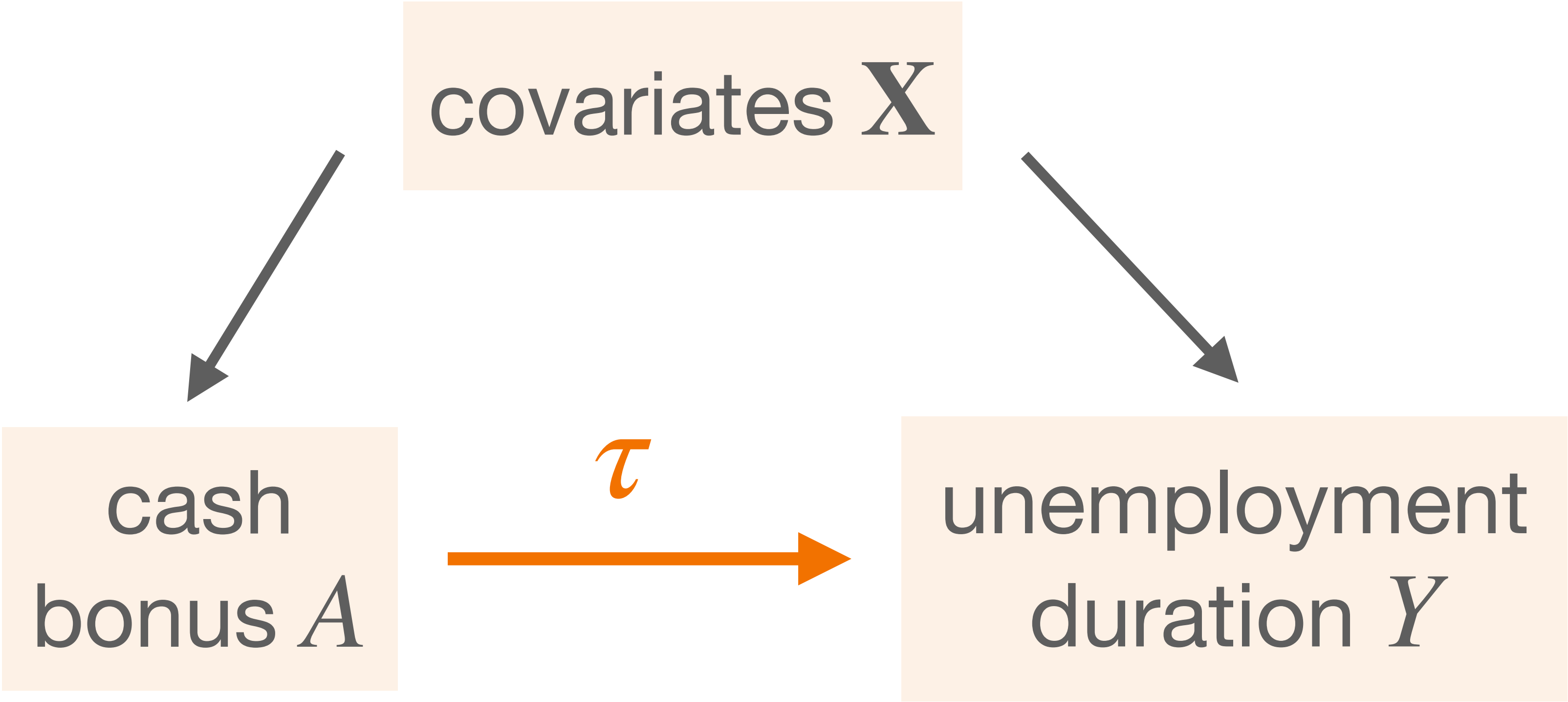

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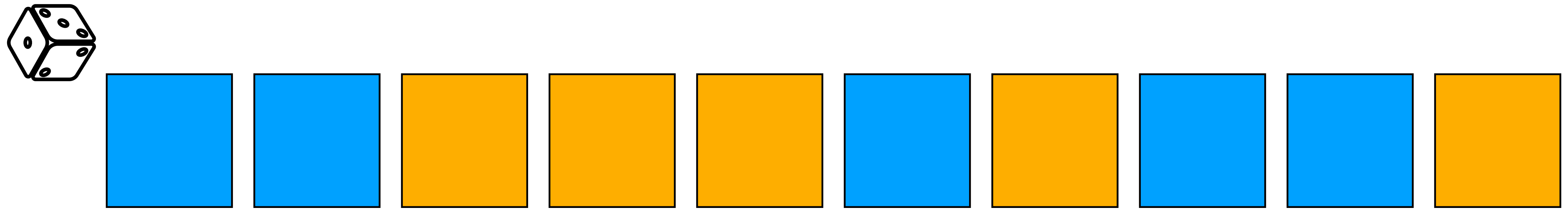

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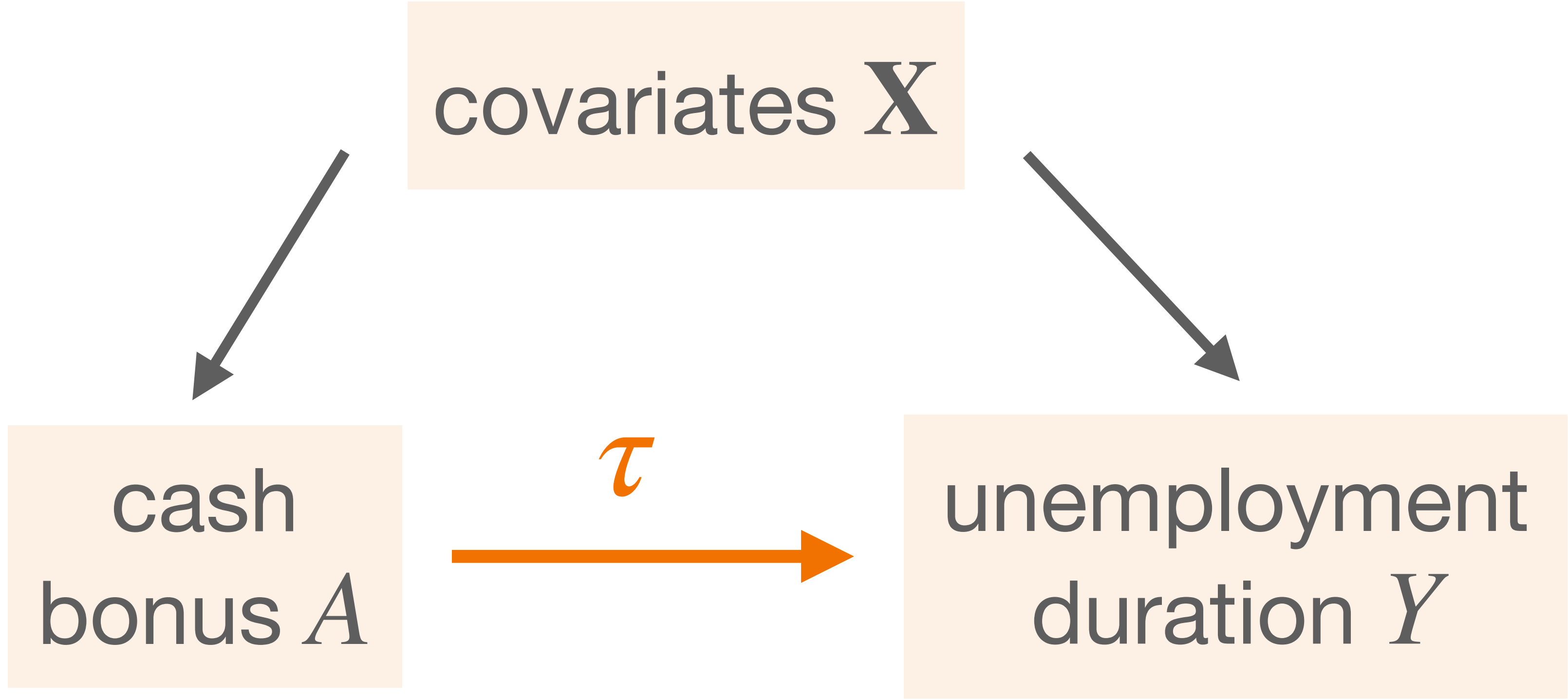

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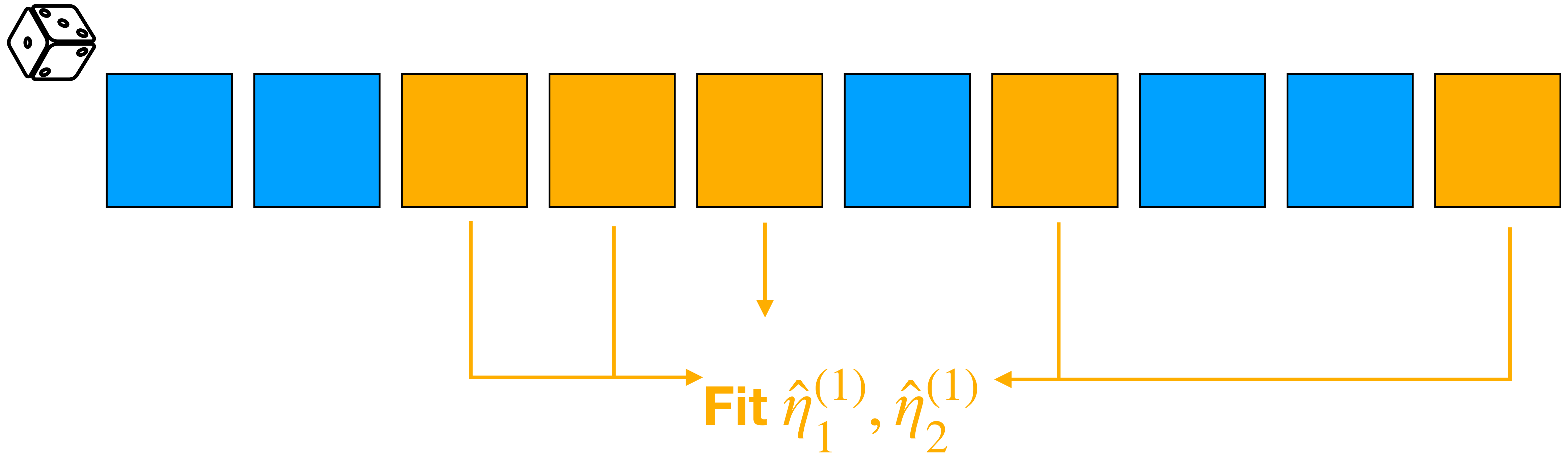

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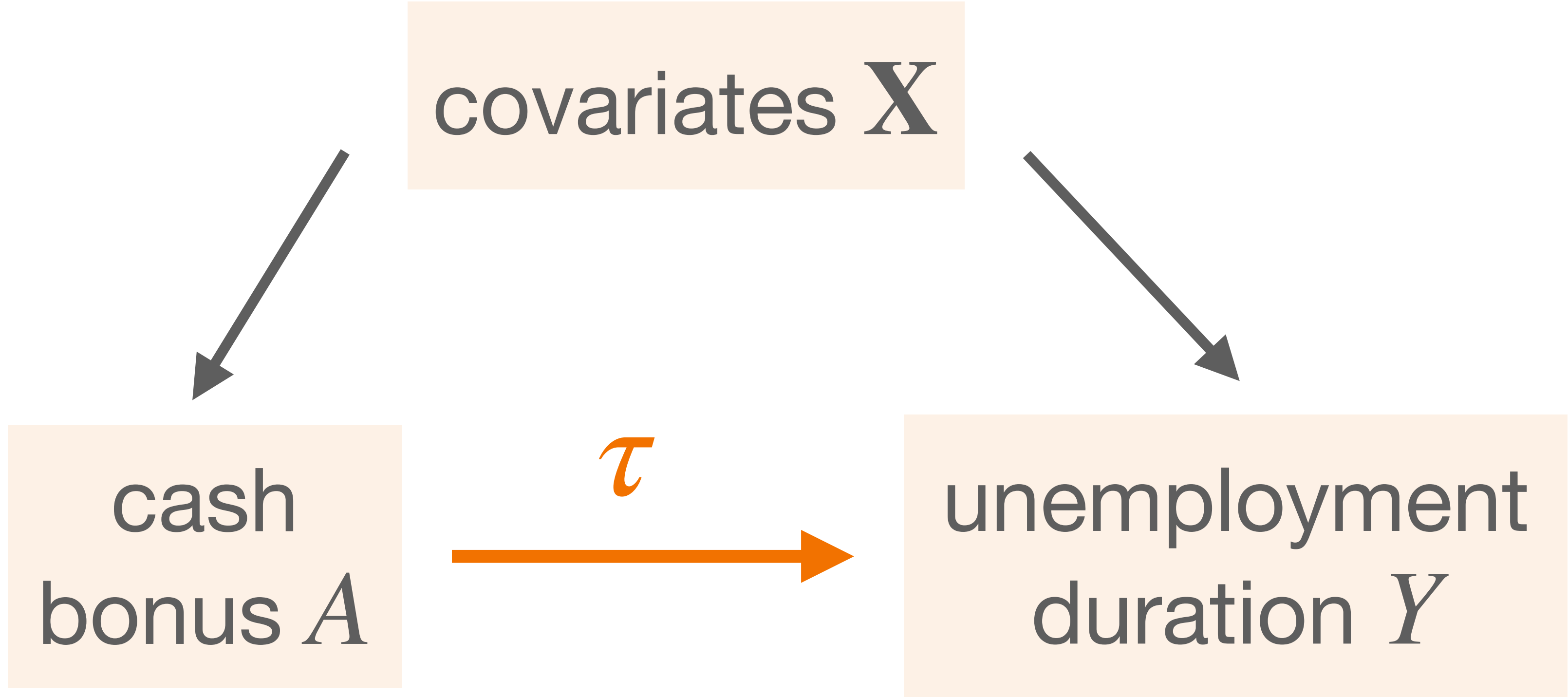

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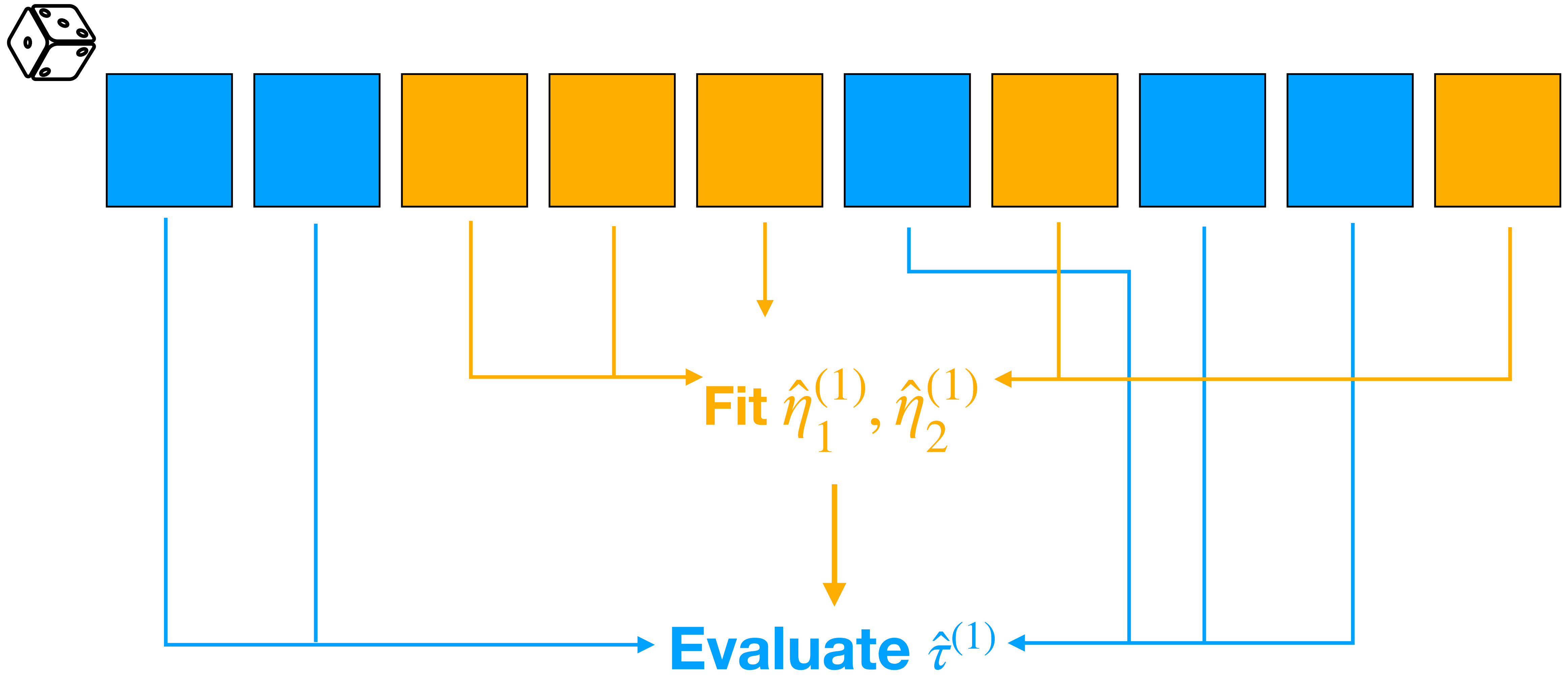
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Evaluate $\hat{\tau}^{(1)}$

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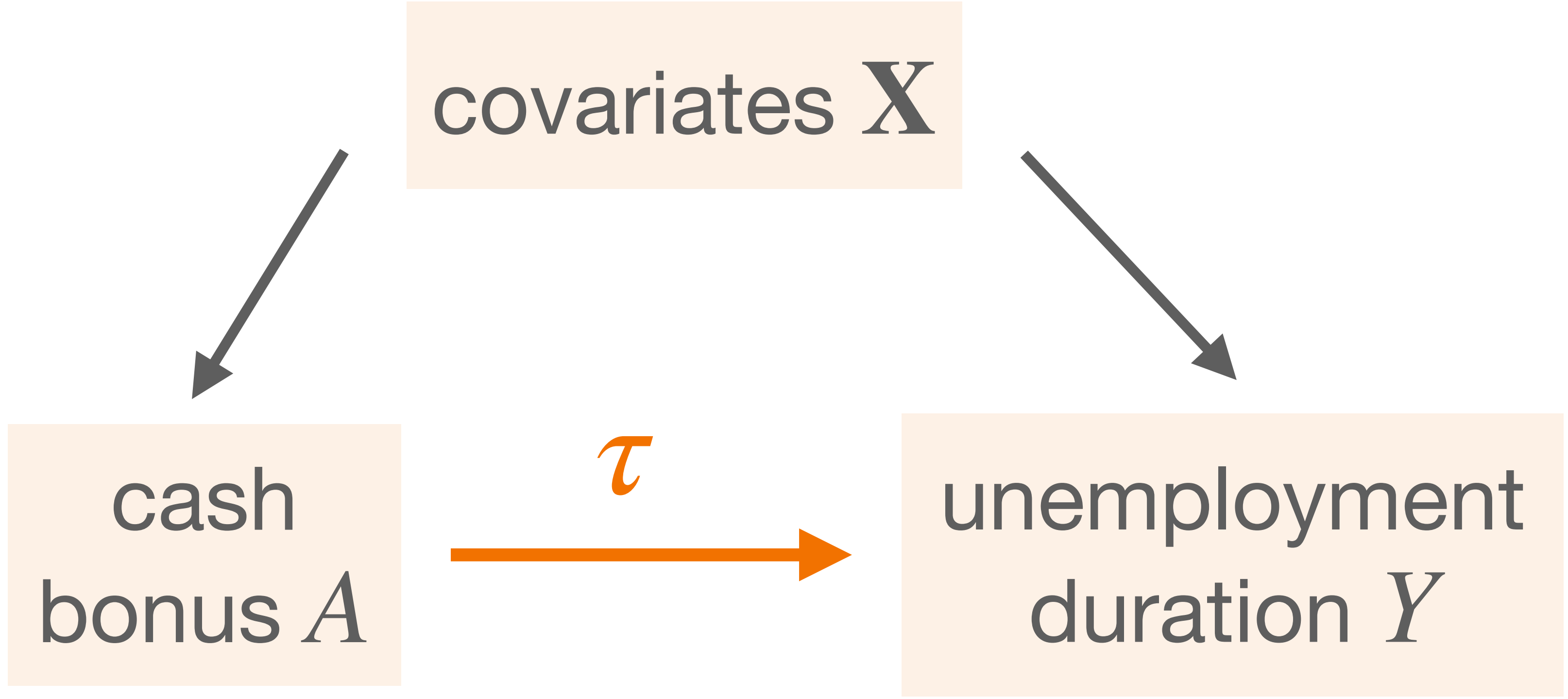

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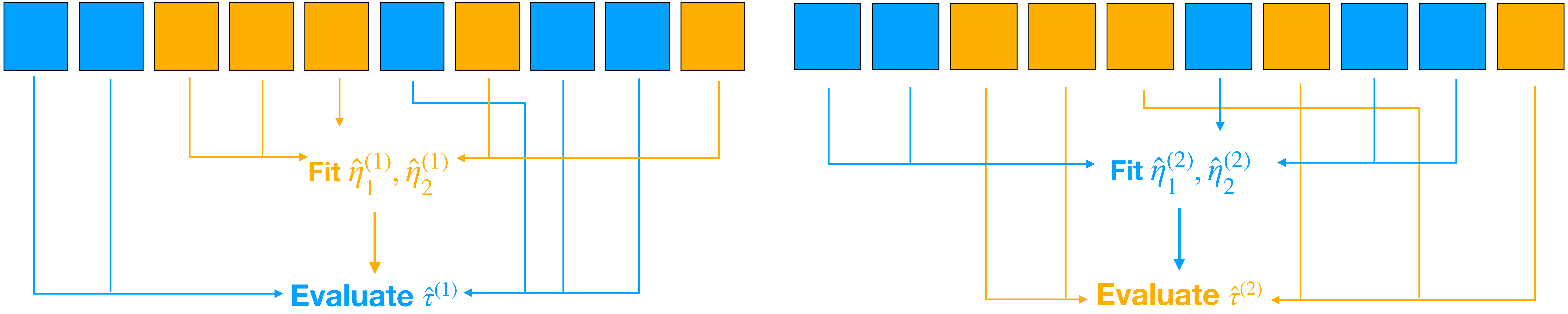
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Fit $\hat{\eta}_1^{(2)}, \hat{\eta}_2^{(2)}$
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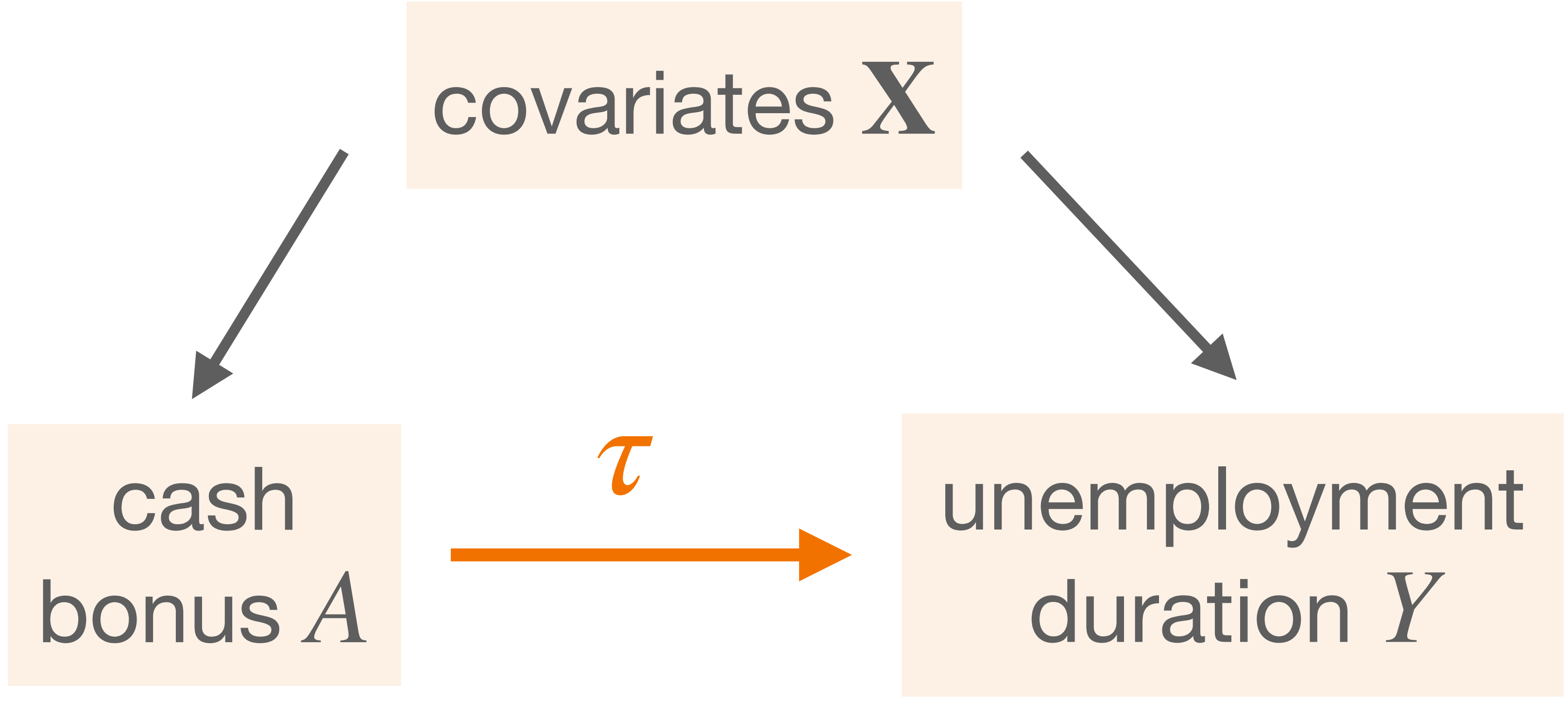

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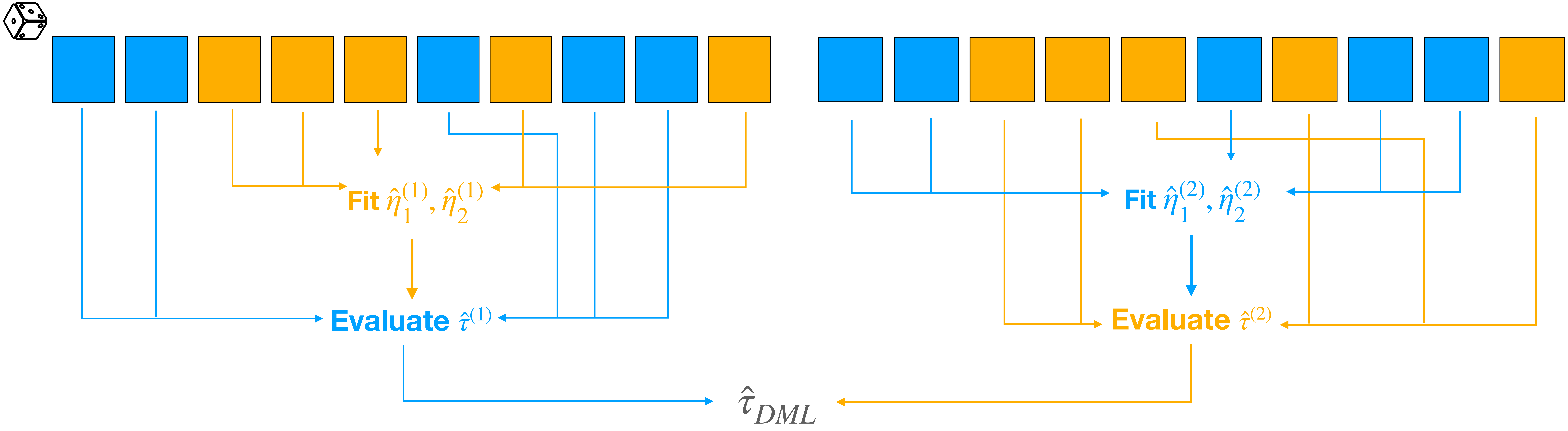

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Evaluate $\hat{\tau}^{(2)}$
$\hat{\tau}_{DML}$

```
> set.seed(42)
```

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```

```
     Estimate. Std. Error t value Pr(>|t|)
tau  -0.1      0.035       -2.86   0.004 **
```

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tau  -0.1      0.035        -2.86   0.004 **
```

```
> set.seed(43)
> dml$fit()
```

```
     Estimate. Std. Error t value Pr(>|t|)
tau  -0.06     0.035        -1.71   0.08 .
```

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```
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tau  -0.1      0.035      -2.86   0.004 **
```

```
> set.seed(43)
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```
     Estimate. Std. Error t value Pr(>|t|)
tau  -0.06     0.035      -1.71   0.08 .
```

```
> set.seed(44)
> dml$fit()
```

```
     Estimate. Std. Error t value Pr(>|t|)
tau  -0.07     0.037      -1.89   0.06 .
```

We find a significant negative effect* ($\hat{\tau} = -0.1$, p-value=0.004)….

* To replicate my analysis, please use “set.seed(42)” (my lucky number).

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Reviewer:

🤔 “To replicate, why must I use your lucky number?”

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Reviewer:

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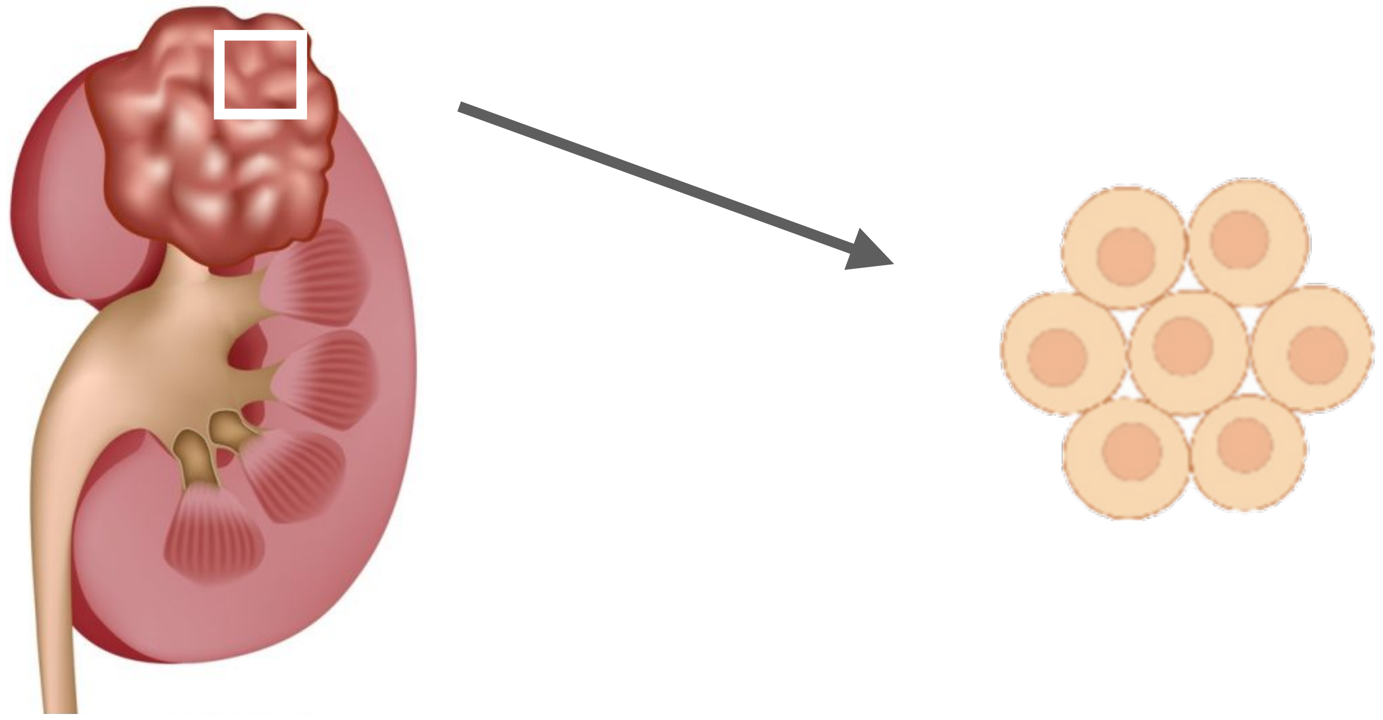
🤔 “How do I know you did not fish for 42?”

Laura, PhD, a cancer biologist
(MS in Statistics)

Laura, PhD, a cancer biologist
(MS in Statistics)



Kidney tumor

🤔 Is there a new subtype of kidney cancer cells?

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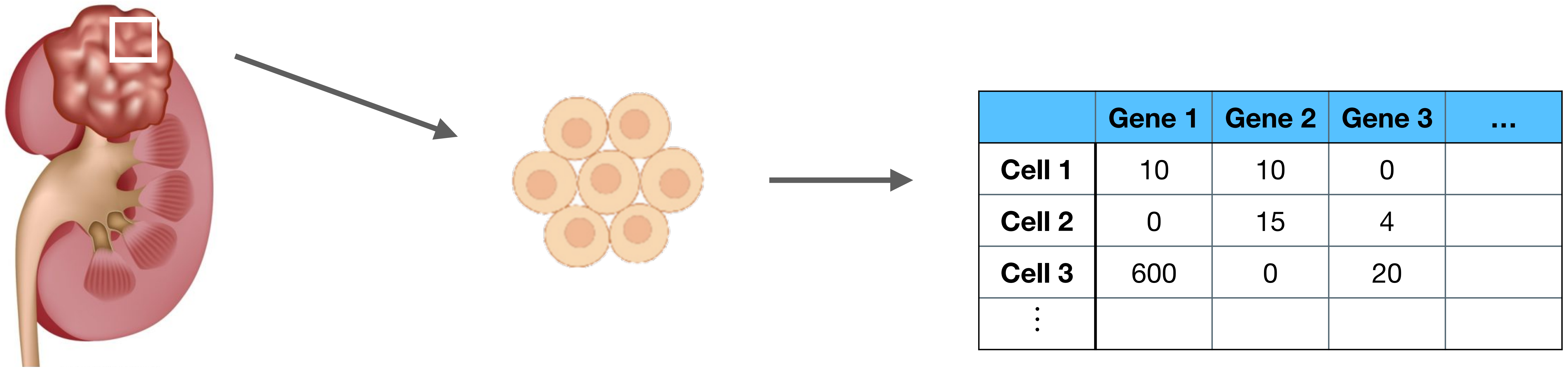

	Gene 1	Gene 2	Gene 3	...
Cell 1	10	10	0	
Cell 2	0	15	4	
Cell 3	600	0	20	
⋮				

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Single-cell RNA read count

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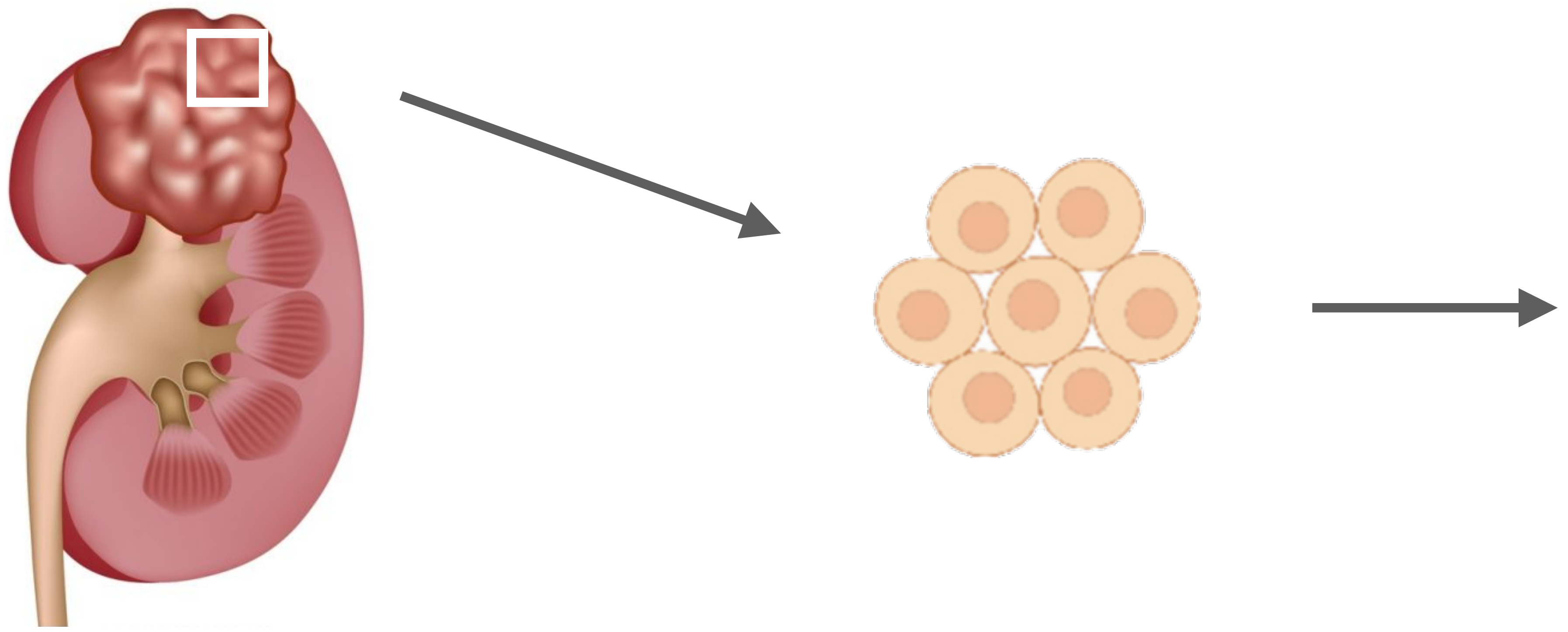

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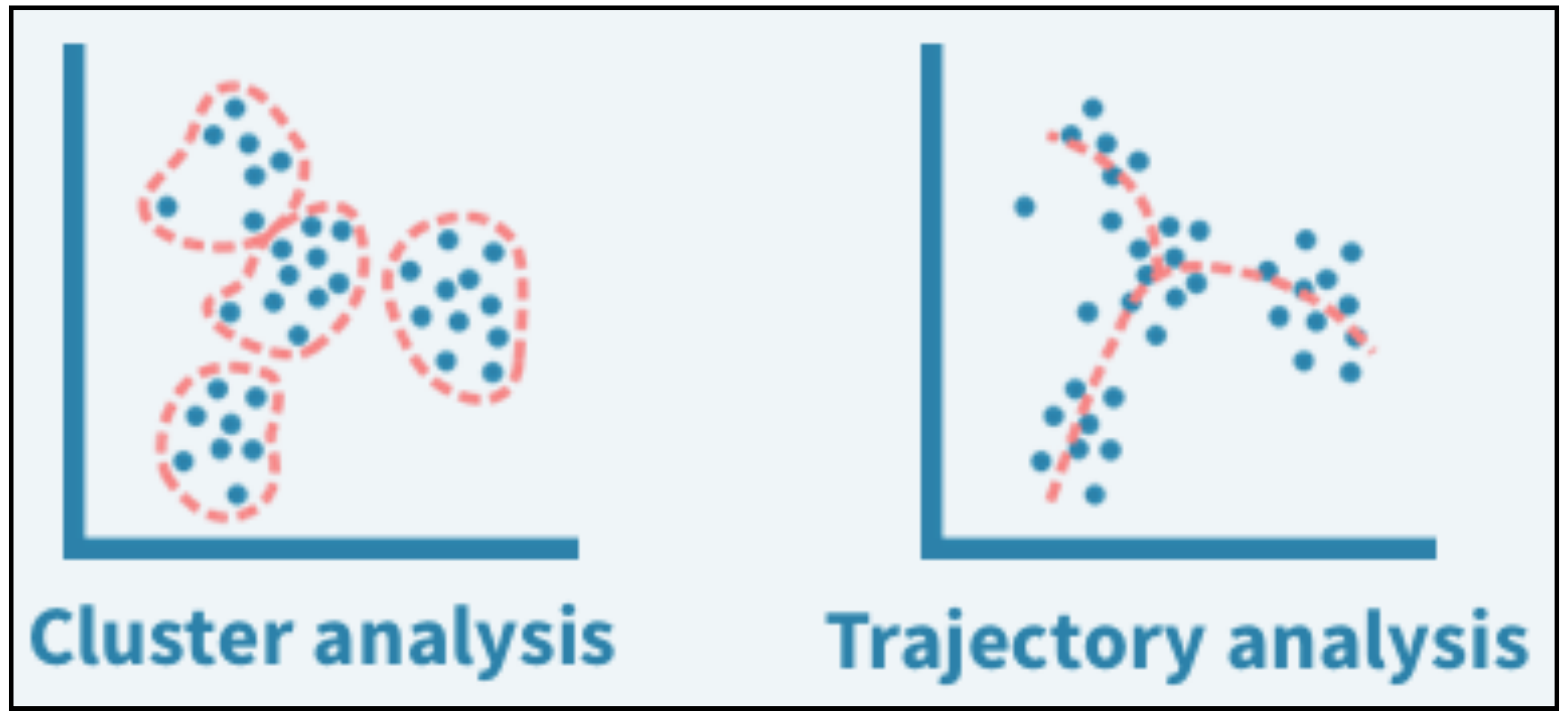
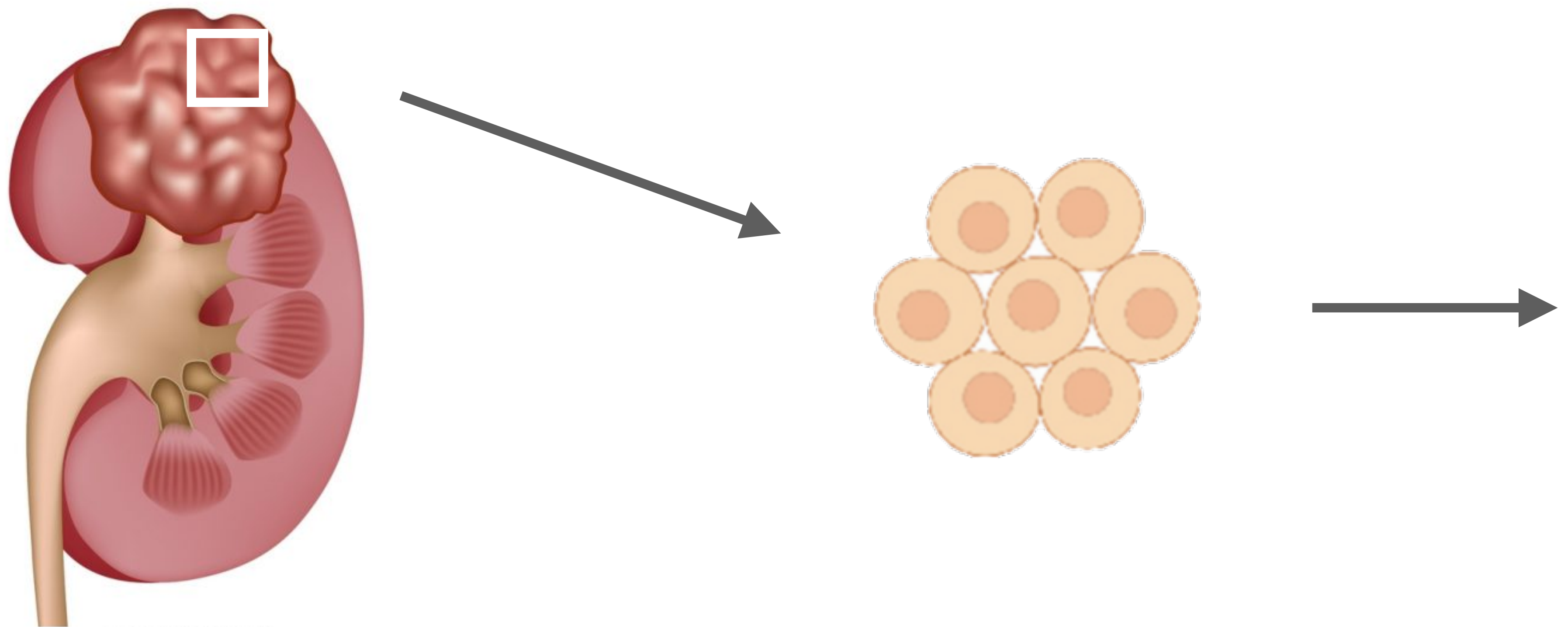


Unsupervised learning

Laura, PhD, a cancer biologist
(MS in Statistics)



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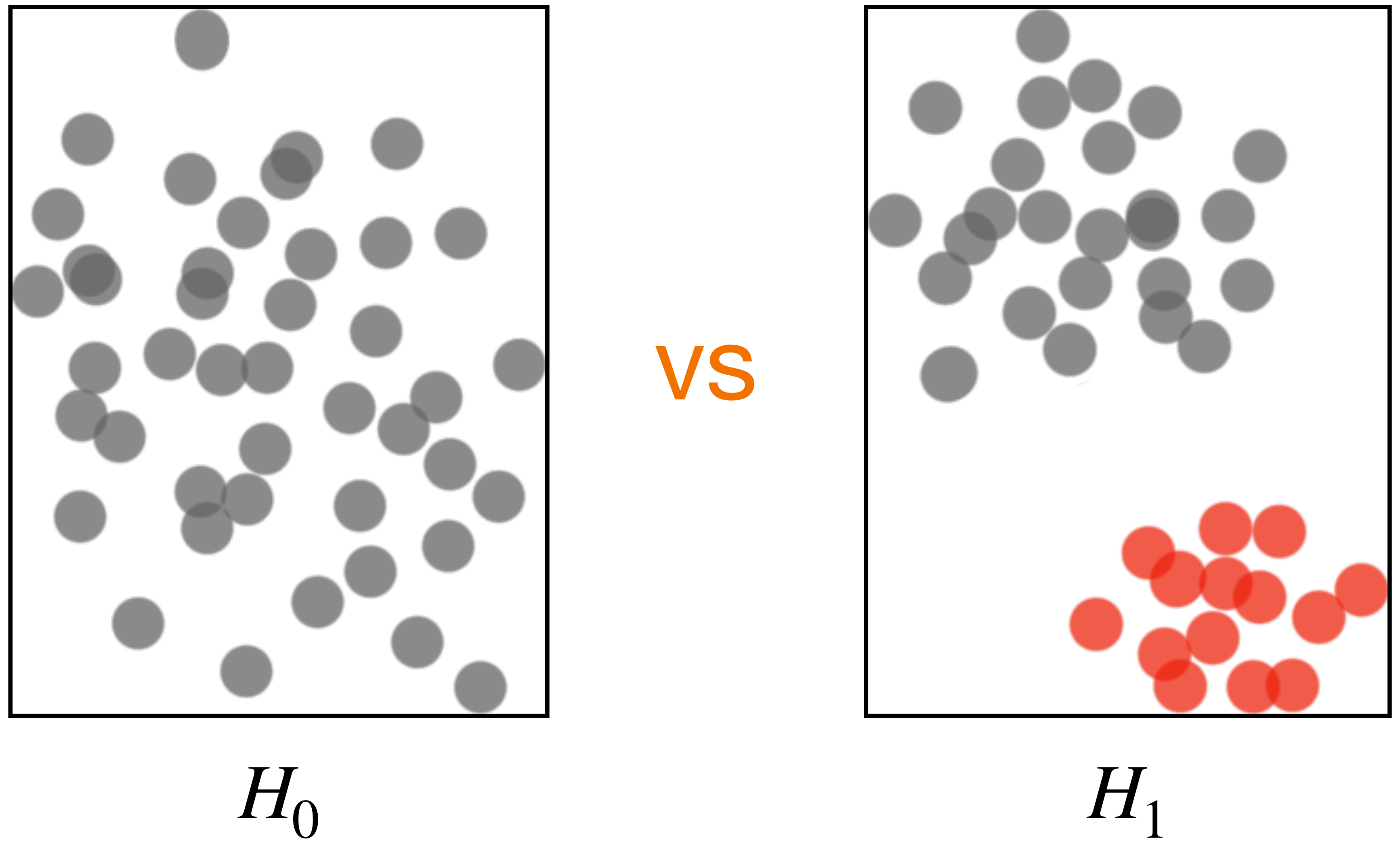

Laura, PhD, a cancer biologist
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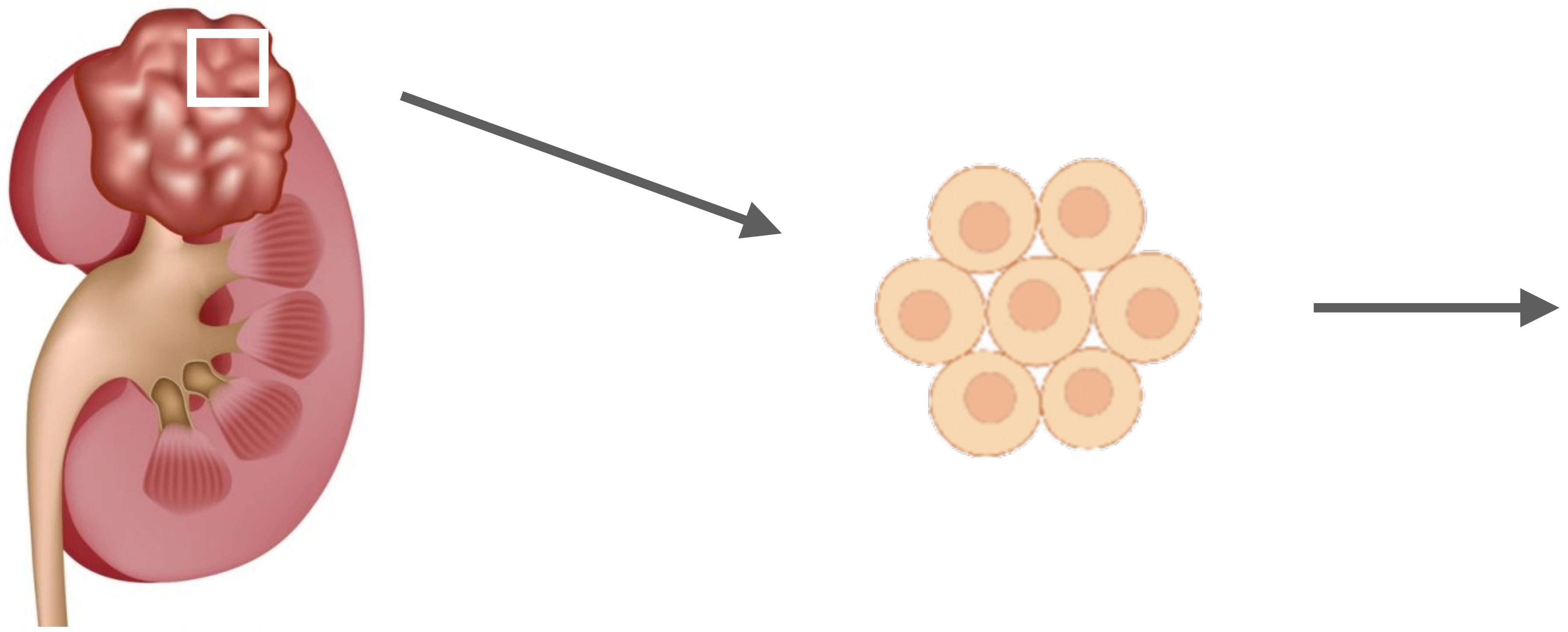

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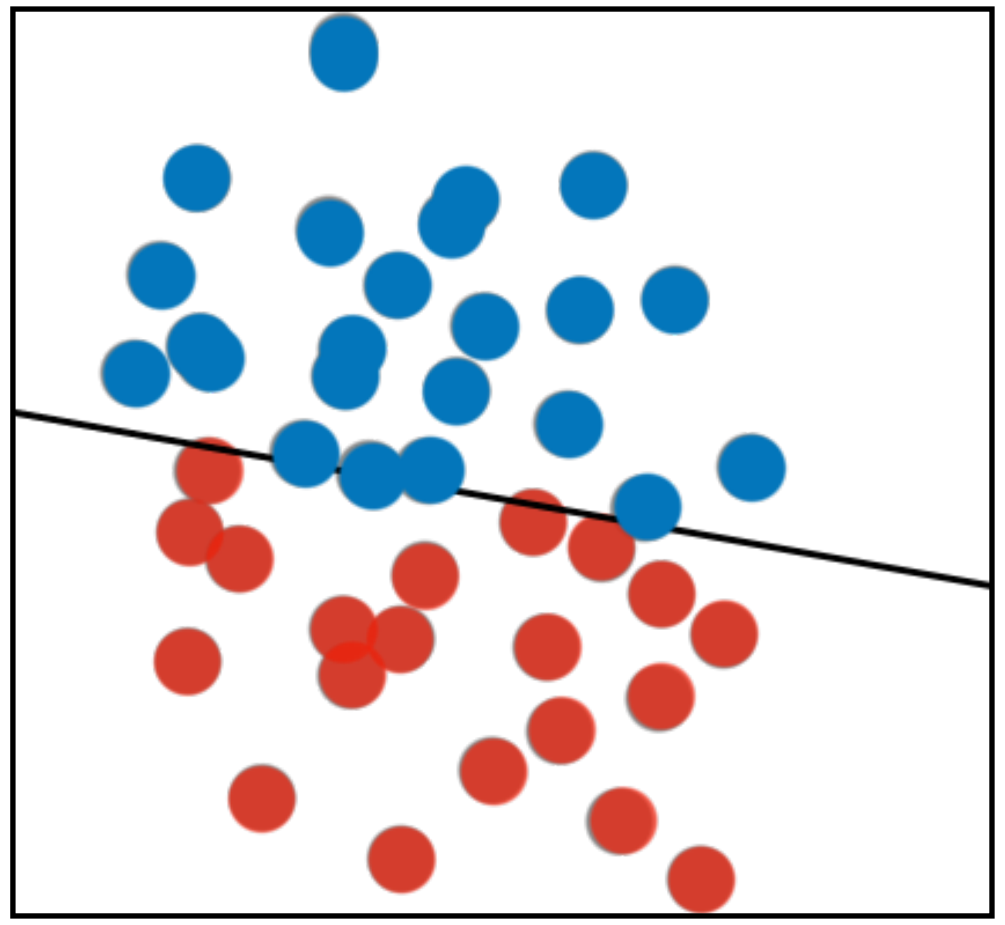
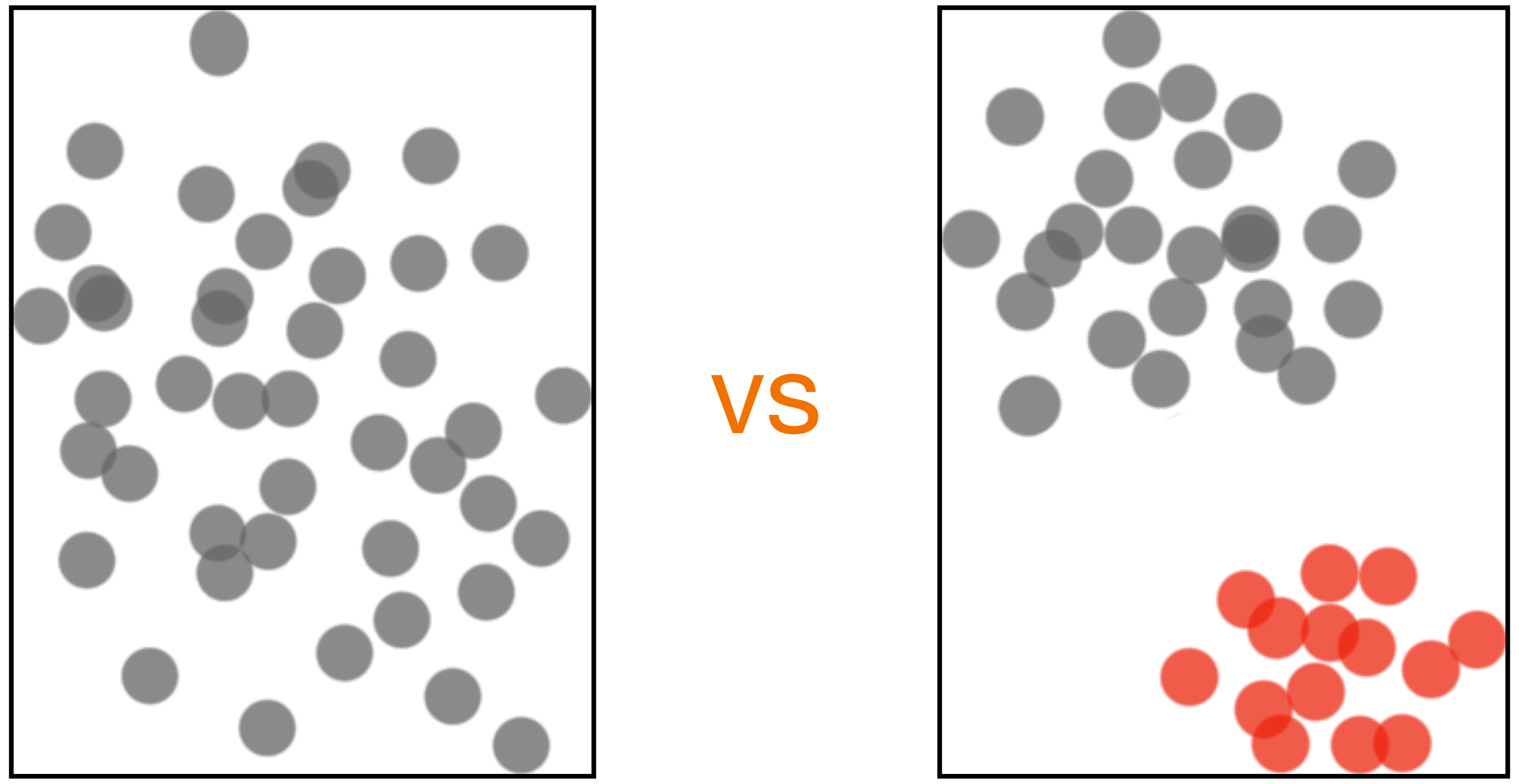
🤔 Is there a new subtype of kidney cancer cells?

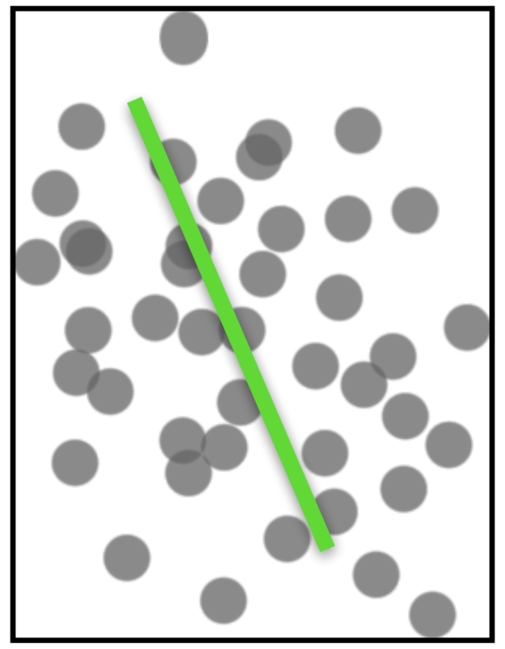
⚠️ Cannot test it with a clustering algorithm.



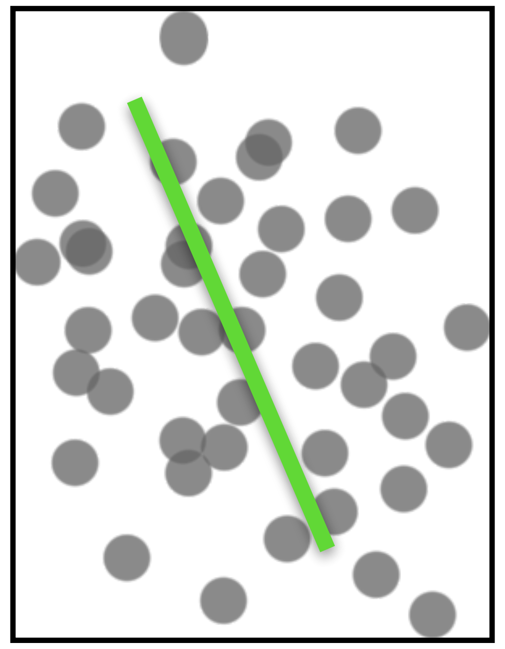
Spurious clusters



H_0 H_1



H_0



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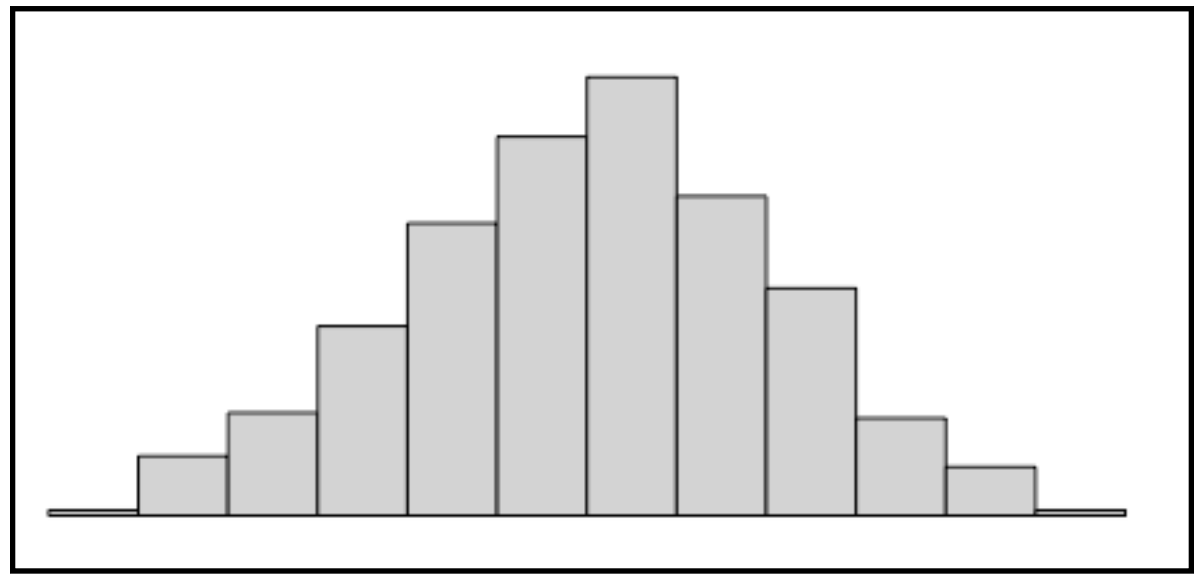

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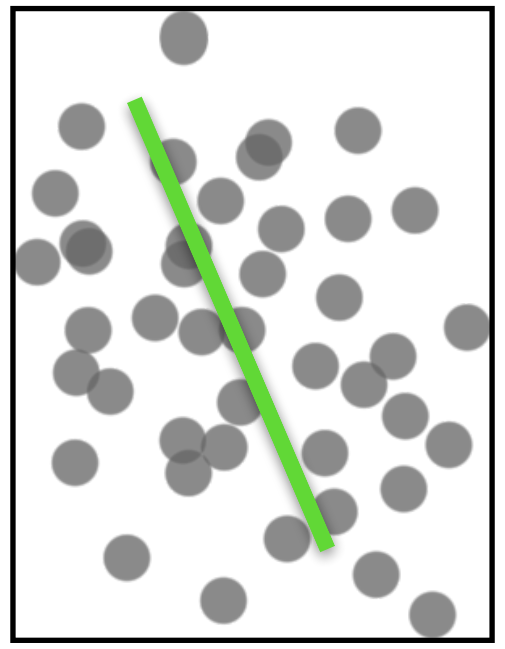

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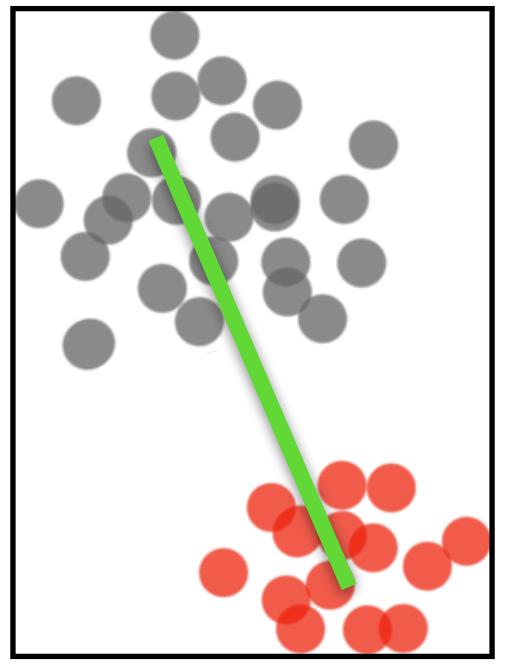

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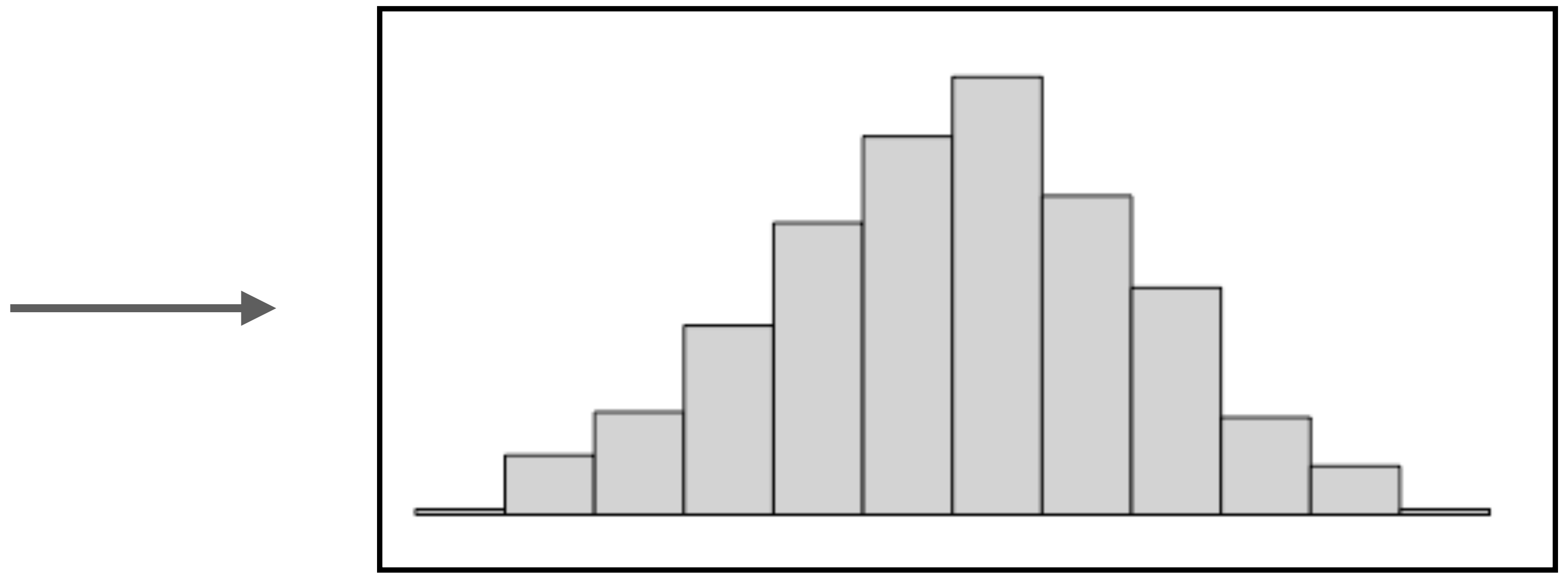
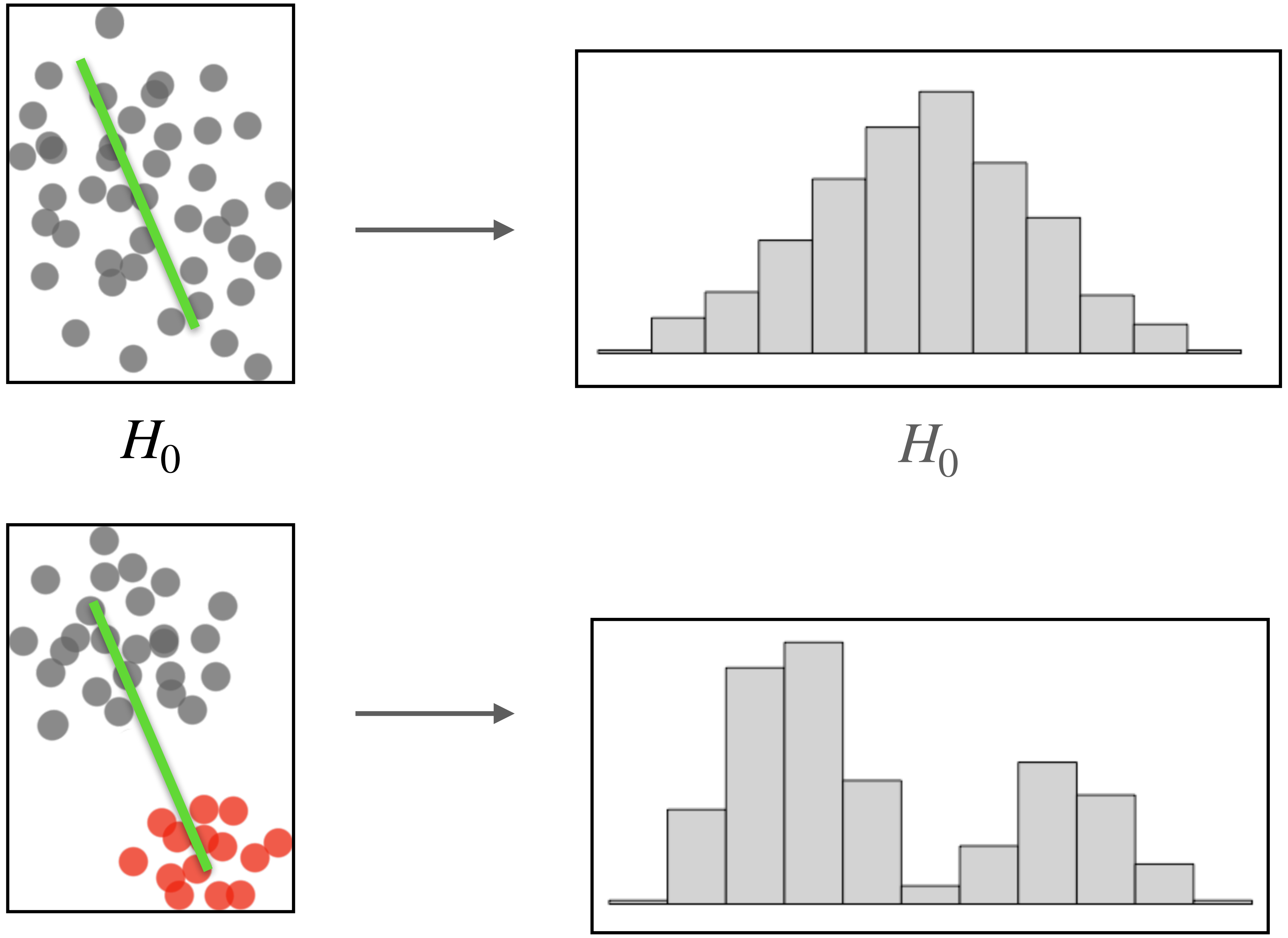
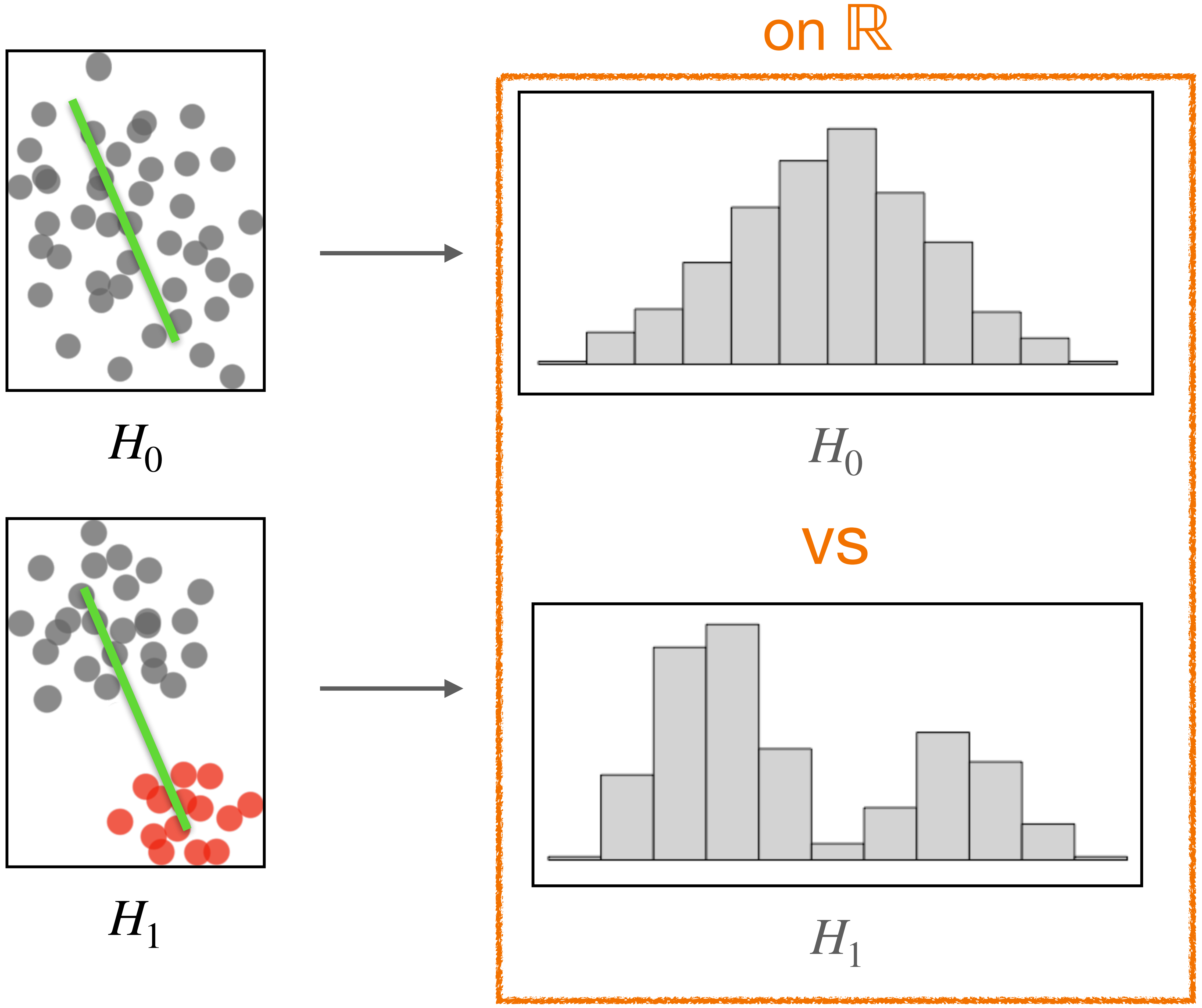
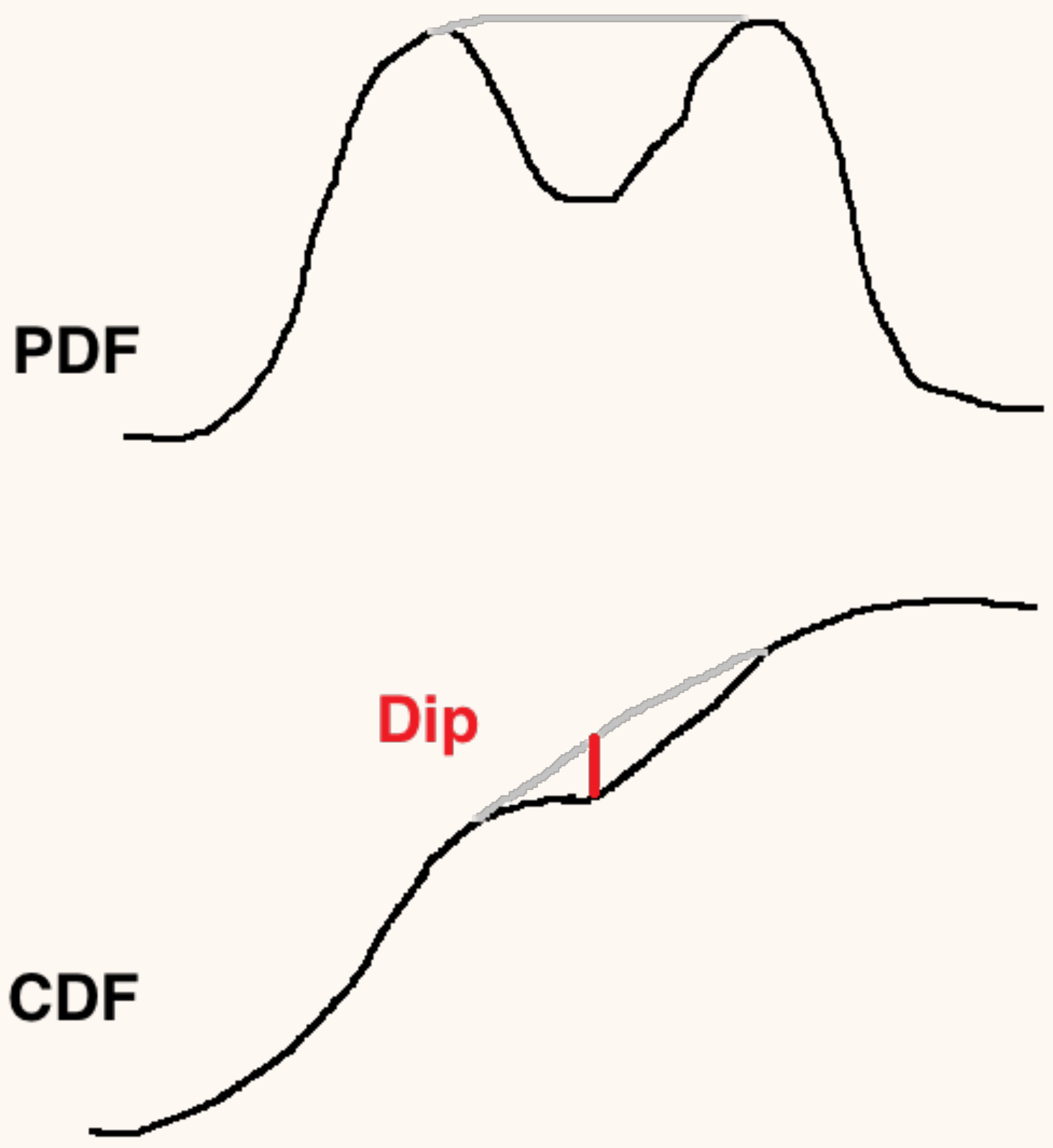


H_0



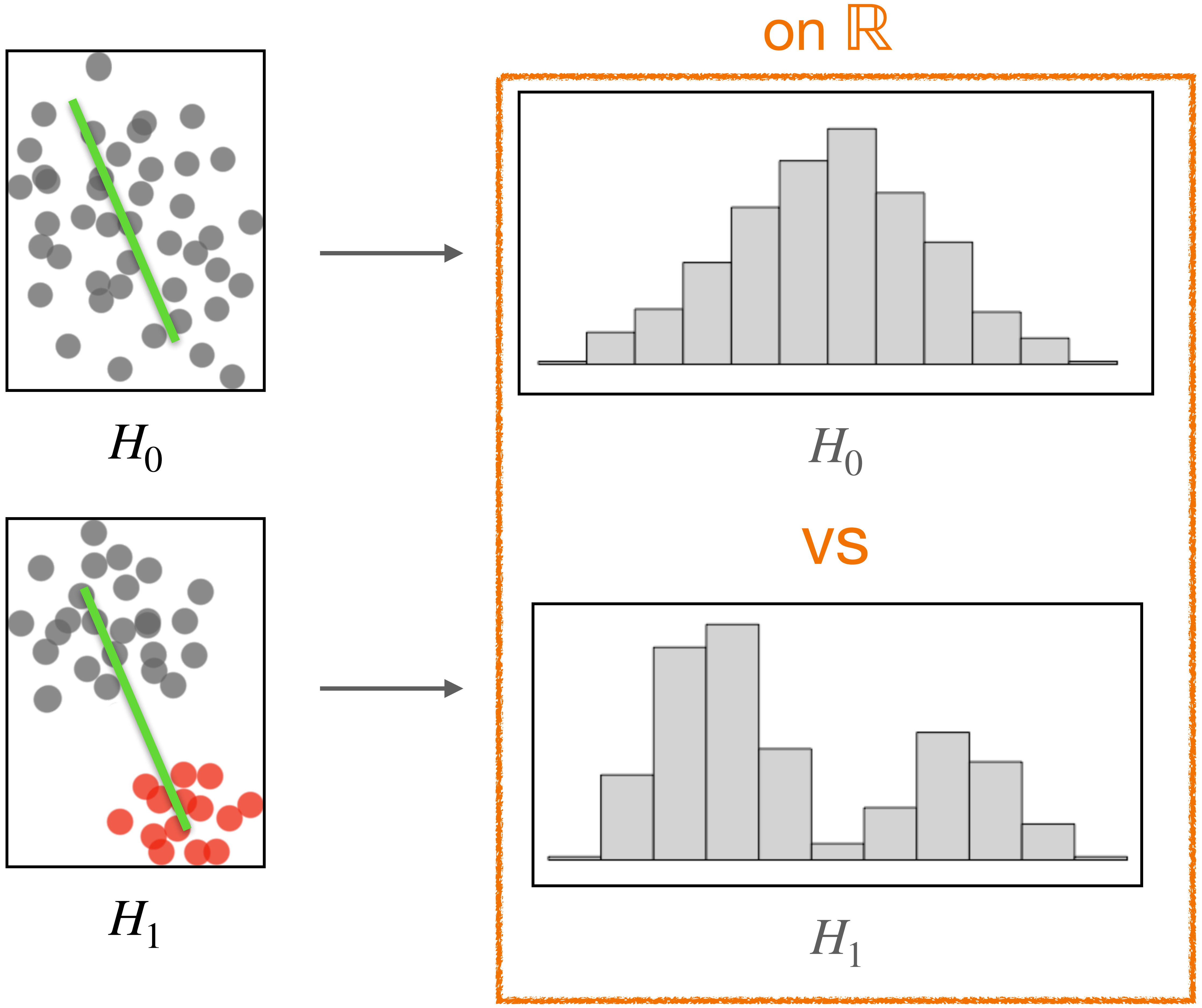
H_0
H_0
H_1
H_1

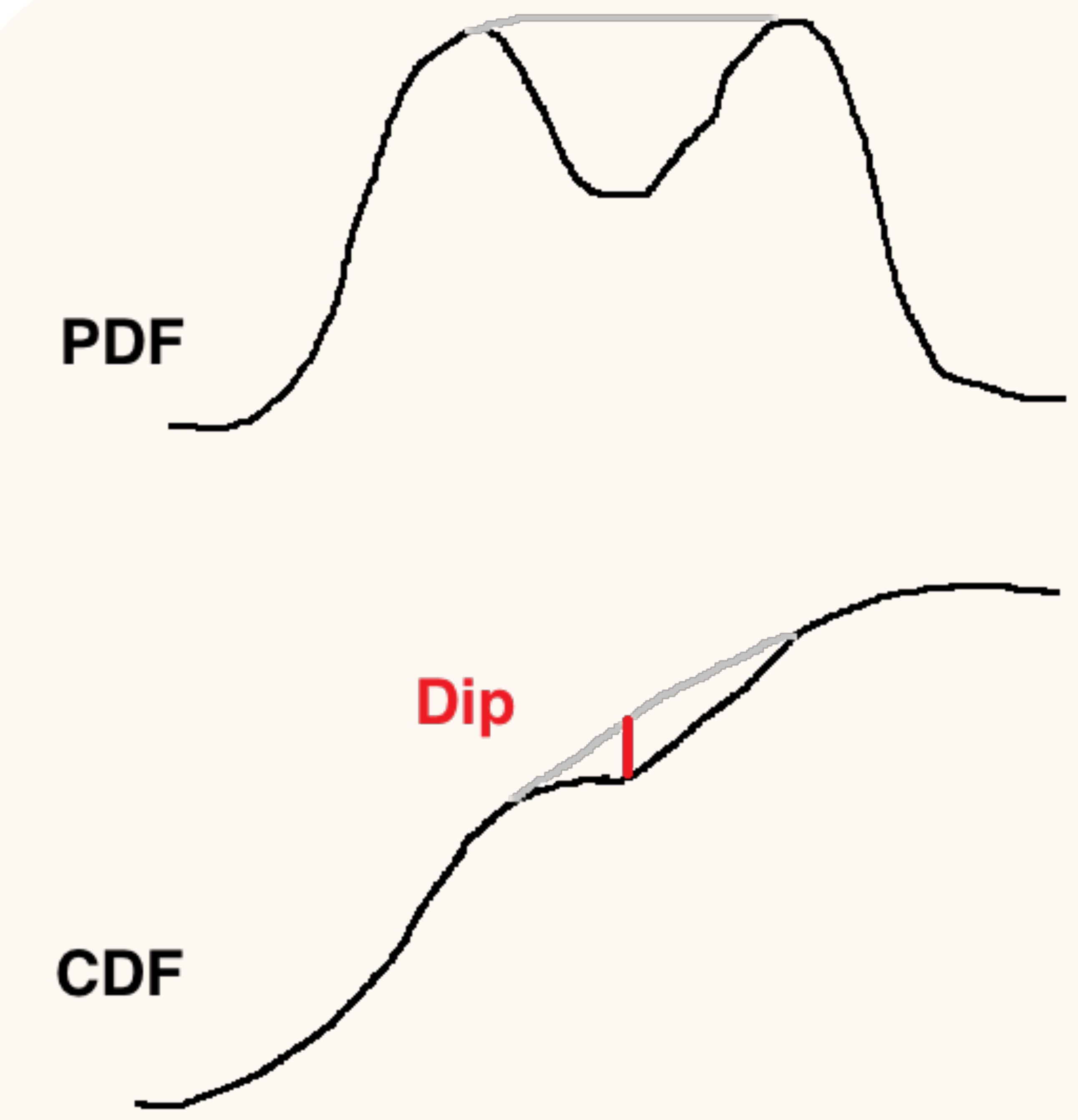




© Edward Ross

J. A. Hartigan & P. M. Hartigan.
The Dip Test of Unimodality.
Annals of Statistics (1985)





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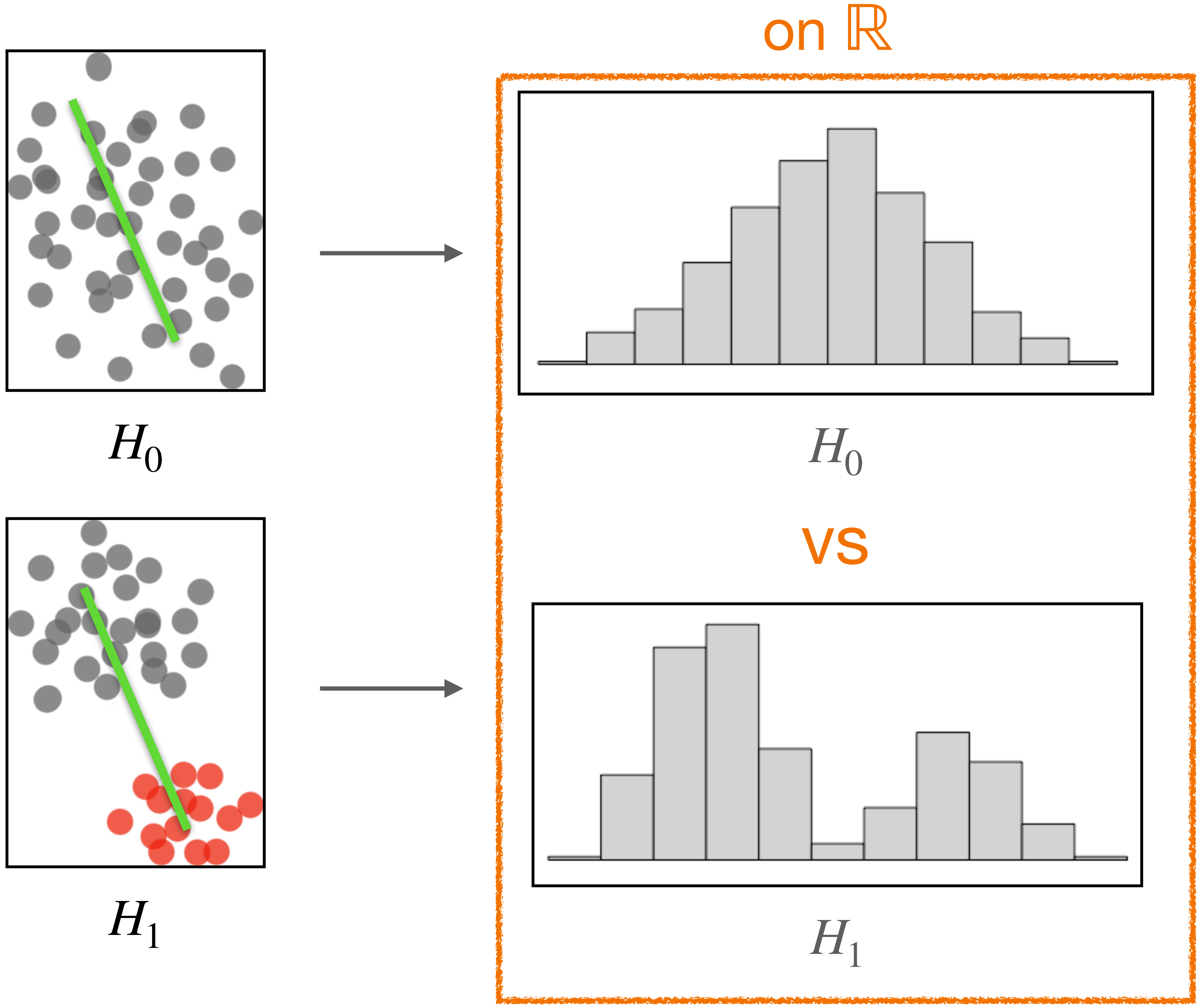
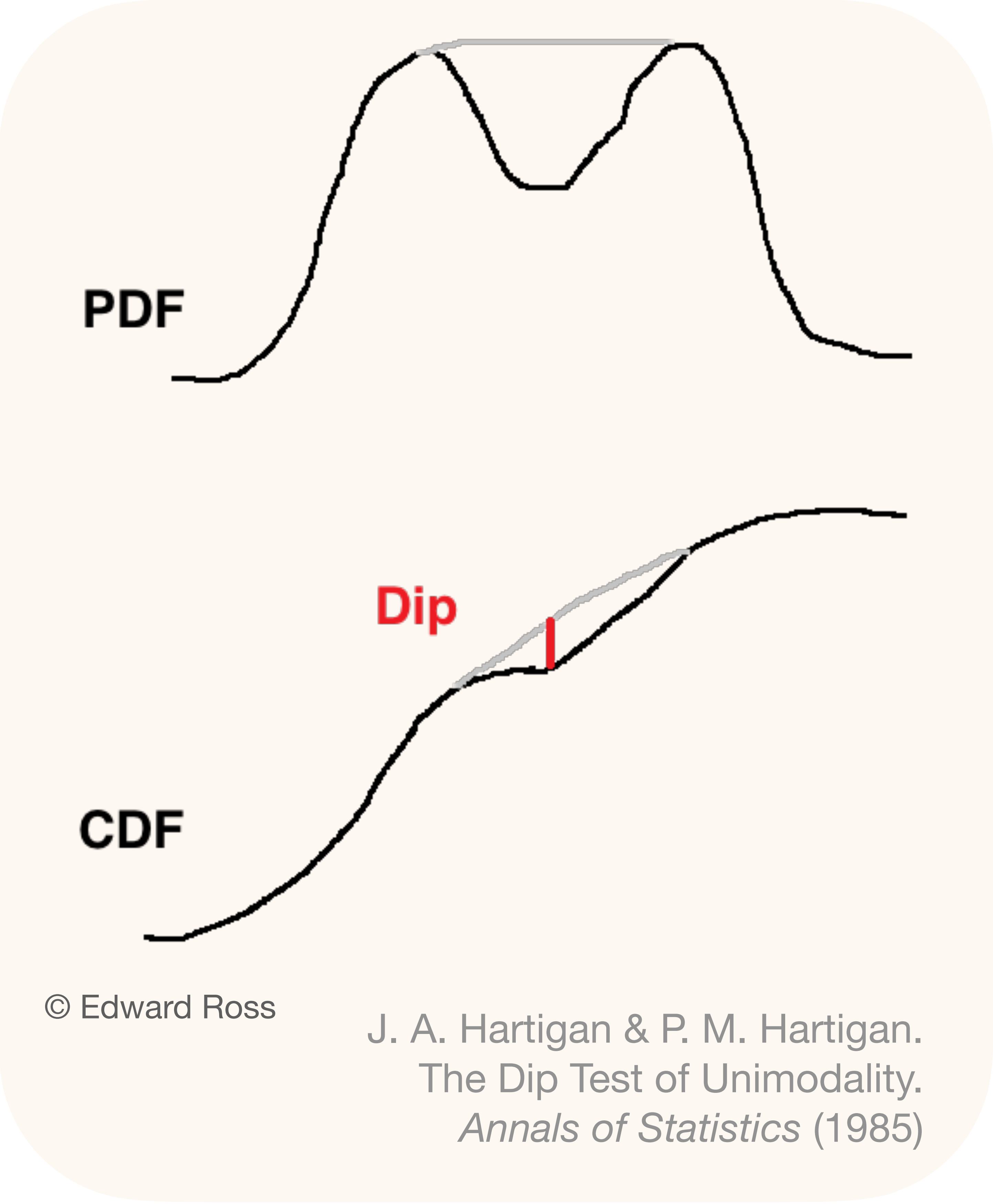
💡 Use clustering (e.g., k-means) to find the direction!





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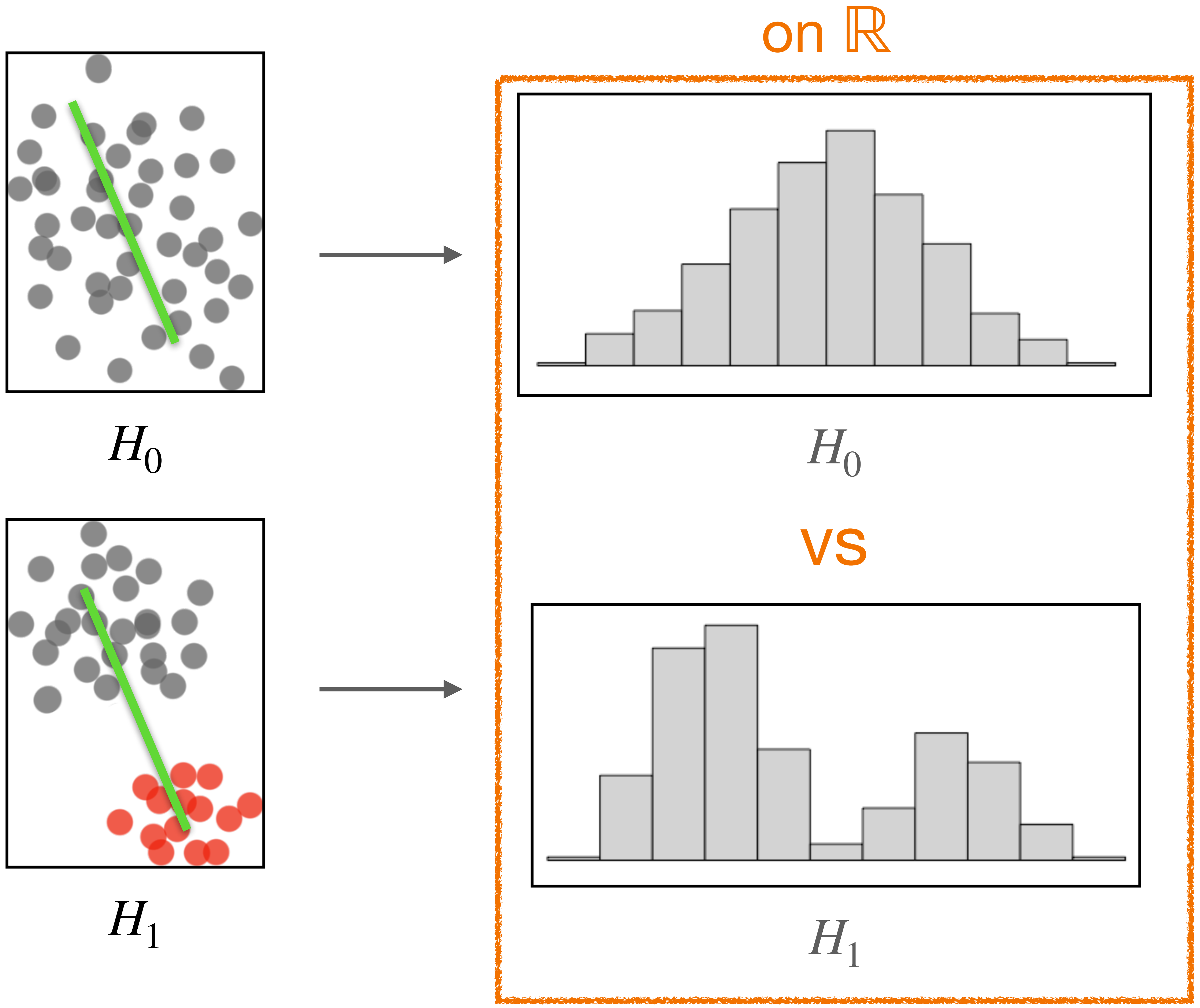
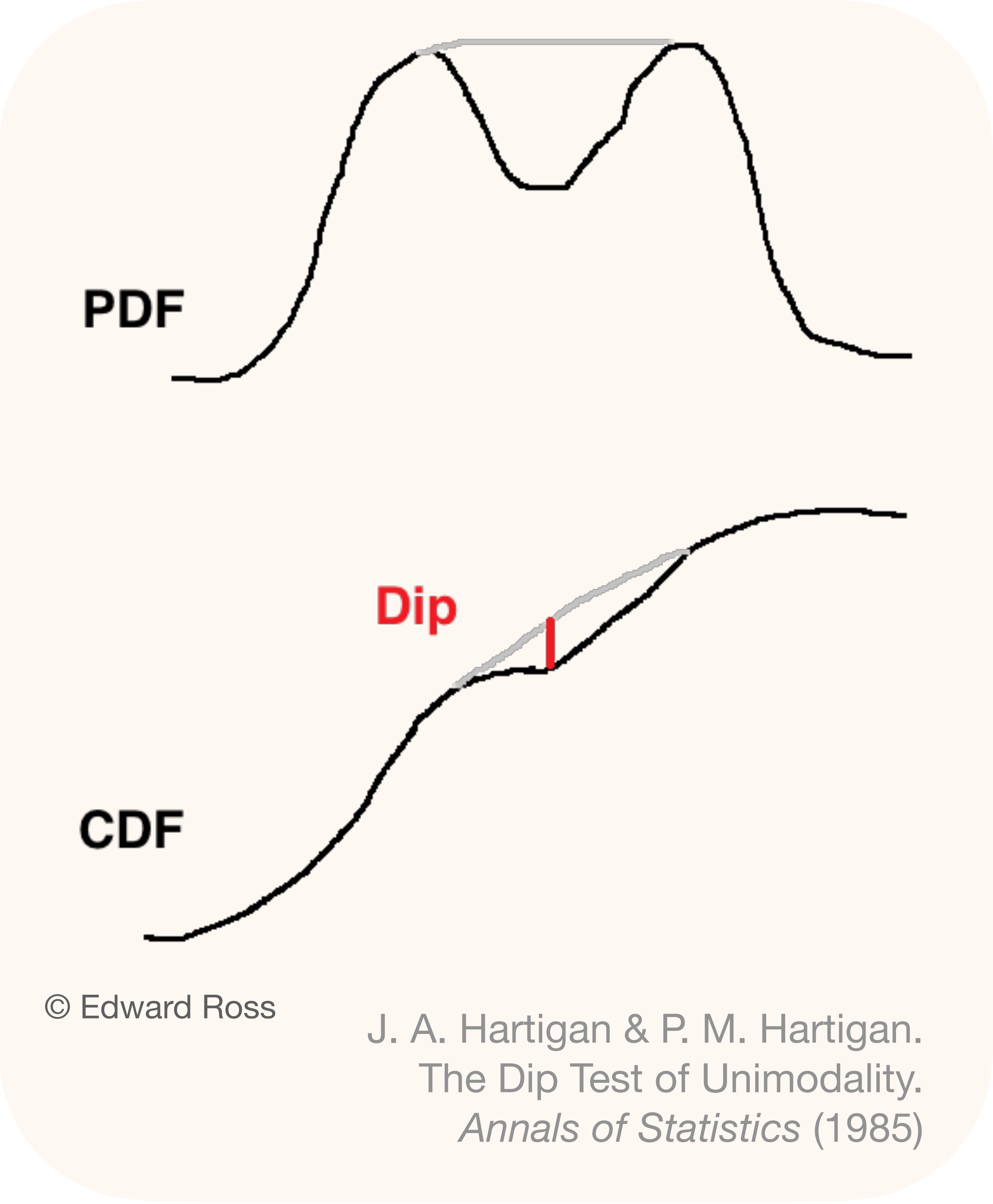
⚠️ Double dipping!





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⚠️ Double dipping!

👉 Data splitting!

Hunt and test!

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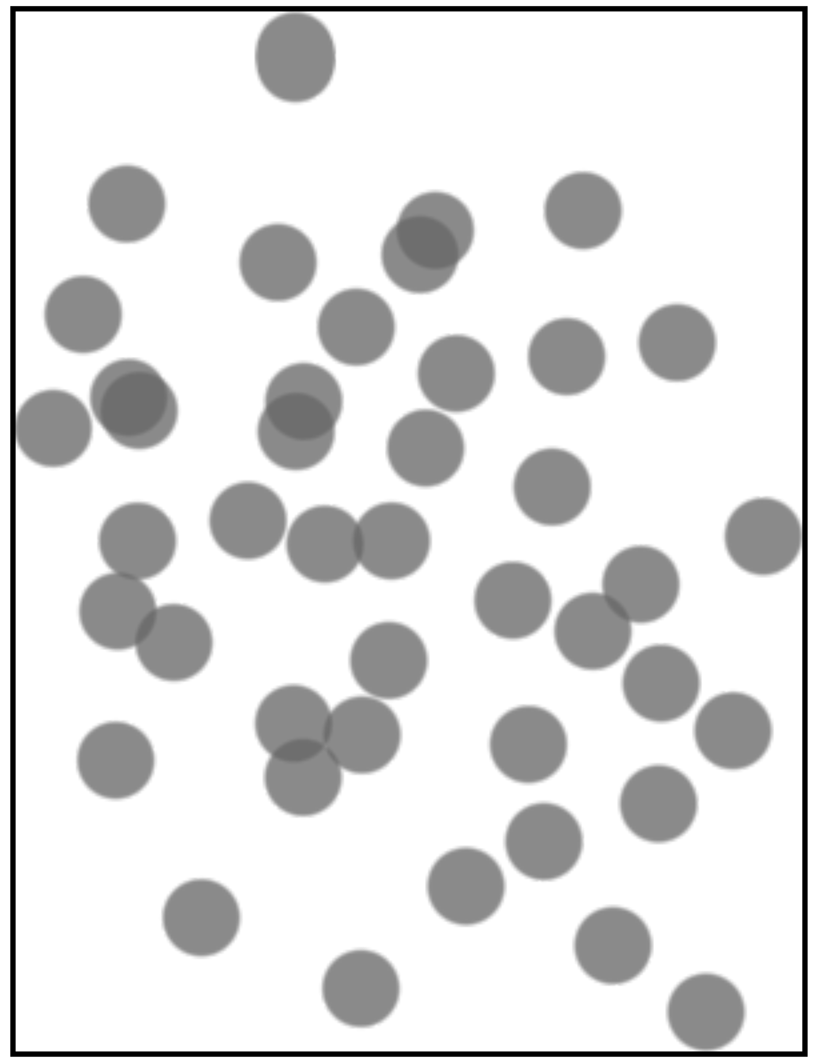

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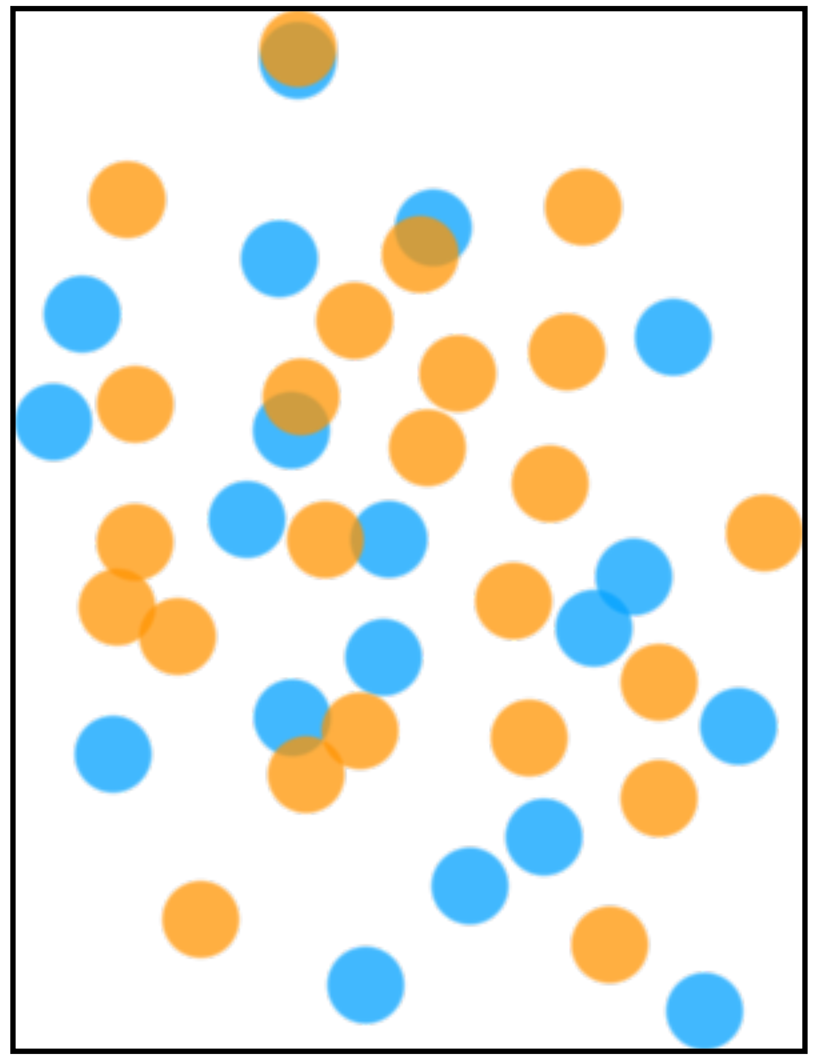

🎲

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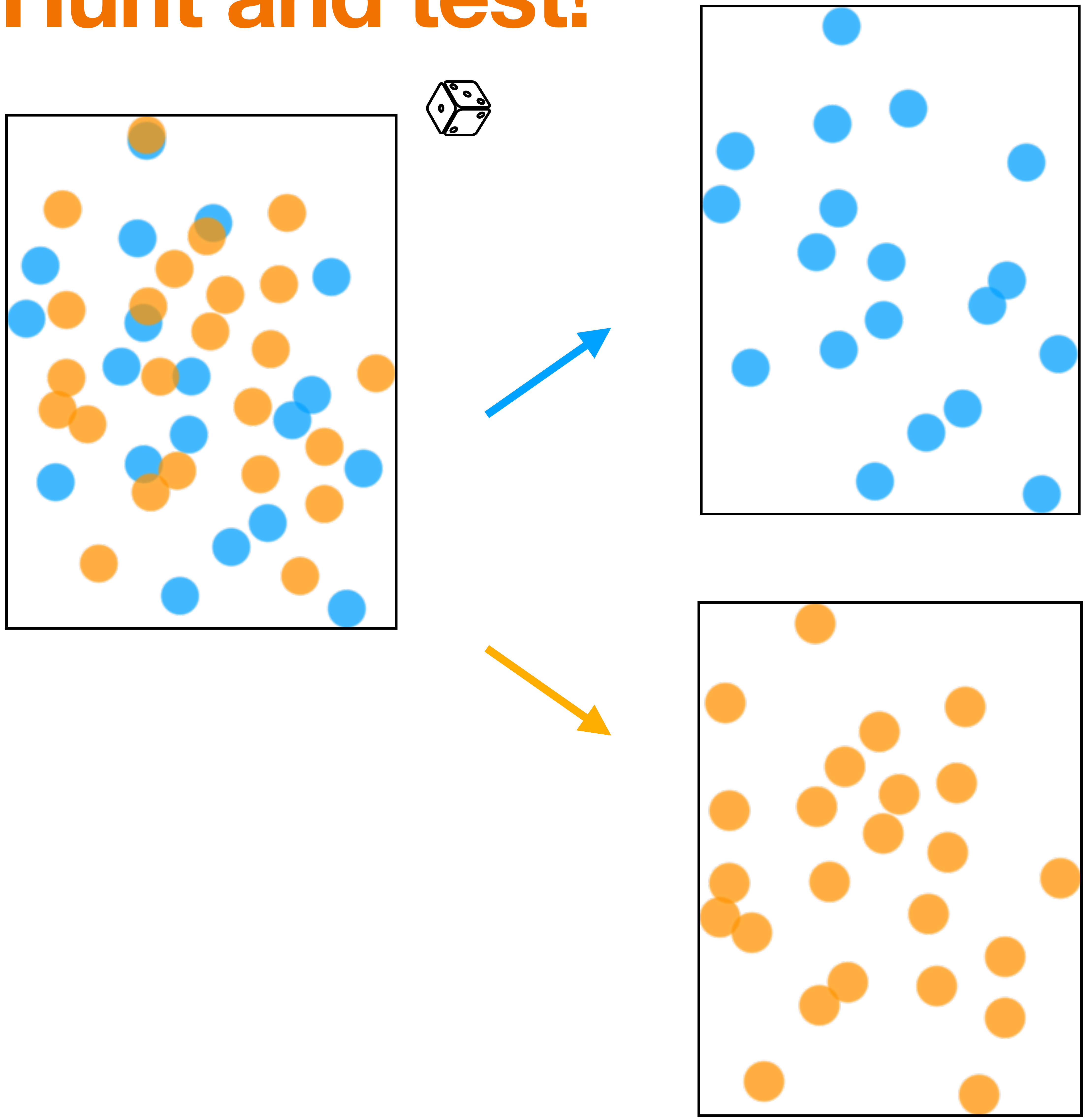

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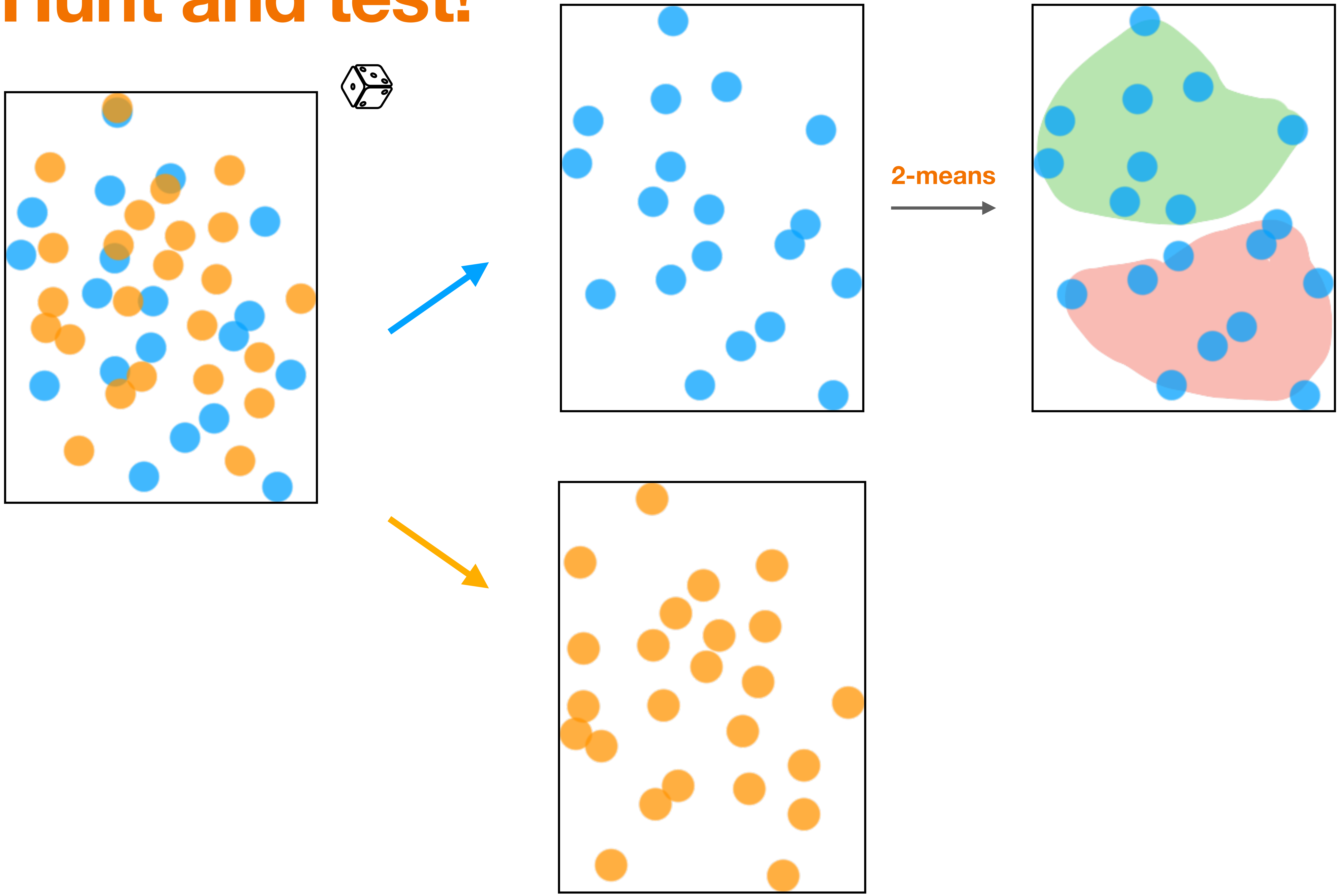
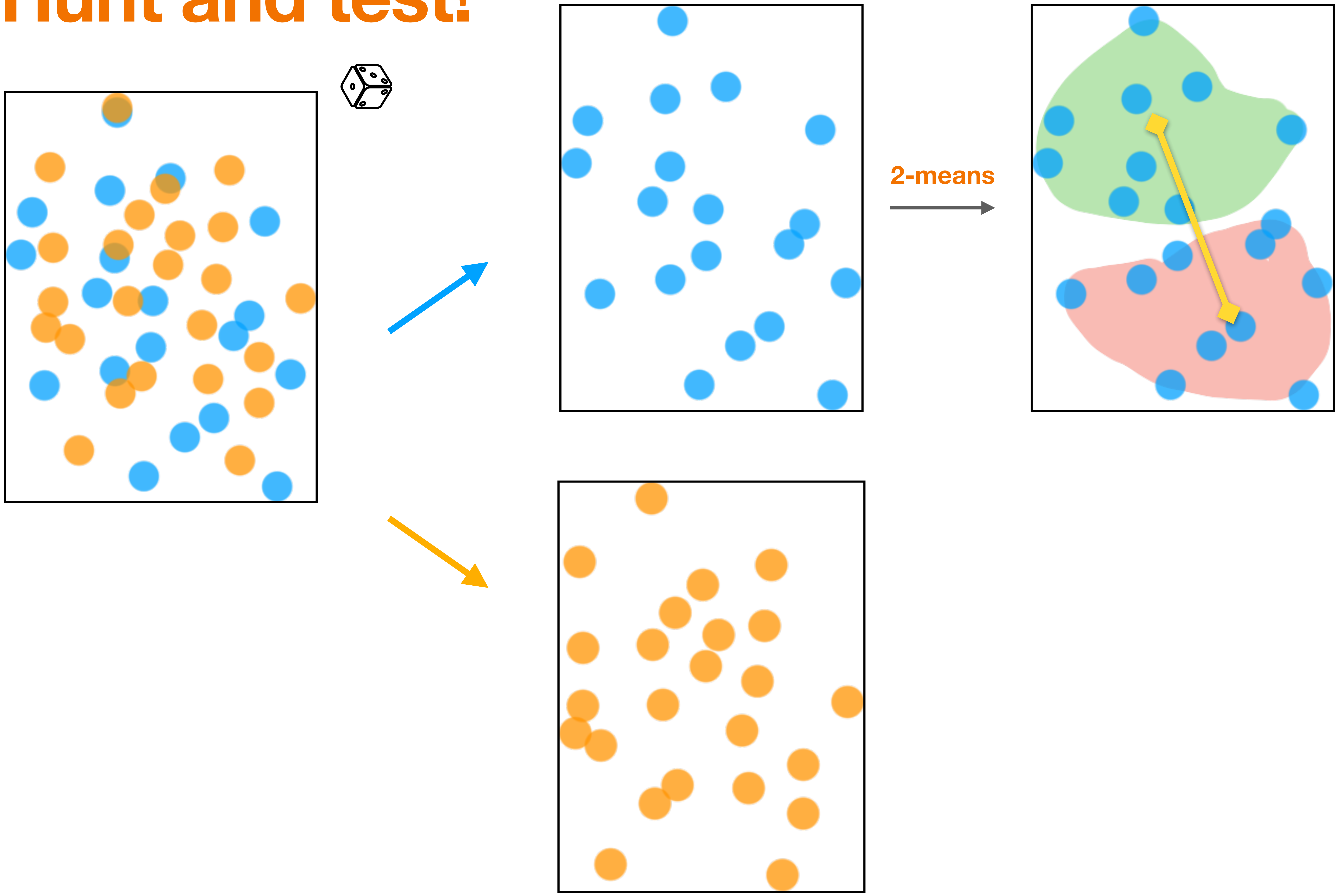


2-means

Hunt and test!



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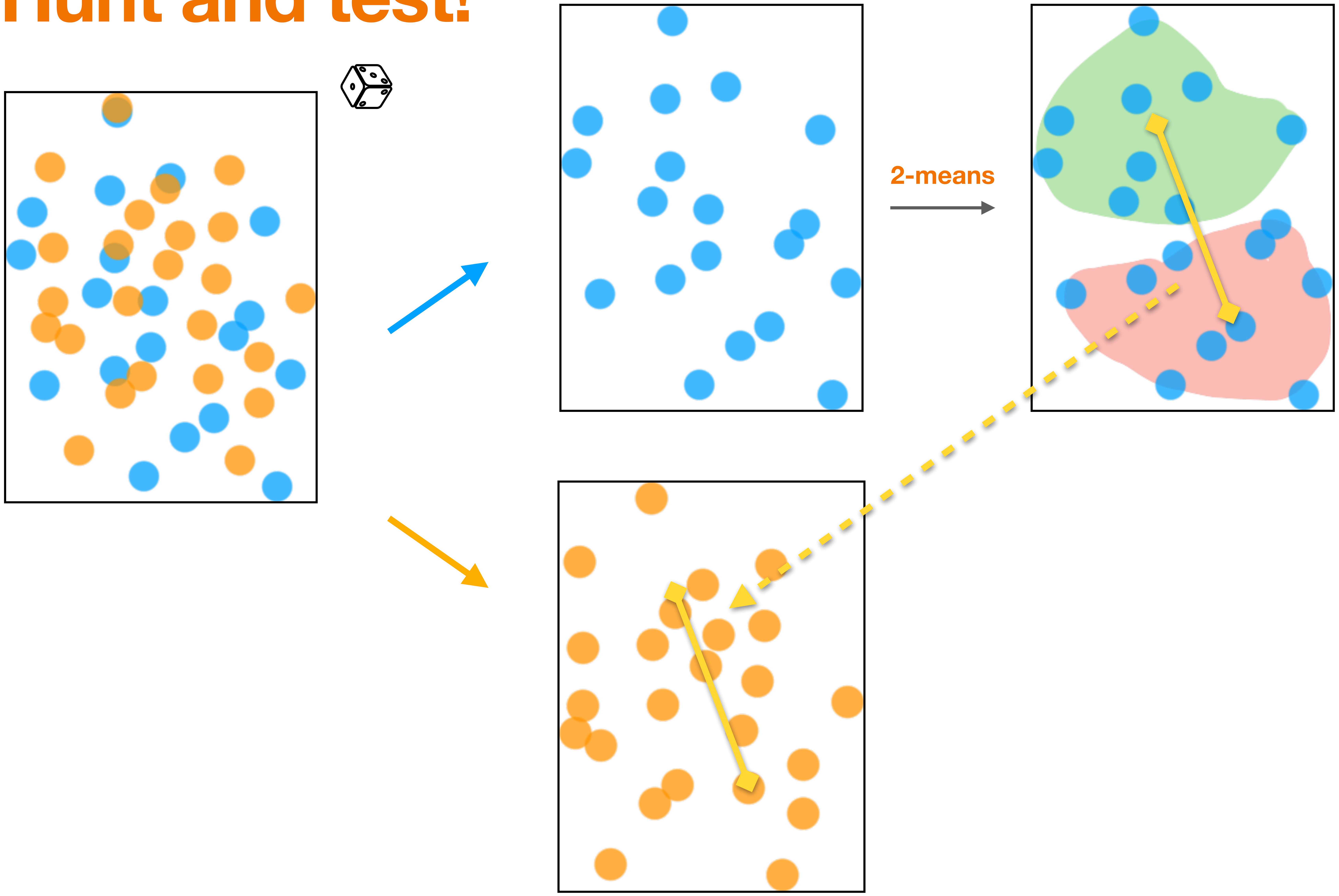

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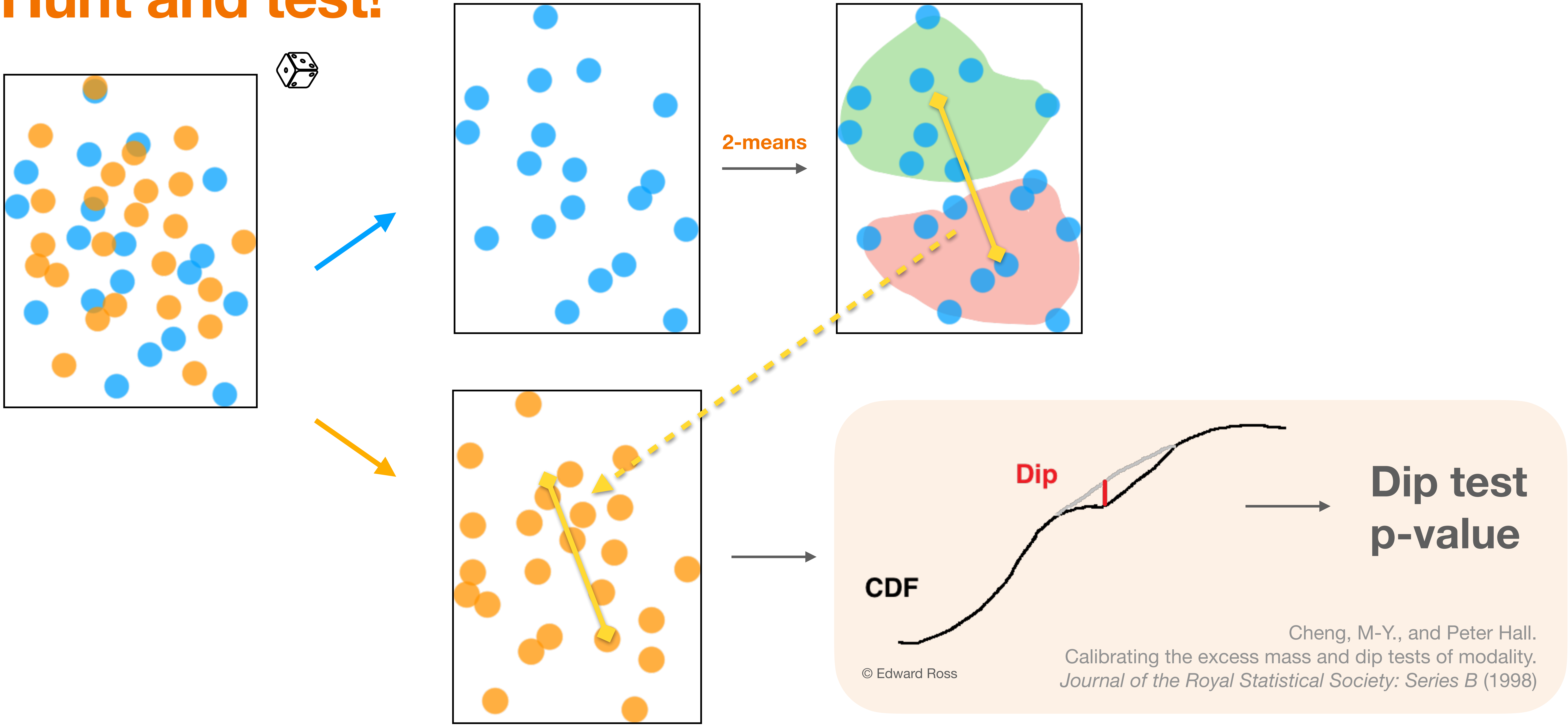

Cheng, M-Y., and Peter Hall.
Calibrating the excess mass and dip tests of modality.
Journal of the Royal Statistical Society: Series B (1998)

```
> replicate(10, hunt.and.test(data))
```

```
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```

```
p value

0.2
0.1    .
0.6
0.3
0.006  ***
0.4
0.7
0.8
0.3
0.06   .
```

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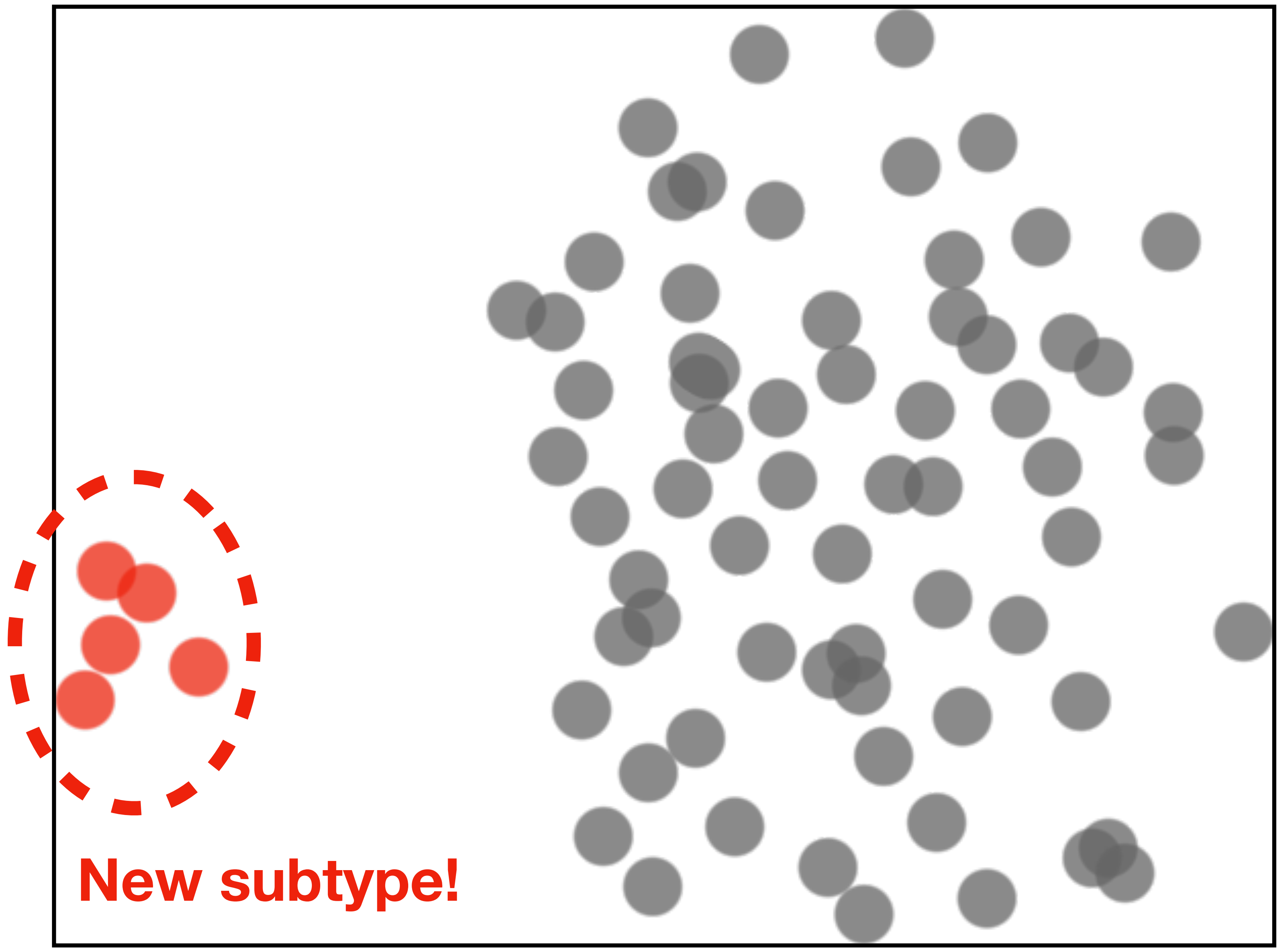

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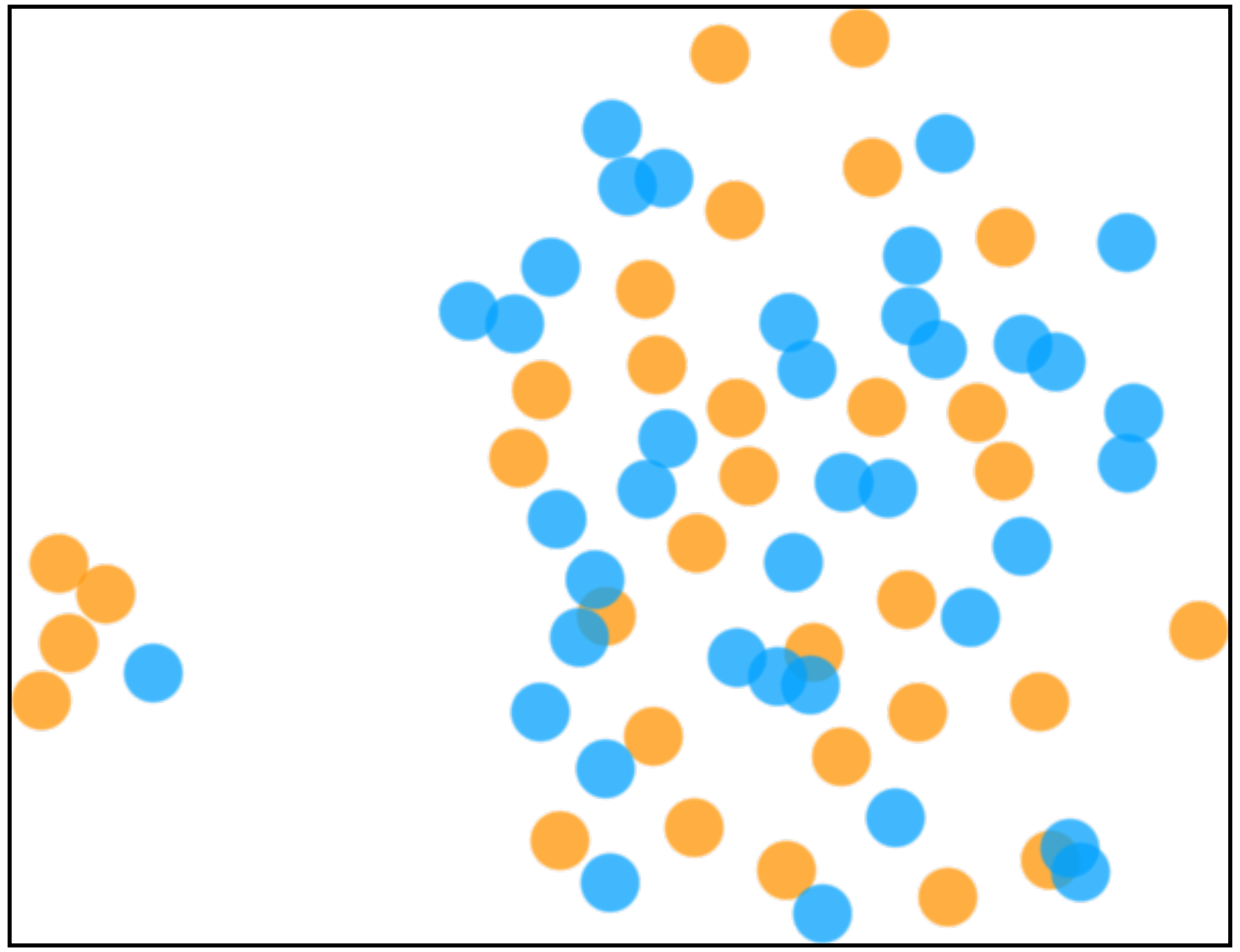

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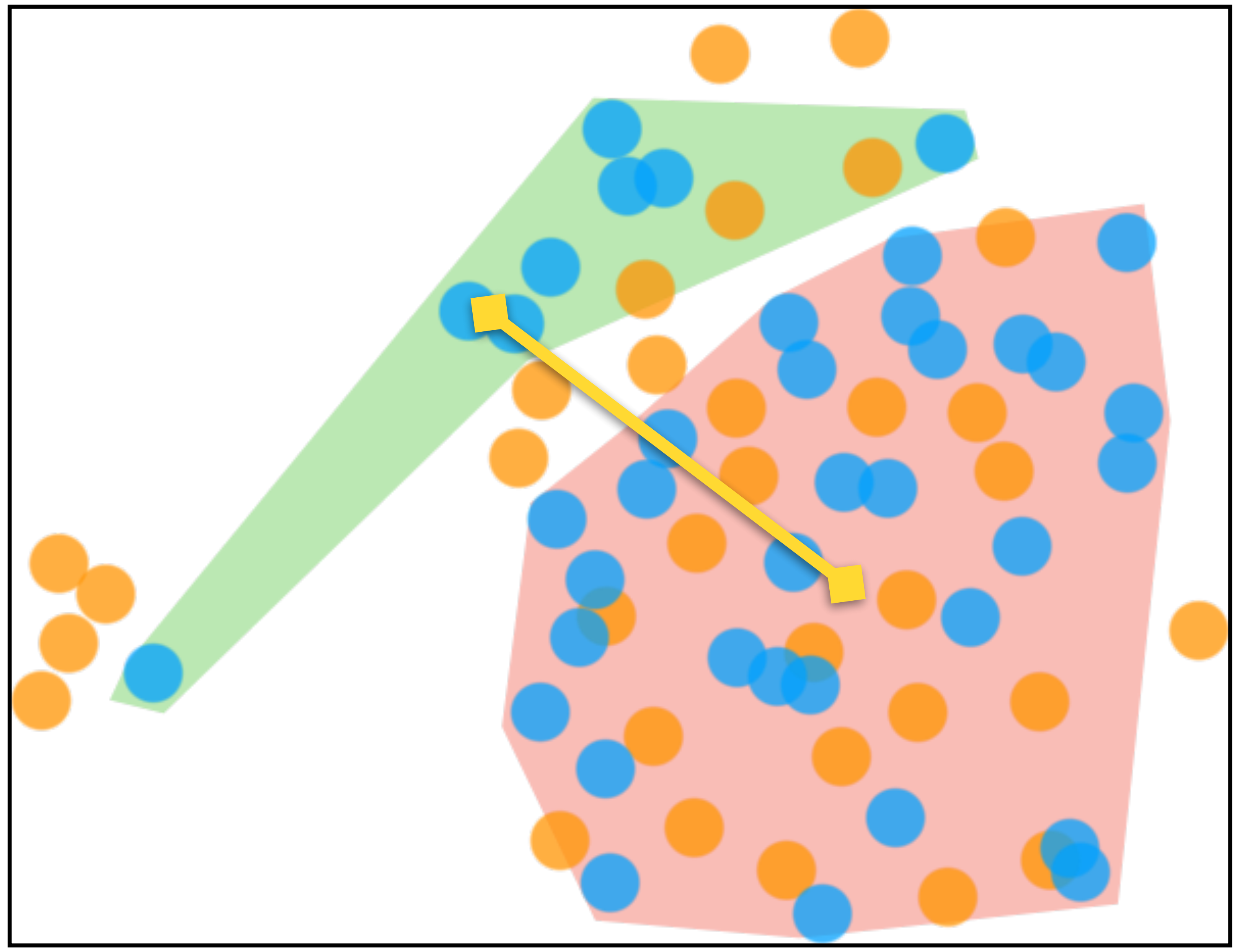

🎲

❌

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```

```
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0.6
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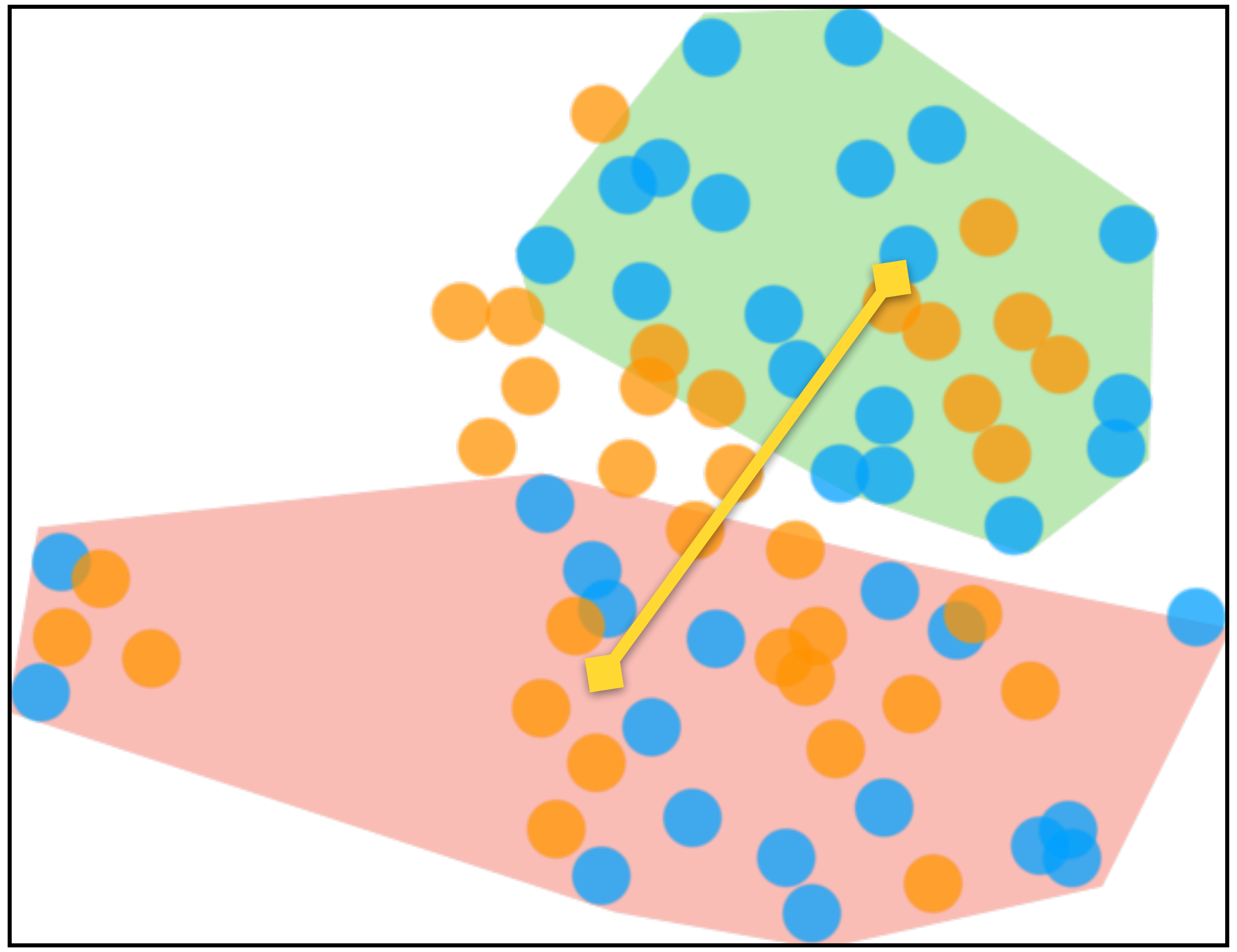

🎲

✗

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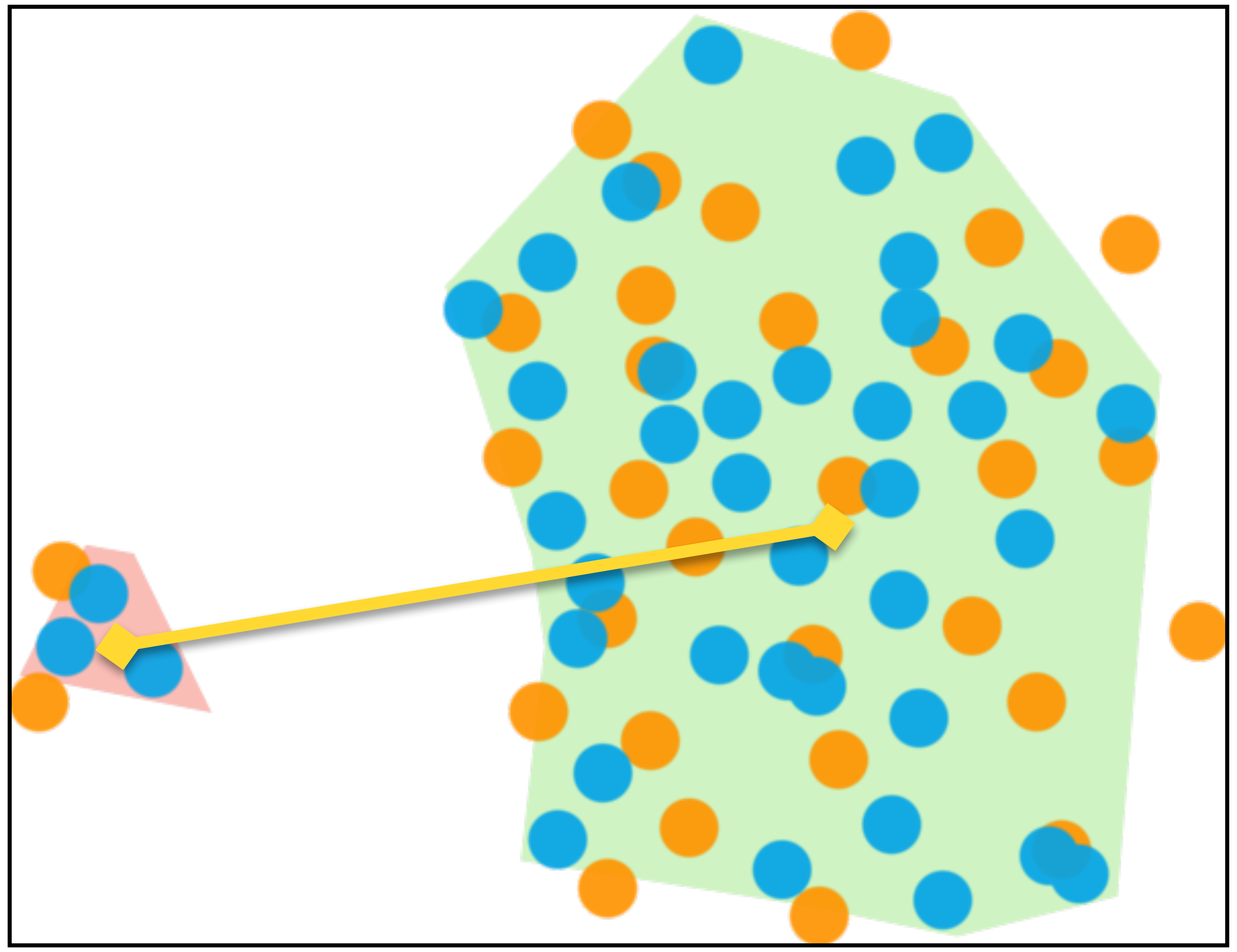

🎲

✅

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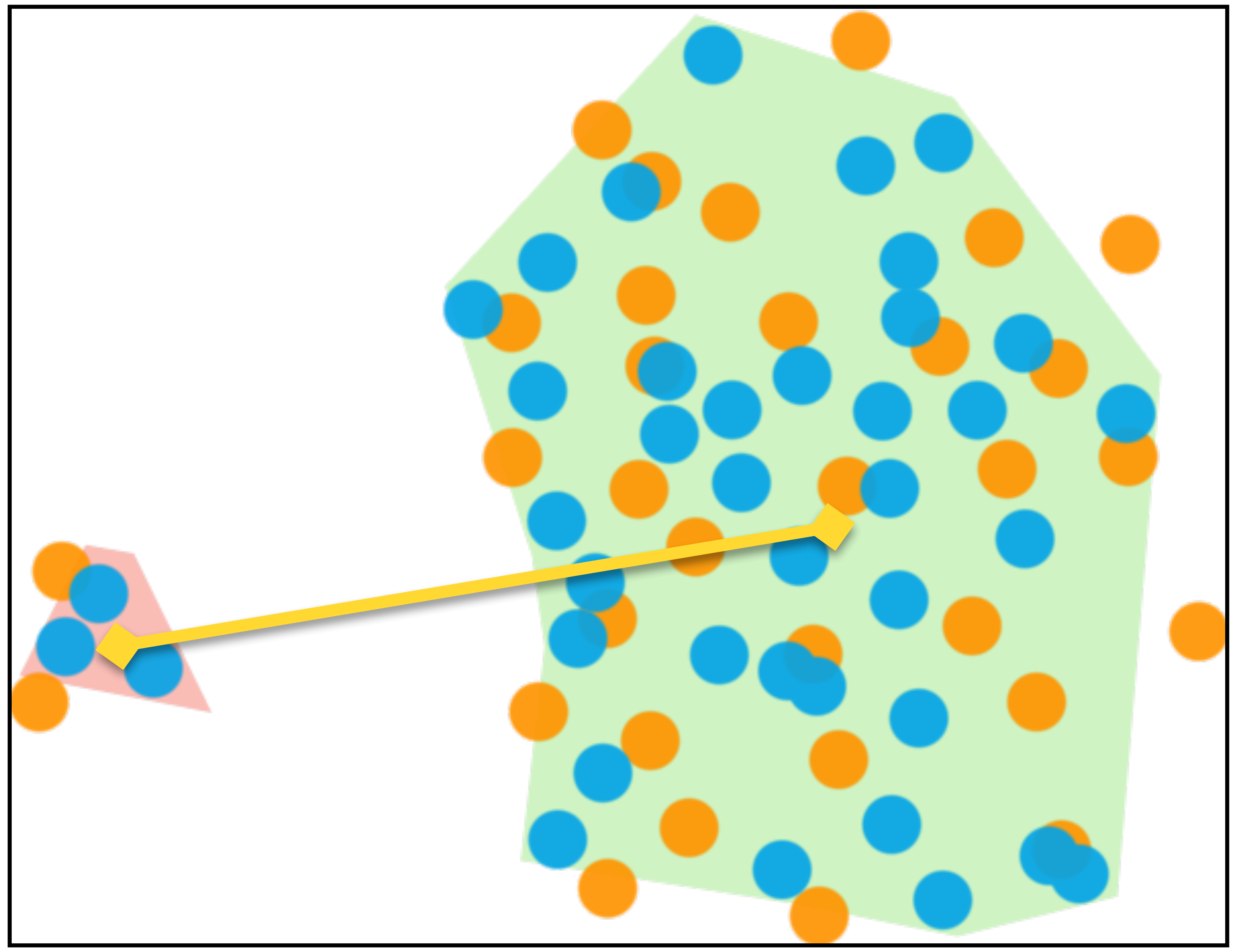

👉 Hunted the wrong direction 9/10 times.

😔 Missed opportunity!

Dilemma of data splitting: Two drawbacks

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Bill

🤔 Raises concern on replicability

Laura

😔 Misses the true signal in data

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⚠️ **High variability conditional on data**

Laura

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⚠️ **Low power**

Dilemma of data splitting: Two drawbacks

Bill

🤔 Raises concern on replicability

⚠️ **High variability conditional on data**

Laura

😔 Misses the true signal in data

⚠️ **Low power**

💡 Use the information from multiple data splits properly!

Outline

- **Setup and main challenge**
- Method: Rank-transformed subsampling
- Applications
  - Hunt and test
  - Improving inference for double machine learning
  - Testing no direct effect in a sequentially randomized trial
- Future directions

Setup: Single split

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IID Data: $X := (X_1, \ldots, X_n) \sim P^n$. Hypothesis testing: $P \in H_0$ vs $P \in H_1$.

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“Single-split” statistic: $T_n(X_1, \ldots, X_n; \Omega)$, where Ω is 🎲 .

- Extra randomness $\Omega \sim P_\Omega$ independent of X.
- Ω is used to split data, perform resampling, etc.

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Assumption. For $P \in H_0$, $T_n(X; \Omega) \to_d F_0$ as $n \to \infty$ unconditionally.

- “unconditionally” = over randomness of both X and Ω
- “conditionally” = over randomness of $\Omega \mid X$

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"Single-split" test: Reject H_0 whenever $T_n \gtrless (\alpha$ quantile of $F_0)$.

⚠️ High conditional variability. ⚠️ Low power.

Setup: Aggregation

“Multiple-split”, exchangeable statistics: Fix X. Draw $\Omega^{(1)}, \ldots, \Omega^{(L)}$ as L independent copies of Ω and let

$$T_n^{(1)} := T_n(X; \Omega^{(1)}), \quad \ldots \quad , T_n^{(L)} := T_n(X; \Omega^{(L)}) \,.$$

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💡 **Aggregated statistic:**

$$S_n := S(T_n^{(1)}, \ldots, T_n^{(L)}),$$

for a chosen aggregation function $S : \mathbb{R}^L \to \mathbb{R}$.

👉 S should be symmetric and Lipschitz in $\|\cdot\|_\infty$. 👉 Examples: $S = $ avg, $S = \min$.

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Aggregated test: Reject H_0 when $S_n = S(T_n^{(1)}, \ldots, T_n^{(L)}) \lessgtr$ **?**

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Aggregated test: Reject H_0 when $S_n = S(T_n^{(1)}, \ldots, T_n^{(L)}) \lessgtr$ ❓

✅ Lower conditional variability and ✅ more power compared to the single-split test: $T_n^{(1)} \gtrless (\alpha \text{ quantile of } F_0)$.

Main challenge

🤔 **Aggregated test:** Reject H_0 when $S_n = S(T_n^{(1)}, \dots, T_n^{(L)}) \lesseqgtr$ **?**

Main challenge

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👉 Under H_0, S_n converges to some unknown distribution that depends on $P \in H_0$.

Typically, S_n will converge to some non-degenerate limit distribution under H_0.

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$X_1, \ldots, X_n \sim \mathcal{N}(\mu, \Sigma)$ in $\mathbb{R}^3$.

Single-split statistic for testing $H_0 : \mu = \mathbf{0}$

$$T_n := \frac{\sqrt{n_2}\hat{\mu}_1^\top \hat{\mu}_2}{\hat{\mu}_1^\top \hat{\Sigma}_2 \hat{\mu}_1} \to_d \mathcal{N}(0,1) \text{ under } H_0.$$

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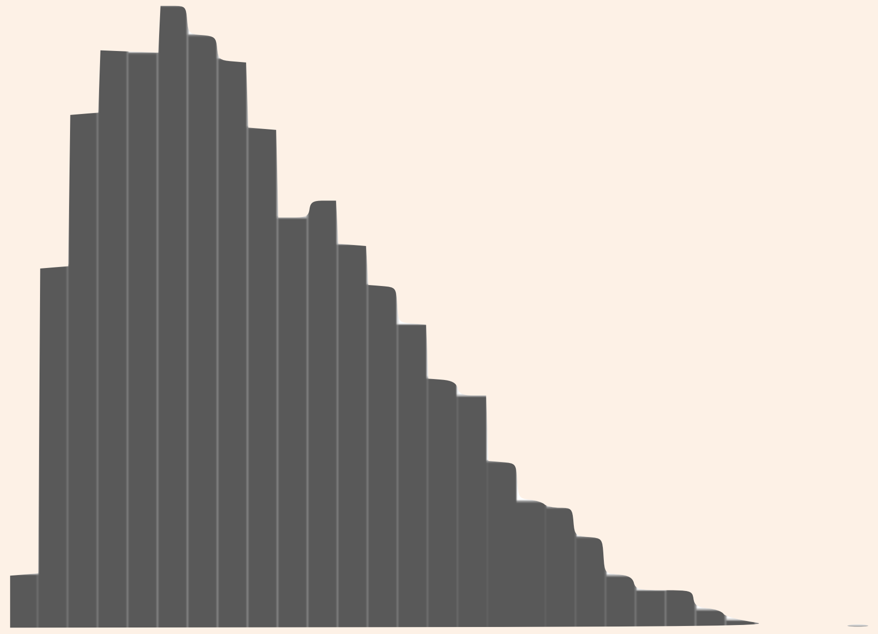

Null distribution of $(T_n^{(1)} + \ldots + T_n^{(200)})/200$

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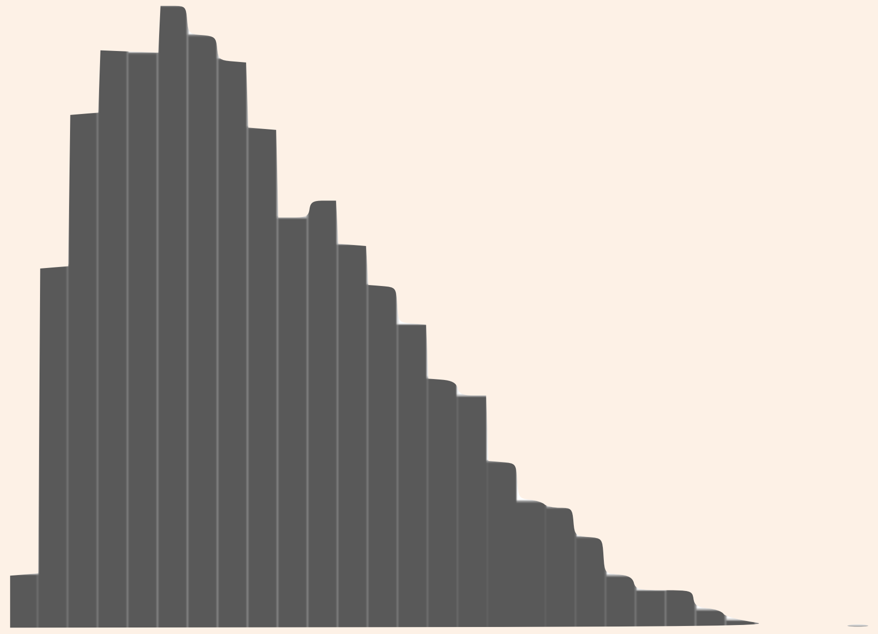

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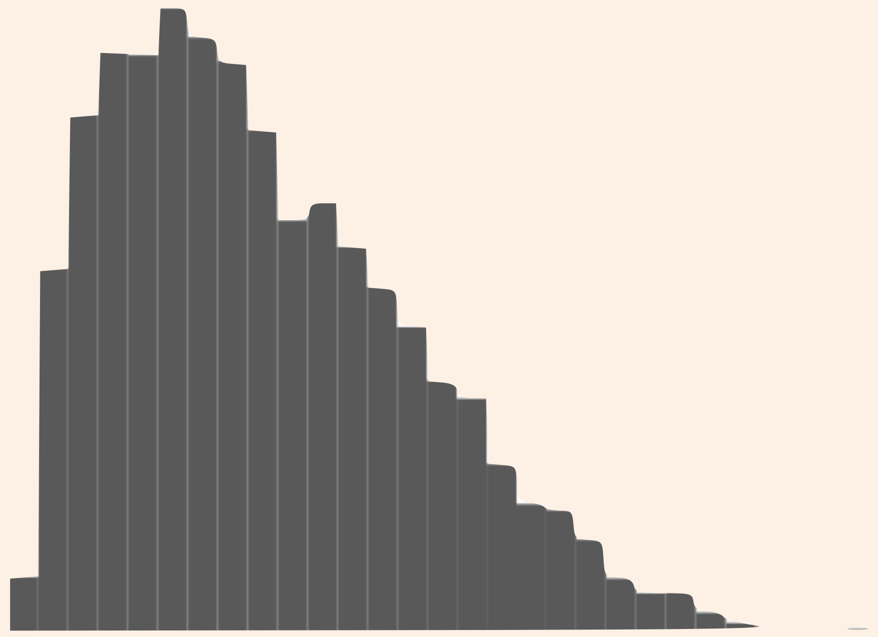

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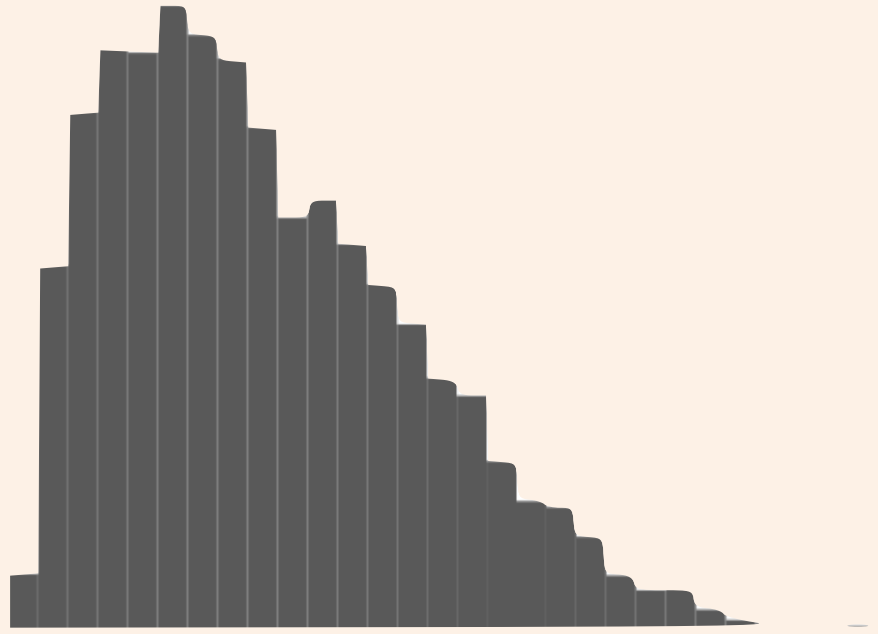

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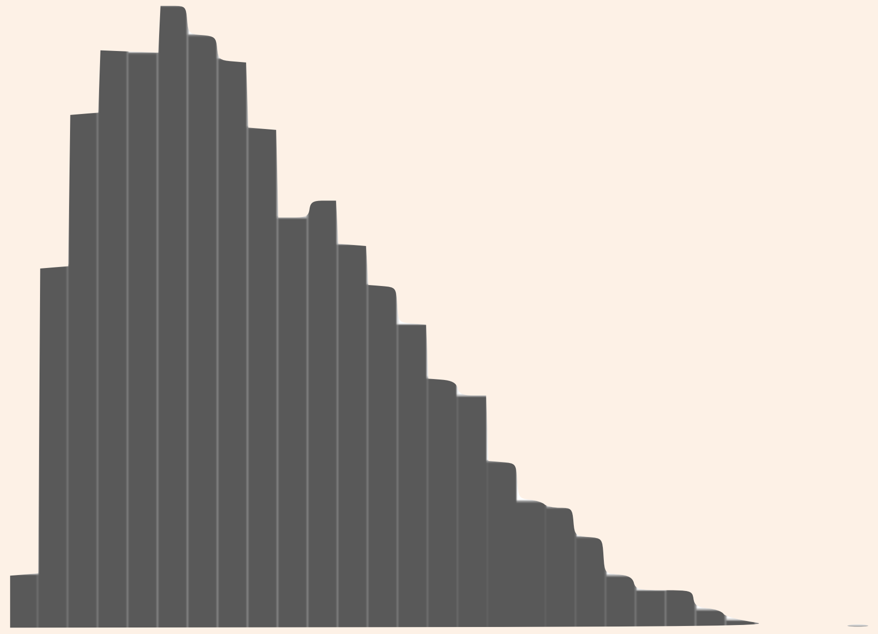

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👉 Symmetry does **not** help. (Choi & Kim, 2022)

Outline

- Setup and main challenge
- **Method: Rank-transformed subsampling**
- Applications
    - Hunt and test
    - Improving inference for double machine learning
    - Testing no direct effect in a sequentially randomized trial
- Future directions

Approach

$(T_n^{(1)}, \ldots, T_n^{(L)})$
under H_0

(1) Marginal: F_0 ✓

Main Challenge

(2) Copula: $C_{n,P}(u_1, \ldots, u_L) = \mathbb{P}\left(F_{n,P}(T_n^{(1)}) \leq u_1, \ldots, F_{n,P}(T_n^{(L)}) \leq u_L\right)$?

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👆 Estimate it **nonparametrically** with **subsampling**!

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$(\widetilde{T}_n^{(1)}, \ldots, \widetilde{T}_n^{(L)})$

Approach

$(T_n^{(1)}, \dots, T_n^{(L)})$ under H_0 $\begin{cases} \text{(1) Marginal: } F_0 \text{ ✅} \\ \text{(2) Copula: } C_{n,P}(u_1,\dots,u_L) = \mathbb{P}\left(F_{n,P}(T_n^{(1)}) \le u_1, \dots, F_{n,P}(T_n^{(L)}) \le u_L\right) \text{ ?} \end{cases}$

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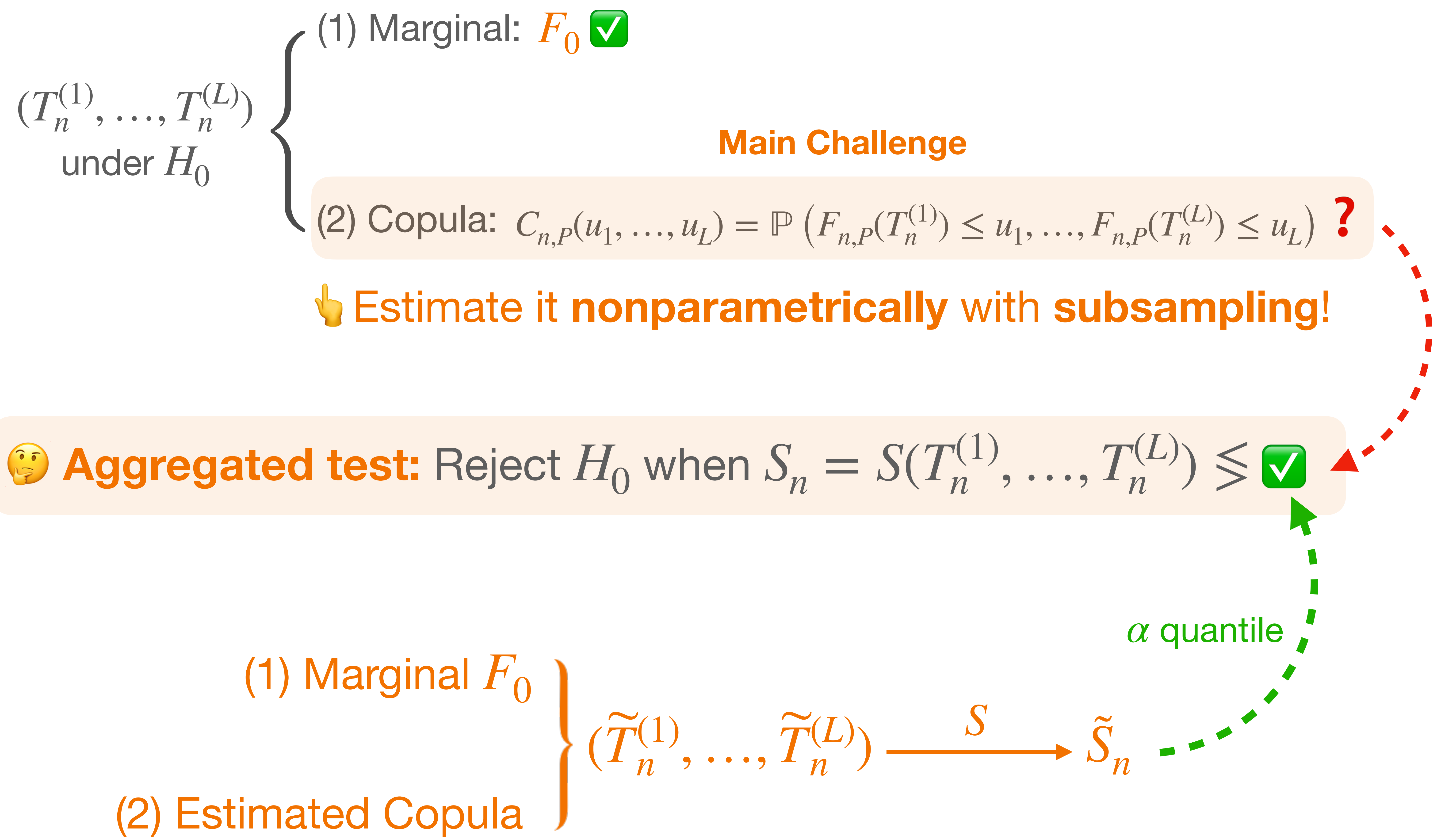
$$\left.\begin{array}{r} \text{(1) Marginal } F_0 \\ \\ \text{(2) Estimated Copula} \end{array}\right\} (\widetilde{T}_n^{(1)}, \dots, \widetilde{T}_n^{(L)}) \xrightarrow{S} \tilde{S}_n$$

Approach



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α quantile

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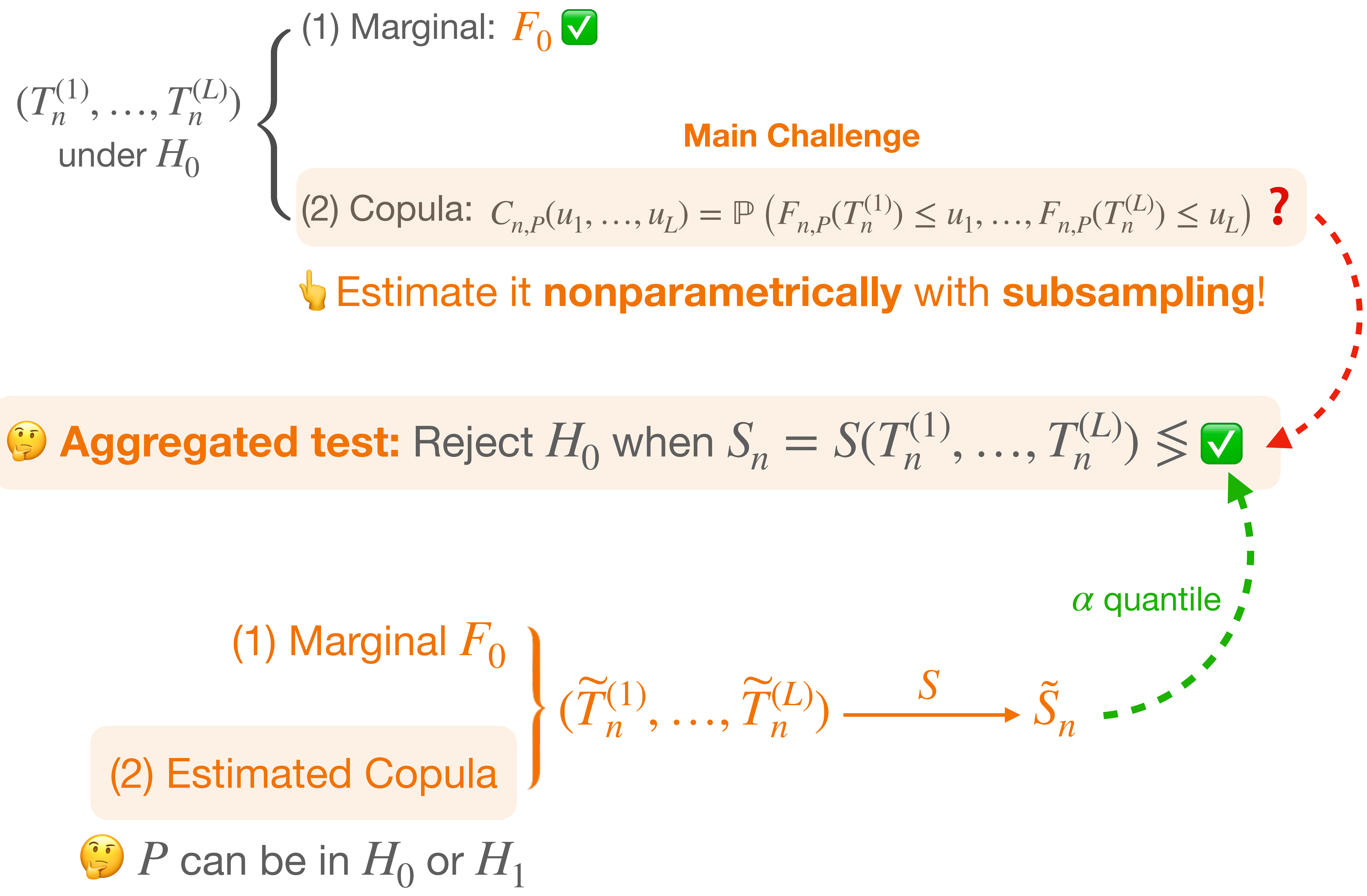
Approach



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α quantile

(1) Marginal F_0

(2) Estimated Copula

$(\widetilde{T}_n^{(1)}, \dots, \widetilde{T}_n^{(L)}) \xrightarrow{S} \tilde{S}_n$

🤔 P can be in H_0 or H_1

Rank-transformed subsampling

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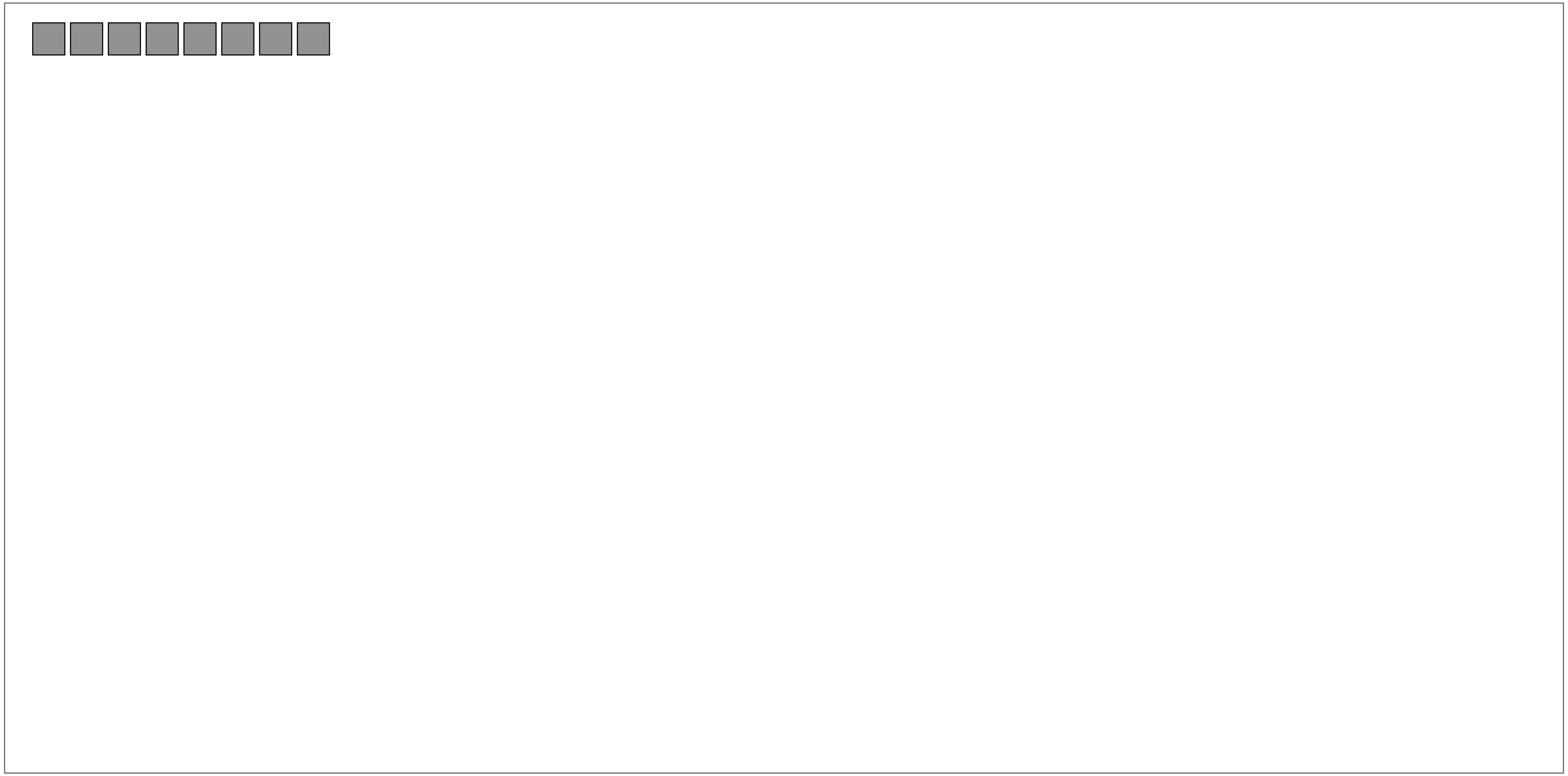
1. Randomly pick B subsamples of size $m = [n/\log n]$

Rank-transformed subsampling



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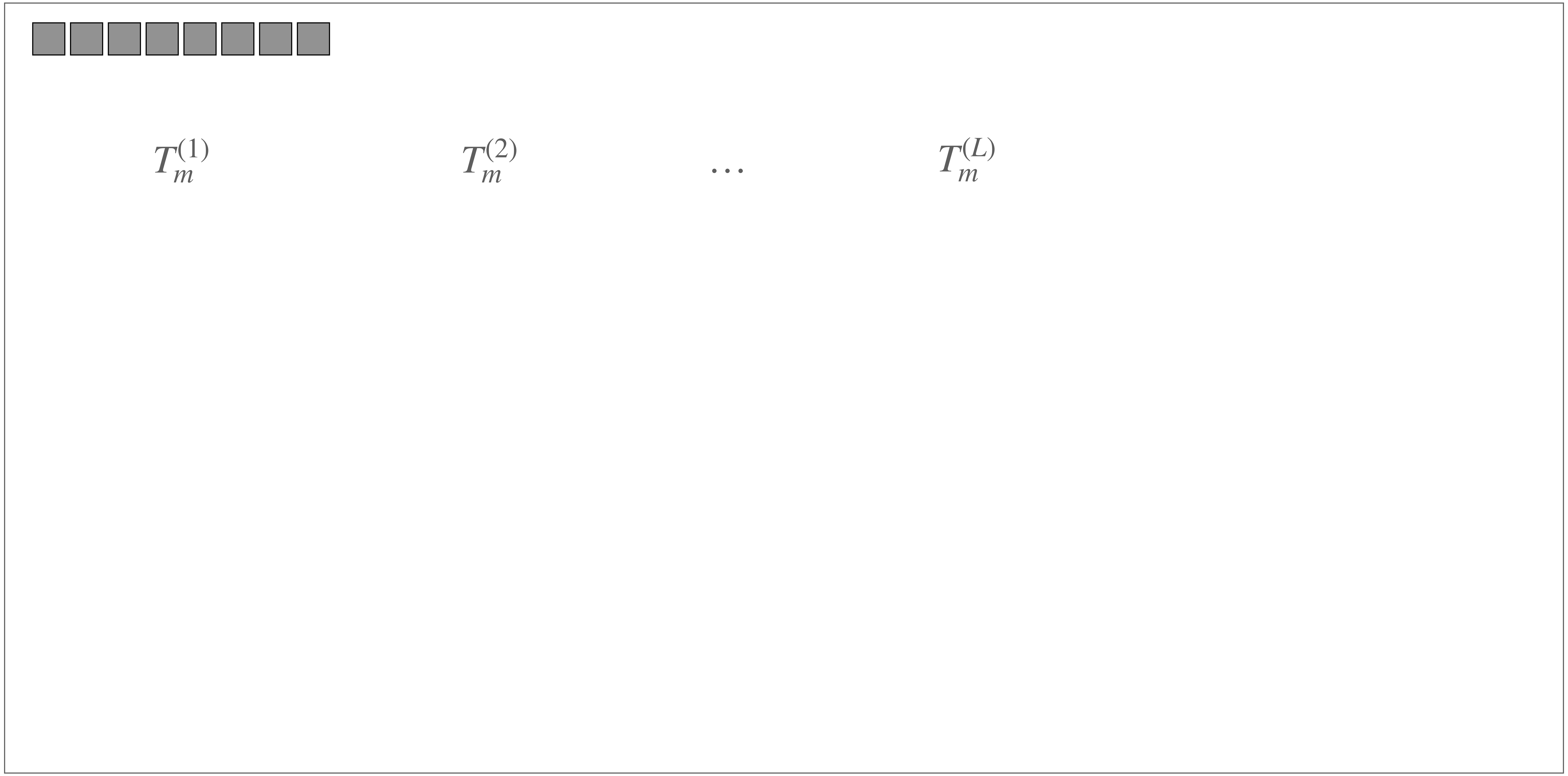

$T_m^{(1)}$ $T_m^{(2)}$ $\dots$ $T_m^{(L)}$

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2. Compute $(T_m^{(1)}, \dots, T_m^{(L)})$ for each subsample

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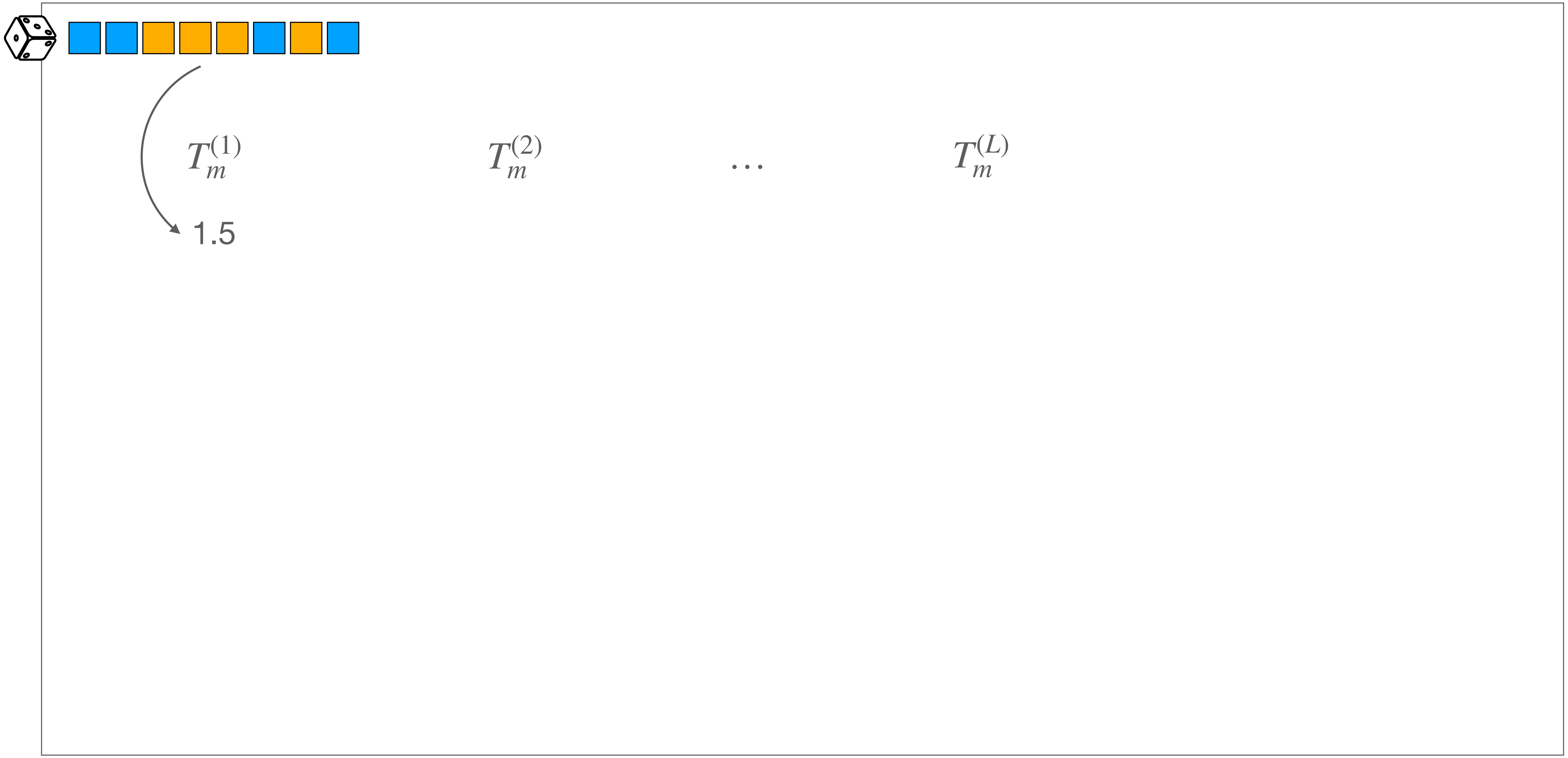

$T_m^{(1)}$ $T_m^{(2)}$ $\dots$ $T_m^{(L)}$

1.5

1. Randomly pick B subsamples of size $m = [n/\log n]$
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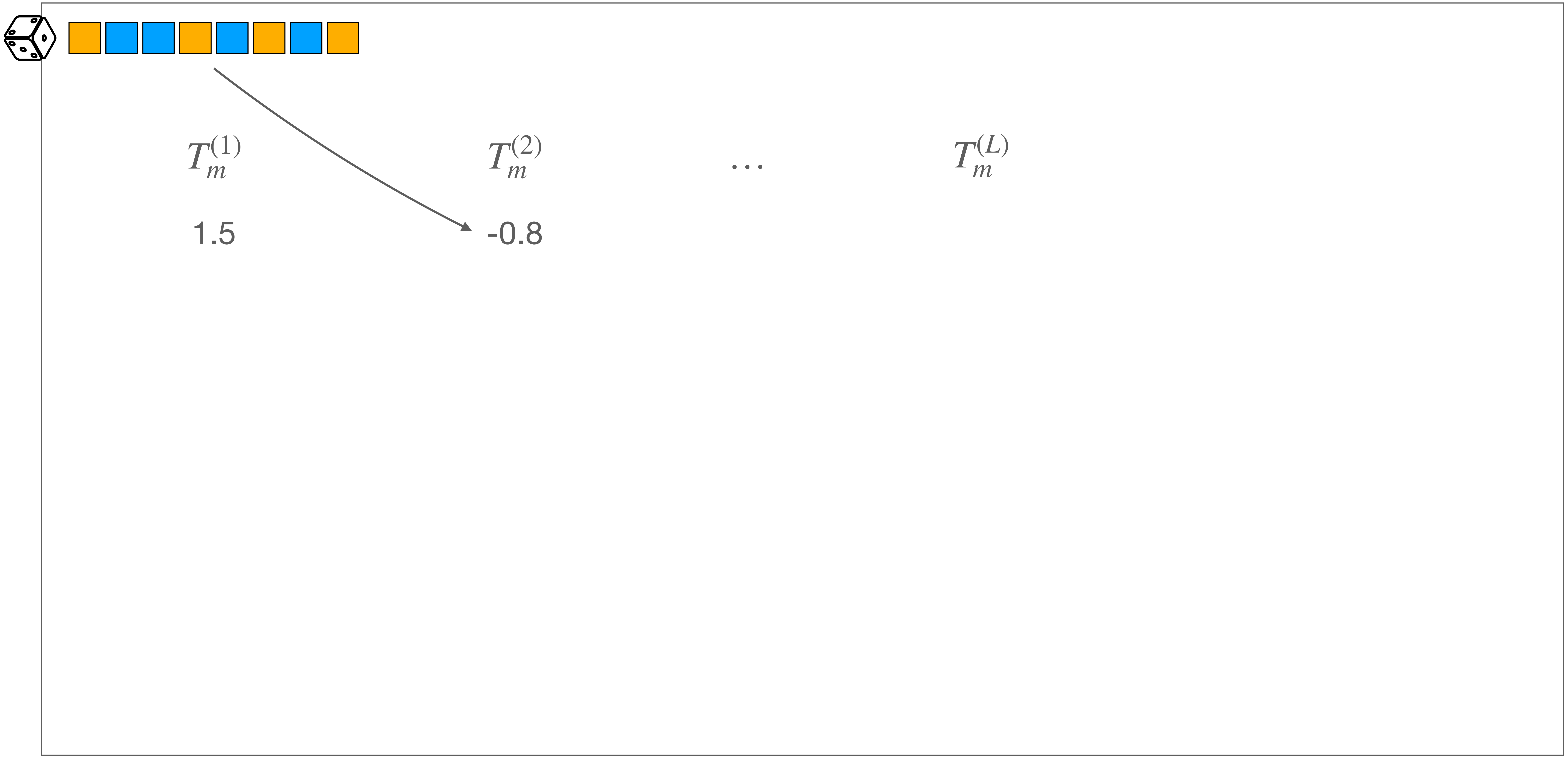
Rank-transformed subsampling



$T_m^{(1)}$ $T_m^{(2)}$ $\dots$ $T_m^{(L)}$

1.5 -0.8

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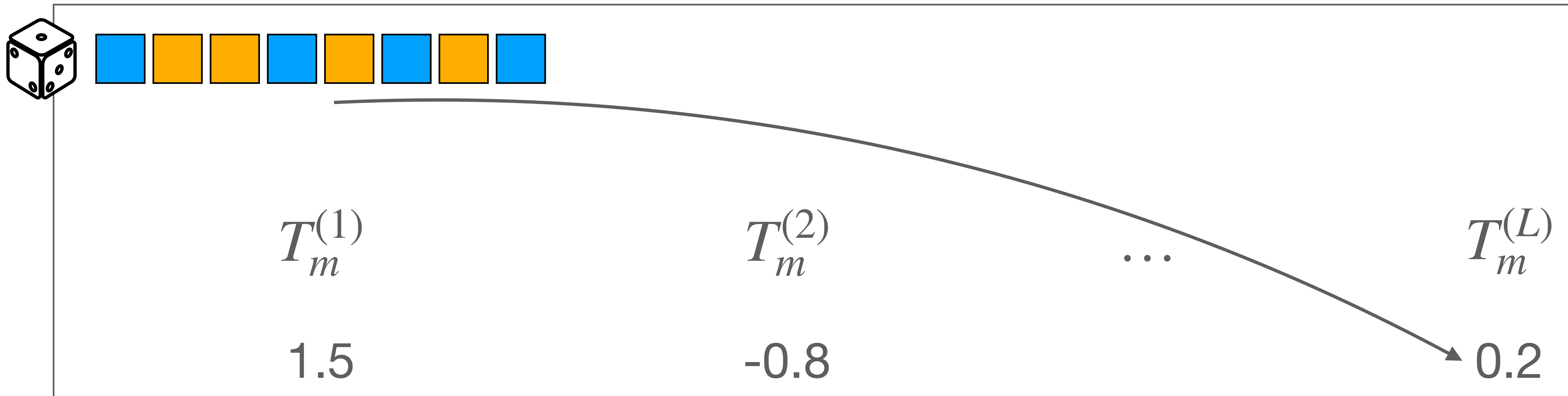

$T_m^{(1)}$ $T_m^{(2)}$ $\dots$ $T_m^{(L)}$

1.5 -0.8 0.2

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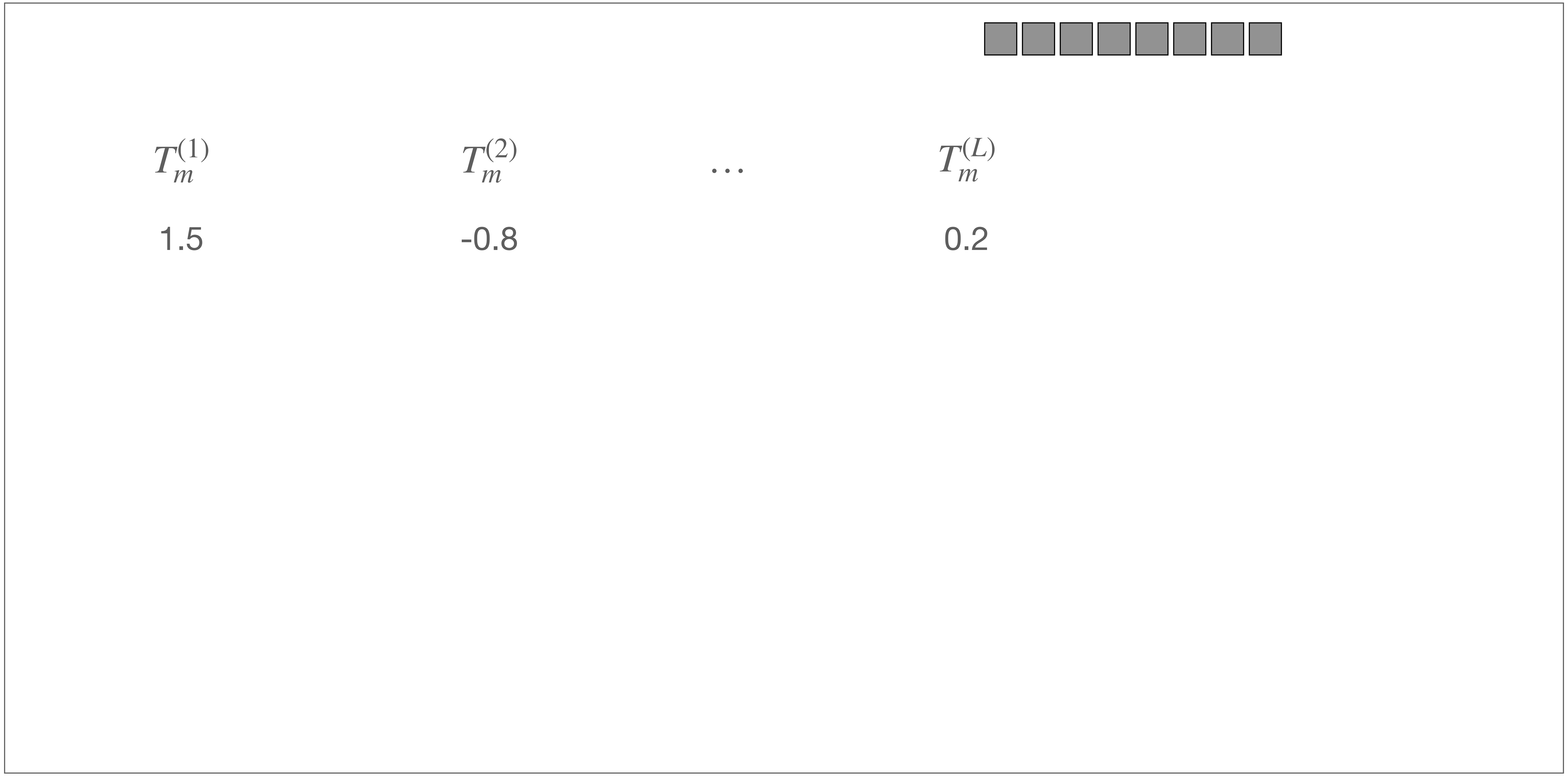

$T_m^{(1)}$	$T_m^{(2)}$	$\dots$	$T_m^{(L)}$
1.5	-0.8		0.2

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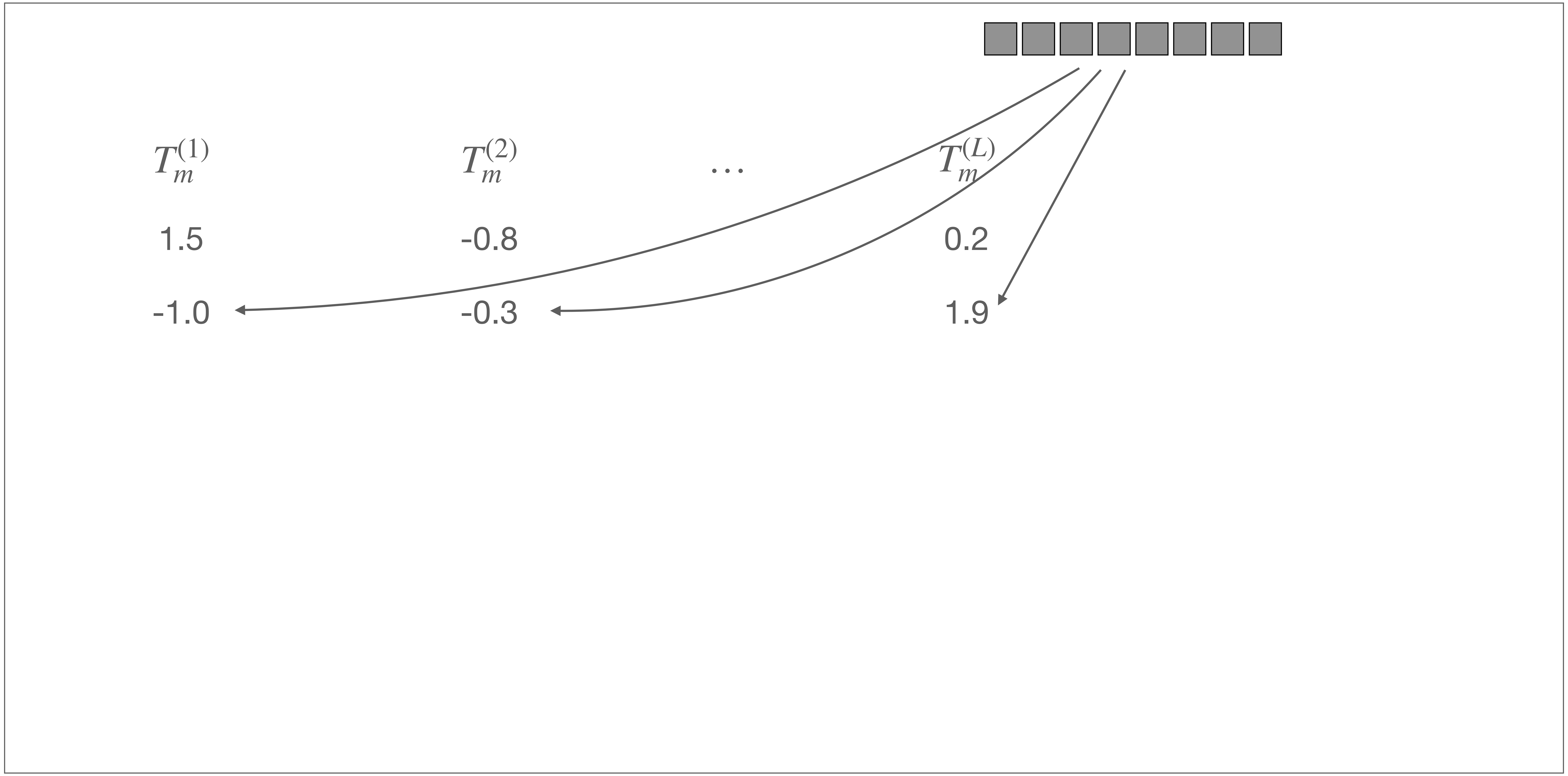

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$T_m^{(1)}$	$T_m^{(2)}$	$\dots$	$T_m^{(L)}$
1.5	-0.8		0.2
-1.0	-0.3		1.9

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2. Compute $(T_m^{(1)}, \dots, T_m^{(L)})$ for each subsample

Rank-transformed subsampling

$T_m^{(1)}$	$T_m^{(2)}$	$\dots$	$T_m^{(L)}$
1.5	-0.8		0.2
-1.0	-0.3		1.9
$\vdots$	$\vdots$		$\vdots$
2.7	0.1		3.0

B rows

L columns

1. Randomly pick B subsamples of size $m = [n/\log n]$
2. Compute $(T_m^{(1)}, \dots, T_m^{(L)})$ for each subsample

Rank-transformed subsampling

$$\begin{array}{c|cccc} & T_m^{(1)} & T_m^{(2)} & \dots & T_m^{(L)} \\ \hline & 1.5 & -0.8 & & 0.2 \\ & -1.0 & -0.3 & & 1.9 \\ \begin{array}{c} B \\ \text{rows} \end{array} & & & & \\ & \vdots & \vdots & & \vdots \\ & 2.7 & 0.1 & & 3.0 \end{array}$$

L columns

1. Randomly pick B subsamples of size $m = [n/\log n]$
2. Compute $(T_m^{(1)}, \dots, T_m^{(L)})$ for each subsample
3. In this $B \times L$ matrix, replace each entry by its rank

Rank-transformed subsampling

$$\begin{array}{c|cccc} & T_m^{(1)} & T_m^{(2)} & \cdots & T_m^{(L)} \\ \hline & 933 & 212 & & 580 \\ & 158 & 380 & & 971 \\ B \text{ rows} & \vdots & \vdots & & \vdots \\ & 990 & 539 & & 998 \end{array}$$

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Rank-transformed subsampling

$$
\begin{array}{c|cccc}
 & T_m^{(1)} & T_m^{(2)} & \cdots & T_m^{(L)} \\
\hline
 & 0.993 & 0.212 & & 0.580 \\
 & 0.158 & 0.380 & & 0.971 \\
B \text{ rows} & & & & \\
 & \vdots & \vdots & & \vdots \\
 & 0.990 & 0.539 & & 0.998
\end{array}
$$

L columns

1. Randomly pick B subsamples of size $m = [n/\log n]$
2. Compute $(T_m^{(1)}, \ldots, T_m^{(L)})$ for each subsample
3. In this $B \times L$ matrix, replace each entry by its rank
4. Normalize the ranks

(Copula estimate)

Rank-transformed subsampling

$$\begin{array}{c|cccc} & \widetilde{T}_m^{(1)} & \widetilde{T}_m^{(2)} & \cdots & \widetilde{T}_m^{(L)} \\ \hline & 1.6 & -0.8 & & 0.1 \\ & -1.1 & -0.2 & & 1.8 \\ B \text{ rows} & \vdots & \vdots & & \vdots \\ & 2.7 & 0.2 & & 2.8 \end{array}$$

L columns

1. Randomly pick B subsamples of size $m = [n/\log n]$
2. Compute $(T_m^{(1)}, \ldots, T_m^{(L)})$ for each subsample
3. In this $B \times L$ matrix, replace each entry by its rank
4. Normalize the ranks

   (Copula estimate)
5. Apply F_0^{-1} entry-wise

   (Enforce the margin)

Rank-transformed subsampling

$$\begin{array}{c|cccc|cc}
 & \widetilde{T}_m^{(1)} & \widetilde{T}_m^{(2)} & \dots & \widetilde{T}_m^{(L)} & \xrightarrow{S} & \tilde{S}_n \\
 & 1.6 & -0.8 & & 0.1 & & 0.5 \\
 & -1.1 & -0.2 & & 1.8 & & -0.1 \\
B \text{ rows} & \vdots & \vdots & & \vdots & & \vdots \\
 & 2.7 & 0.2 & & 2.8 & & 1.2
\end{array}$$

L columns

1. Randomly pick B subsamples of size $m = [n/\log n]$
2. Compute $(T_m^{(1)}, \dots, T_m^{(L)})$ for each subsample
3. In this $B \times L$ matrix, replace each entry by its rank
4. Normalize the ranks **(Copula estimate)**
5. Apply F_0^{-1} entry-wise **(Enforce the margin)**
6. Aggregate

Rank-transformed subsampling

$$\begin{array}{c|cccc|c}
 & & & & & ✅ \\
 & \widetilde{T}_m^{(1)} & \widetilde{T}_m^{(2)} & \cdots & \widetilde{T}_m^{(L)} & \tilde{S}_n \\
 & 1.6 & -0.8 & & 0.1 & 0.5 \\
 & -1.1 & -0.2 & & 1.8 & -0.1 \\
B \text{ rows} & & & & & \\
 & \vdots & \vdots & & \vdots & \vdots \\
 & 2.7 & 0.2 & & 2.8 & 1.2
\end{array}$$

L columns

1. Randomly pick B subsamples of size $m = [n/\log n]$
2. Compute $(T_m^{(1)}, \ldots, T_m^{(L)})$ for each subsample
3. In this $B \times L$ matrix, replace each entry by its rank
4. Normalize the ranks **(Copula estimate)**
5. Apply F_0^{-1} entry-wise **(Enforce the margin)**
6. Aggregate
7. Use upper α quantile of $\tilde{S}_n$ as critical value

Rank-transformed subsampling: under H_0

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$L = 2$, $F_0 =$ unif$(0,1)$

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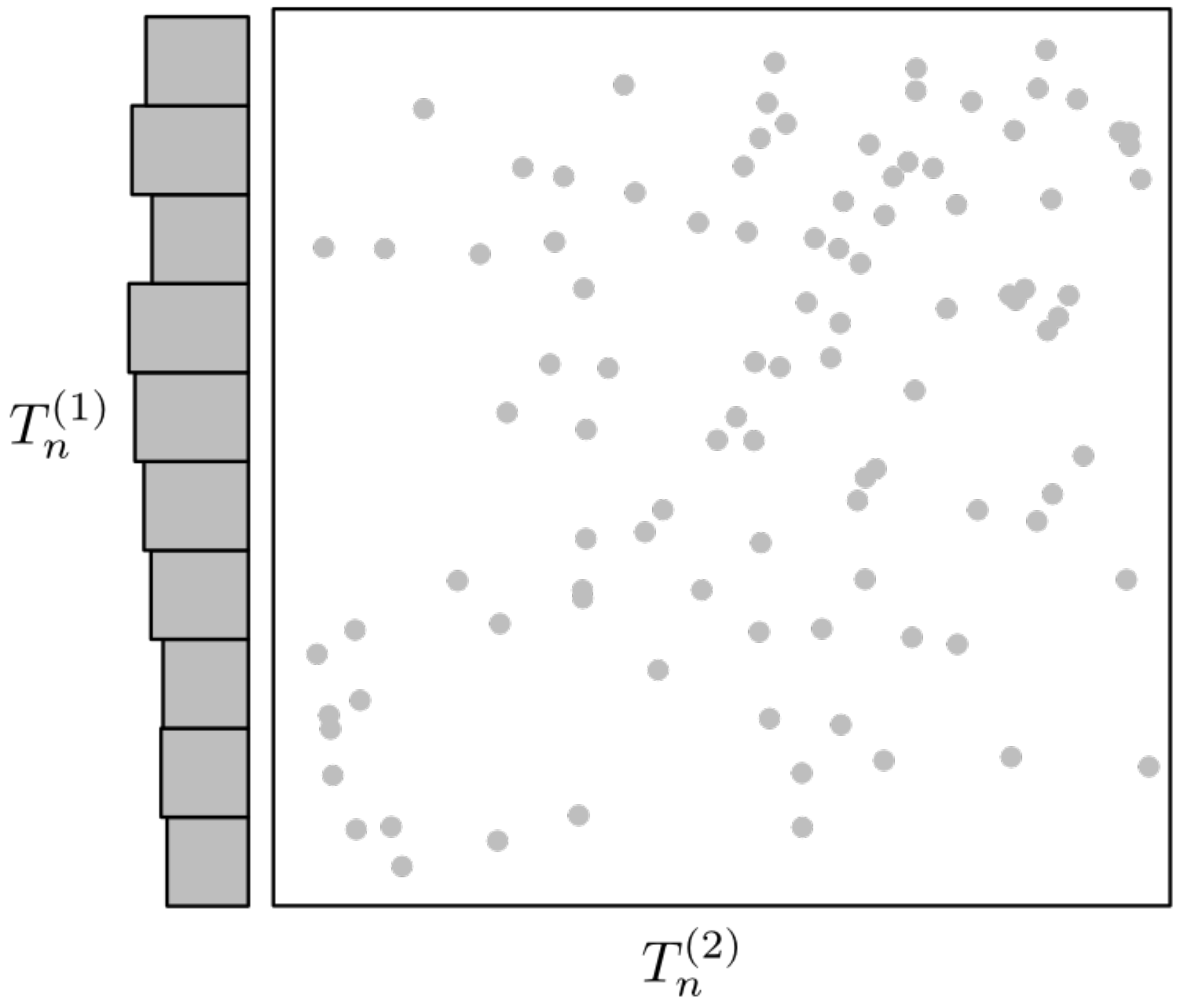

before rank transform

Rank-transformed subsampling: under H_0

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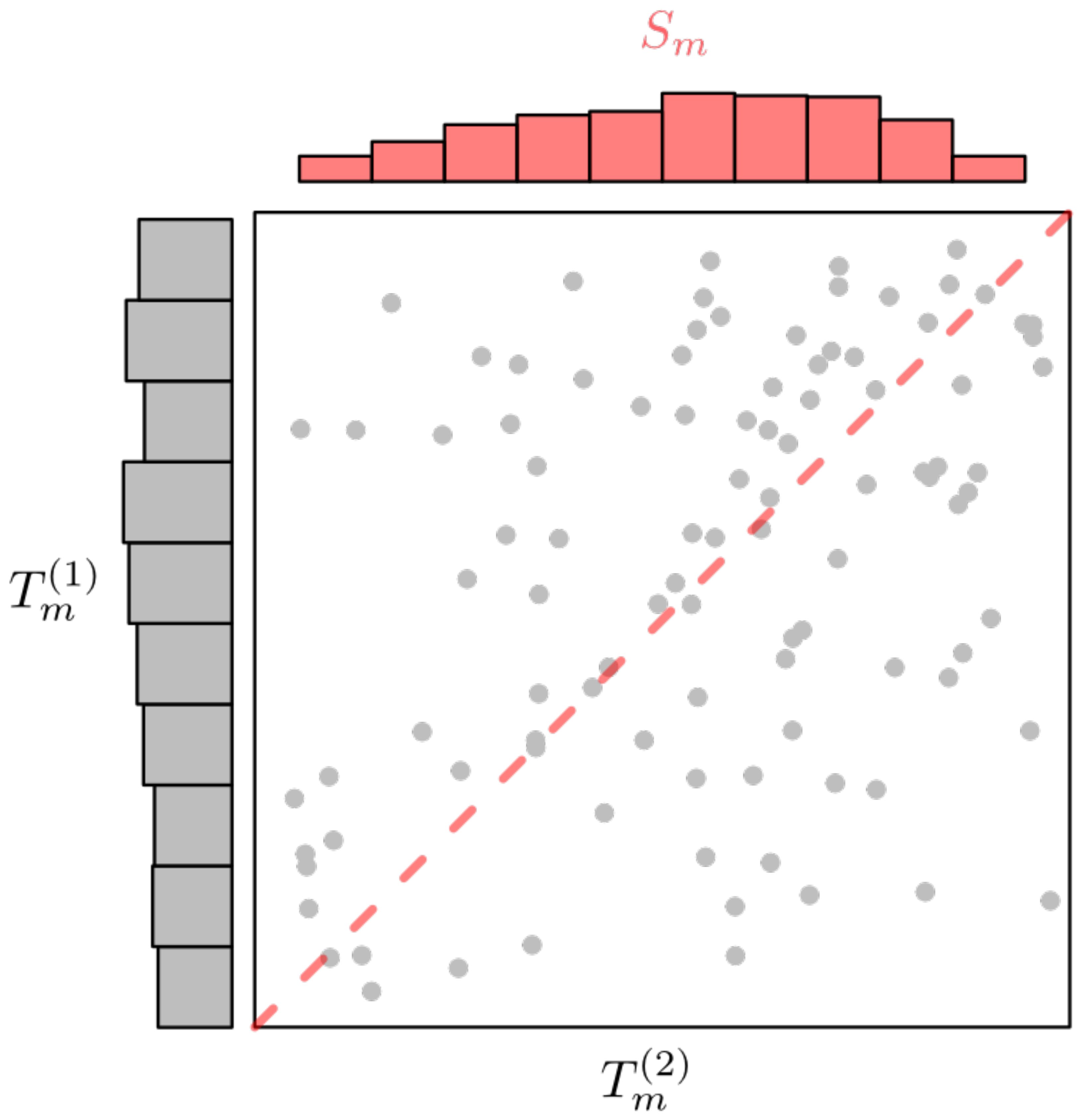
$S =$ avg



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Rank-transformed subsampling: under H_0

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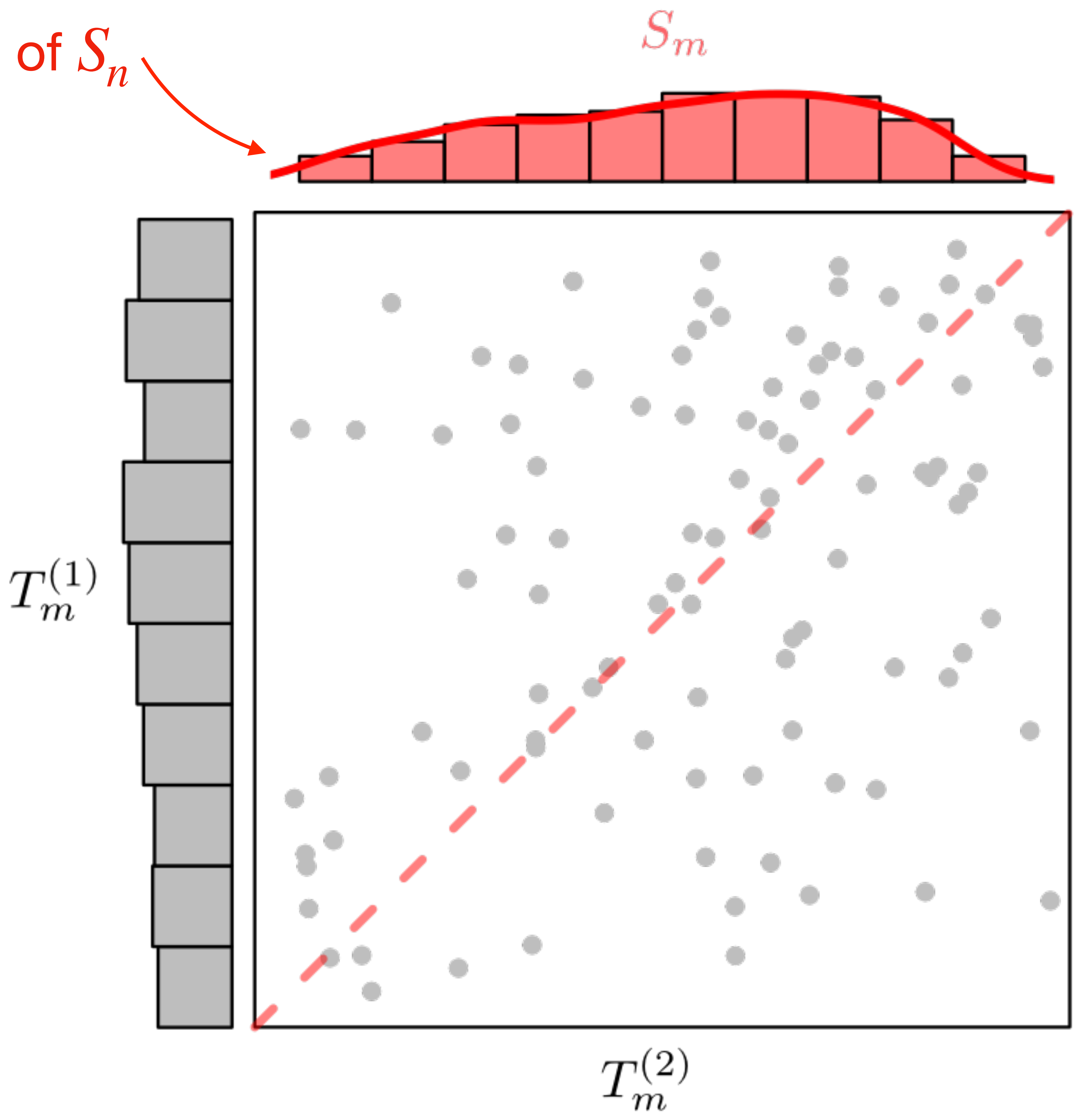
Null distribution of S_n



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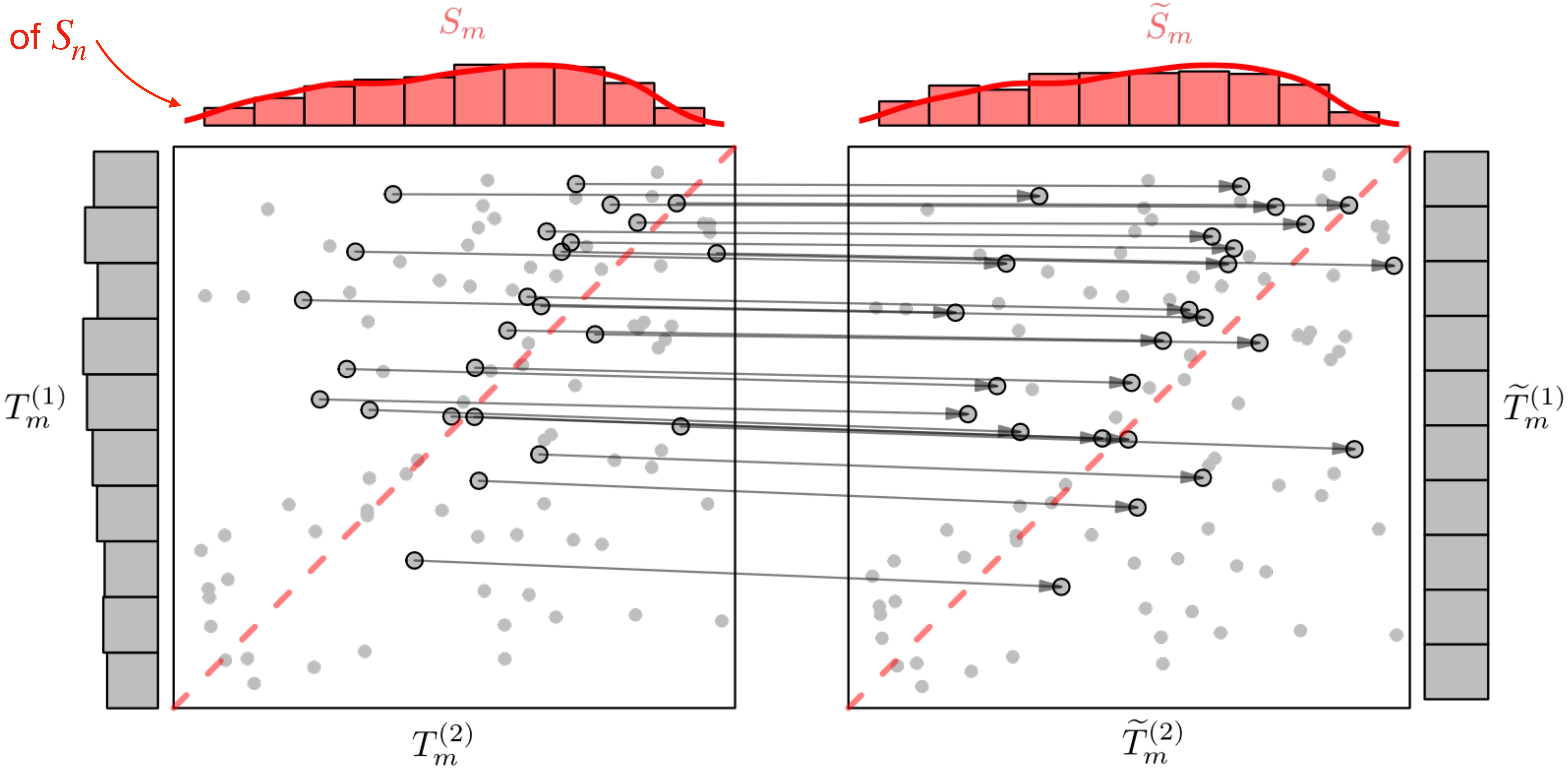

before rank transform

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Theory: under H_0

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A1. For $P \in H_0$, $T_n(X;\Omega) \to_d F_0 \in \{\text{unif}(0,1), \mathcal{N}(0,1)\}$ as $n \to \infty$.

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Then, under A1, our test is pointwise asymptotically level α.

✅ **Not conservative**

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Theorem Suppose $S(\cdot)$ is symmetric and Lipschitz. Suppose the aggregated S_n has a continuous asymptotic law under H_0.
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Further, if T_n and S_n converge to their respective limit distributions uniformly over H_0, then our test is uniformly asymptotic level α.

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Rank-transformed subsampling: Local alternative

$L = 2$, $F_0 = \text{unif}(0,1)$

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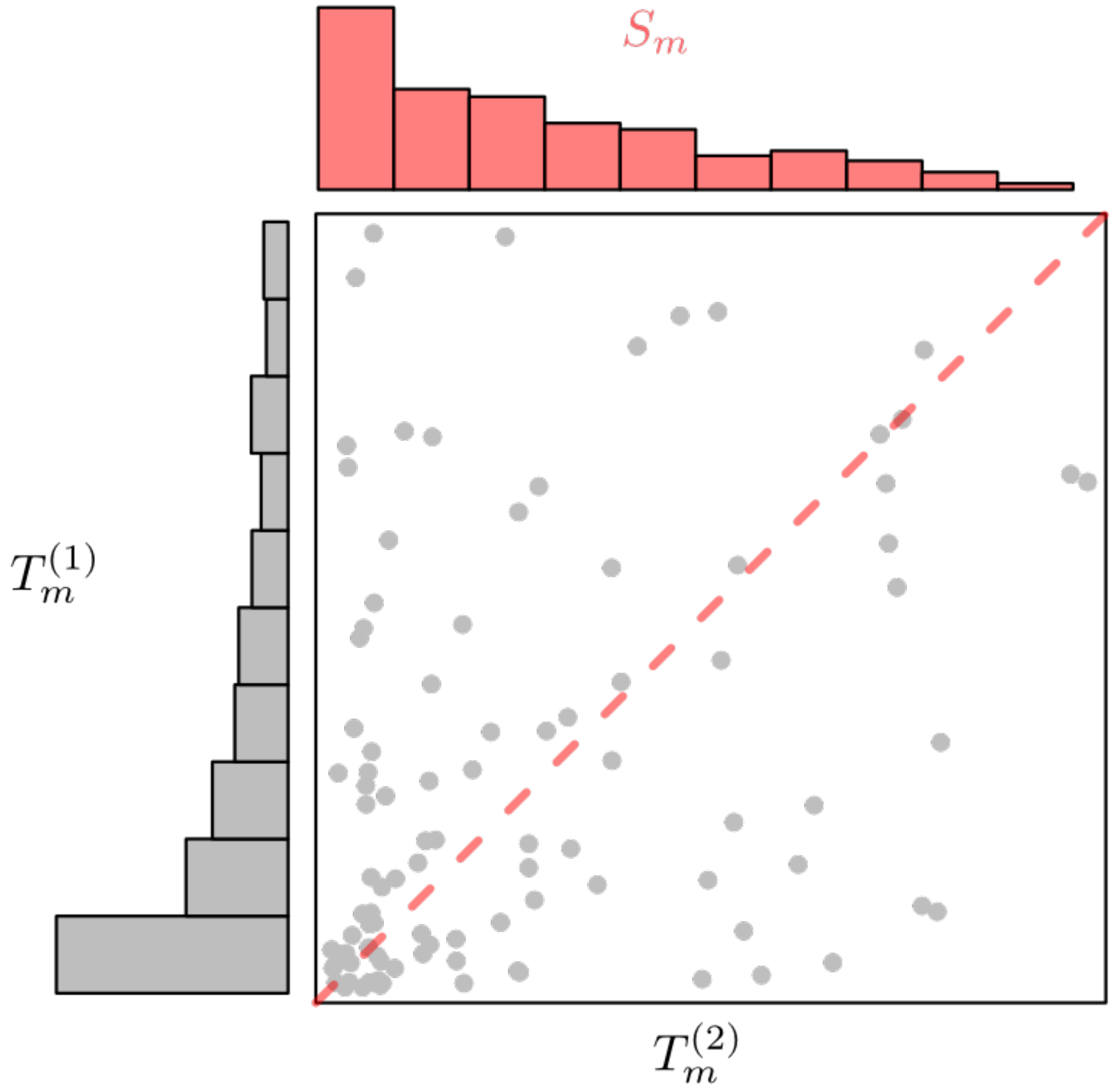

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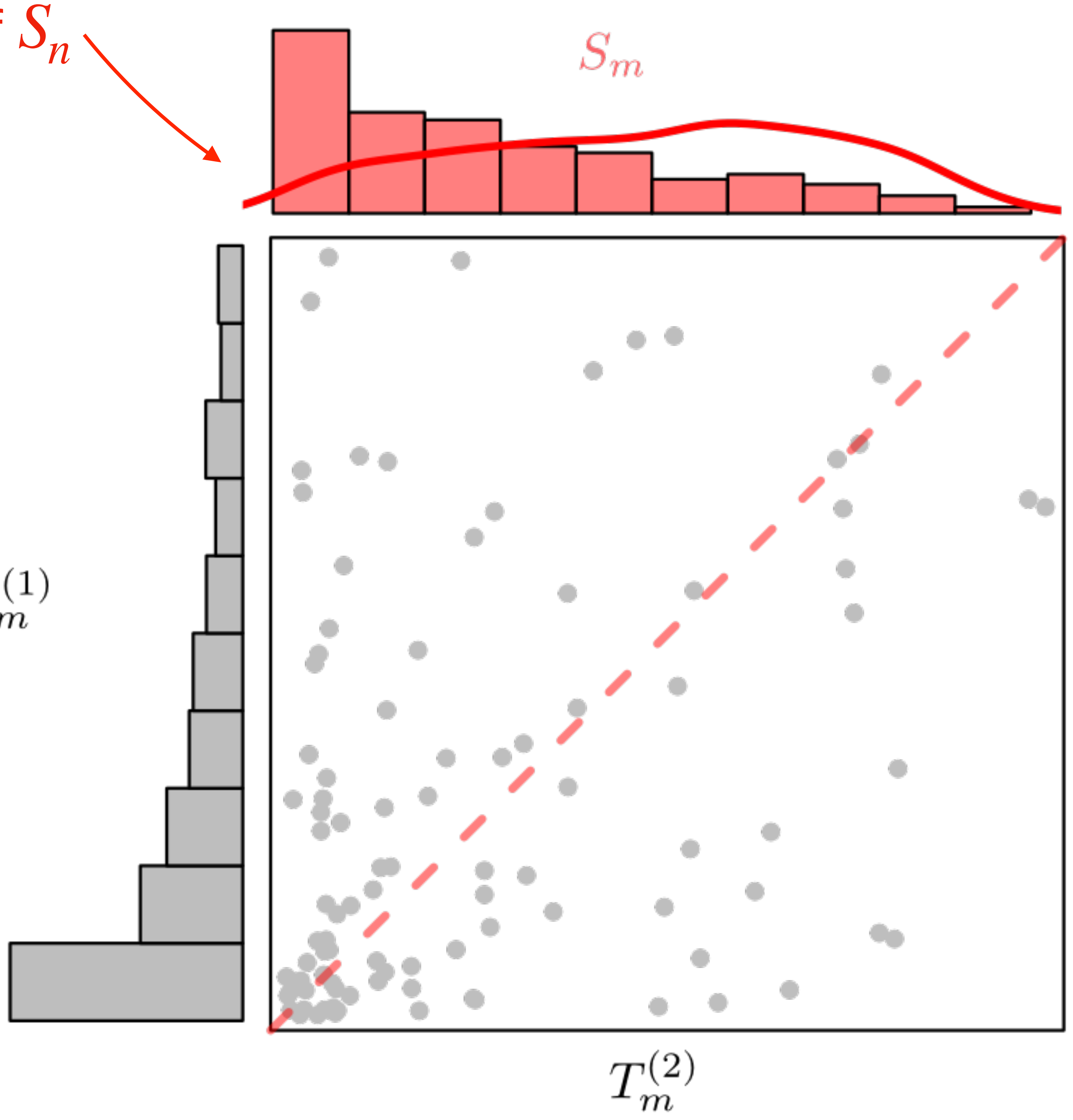

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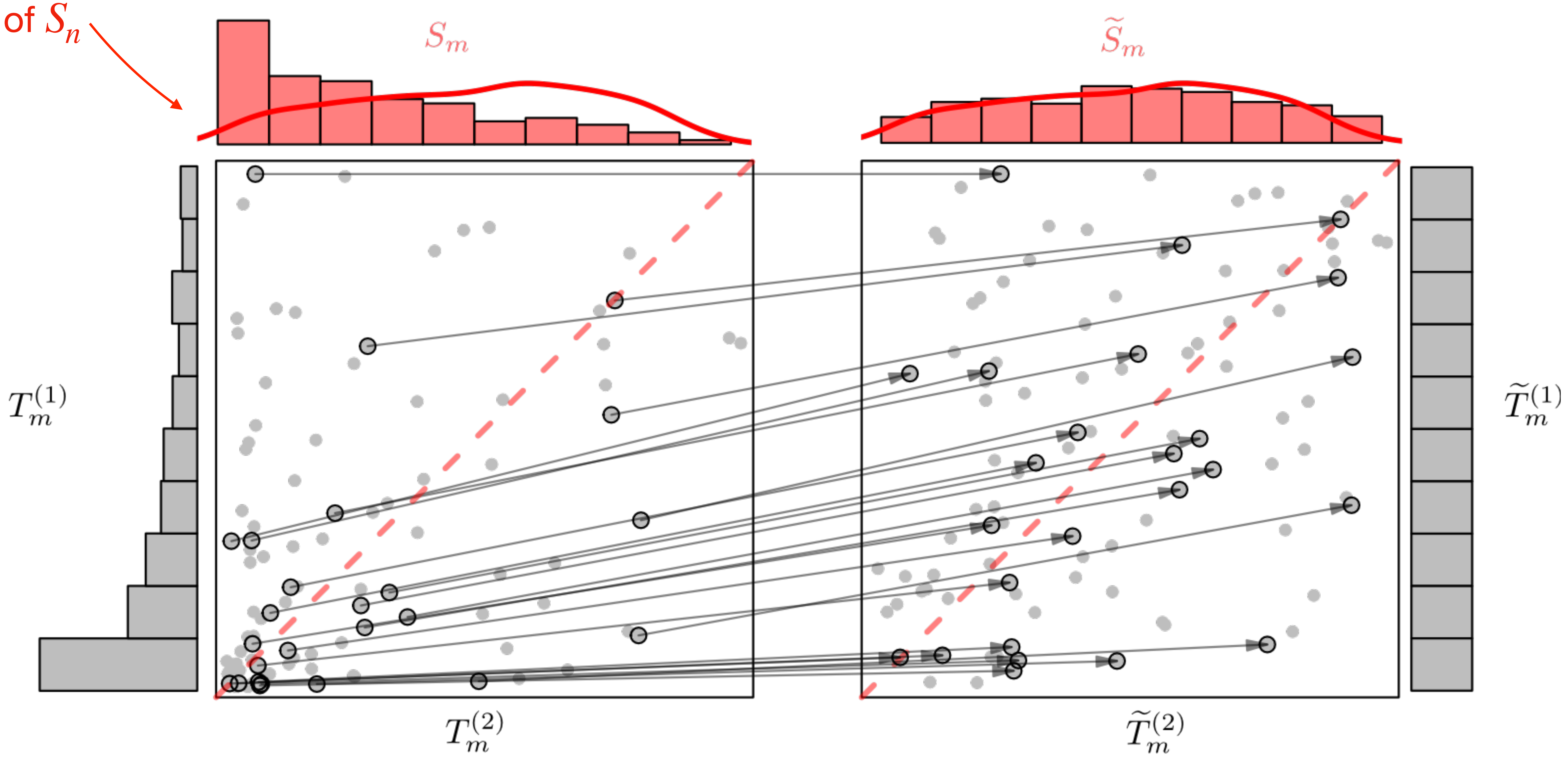

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Rank-transformed subsampling: Local alternative

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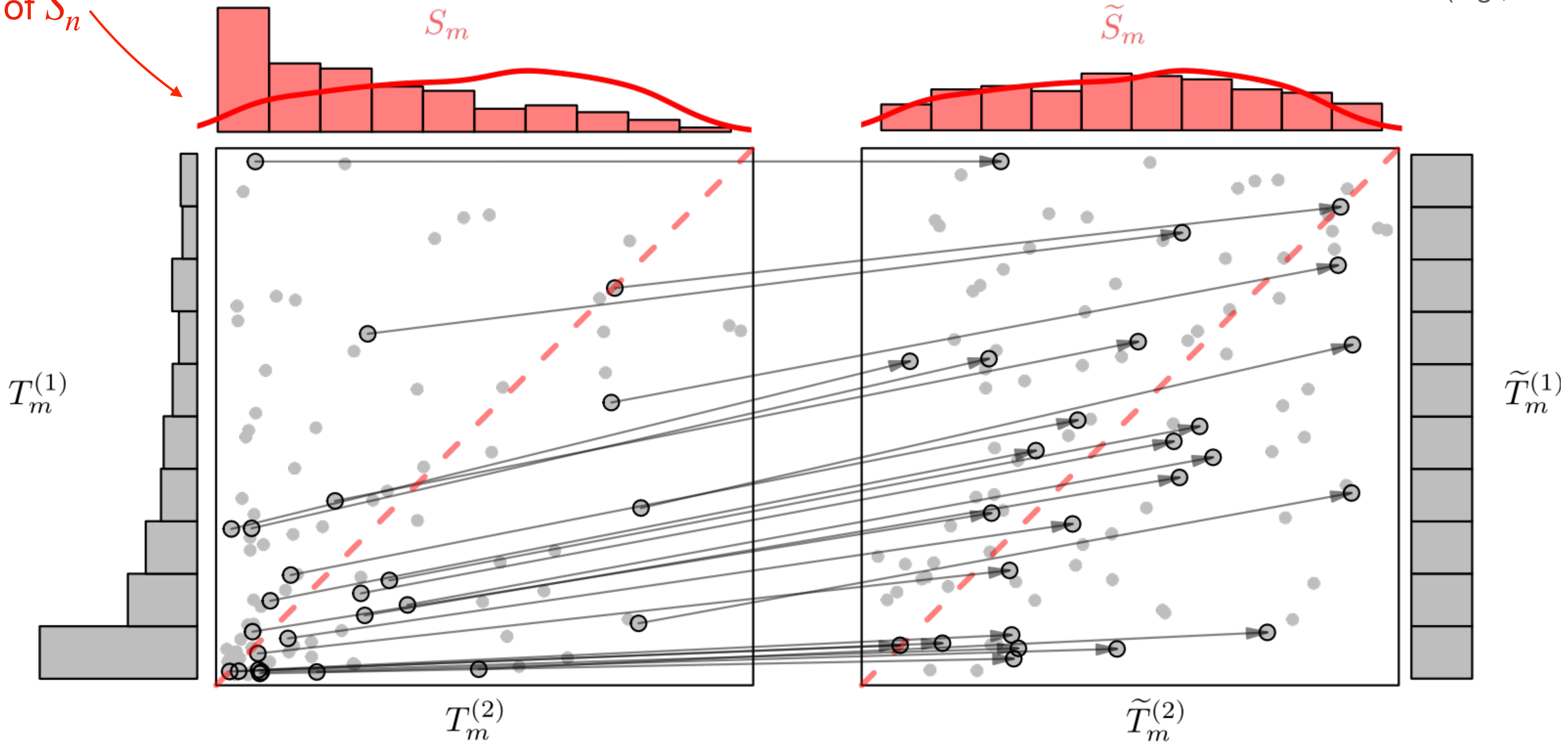
💡 **Intuition:** copula under the null ≈ copula under local alternatives

(e.g., Le Cam's 3rd Lemma)

Null distribution of S_n



before rank transform

after rank transform

Theory: Local power

Theory: Local power

Theorem (informal) Fix $P_0 \in H_0$.

If the copula of $(T_n^{(1)}, \ldots, T_n^{(L)})$ converges in a locally uniform fashion at P_0, then for P_0's local alternatives,

| Power(our test) - Power(oracle test) | $\to 0,$

where the oracle test has access to S_n's null distribution under P_0.

💡 For example, when Le Cam's 3rd lemma is applicable to $(T_n^{(1)}, \ldots, T_n^{(L)})$.

Outline

- Setup and main challenge
- Method: Rank-transformed subsampling
- Applications
  - **Hunt and test**
  - Improving inference for double machine learning
  - Testing no direct effect in a sequentially randomized trial
- Future directions

Hunt and test

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👉 Test hypothesis of the form $H_0 = \cap_d H_0(d)$, where each $H_0(d)$ is relatively easy to test.

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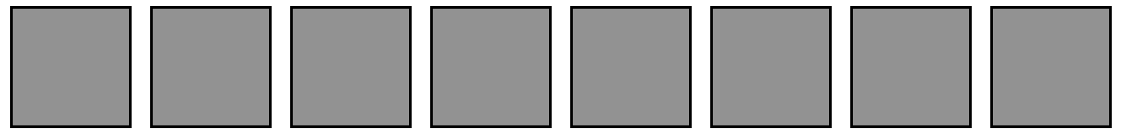

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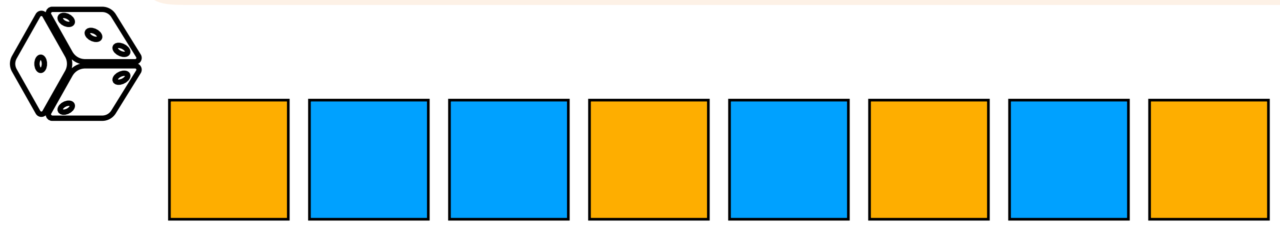

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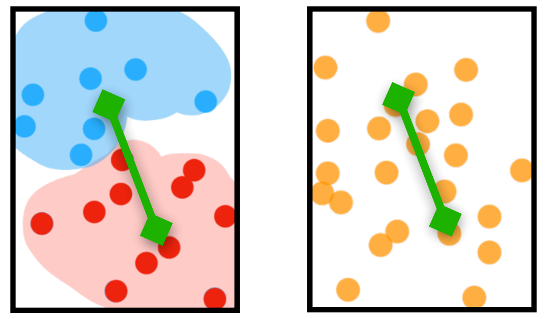
(1) Find $\hat{d}$ by running 2-means on 🟦🟦🟦🟦 .

(2) Compute T_n := dip test p-value on 🟧🟧🟧🟧.

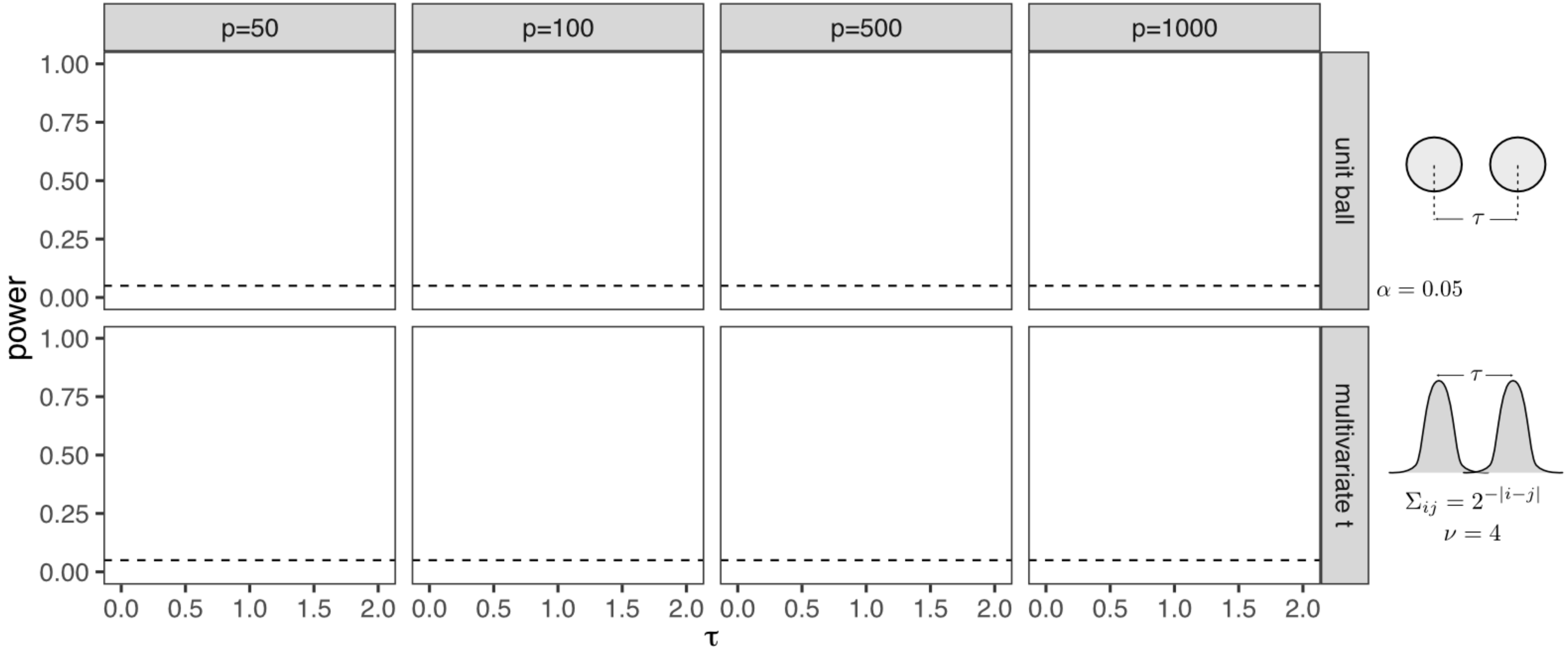
Cheng, M-Y., and Peter Hall. "Calibrating the excess mass and dip tests of modality." JRSS-B (1998)



⚠️ Low power

Hunt and test: Detecting cancer subtypes

Simulation in $\mathbb{R}^p$



Hunt and test: Detecting cancer subtypes

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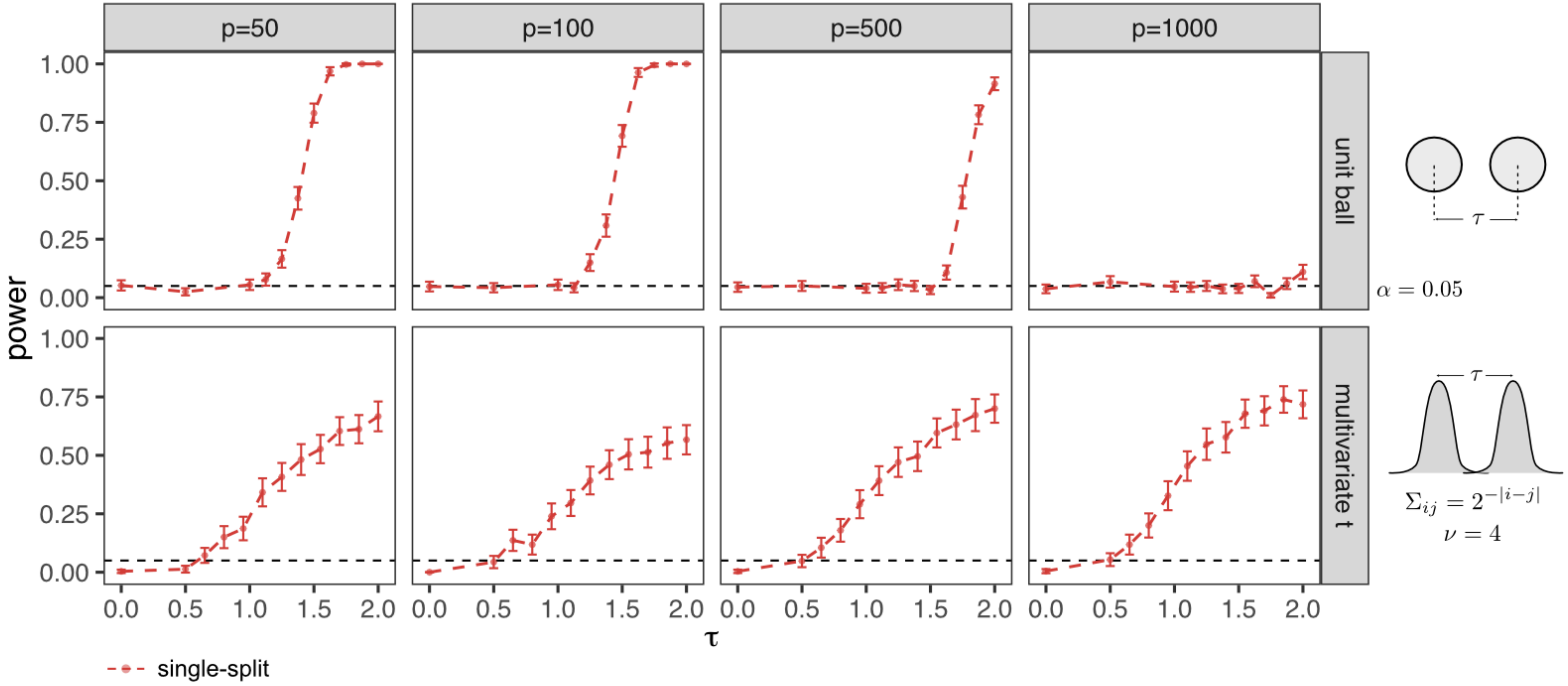

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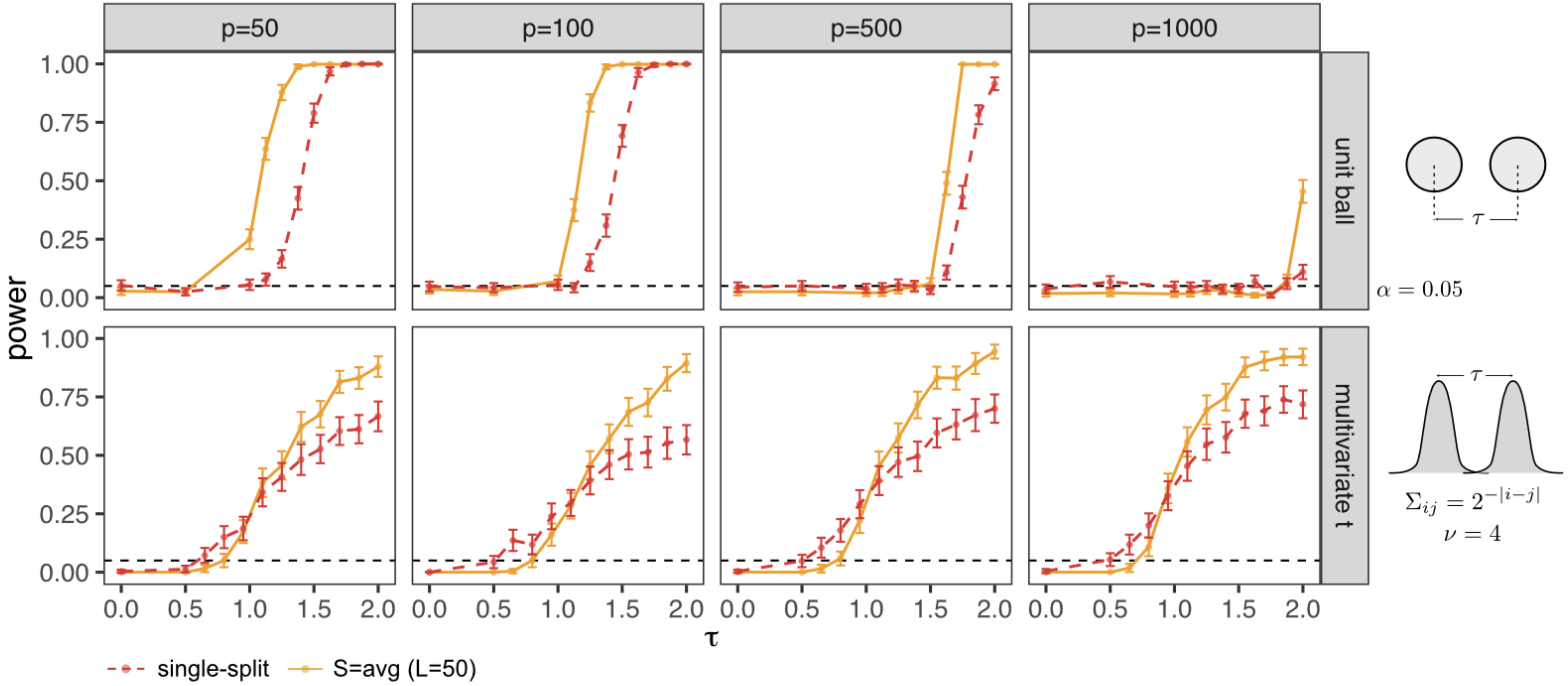

- Rank-transform subsampling maintains the correct level and significantly improves power.

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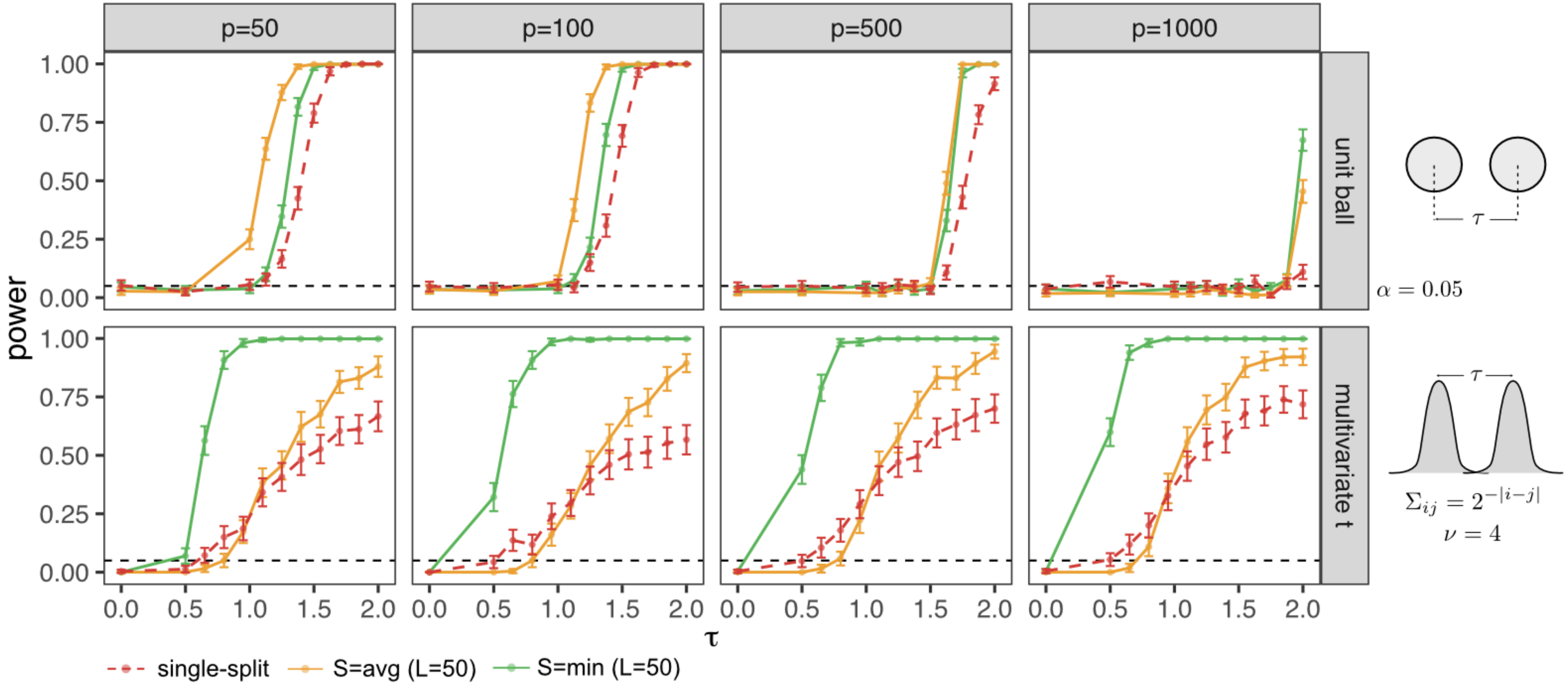

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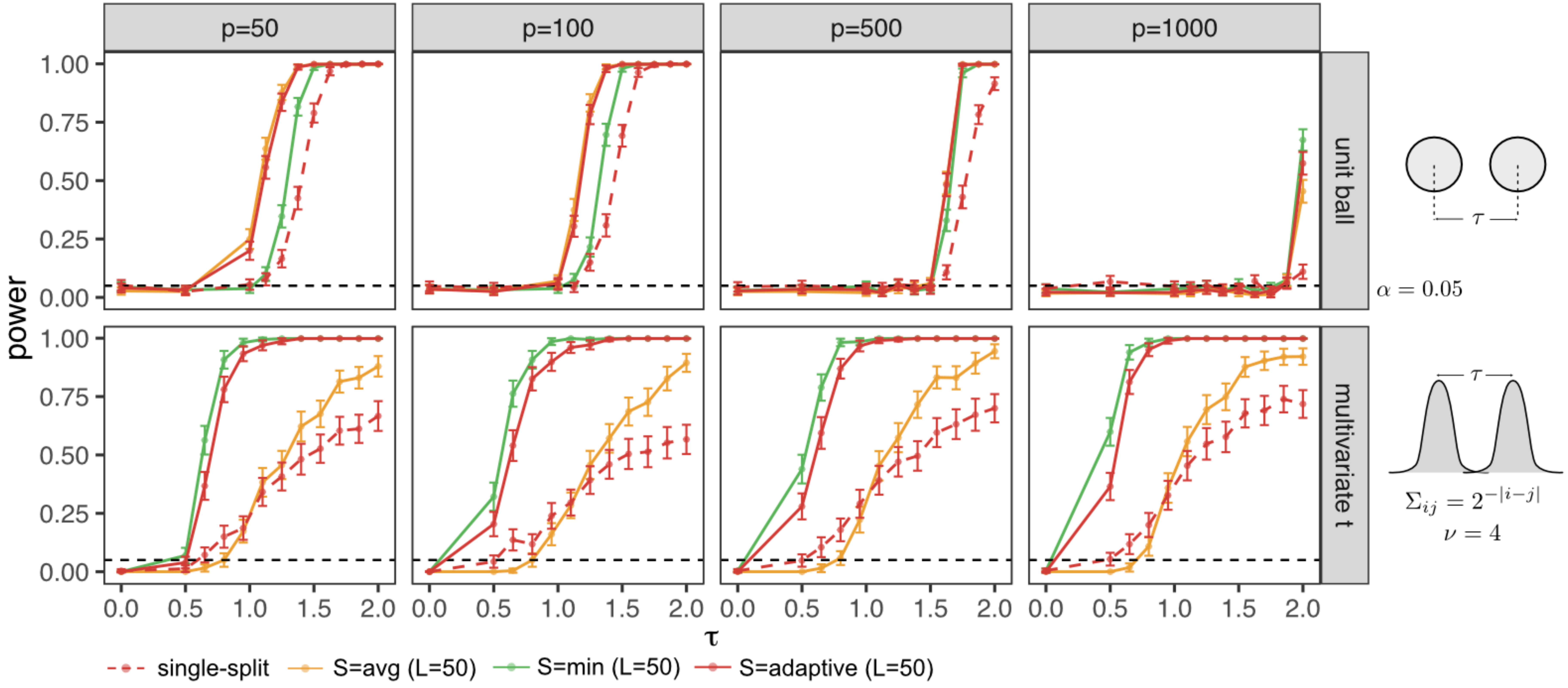

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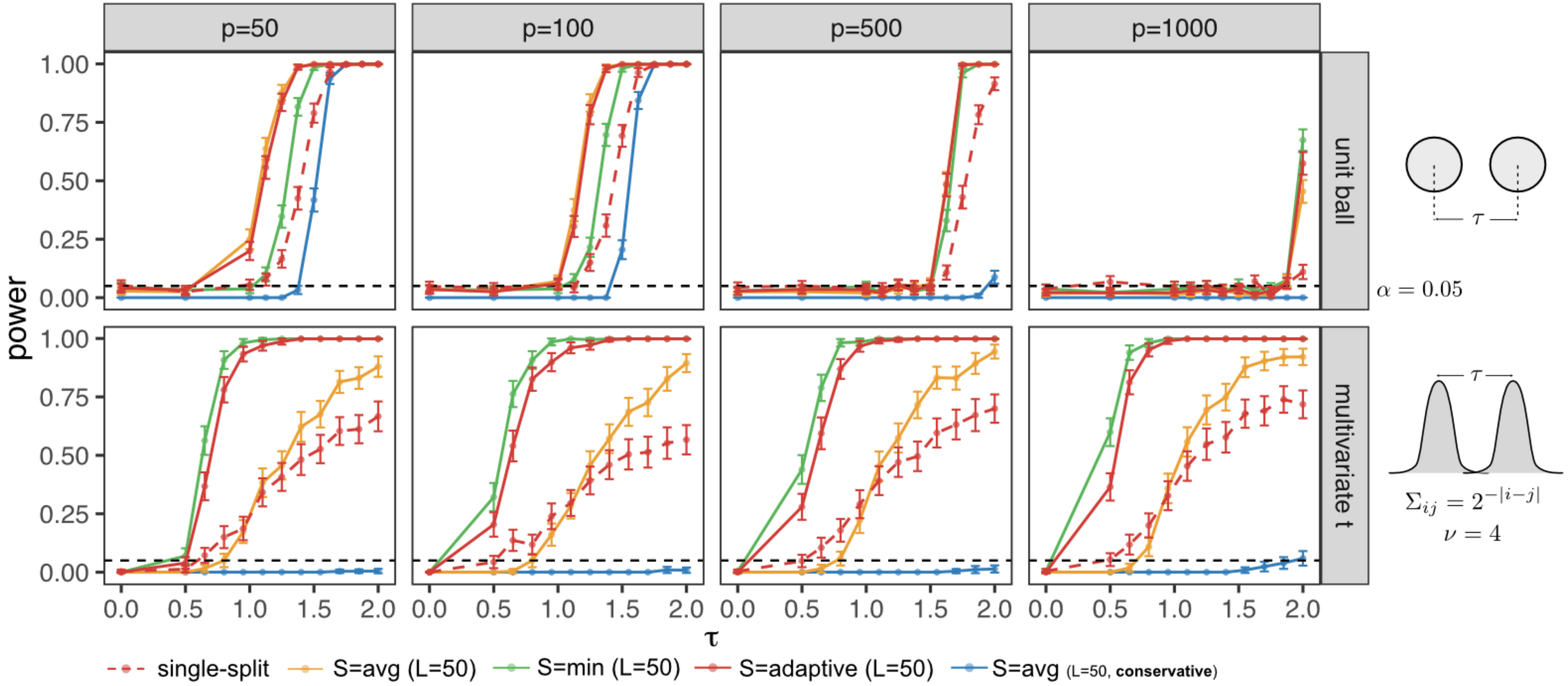

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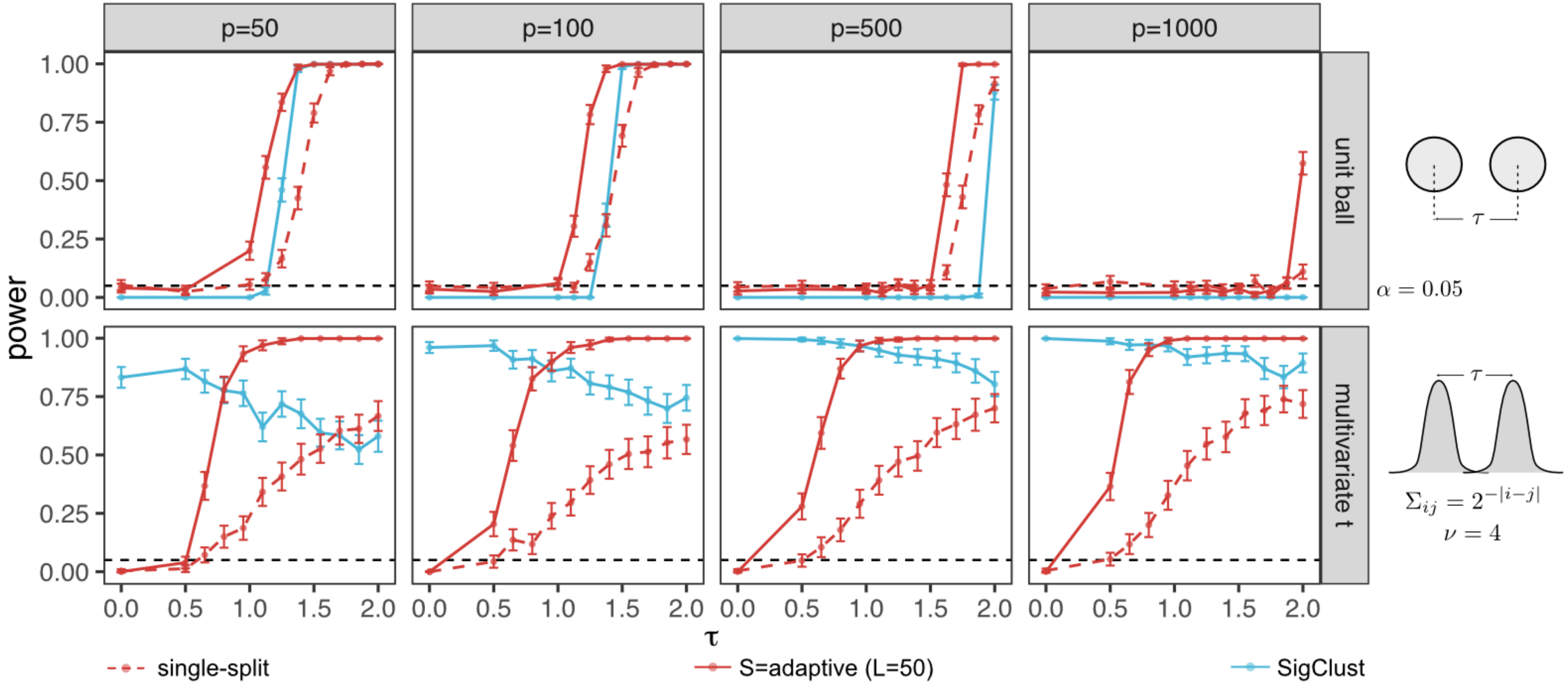

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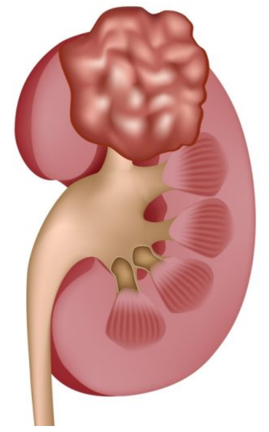
- Conservatively averaged p-value is not competitive.
- SigClust: for unit balls, it loses power as p increases; for multivariate t, it does not control type-I error.

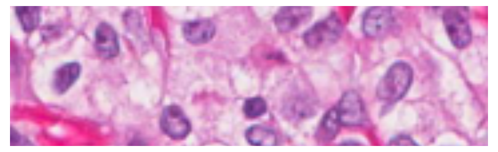
Yufeng Liu, David Neil Hayes, Andrew Nobel, and J. S Marron.
Statistical significance of clustering for high-dimension, low–sample size data.
Journal of the American Statistical Association (2008).
https://CRAN.R-project.org/package=sigclust

Hunt and test: Detecting cancer subtypes

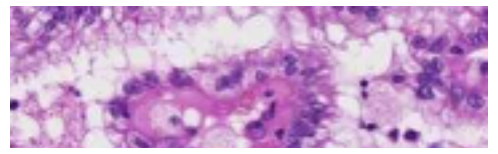
ICGC/TCGA Pan-Cancer dataset



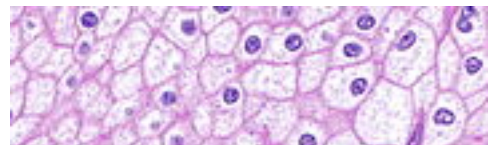
111 Kidney Cancer
(Renal Cell Carcinoma)
Cases



37 Clear Cell (cc)



31 Papillary (P)



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Hunt and test: Detecting cancer subtypes

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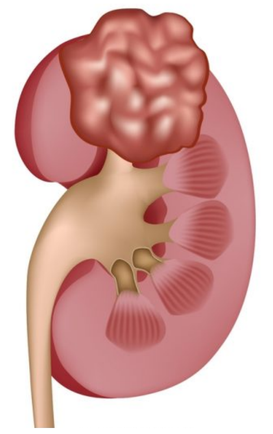

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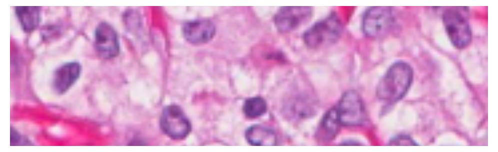

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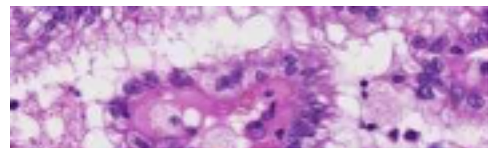

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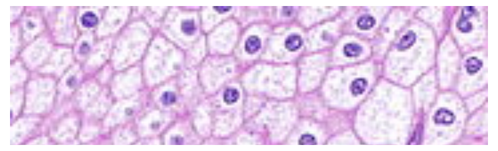

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Selected 1000 genes by comparing to control

	Gene 1	**Gene 2**	**Gene 3**	**...**
Cell 1	-1.2	0.5	6.2	
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⋮				

Normalized mRNA expression

Hunt and test: Detecting cancer subtypes

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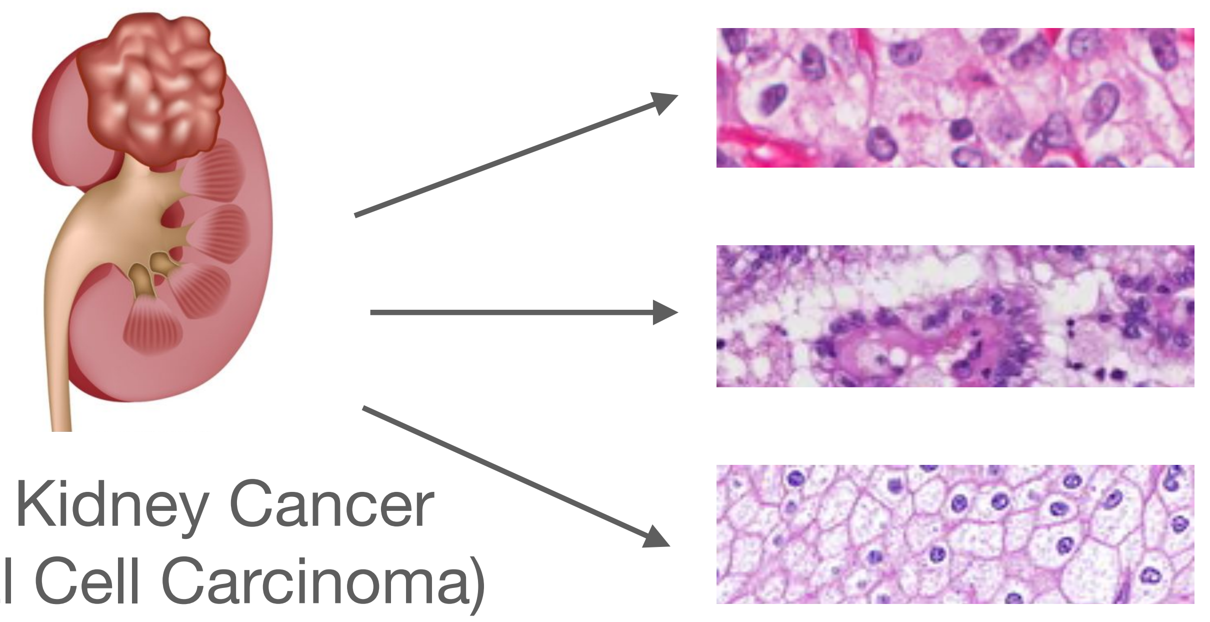

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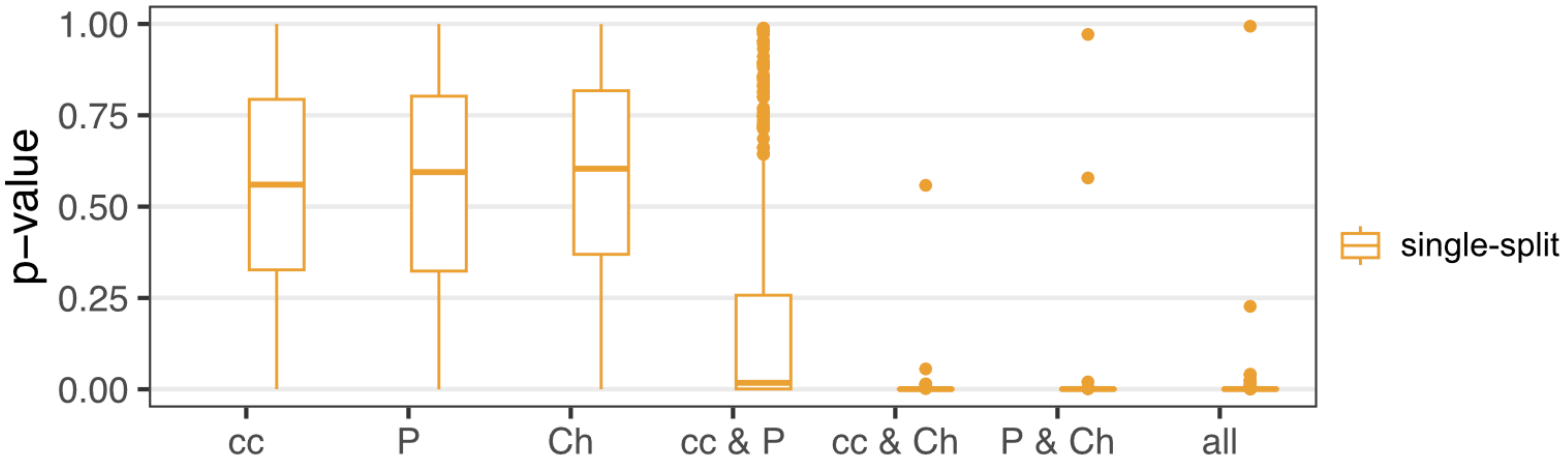

Hunt and test: Detecting cancer subtypes

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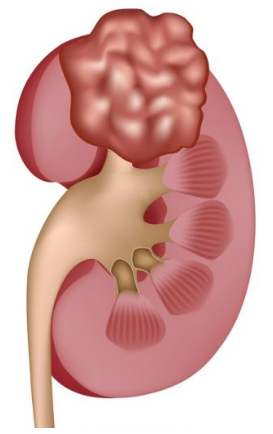

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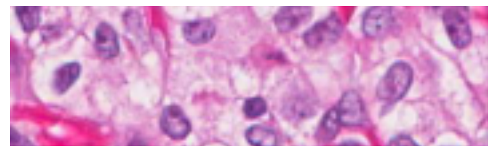

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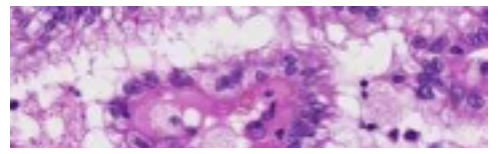

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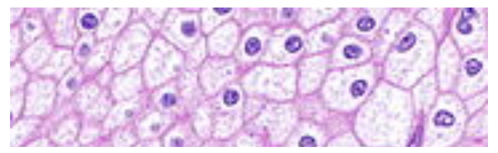

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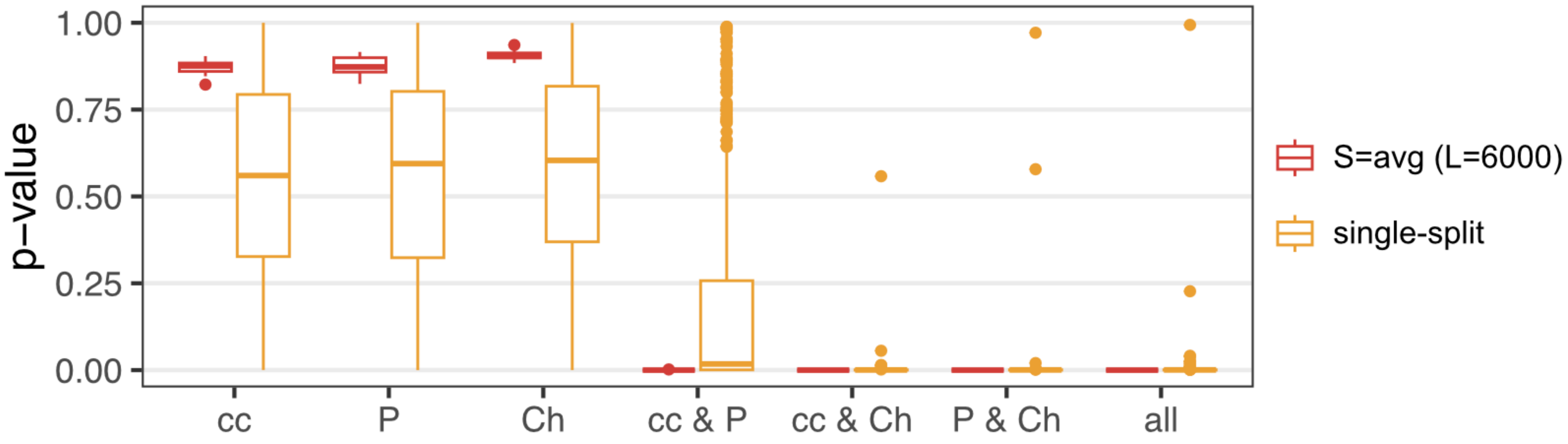

Hunt and test: Detecting cancer subtypes

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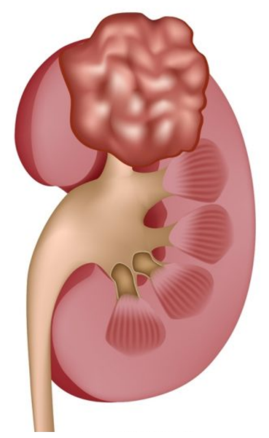

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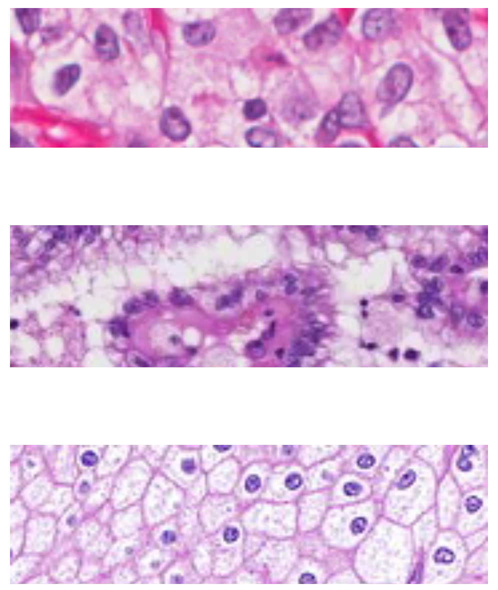

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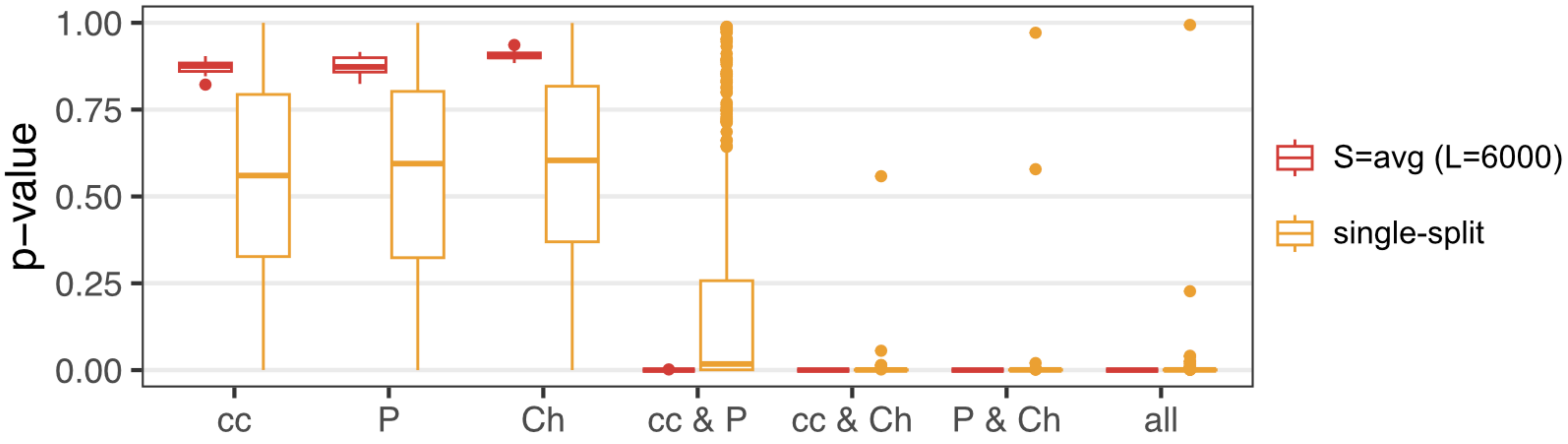

Happy Laura

Other hunt-and-test / data-split procedures

- Testing multiple sample (Cox, 1975)
- Split conformal prediction (Lei et al., 2018; Solari & Djordjilović, 2022)
- Goodness-of-fit testing (Janková et al., 2020)
- Conditional (mean) independence testing (Scheidegger et al., 2021; Lundborg et al., 2022)
- Dimension-agnostic inference (Kim & Ramdas, 2020)

  …

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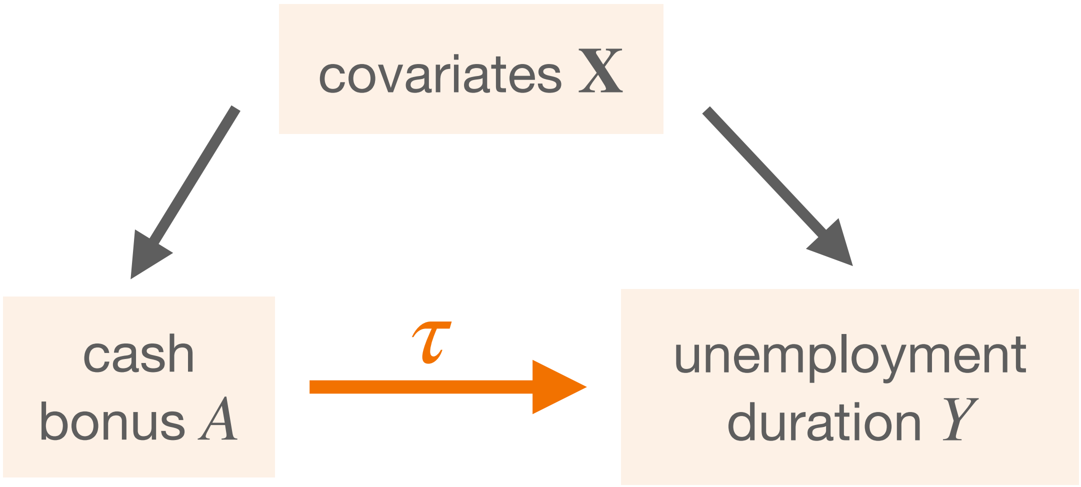
Bill

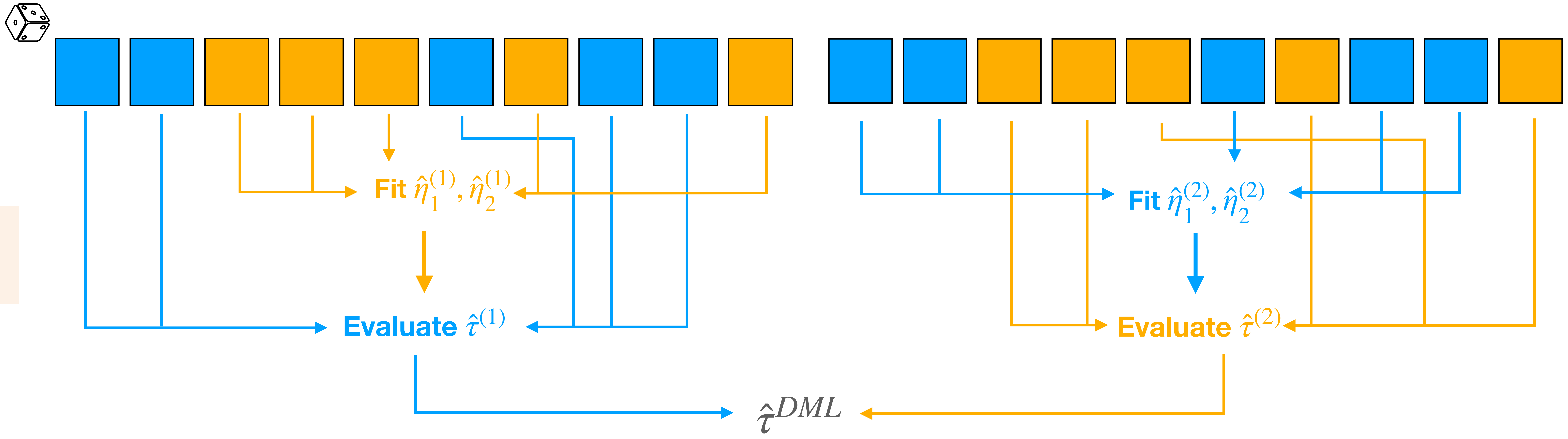


covariates $\mathbf{X}$

cash bonus A

τ

unemployment duration Y



Fit $\hat{\eta}_1^{(1)}, \hat{\eta}_2^{(1)}$

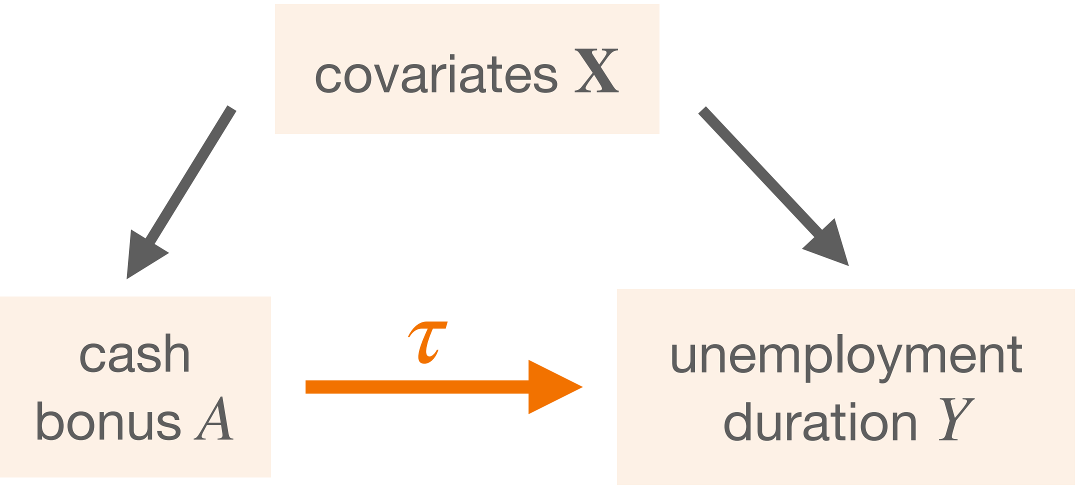
Evaluate $\hat{\tau}^{(1)}$

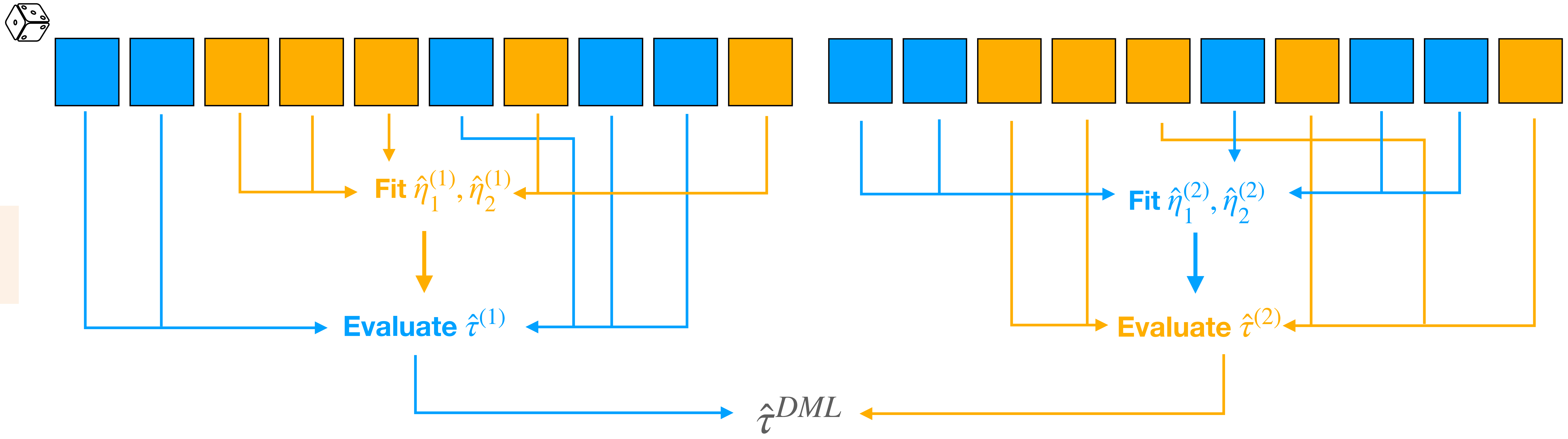
Fit $\hat{\eta}_1^{(2)}, \hat{\eta}_2^{(2)}$

Evaluate $\hat{\tau}^{(2)}$

$\hat{\tau}^{DML}$

Bill



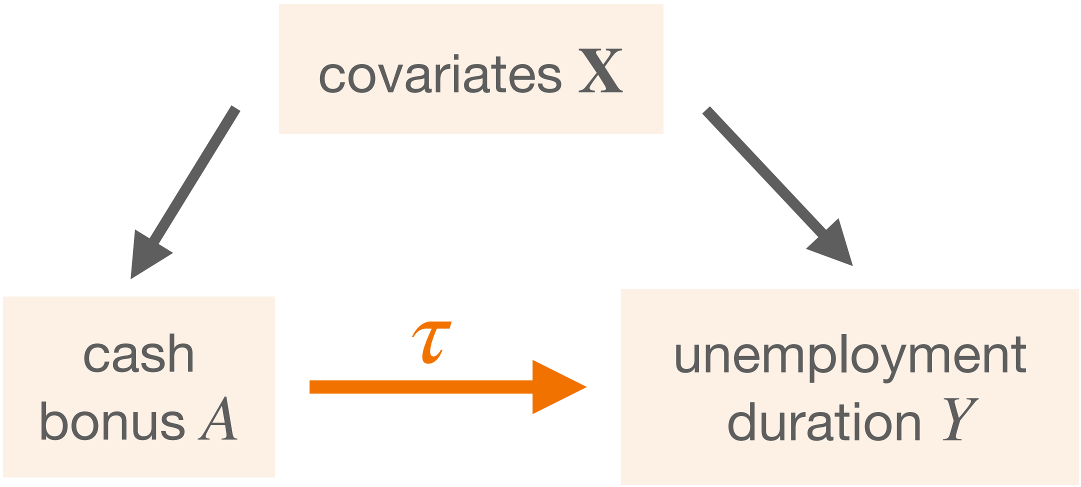

Fit $\hat{\eta}_1^{(1)}, \hat{\eta}_2^{(1)}$
Fit $\hat{\eta}_1^{(2)}, \hat{\eta}_2^{(2)}$
Evaluate $\hat{\tau}^{(1)}$
Evaluate $\hat{\tau}^{(2)}$
$\hat{\tau}^{DML}$

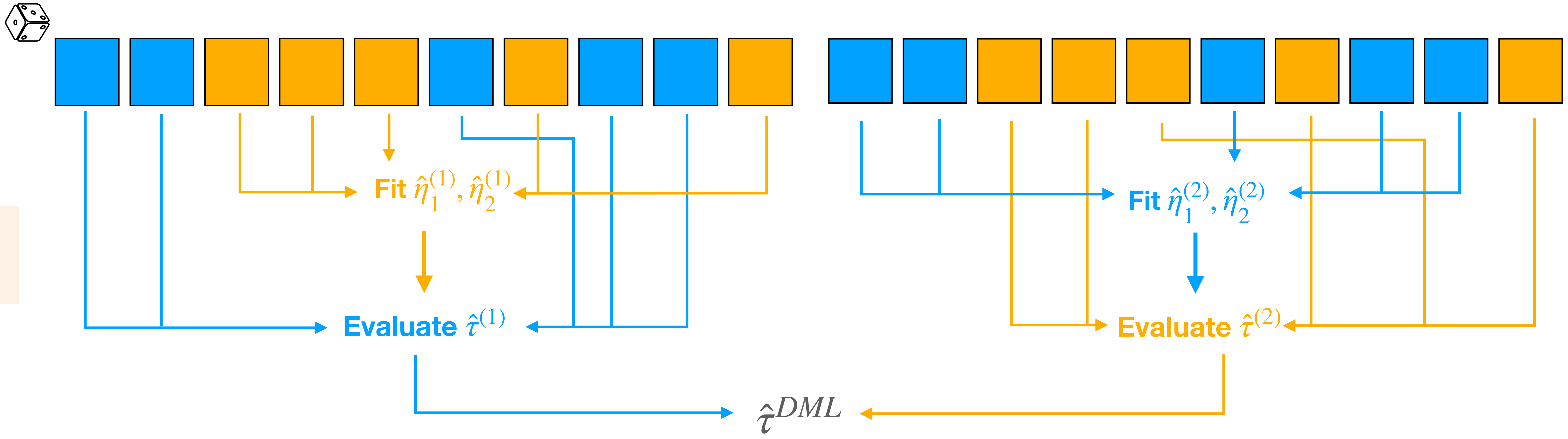
```
> set.seed(42)
> dml$fit()
      Estimate. Std. Error t value Pr(>|t|)
tau   -0.1      0.035       -2.86  0.004 **
```

```
> set.seed(43)
> dml$fit()
      Estimate. Std. Error t value Pr(>|t|)
tau   -0.06     0.035       -1.71  0.08 .
```

Problem 1. Conditional variability due to data splitting

Bill

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```
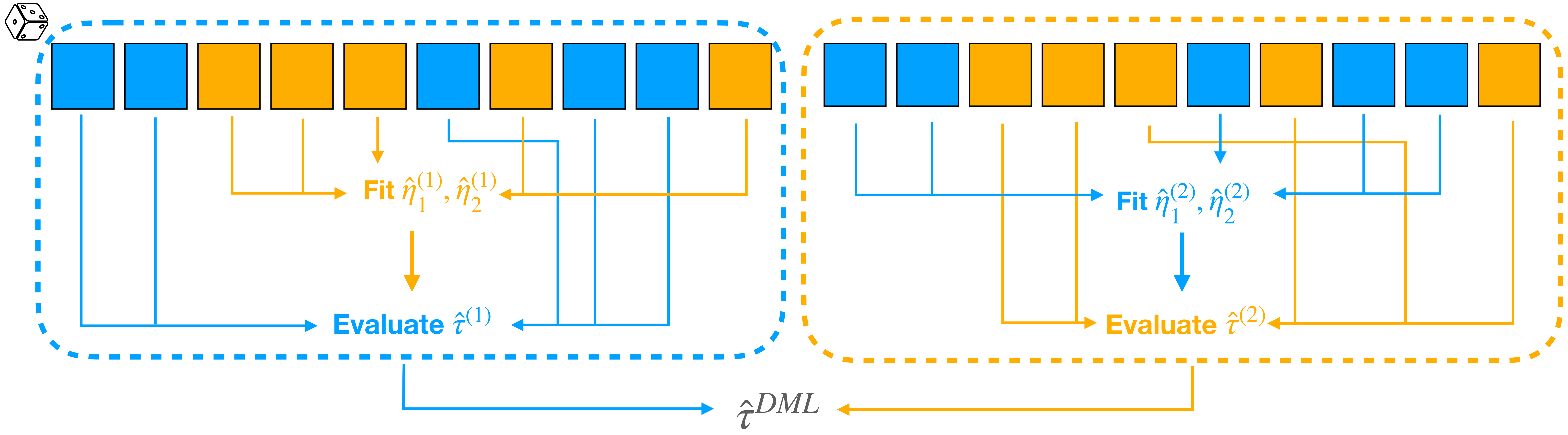

Problem 1. Conditional variability due to data splitting

Problem 2. DML Std. Error tends to be too small

👉 It ignores cross-fold correlation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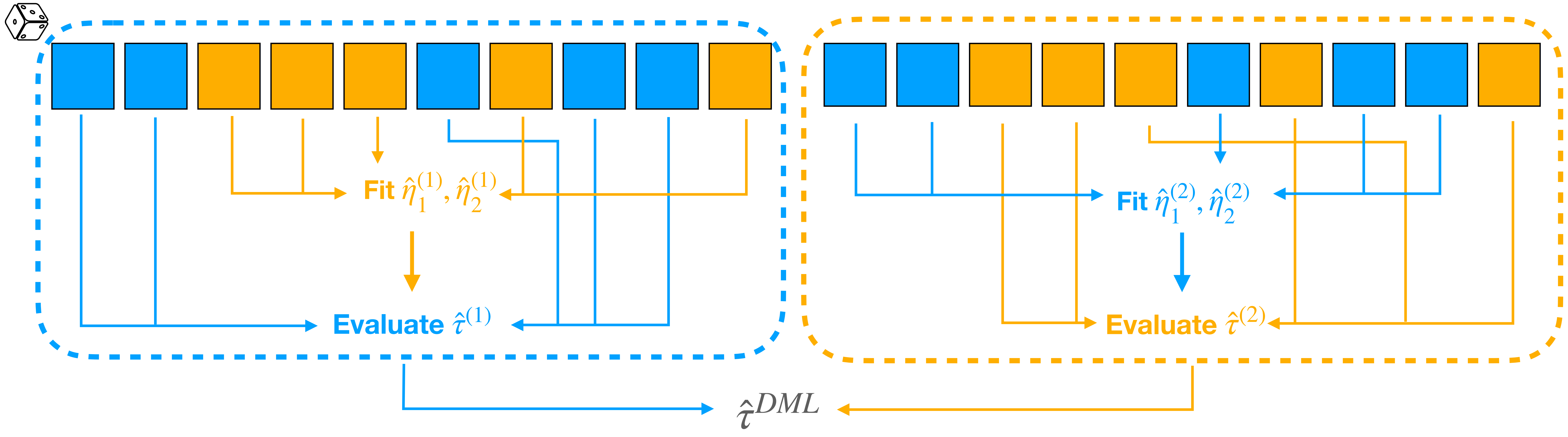
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💡 Each fold defines a "single-split" statistic $T_n^{(1)} := \dfrac{\sqrt{n/2}(\hat{\tau}_1^{(1)} - \tau)}{\sigma} \to_d \mathcal{N}(0,1)$

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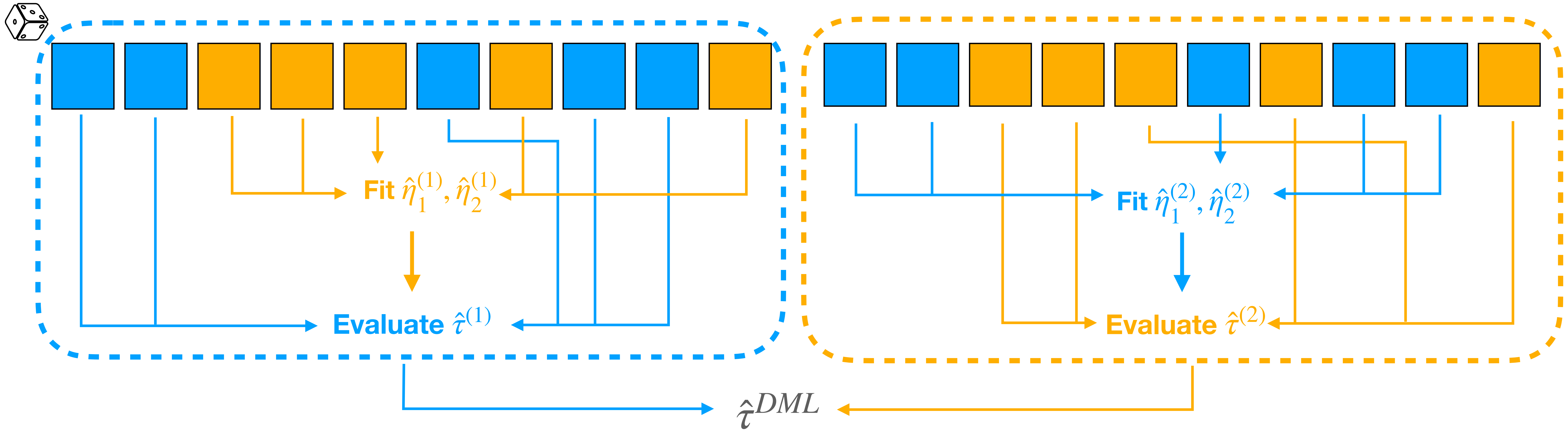

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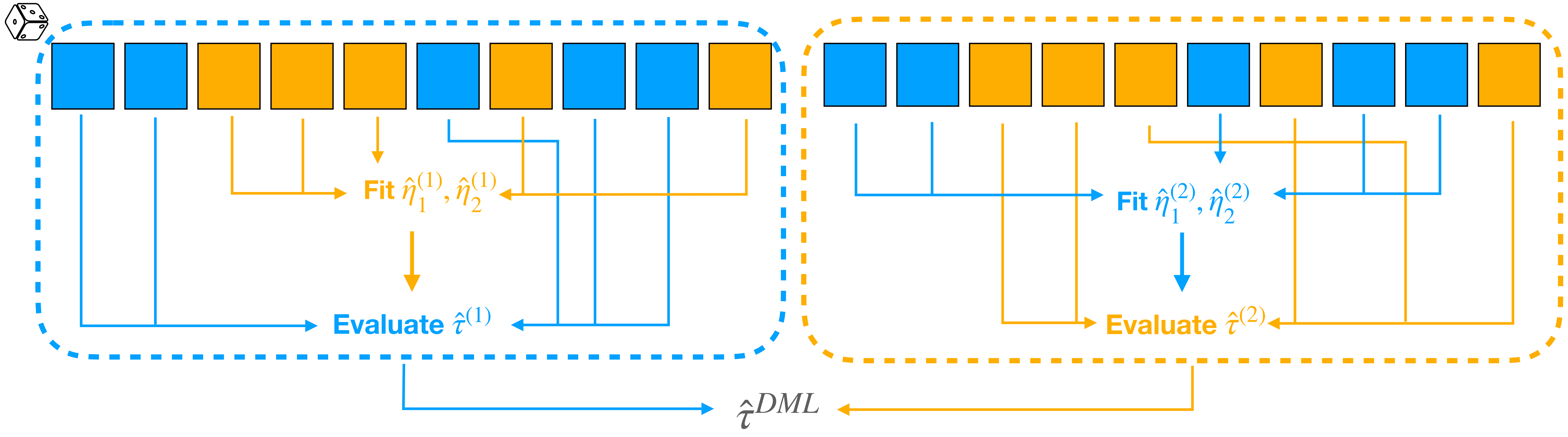
DML CLT: $$\frac{\sqrt{n}(\hat{\tau}_{\text{DML}} - \tau)}{\sigma} = \frac{1}{\sqrt{2}}(T_n^{(1)} + T_n^{(2)}) \to \mathcal{N}(0,1)\,.$$

🤔 Under conditions required by DML, between-fold correlation $\rho \to 0$.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⚠️ For finite sample, $\rho > 0$.

	Std. Error
DML	$\sigma/\sqrt{n}$
Actual	$\sigma\sqrt{1+\rho(L-1)}\;/\sqrt{n}$

Improved DML inference

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💡 Rank-transformed subsampling **automatically accounts for ρ.**

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👉 Can be performed without knowing τ or σ:

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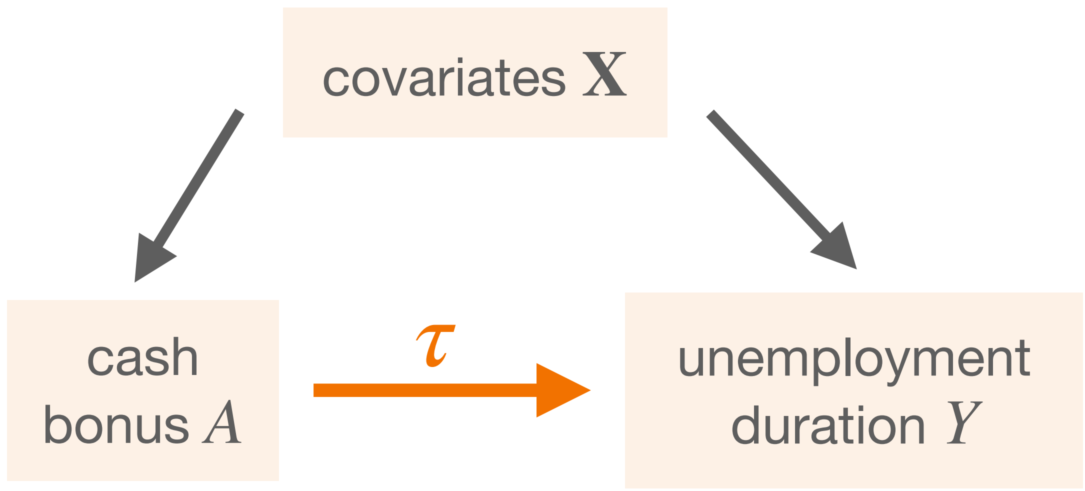

covariates $\mathbf{X}$

cash bonus A

τ

unemployment duration Y

Table 1: Coverage of nominal 95% confidence intervals

method	$n = 500$		$n = 1000$		$n = 2000$	
	$L = 2$	$L = 5$	$L = 2$	$L = 5$	$L = 2$	$L = 5$
$\rho(L-1)$	0.46	0.31	0.36	0.18	0.25	0.14
Corrected	0.94	0.93	0.95	0.95	0.96	0.95
DML	0.86	0.88	0.88	0.92	0.91	0.92

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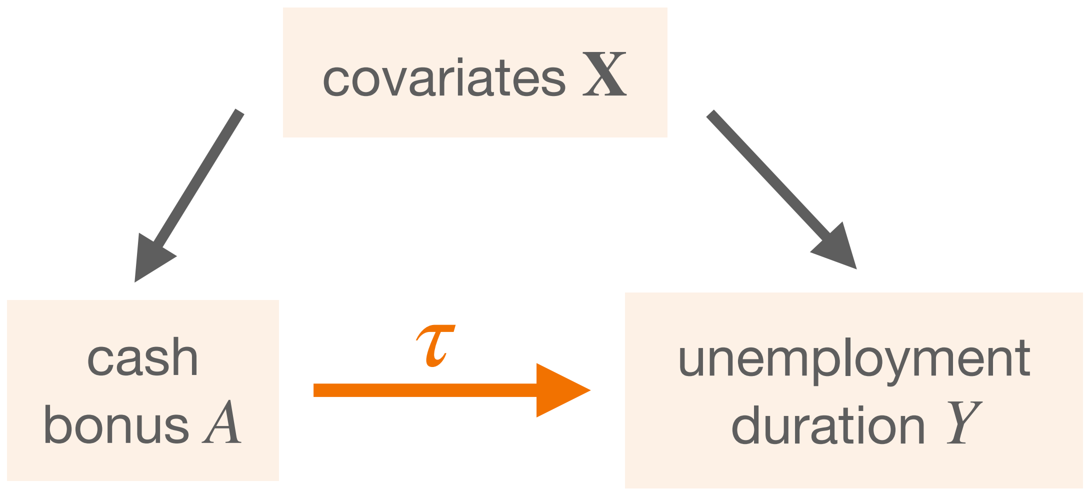

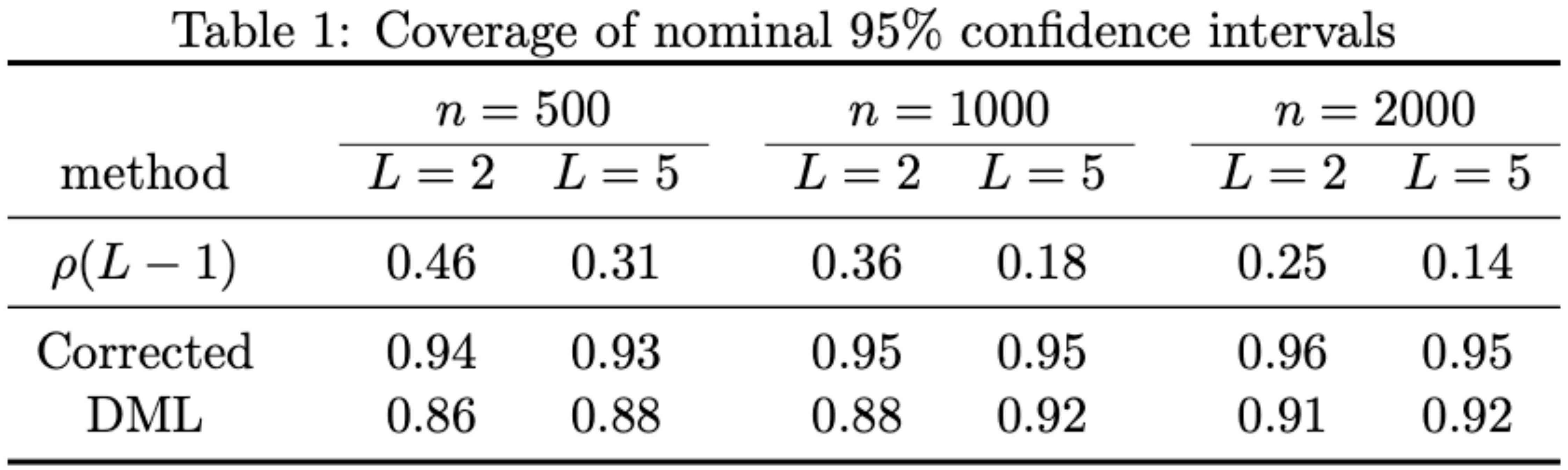
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✅ Calibrated CI’s by accounting for correlation.

✅ Improved replicability by averaging over data splits.

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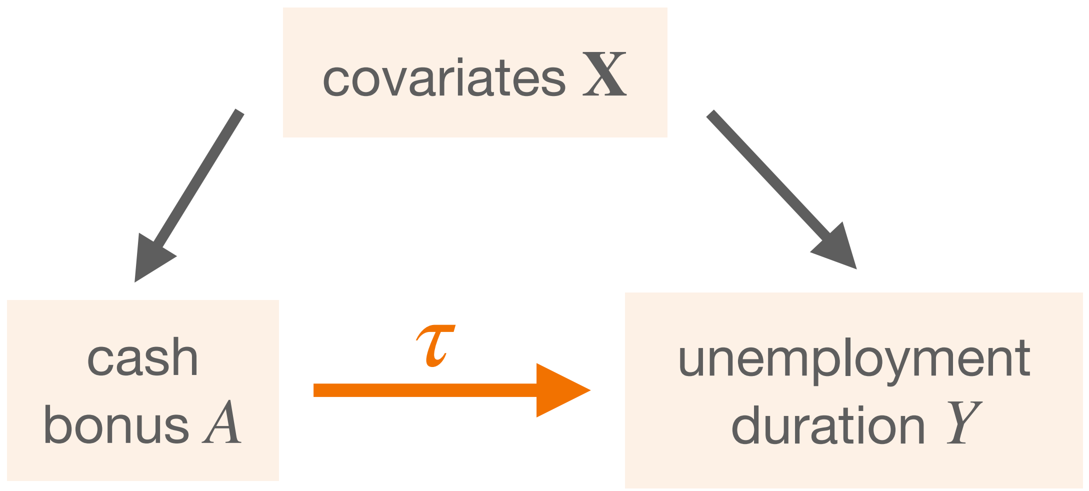

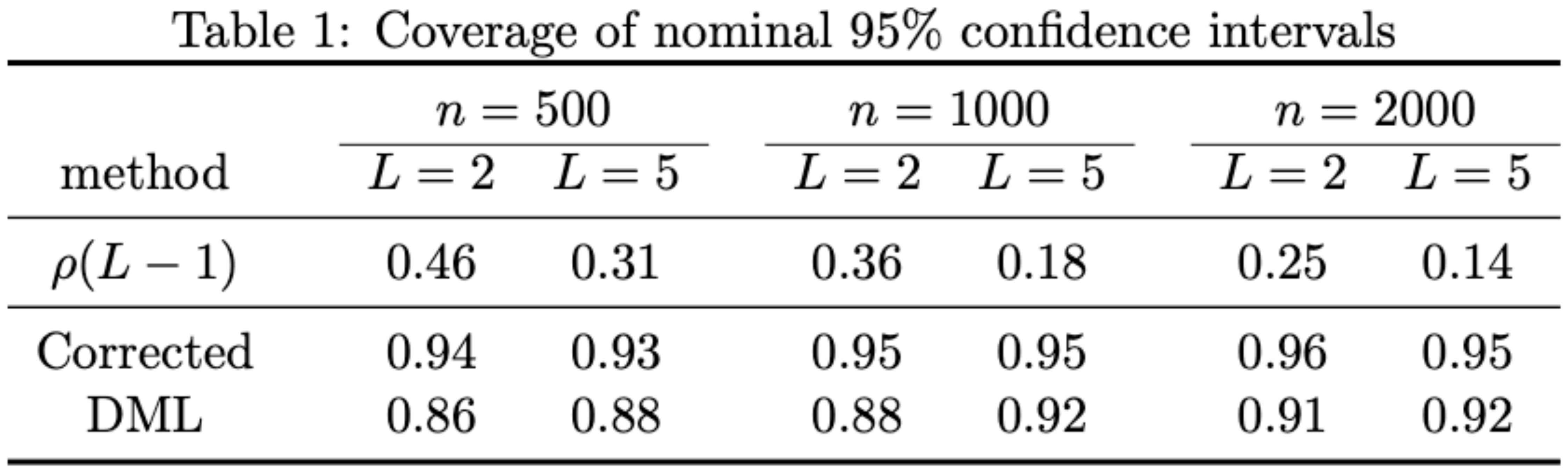

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Relieved Bill

✅ Calibrated CI's by accounting for correlation.

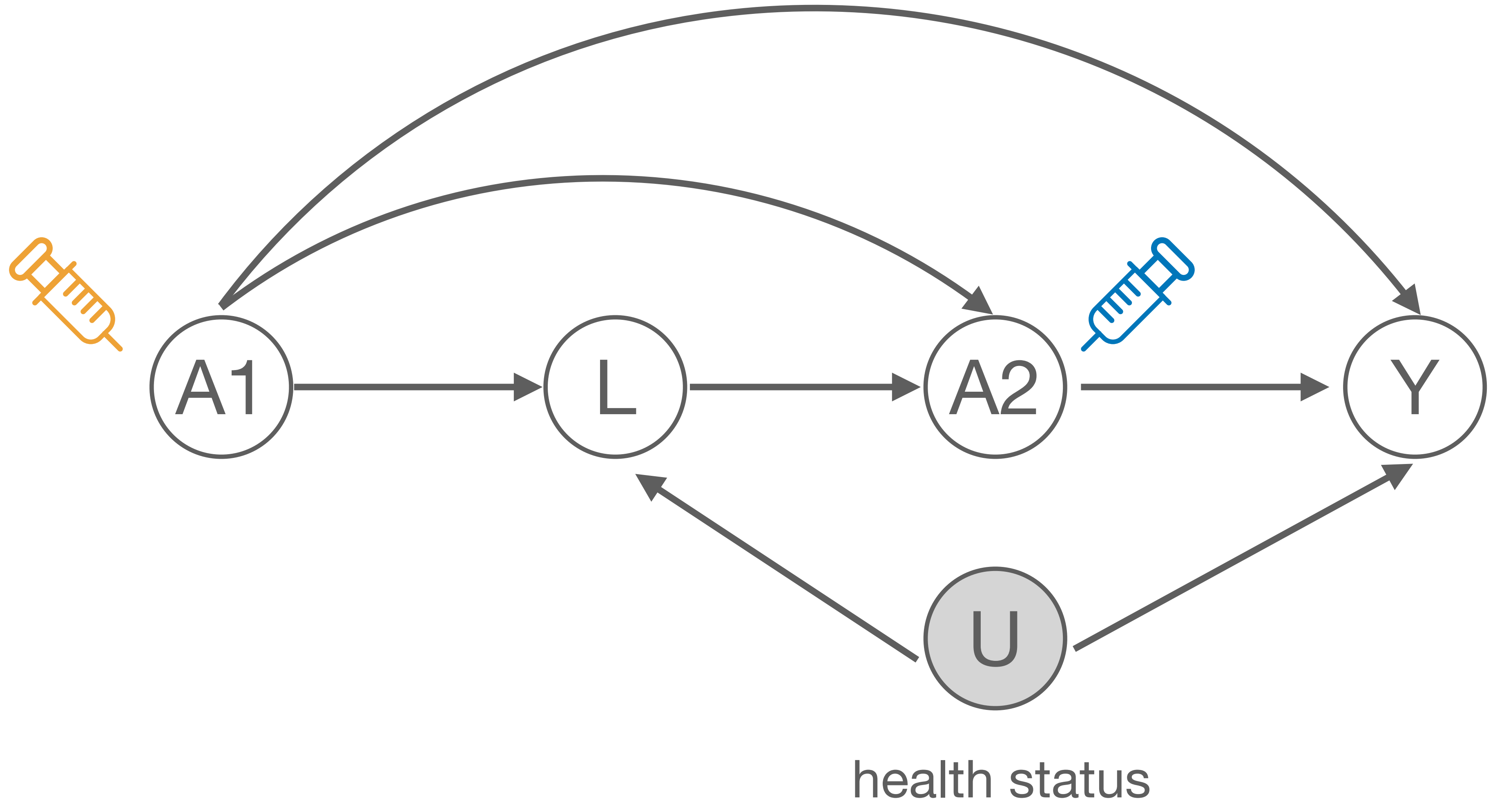
✅ Improved replicability by averaging over data splits.

Outline

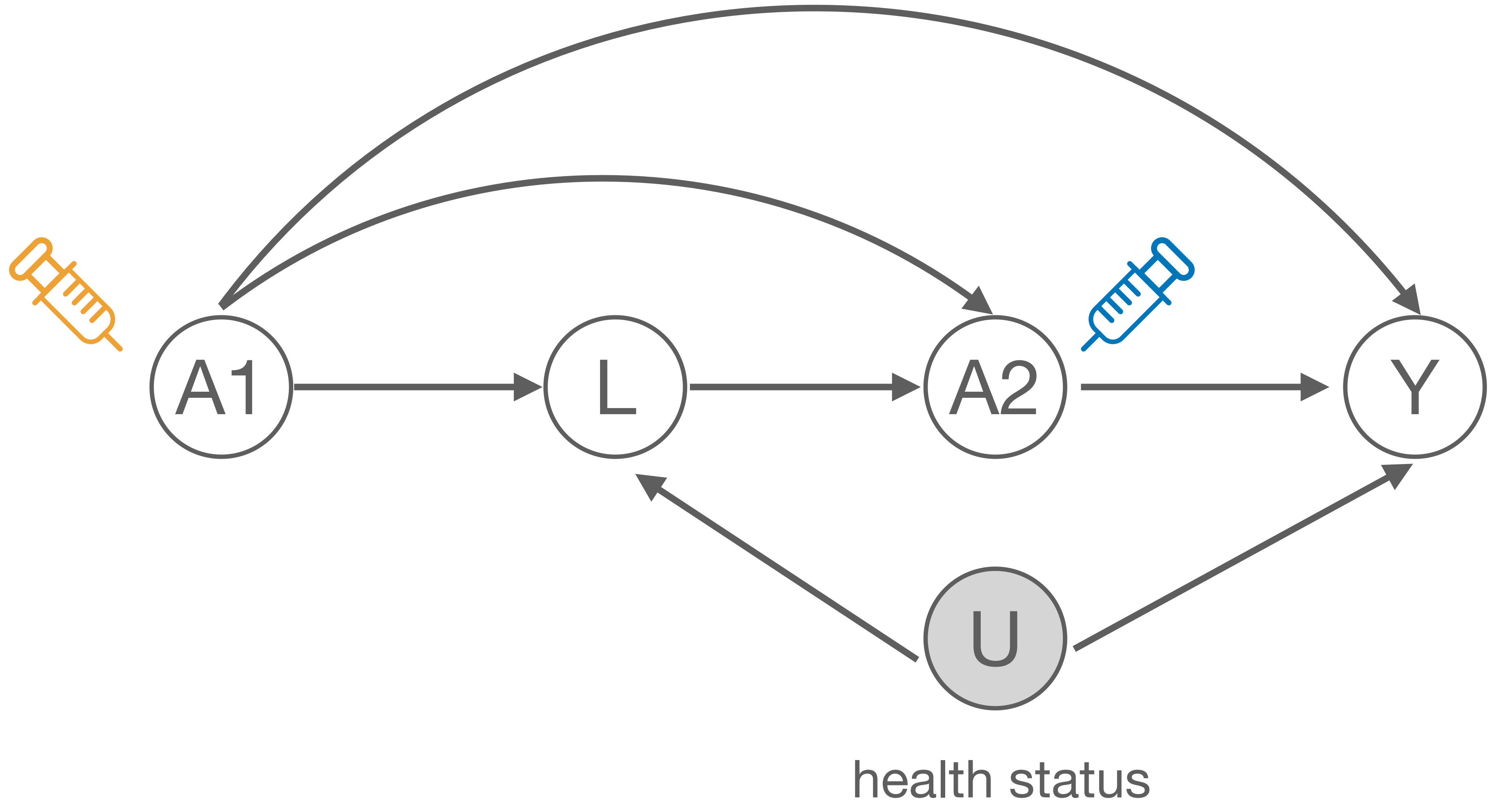
- Setup and main challenge
- Method: Rank-transformed subsampling
- Applications
    - Hunt and test
    - Improving double machine learning
    - **Testing no direct effect in a sequentially randomized trial**
- Future directions

Sequentially randomized trial

Sequentially randomized trial

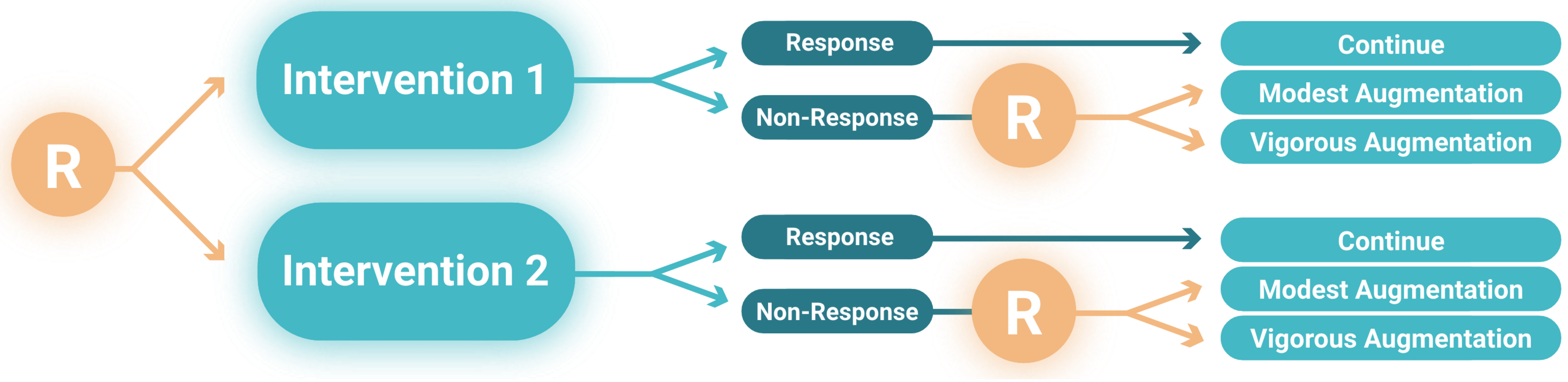


Sequentially randomized trial



- SMART trials

(Murphy, 2005; Murphy et al., 2006)



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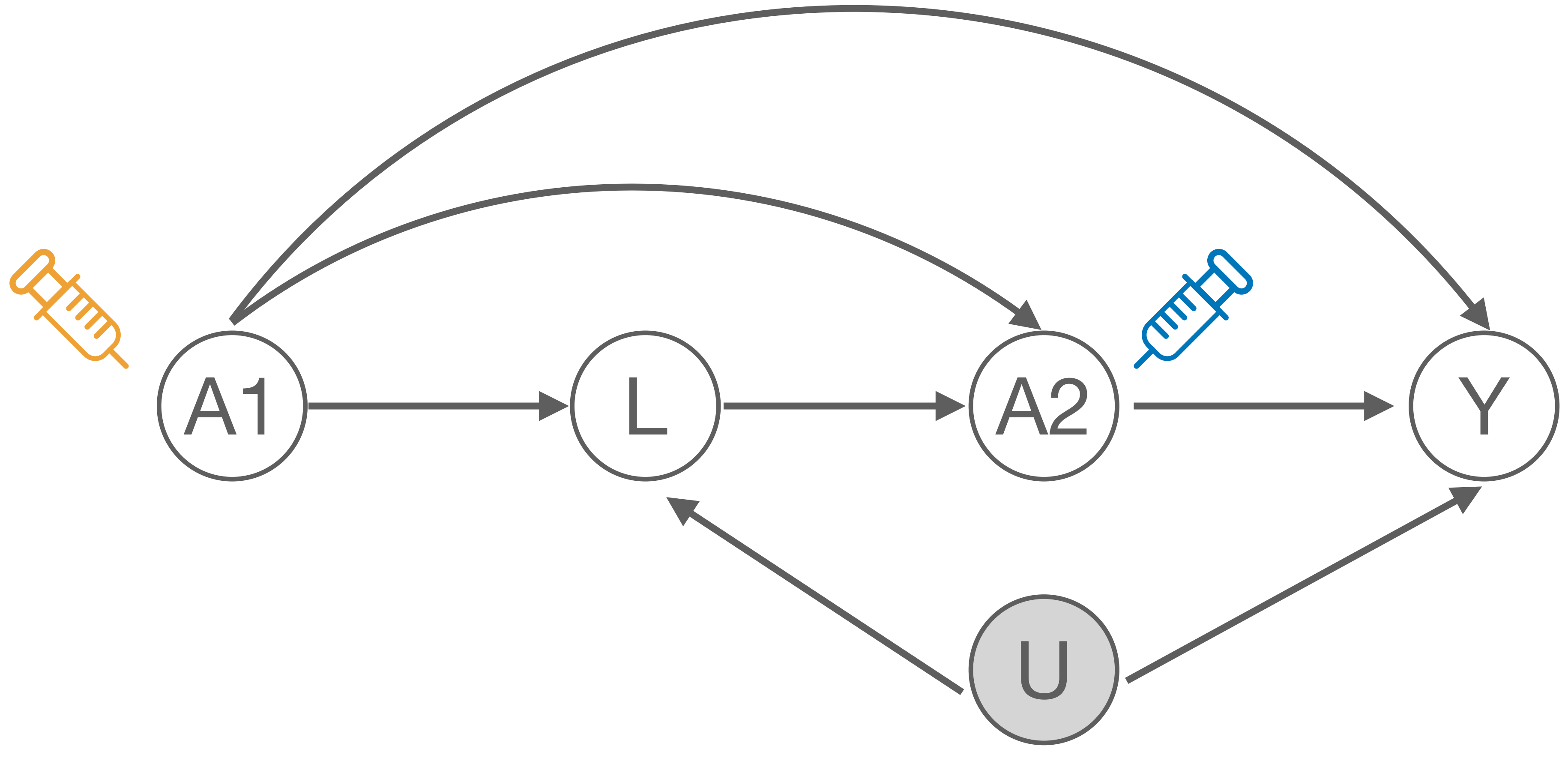
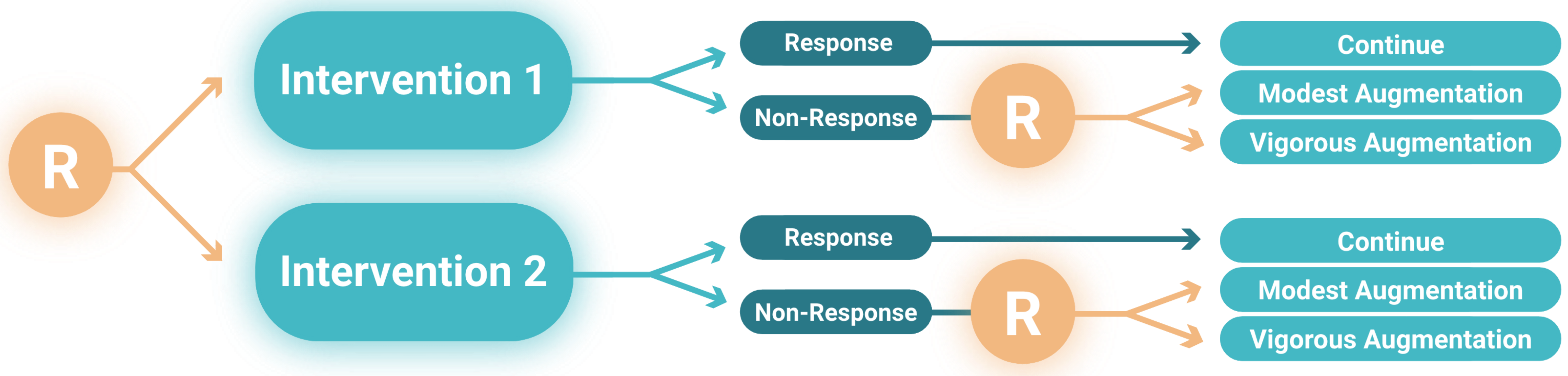
Sequentially randomized trial



health status

- SMART trials

(Murphy, 2005; Murphy et al., 2006)



R

Intervention 1

Response

Non-Response

R

Continue

Modest Augmentation

Vigorous Augmentation

Intervention 2

Response

Non-Response

R

Continue

Modest Augmentation

Vigorous Augmentation

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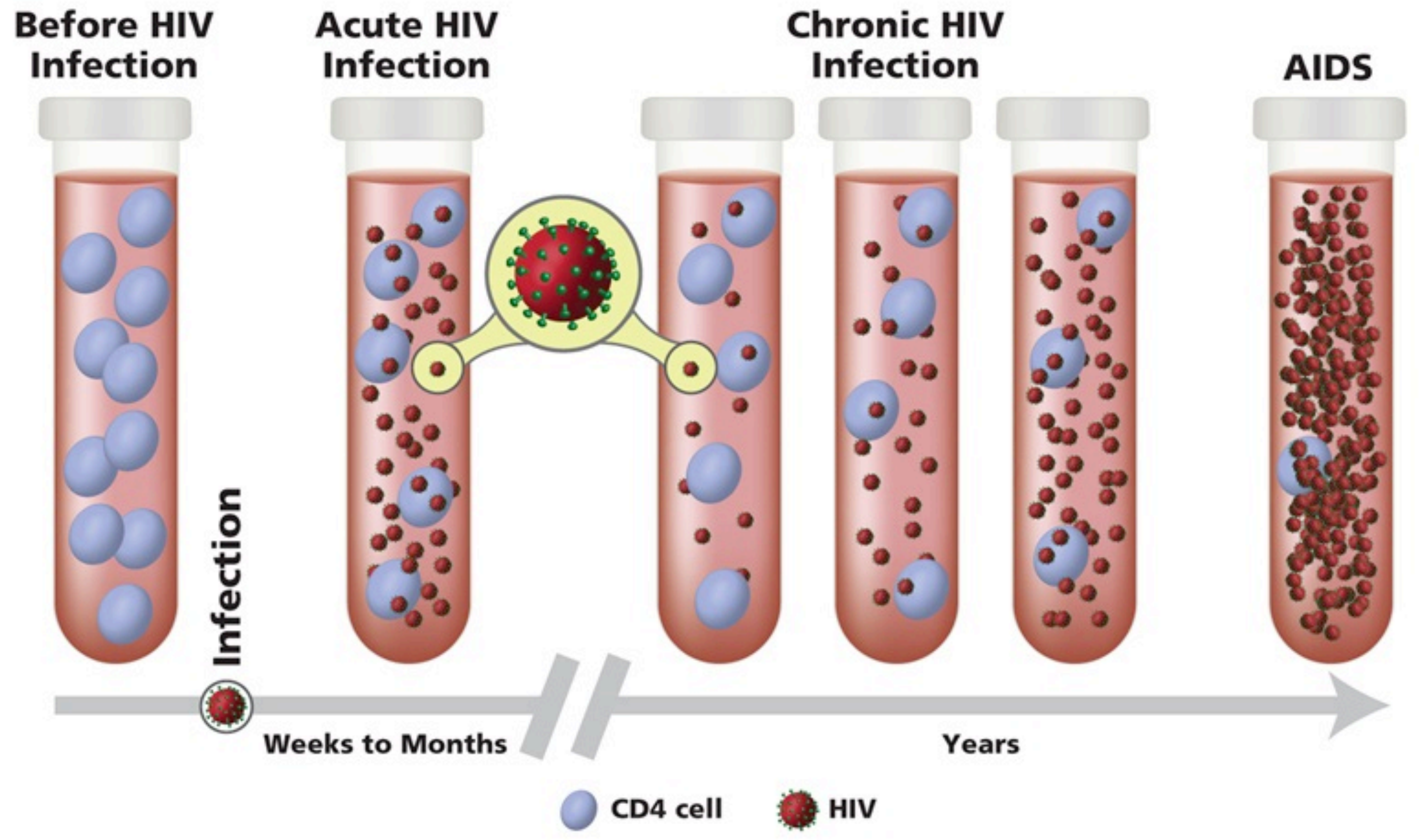
- Observational / follow-up studies

HIV studies: A_1, A_2: antiretroviral therapy; L, Y: CD4 cell counts



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Sharp null of no direct effect

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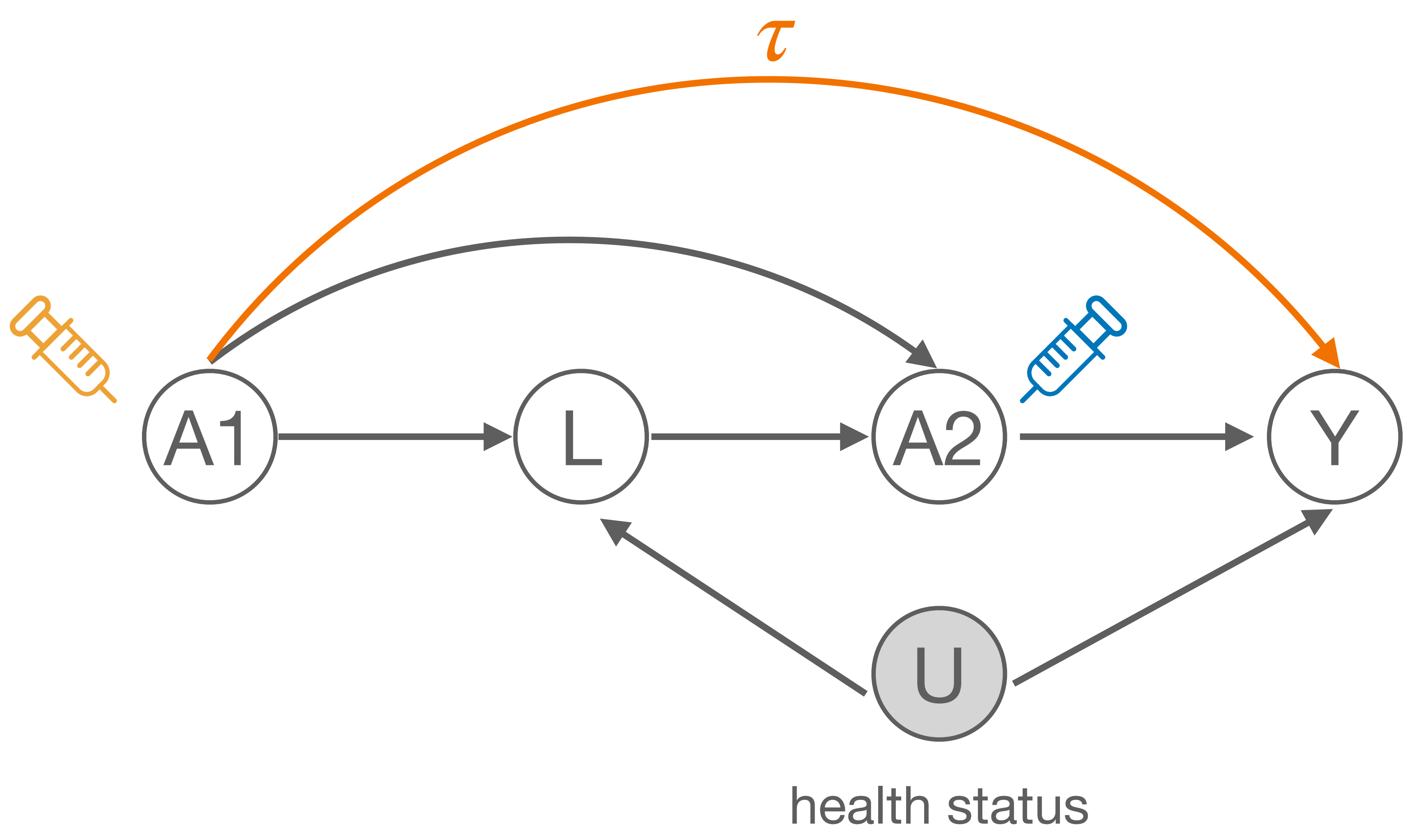
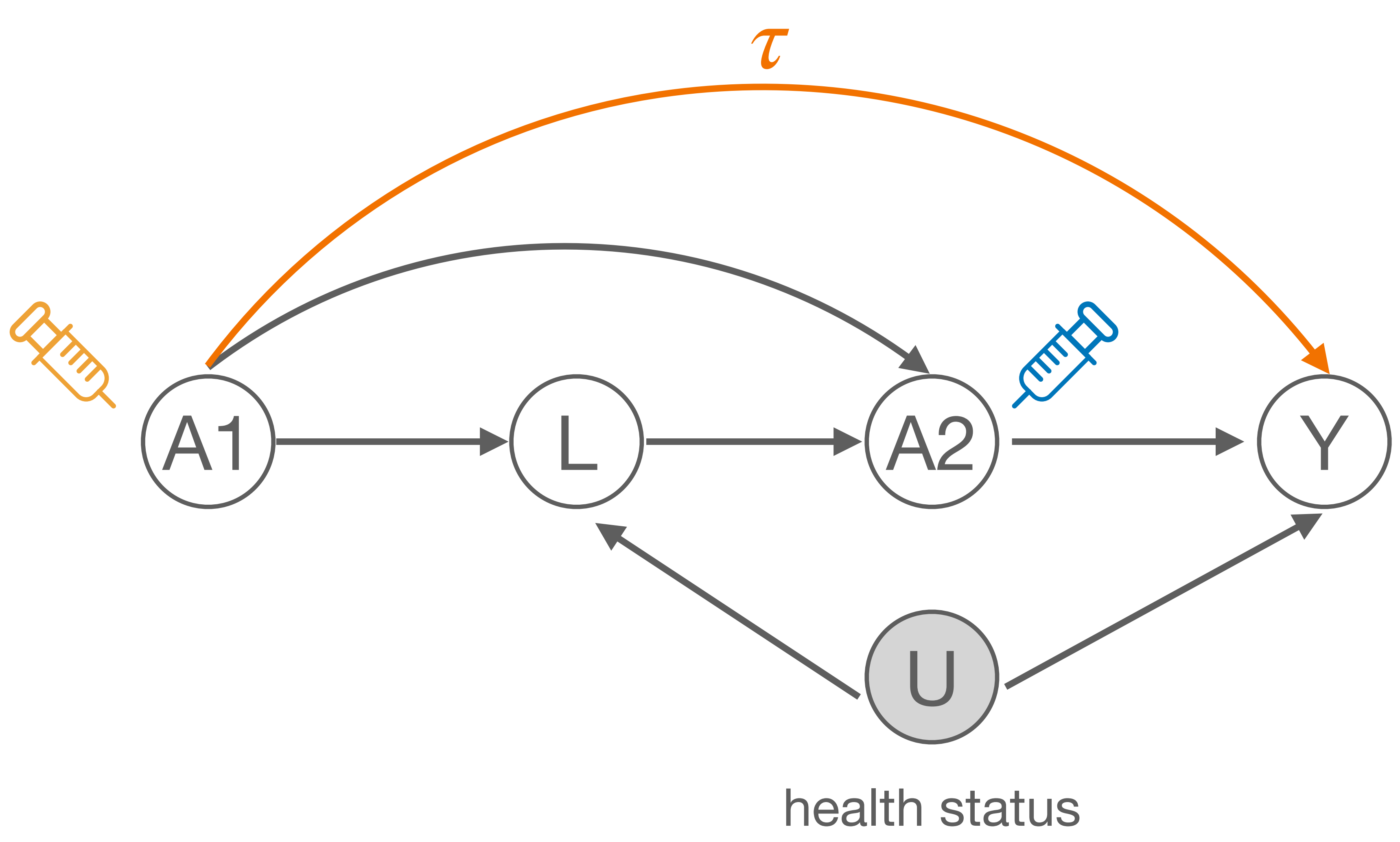


τ: the direct effect of A_1 on Y (i.e., not through A_2).

Sharp null of no direct effect



τ: the direct effect of A_1 on Y (i.e., not through A_2).

Sharp null hypothesis H_0: $\tau_i \equiv 0$ for every individual i.

* More precisely, $Y_i(1,0) - Y_i(0,0) \equiv 0$ and $Y_i(1,1) - Y_i(0,1) = 0$ for every i. $Y_i(a_1, a_2)$ is the potential outcome had subject i taken treatments (a_1, a_2).

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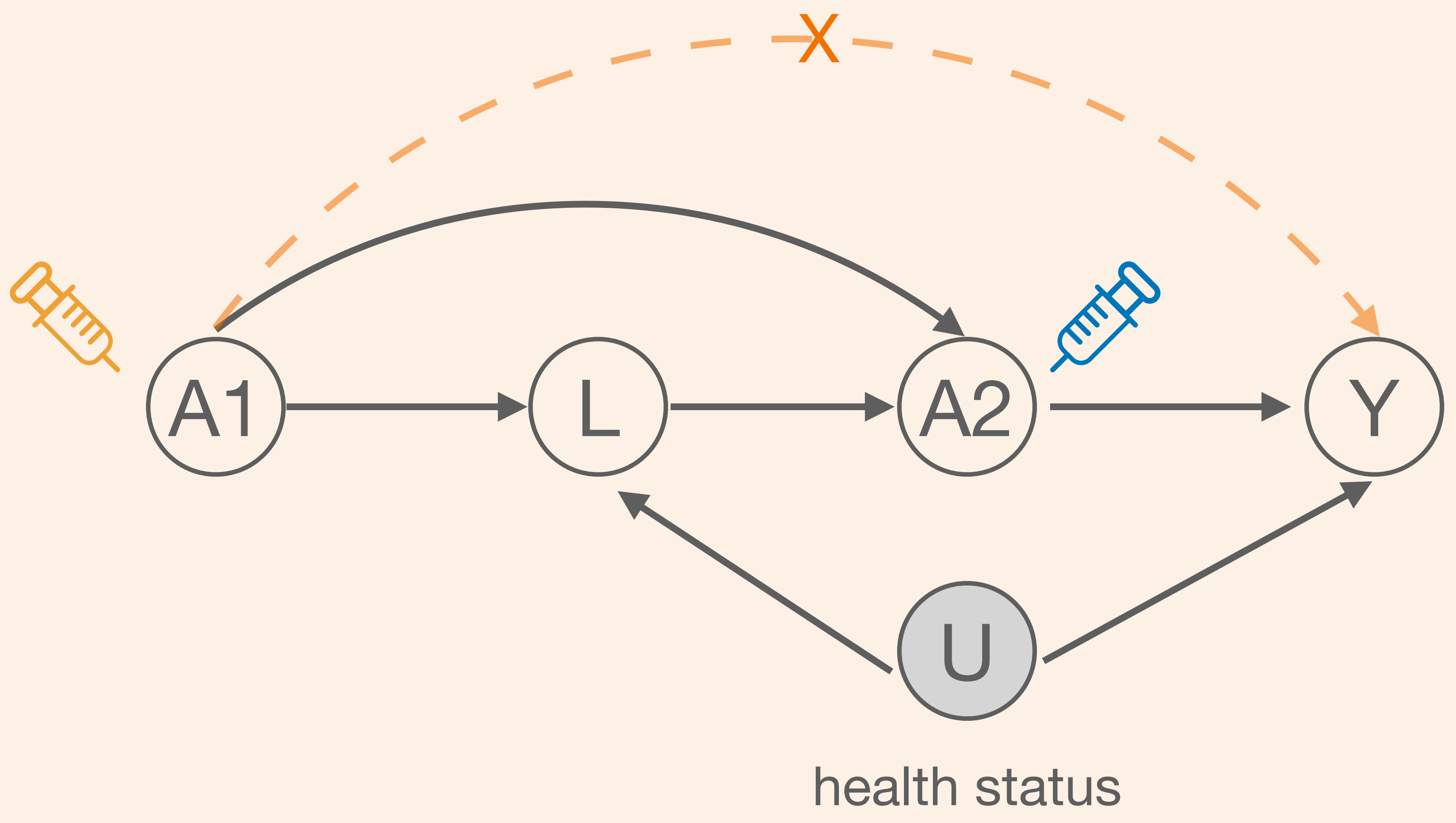

Graph under the sharp null H_0

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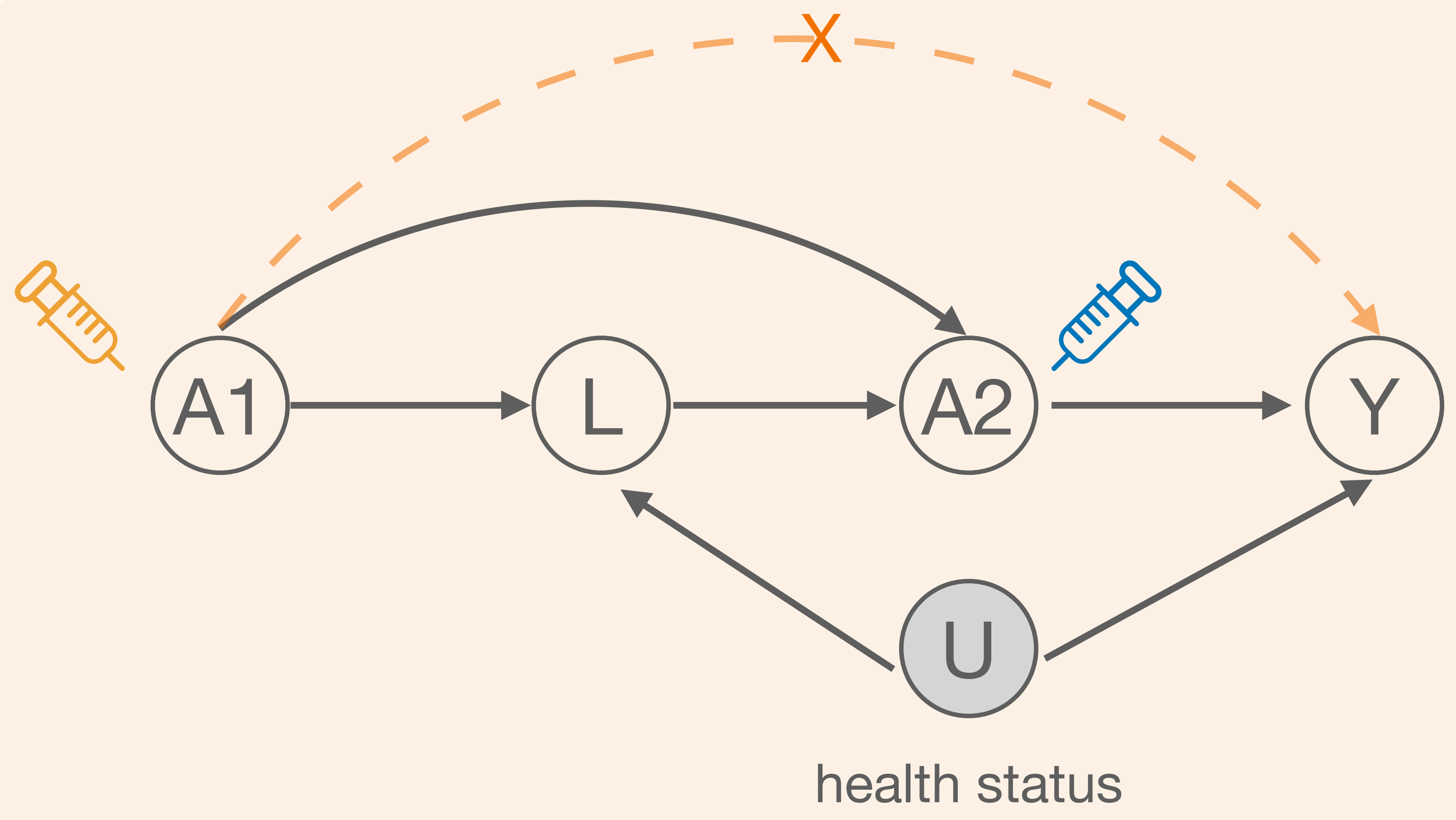

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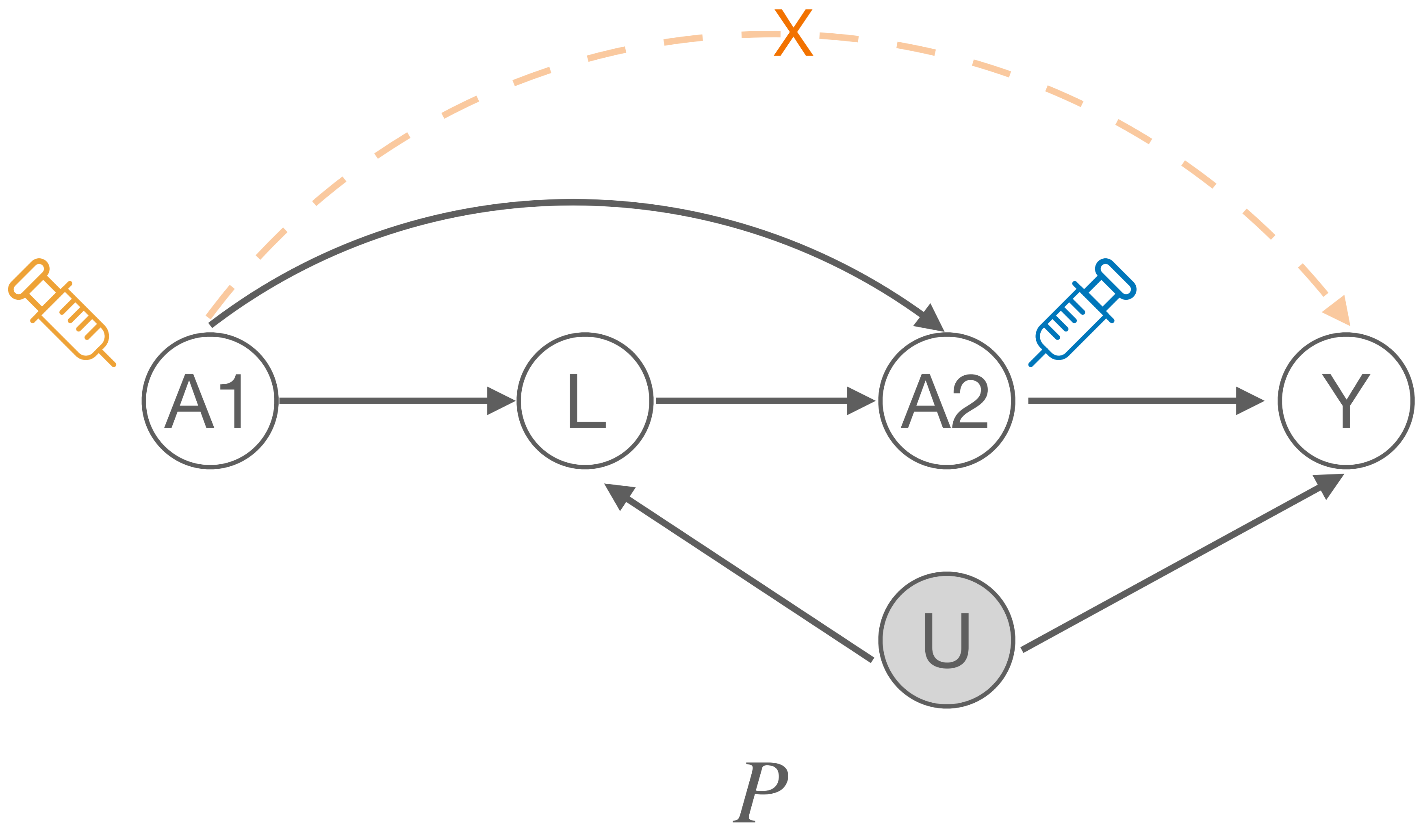
🤔 H_0 cannot be formulated as an independence or conditional independence.

Testing the sharp null

Sequentially randomized trial under the sharp null



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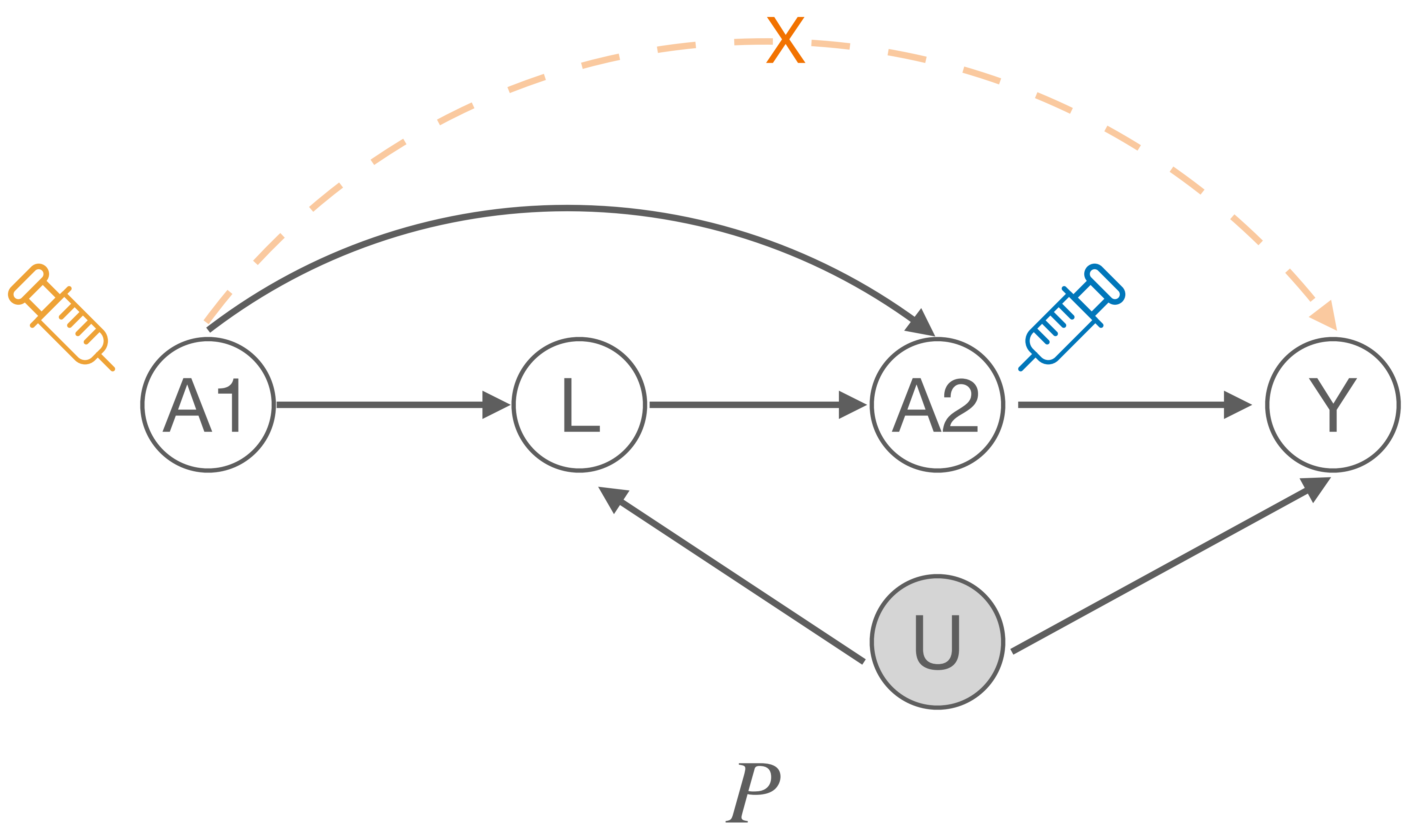
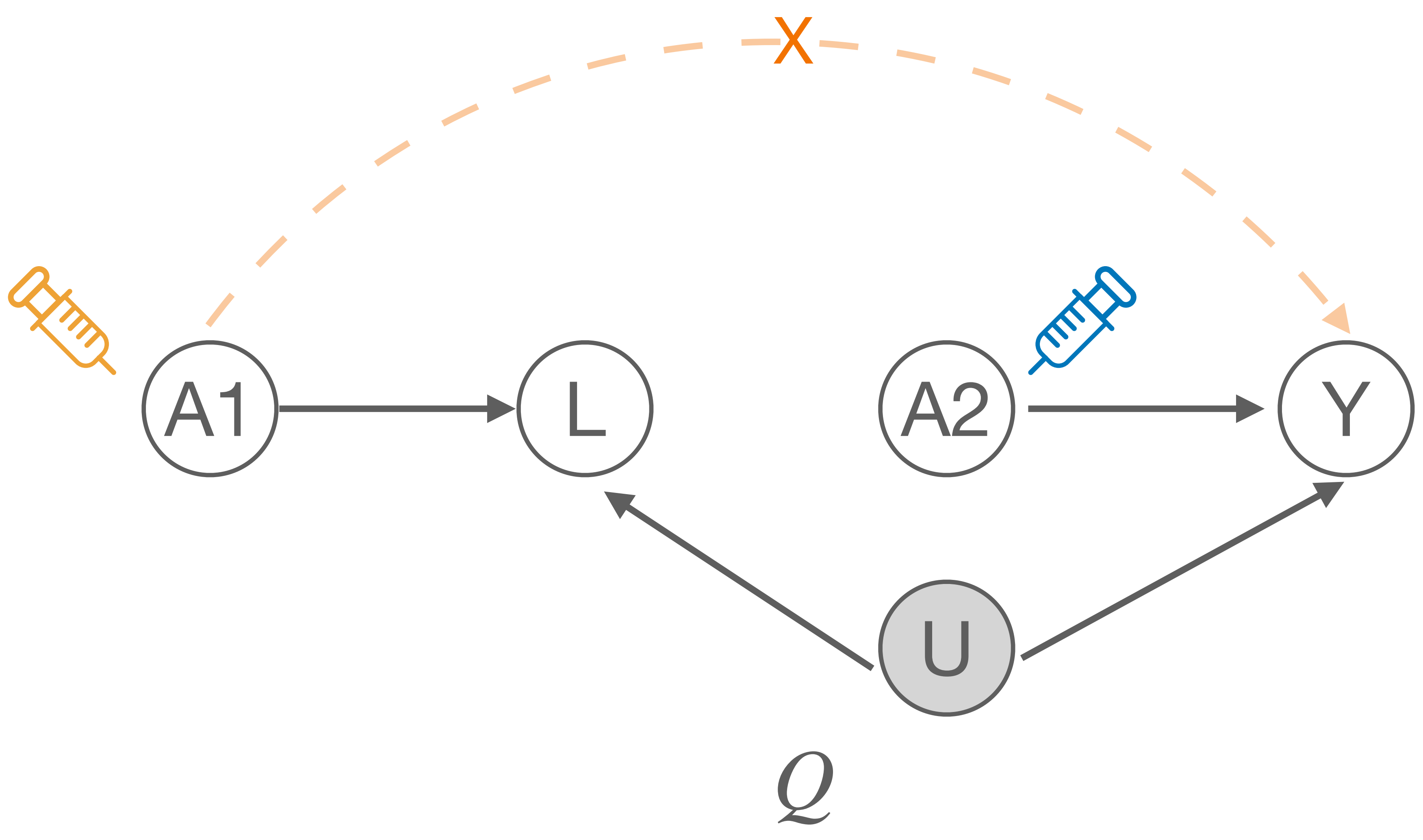


Completely randomized trial under the sharp null



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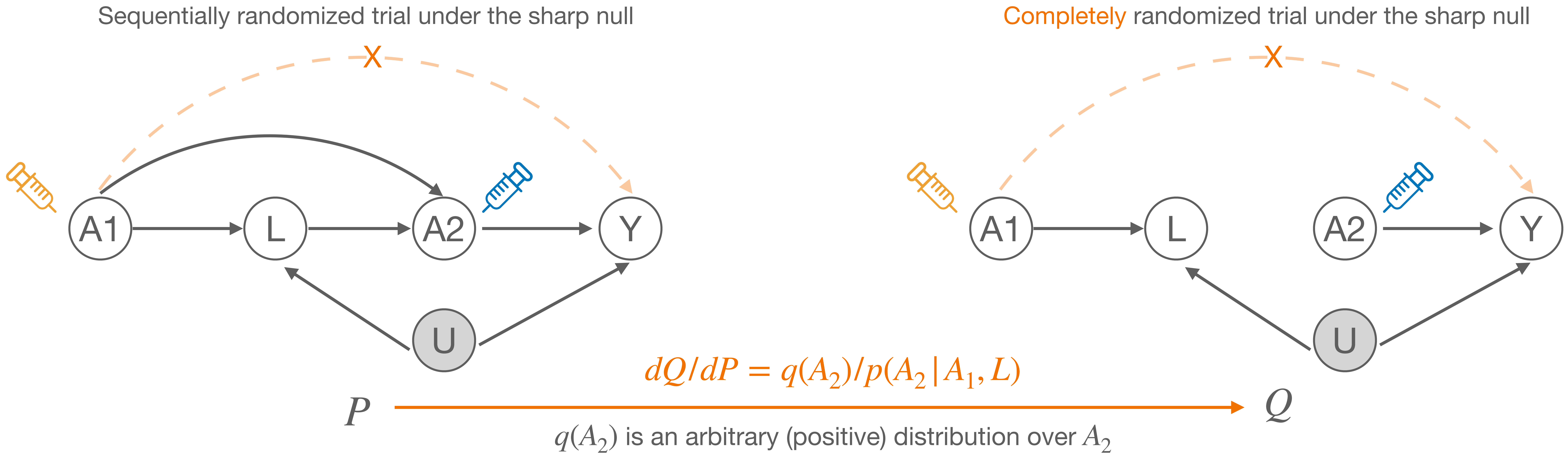


Sequentially randomized trial under the sharp null

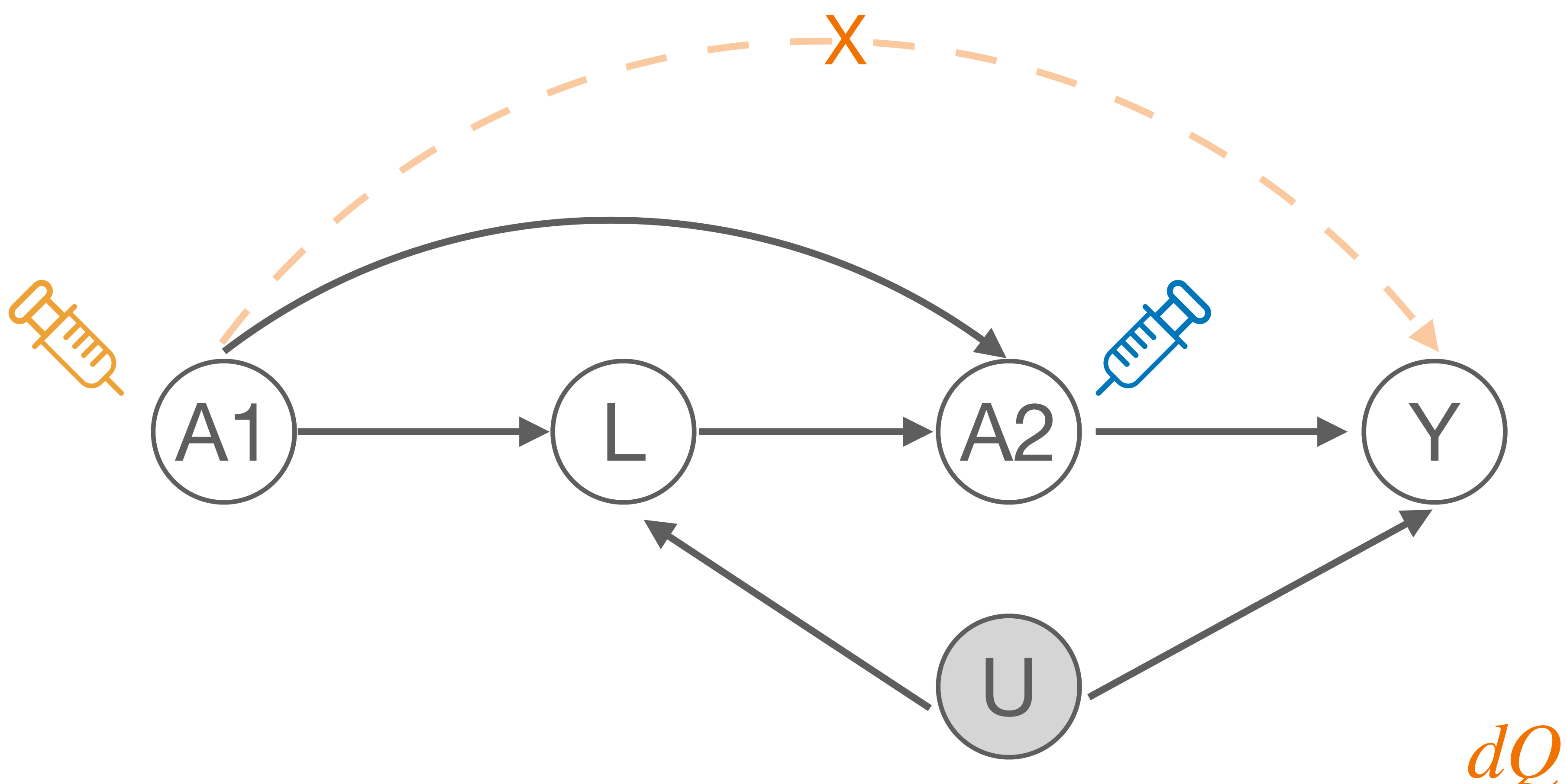
Completely randomized trial under the sharp null

$$dQ/dP = q(A_2)/p(A_2\,|\,A_1, L)$$

$q(A_2)$ is an arbitrary (positive) distribution over A_2

Testing the sharp null

Sequentially randomized trial under the sharp null



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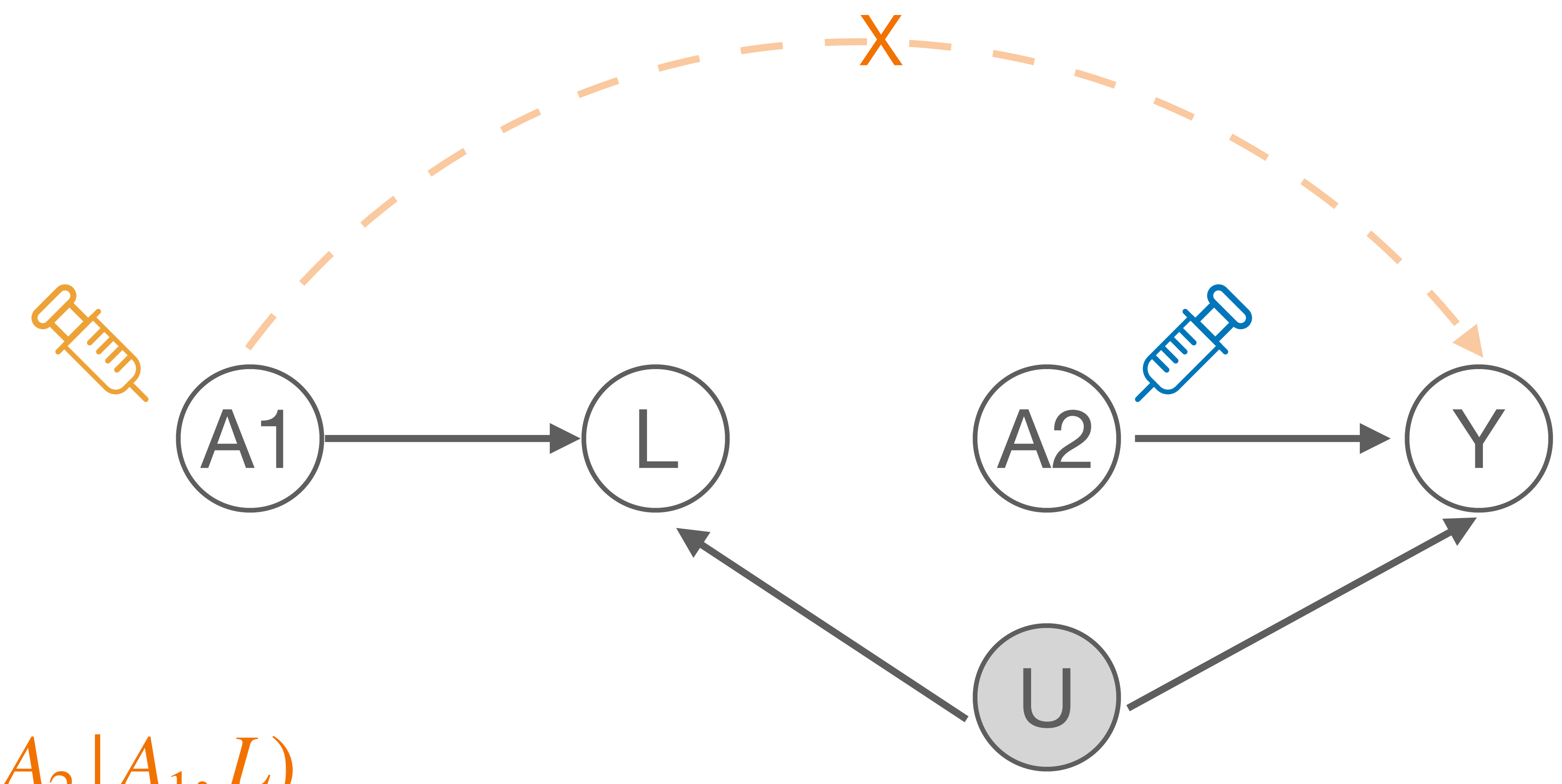

$$P \xrightarrow[q(A_2)\text{ is an arbitrary (positive) distribution over }A_2]{dQ/dP = q(A_2)/p(A_2\,|\,A_1,L)} Q$$

💡 Sharp null H_0: $A_1 \perp\!\!\!\perp Y\ (Q),\ dQ/dP = q(A_2)/p(A_2\,|\,A_1,L)$.

Testing the sharp null

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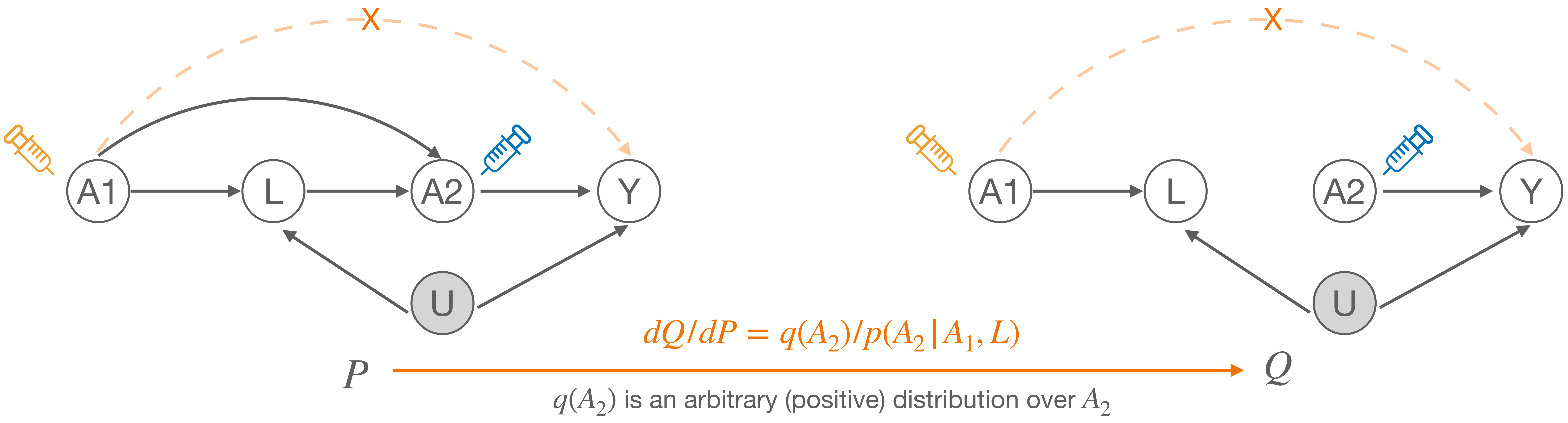

$dQ/dP = q(A_2)/p(A_2 \mid A_1, L)$

$P \xrightarrow{\qquad} Q$

$q(A_2)$ is an arbitrary (positive) distribution over A_2

💡 Sharp null H_0: $A_1 \perp\!\!\!\perp Y \ (Q),\ dQ/dP = q(A_2)/p(A_2 \mid A_1, L)$.

👉 This is a generalized / “dormant” independence, aka. Verma constraint on P.

Robins (1986, 1999), Verma & Pearl (1990), Wermuth & Cox (2008), Richardson et al. (2017)

An instance of “distribution shift”.

Testing generalized (conditional) independence

Testing generalized (conditional) independence

A lot of recent progress in independence / conditional independence testing.

Independence: kernel embedding (Gretton et al., 2005, 2007), rank correlation coefficients (Bergsma & Dassios, 2014; Drton et al., 2020; Shi et al., 2021), optimal rates via U-statistics (Berrett et al., 2021), optimal transport (Liu et al., 2022), etc.

Conditional Independence: kernel method (Zhang et al., 2011), generalized covariance measure (Shah & Peters, 2020; Scheidegger et al., 2022), copula (Petersen & Hansen, 2021), projected covariance (Lundborg et al., 2022), model-X (Candès et al., 2018; Berrett et al., 2020), etc.

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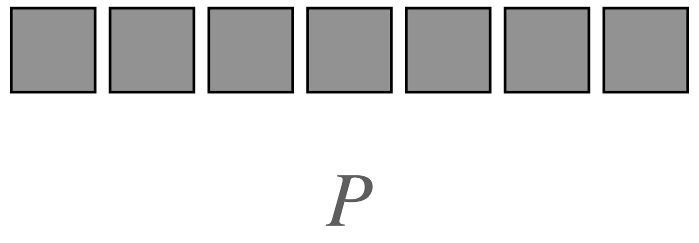

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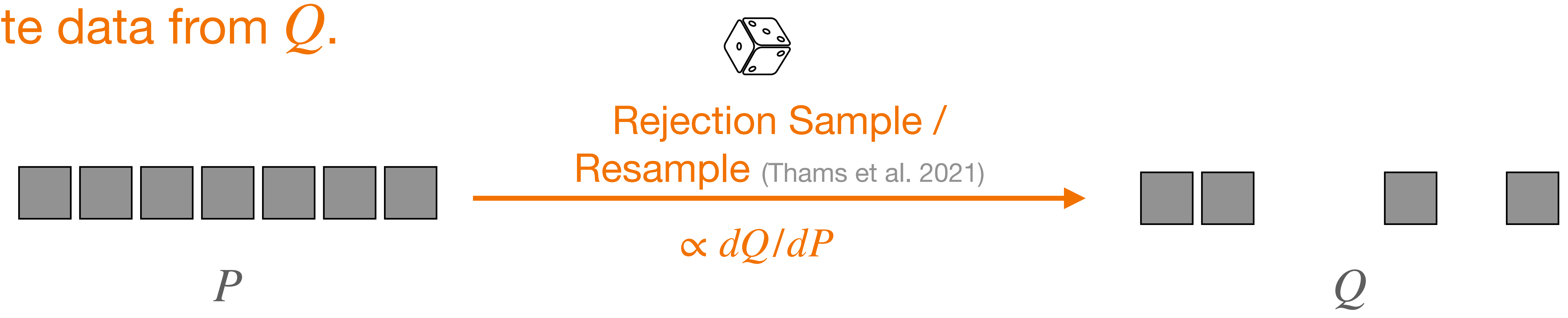

Rejection Sample / Resample (Thams et al. 2021)

$\propto dQ/dP$

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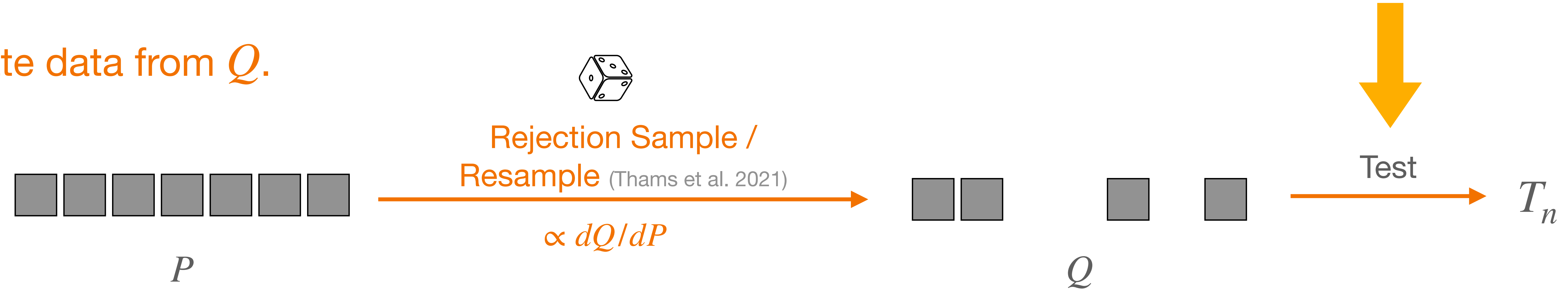


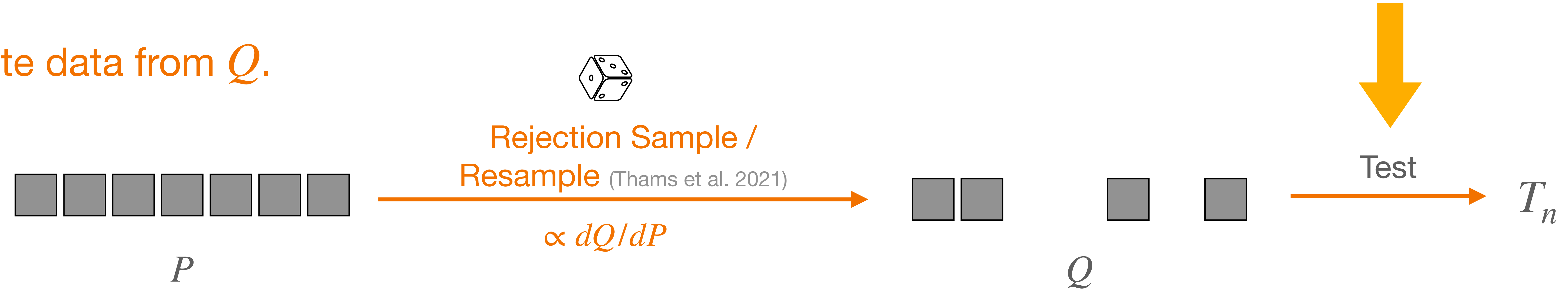
Testing generalized (conditional) independence

A lot of recent progress in independence / conditional independence testing.

Independence: kernel embedding (Gretton et al., 2005, 2007), rank correlation coefficients (Bergsma & Dassios, 2014; Drton et al., 2020; Shi et al., 2021), optimal rates via U-statistics (Berrett et al., 2021), optimal transport (Liu et al., 2022), etc.

Conditional Independence: kernel method (Zhang et al., 2011), generalized covariance measure (Shah & Peters, 2020; Scheidegger et al., 2022), copula (Petersen & Hansen, 2021), projected covariance (Lundborg et al., 2022), model-X (Candès et al., 2018; Berrett et al., 2020), etc.

💡 We can simulate data from Q.



	Need re-calibration	Reduced sample size	Randomized
Sampling	No	Yes	Yes
Inverse probability weighting (IPW)	Yes	No	No

Simulation: Linear SEM

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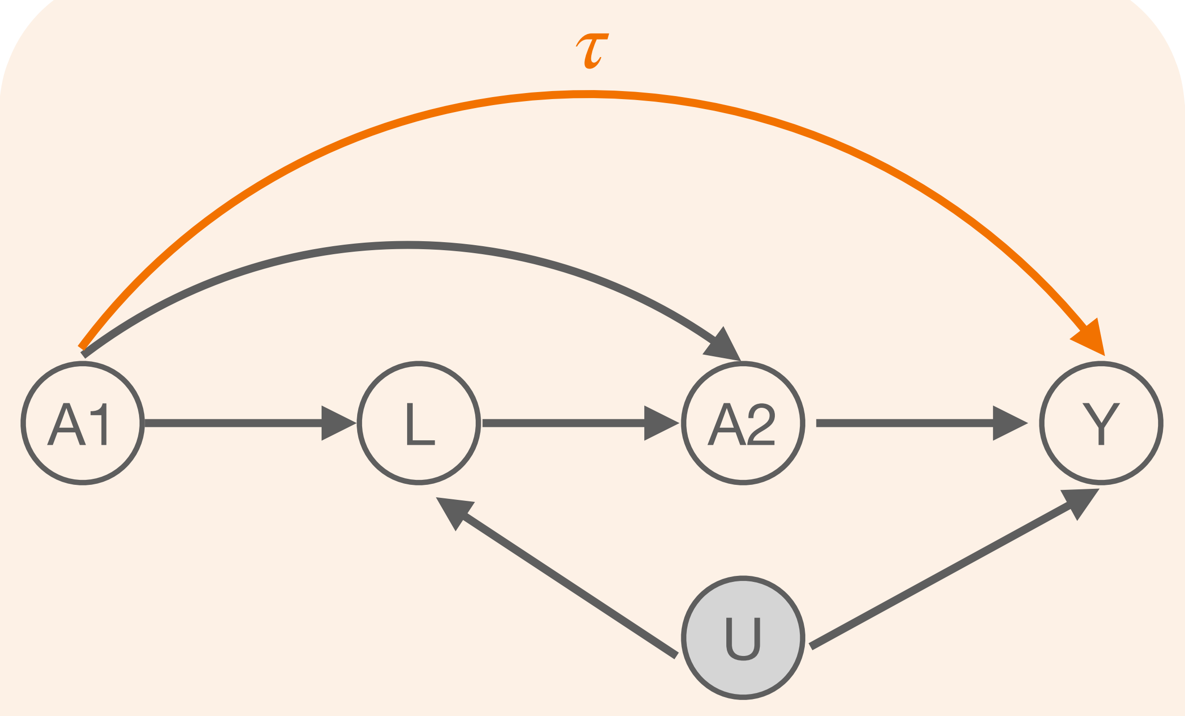
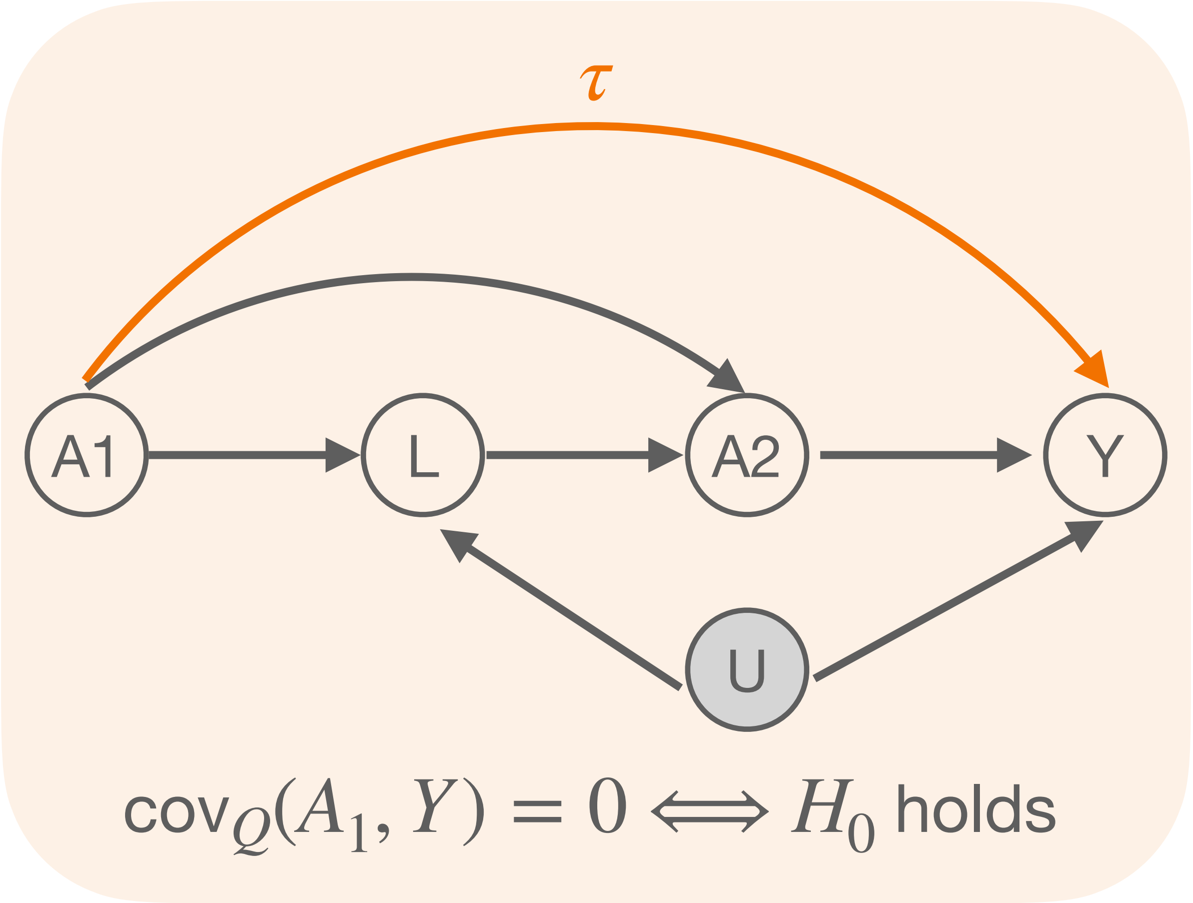


$\mathrm{cov}_Q(A_1, Y) = 0 \iff H_0$ holds

Simulation: Linear SEM



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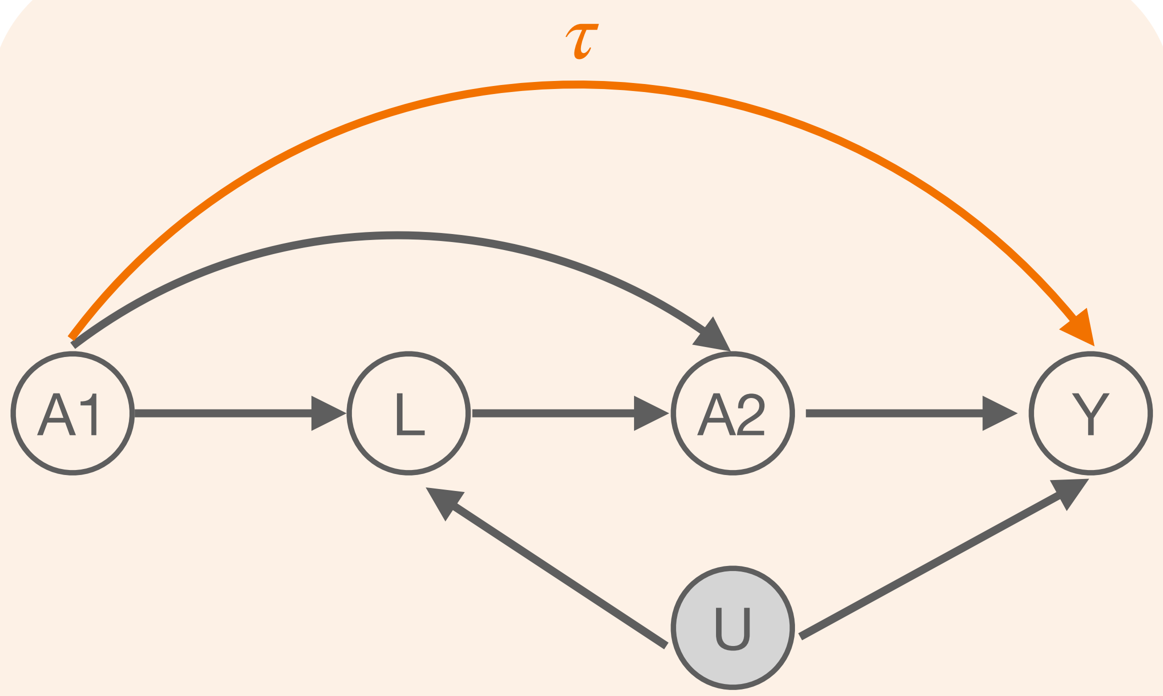
(1) Rej. Sample + Permutation

Simulation: Linear SEM



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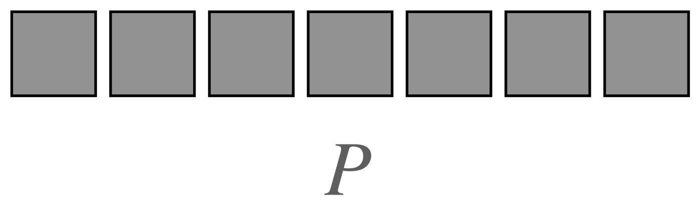

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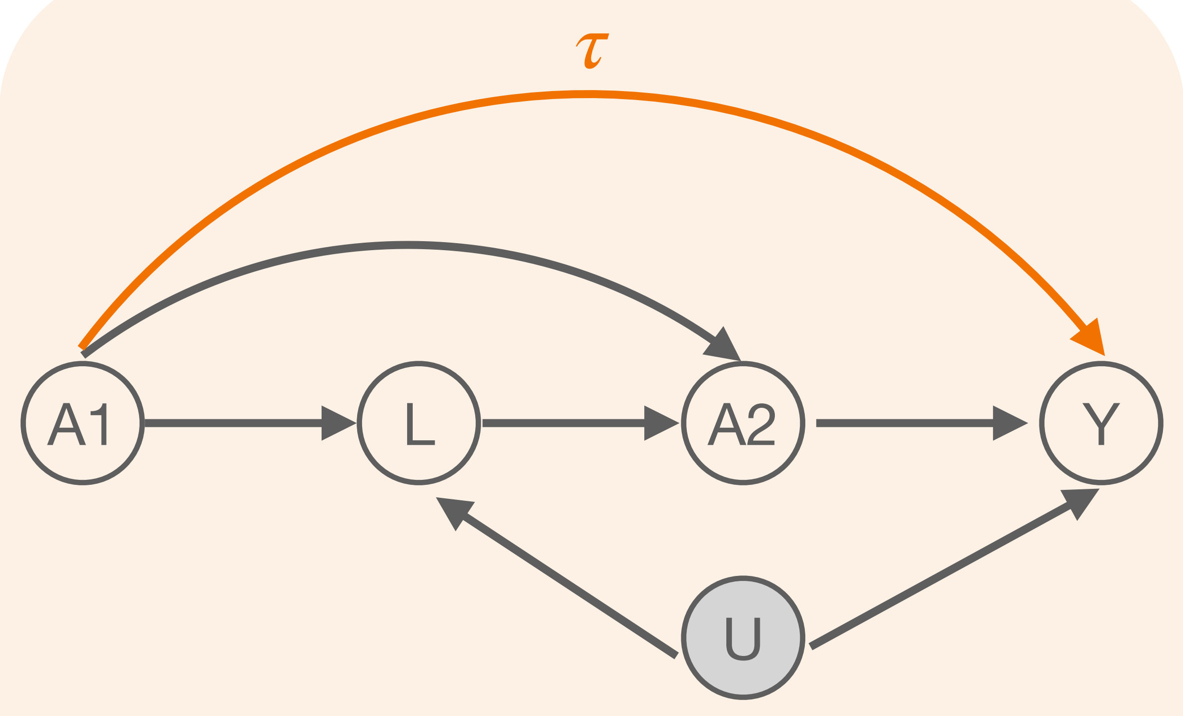

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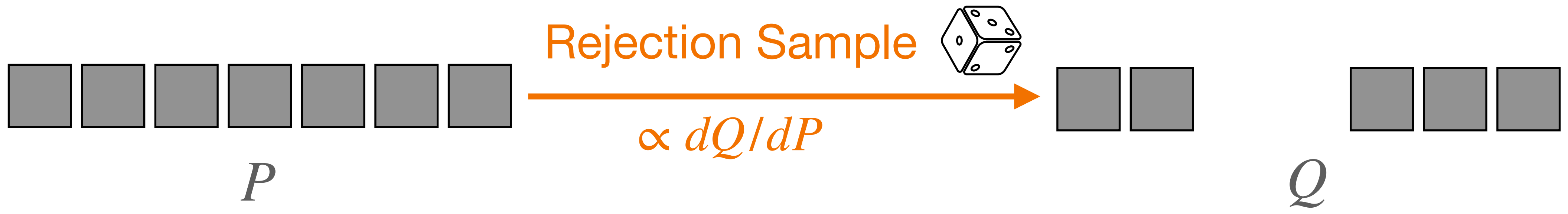
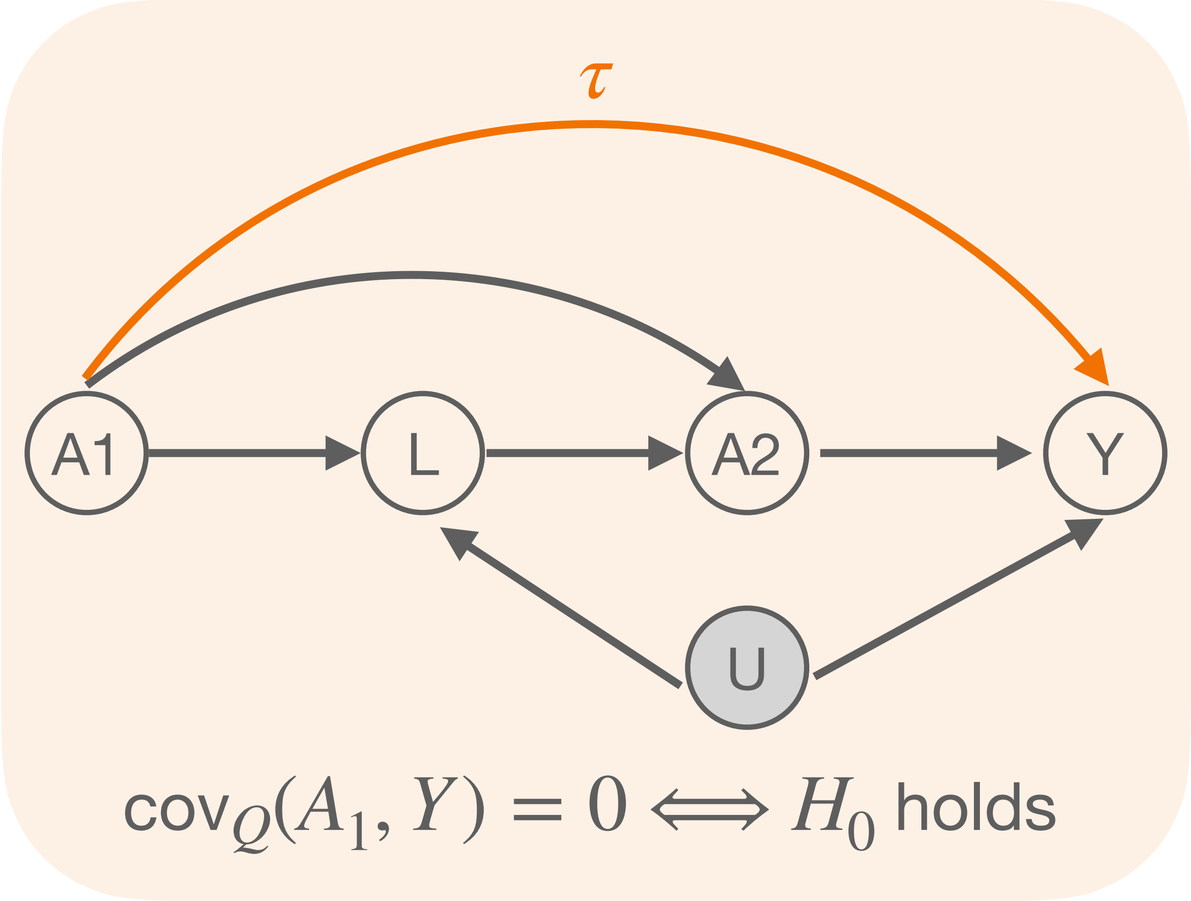

Rejection Sample

$\propto dQ/dP$

P

Q

Simulation: Linear SEM



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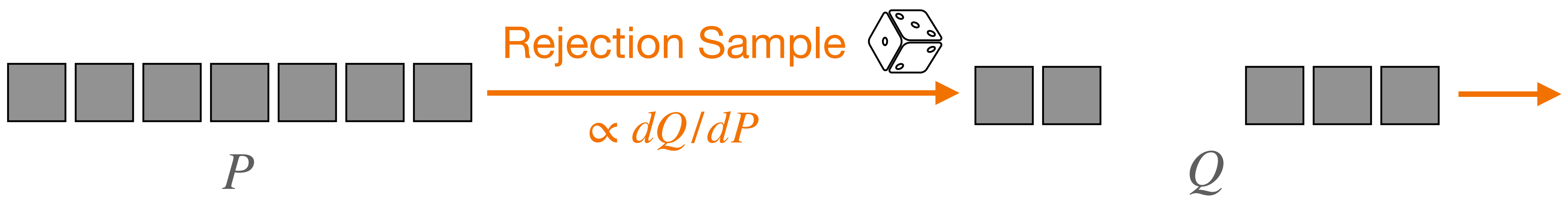


Rejection Sample

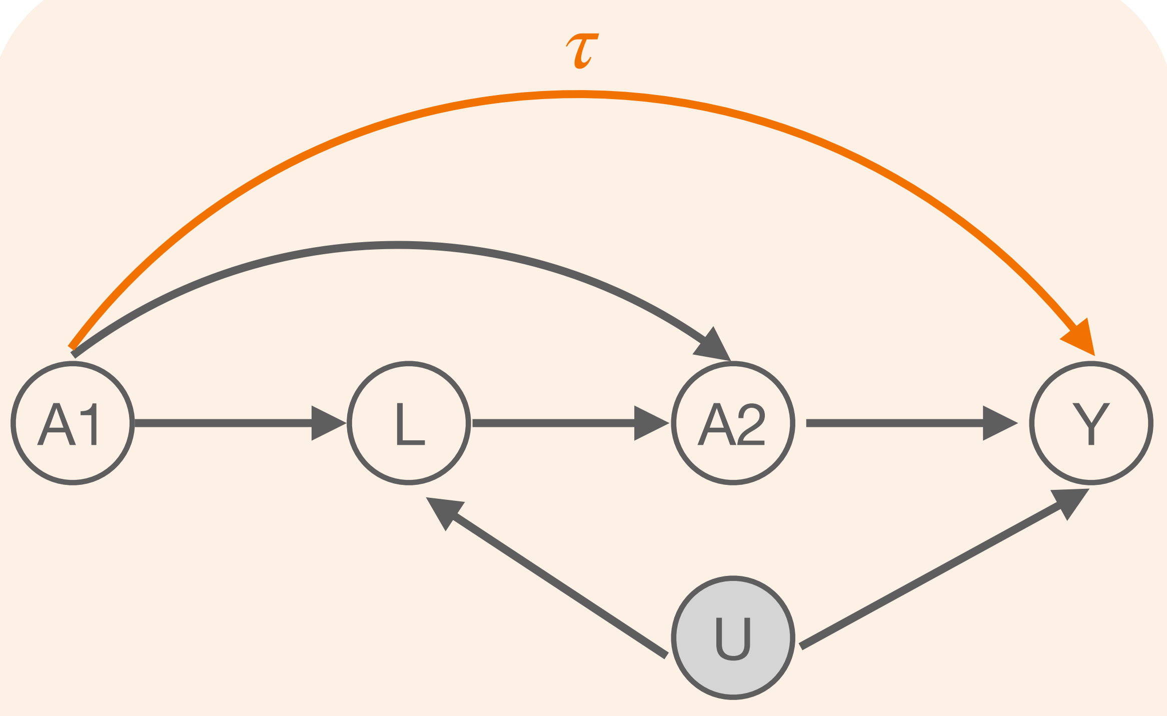
$\propto dQ/dP$

P

Q

T_n := Perm. p-value of $\mathrm{cov}_Q(A_1, Y)$

Simulation: Linear SEM



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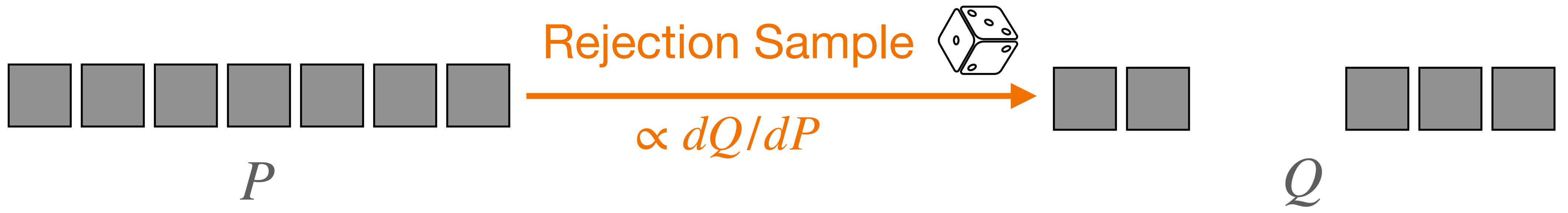

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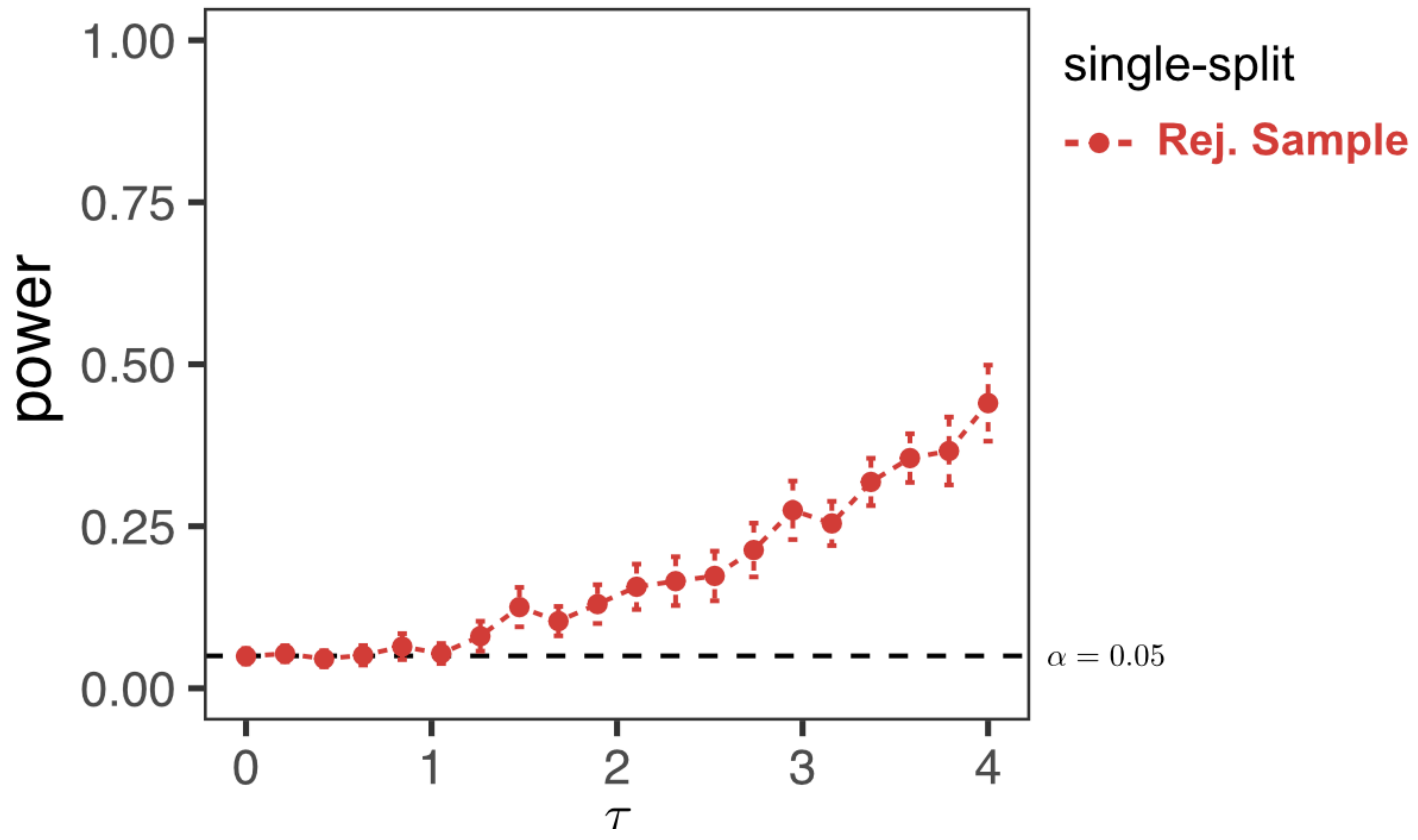

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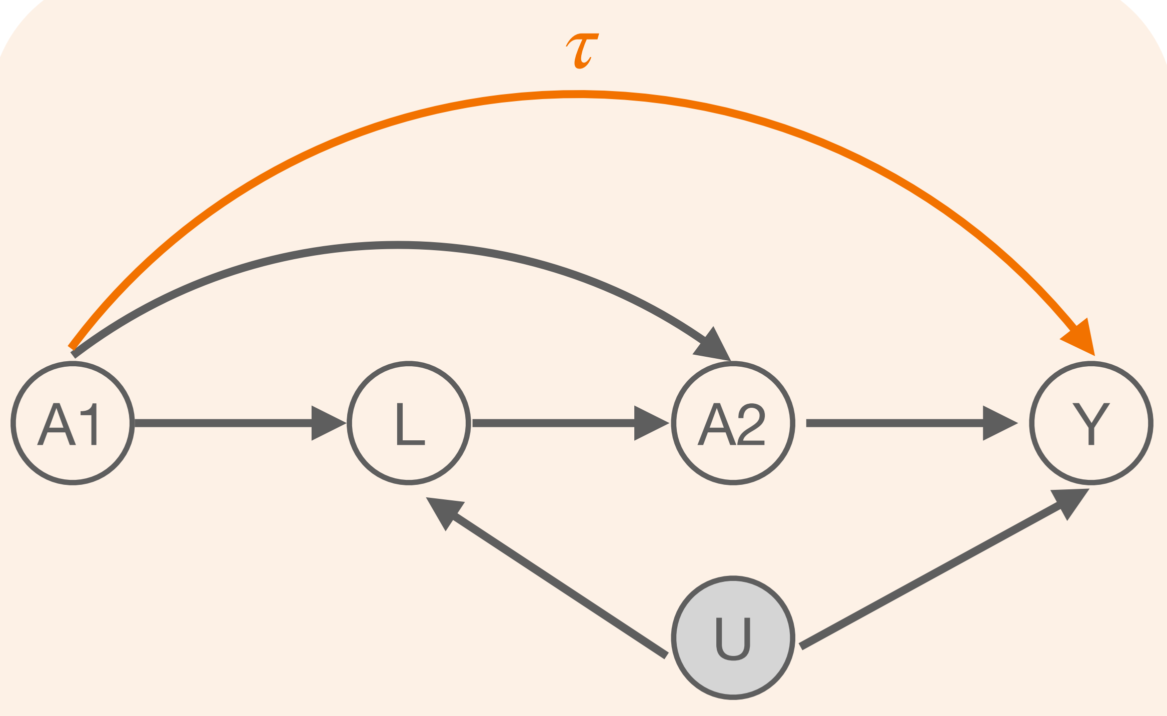

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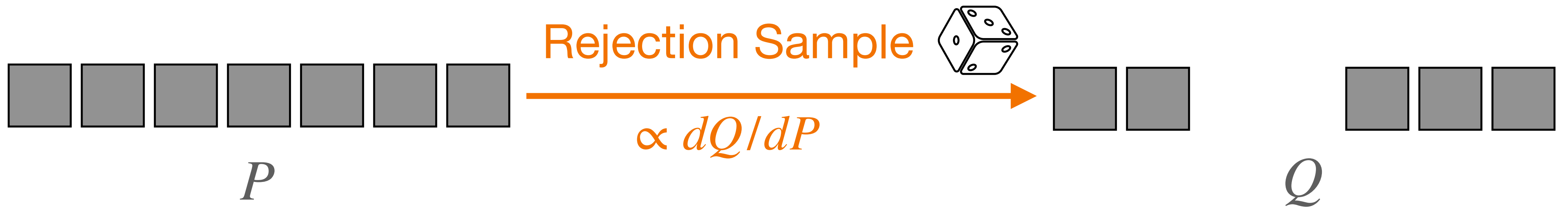
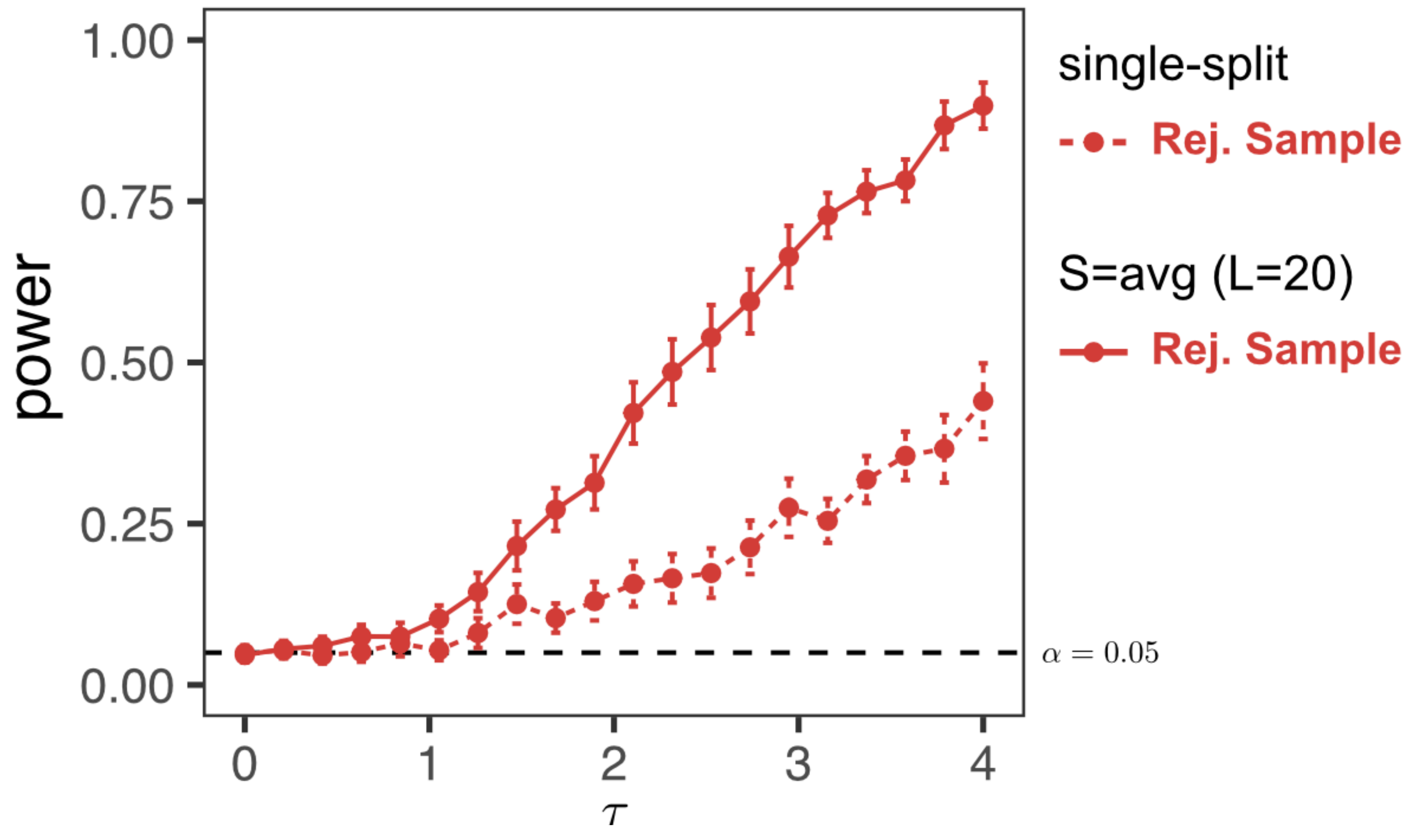


→ T_n := Perm. p-value of $\mathrm{cov}_Q(A_1, Y)$



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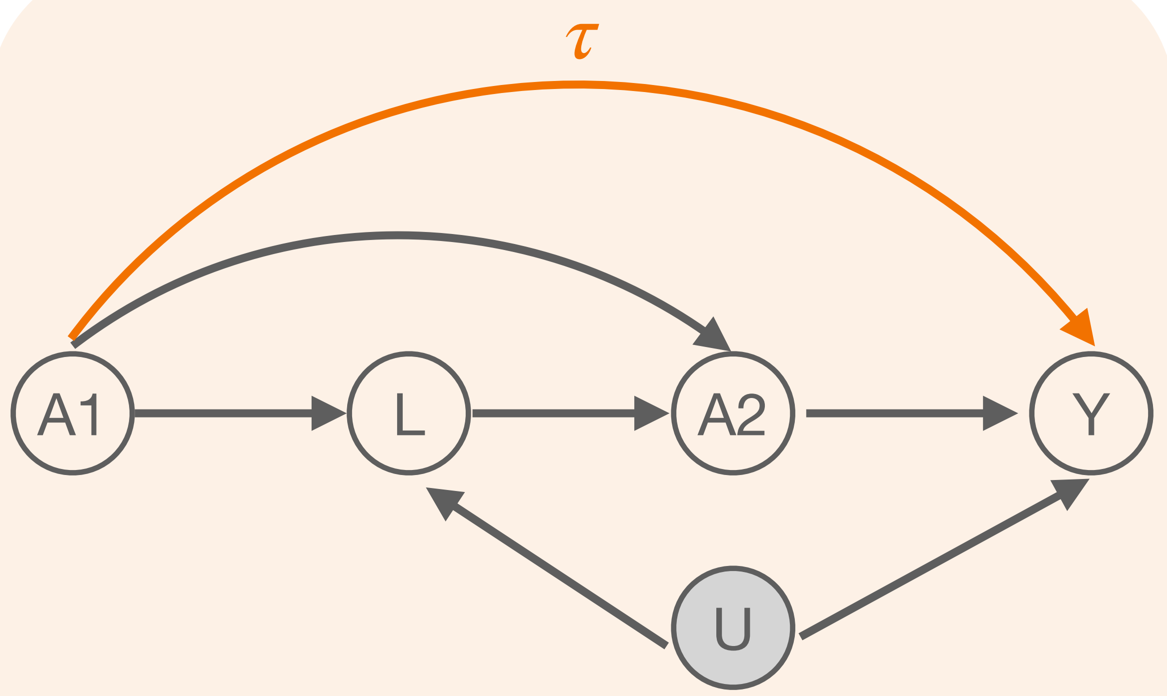

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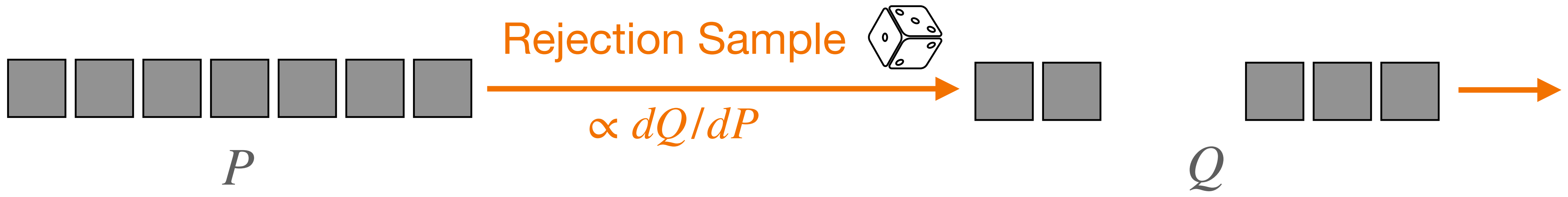
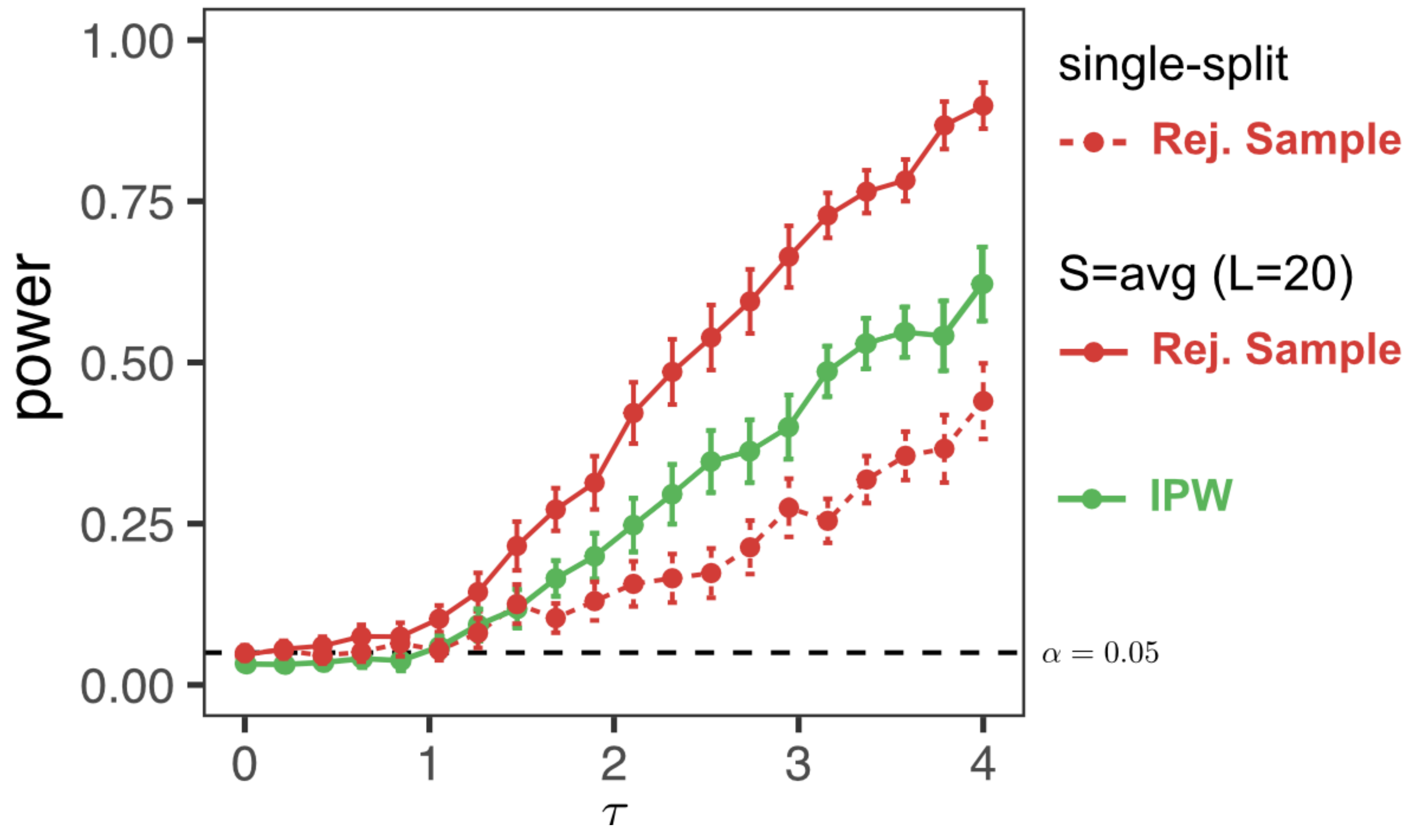


$T_n :=$ Perm. p-value of $\mathrm{cov}_Q(A_1, Y)$

(2) IPW for $\mathrm{cov}_Q(A_1, Y)$ (Robins, 1999)

$$Z_i := \frac{Y_i(A_{1,i} - \mathbb{E}A_1)}{P(A_{2,i} \mid L_i, A_{1,i})}, \qquad \chi_n := \frac{\sum_i Z_i}{\sqrt{\sum_i Z_i^2}} \to_d \mathcal{N}(0,1)\,.$$



Theme so far

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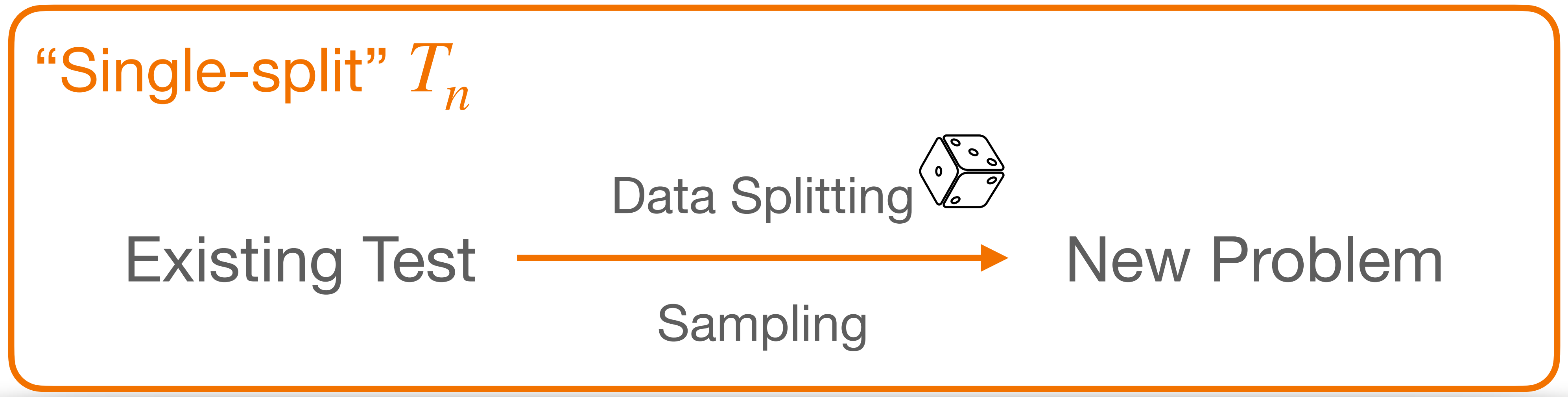
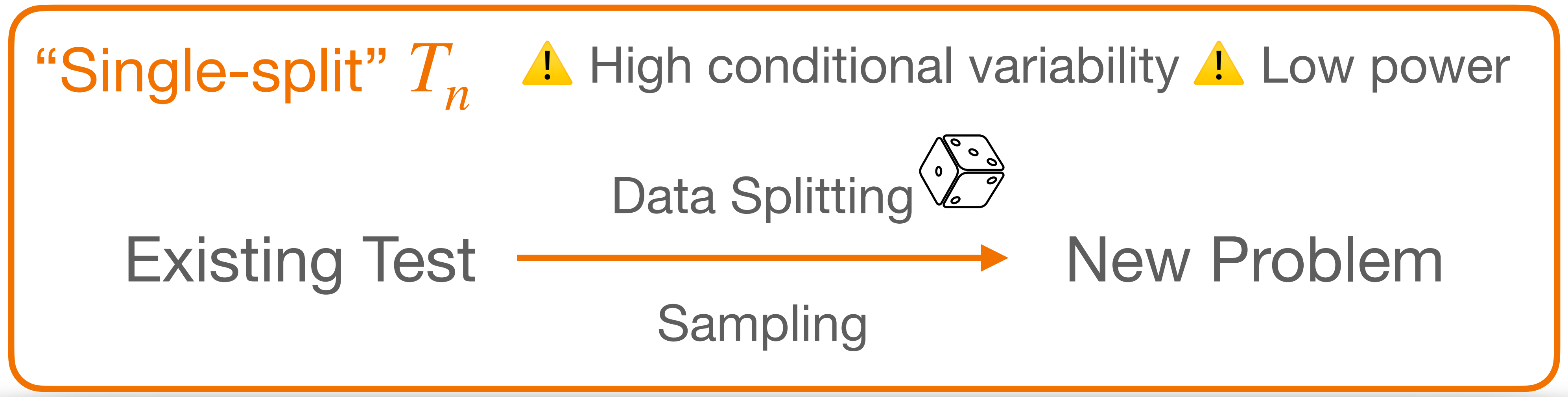


“Single-split” T_n

Existing Test $\xrightarrow[\text{Sampling}]{\text{Data Splitting}}$ New Problem

Theme so far

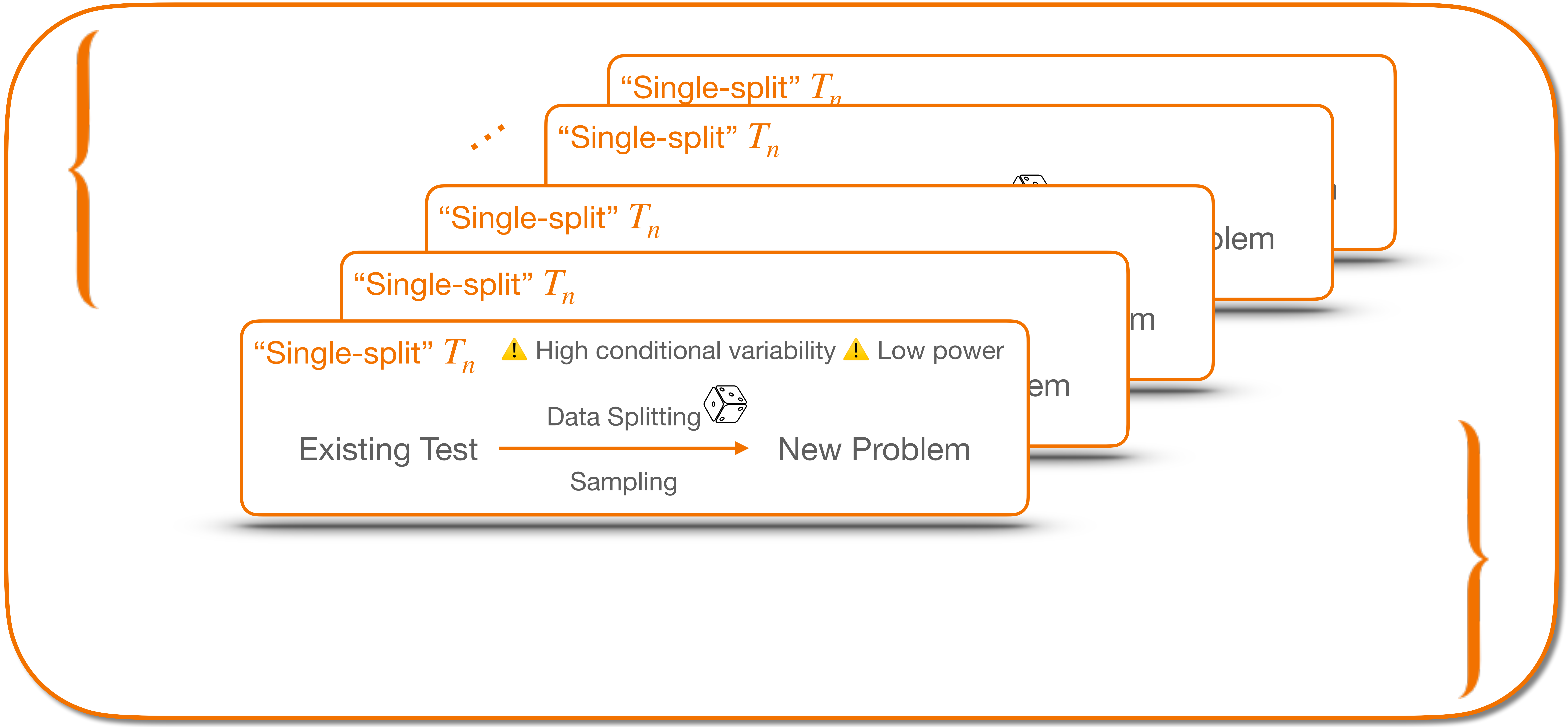


“Single-split” T_n ⚠ High conditional variability ⚠ Low power

$$\text{Existing Test} \xrightarrow[\text{Sampling}]{\text{Data Splitting}} \text{New Problem}$$

Theme so far

Meta-algorithm: **Rank-transformed Subsampling**



“Single-split” T_n

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“Single-split” T_n ⚠ High conditional variability ⚠ Low power

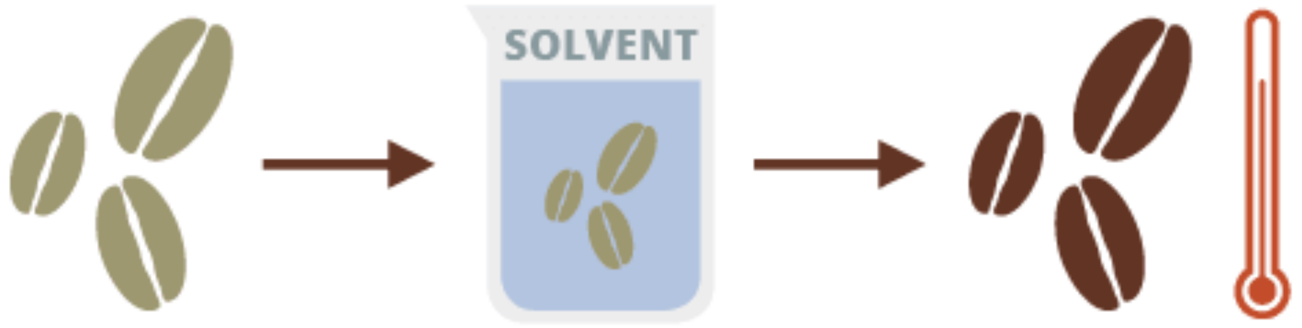
$$\text{Existing Test} \xrightarrow[\text{Sampling}]{\text{Data Splitting}} \text{New Problem}$$

Reduces (conditional) variability & Boosts power!

Outline

- Setup and main challenge
- Method: Rank-transformed subsampling
- Applications
    - Hunt and test
    - Improving double machine learning
    - Testing no direct effect of a sequentially randomized trial
- **Future directions**

Harness extra randomness



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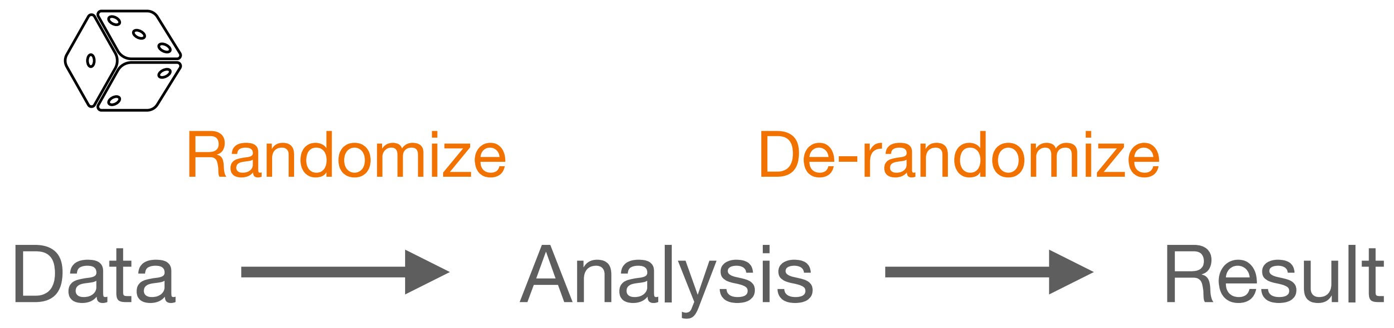
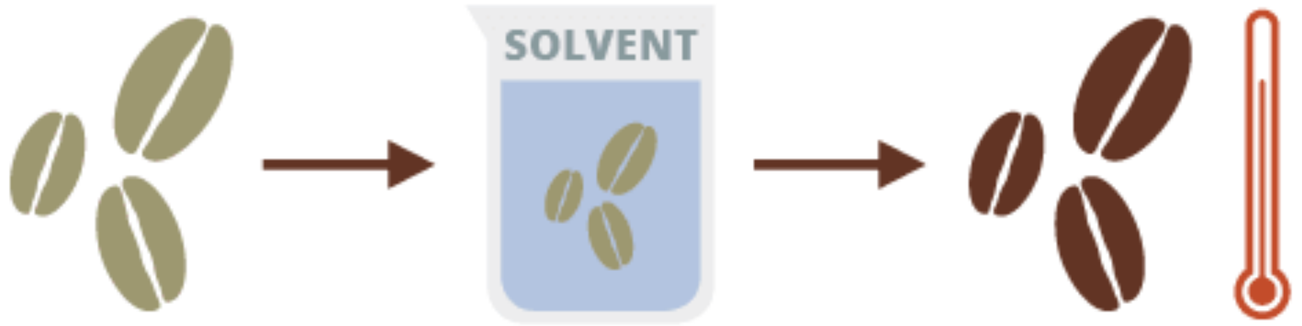


Randomize

De-randomize

Data → Analysis → Result

Harness extra randomness



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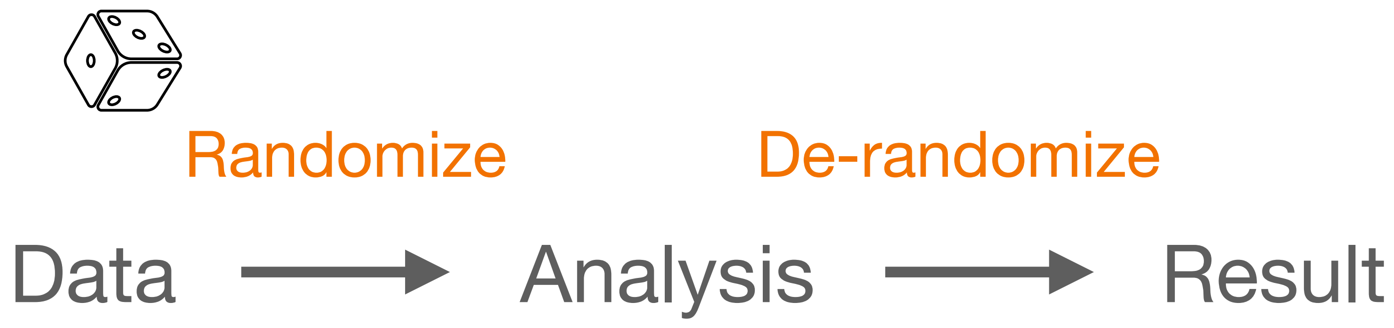

👉 Flexible goodness-of-fit

e.g., quantile regression

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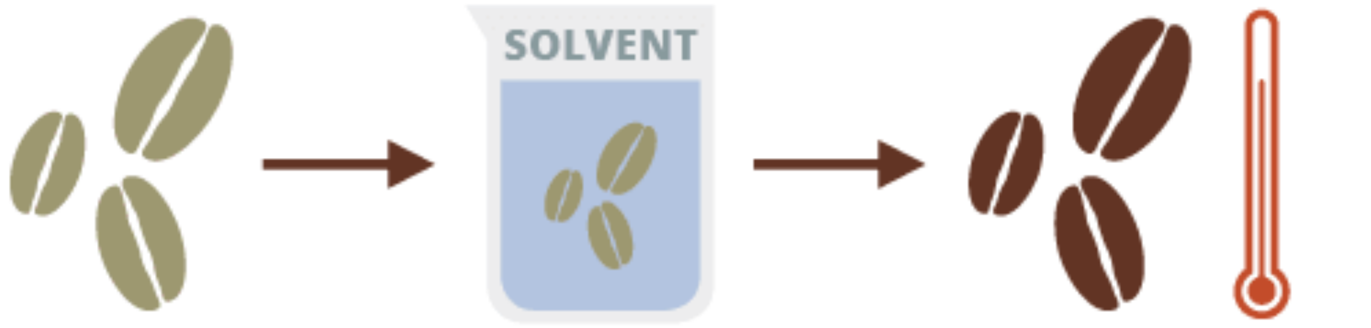

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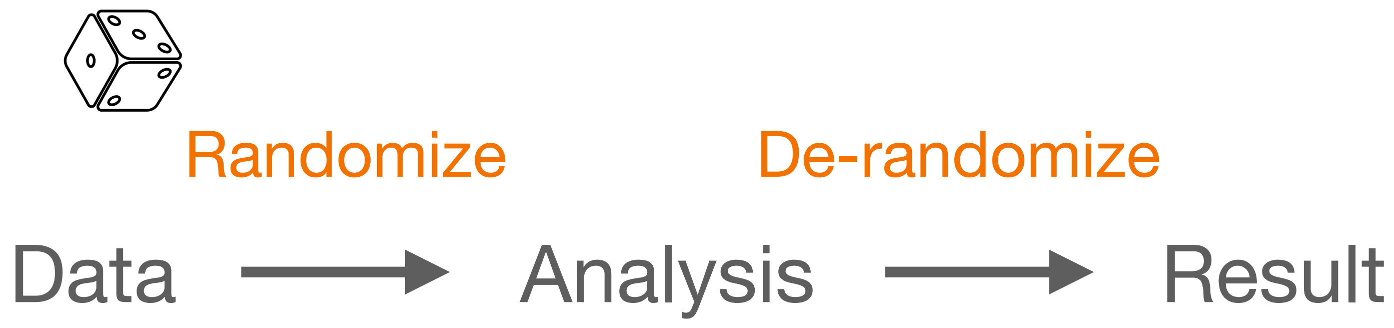

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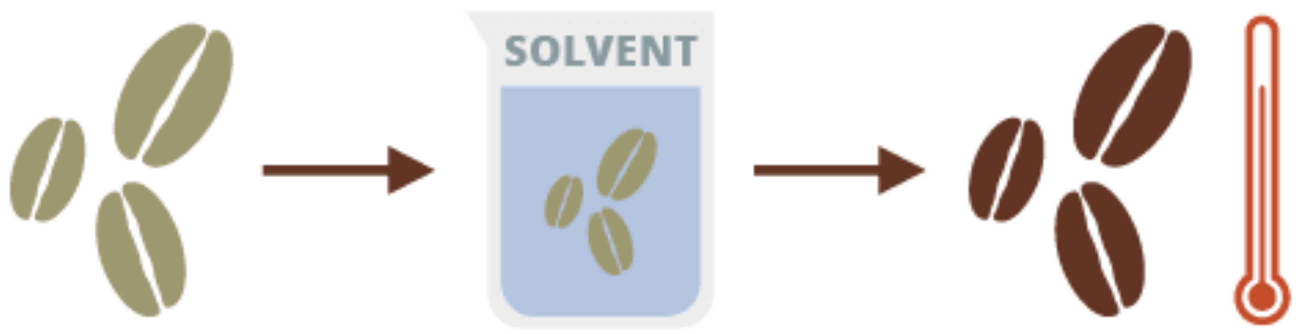

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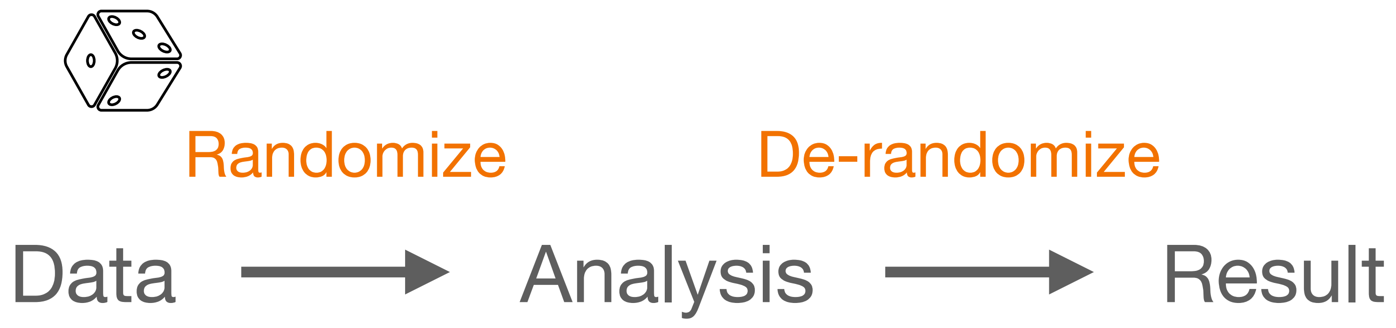
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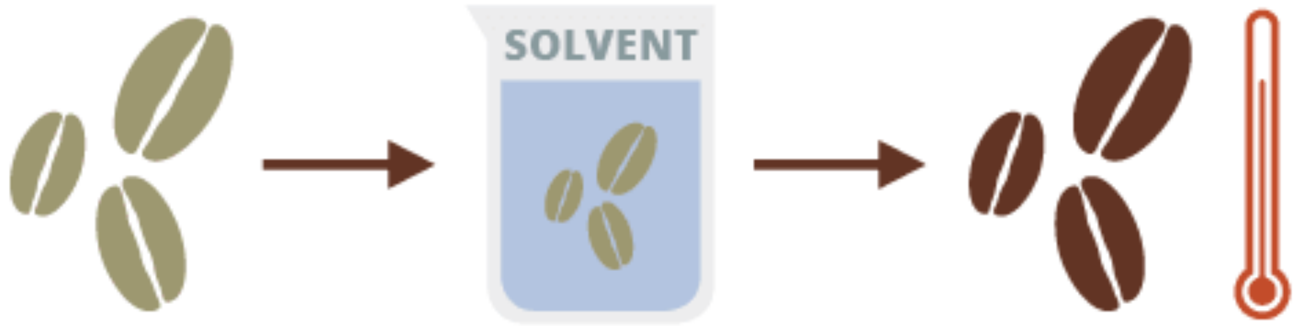

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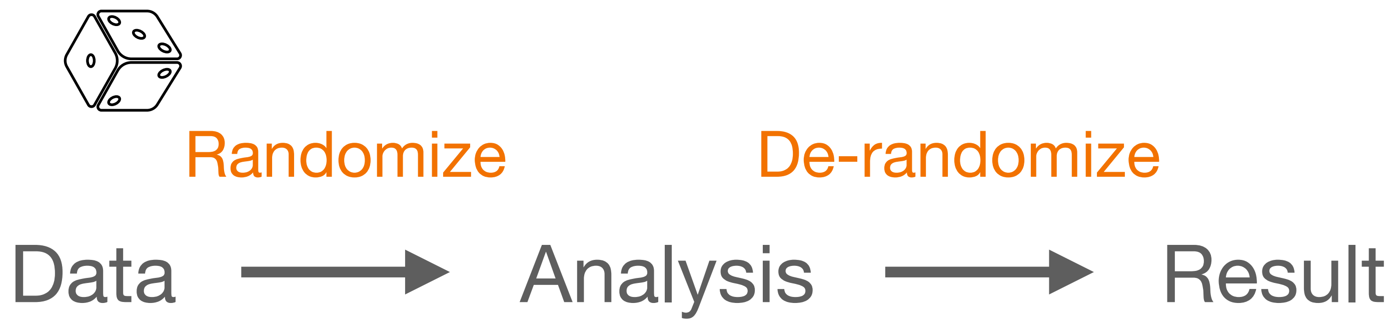

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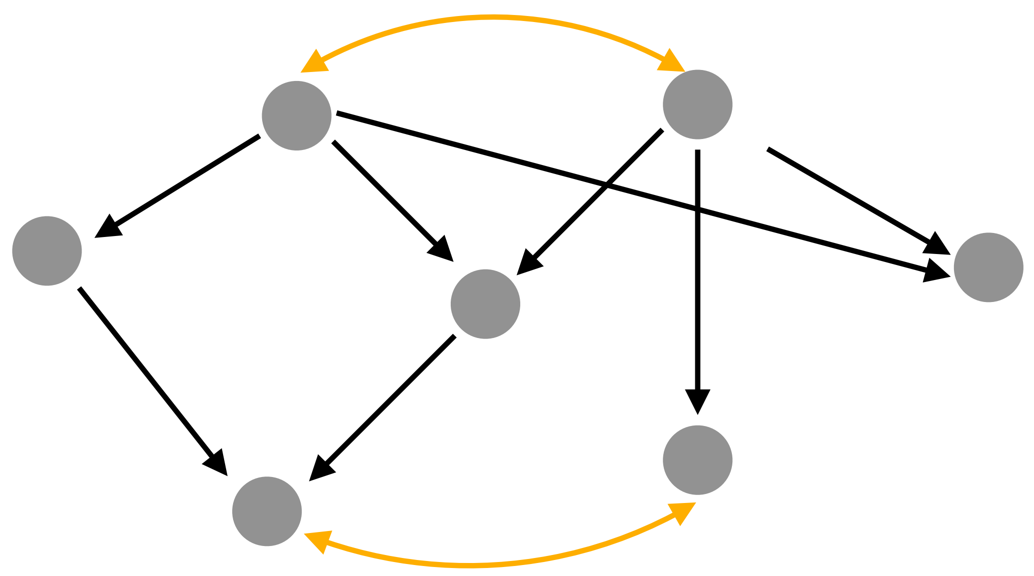
👉 Causal inference & causal discovery

- Observed distribution → Intervened distribution

Empowering causal discovery

	Gene 1	Gene 2	Gene 3	...
Cell 1	10	10	0	
Cell 2	0	15	4	
Cell 3	600	0	20	
⋮				



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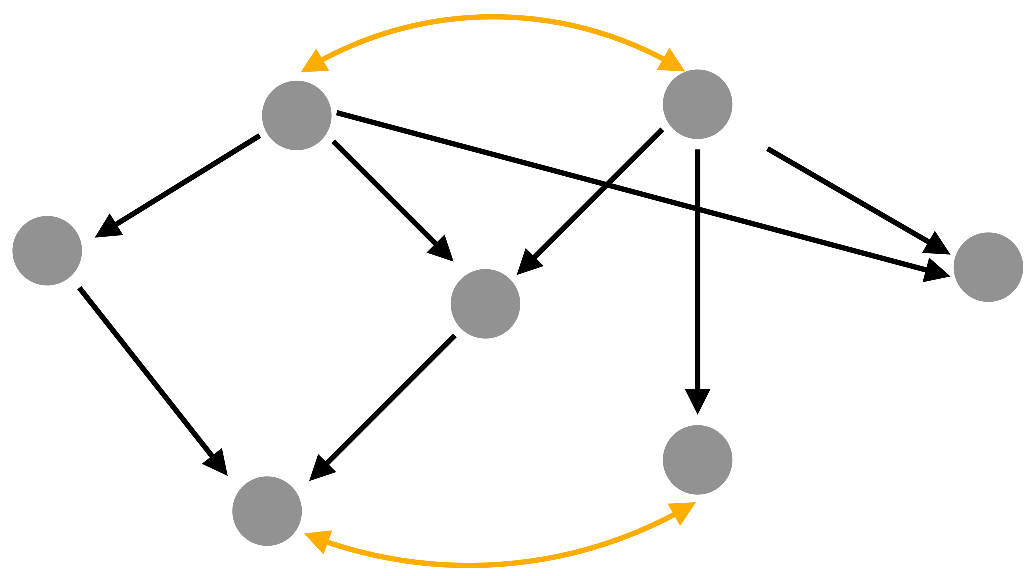

🙁 **State of the art:** cannot utilize generalized conditional independence.

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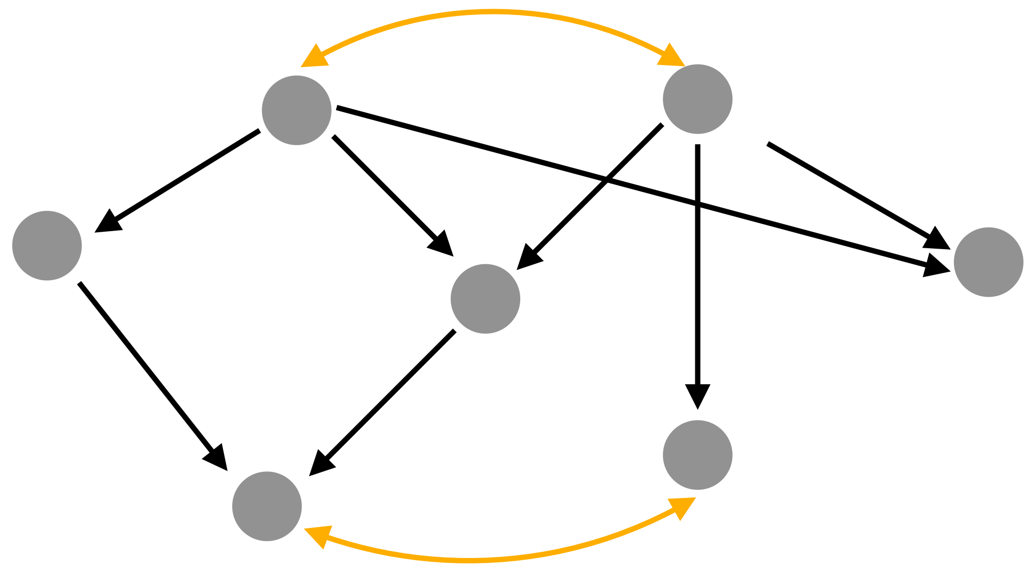

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💡 Generalized conditional independence can be very informative about the graph!

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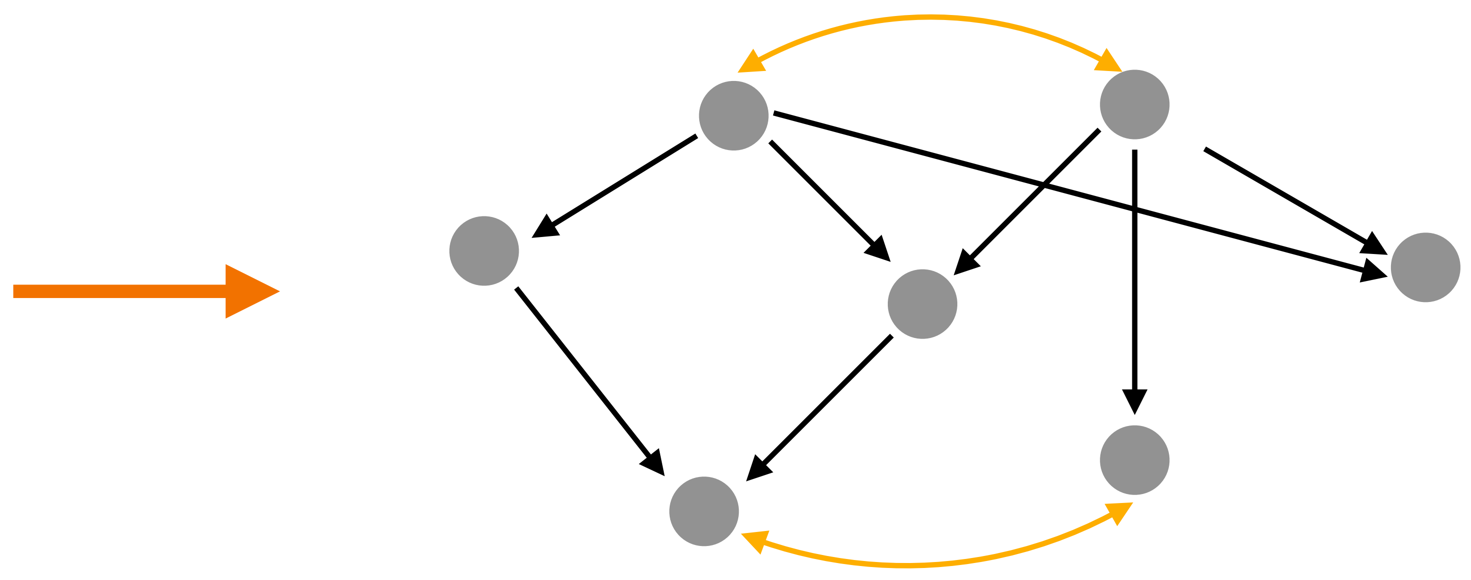

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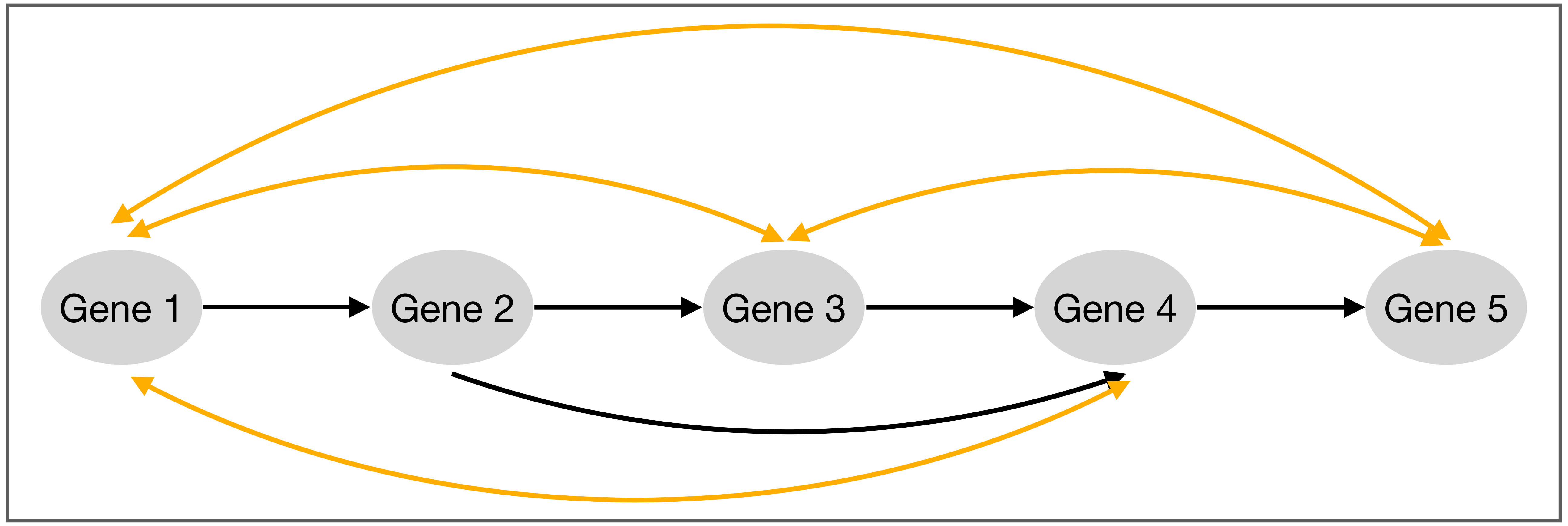
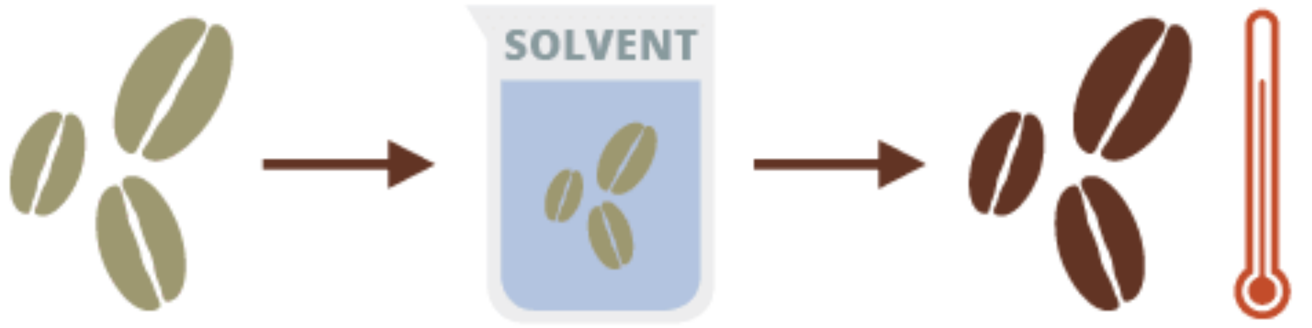


😮 Uniquely identified (from ~30,000 possibilities) from one single generalized conditional independence constraint!

Robins. Interview with Jamie Robins. *Observational Studies* (2022).

Harness extra randomness



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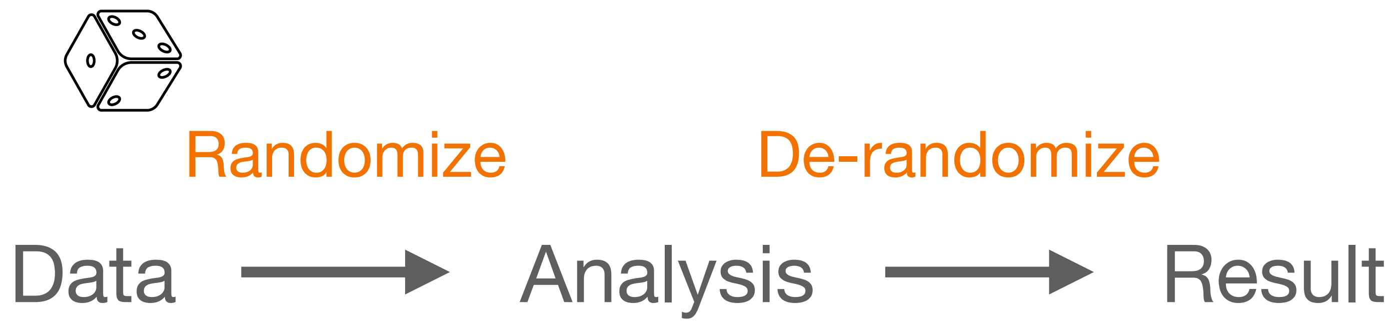

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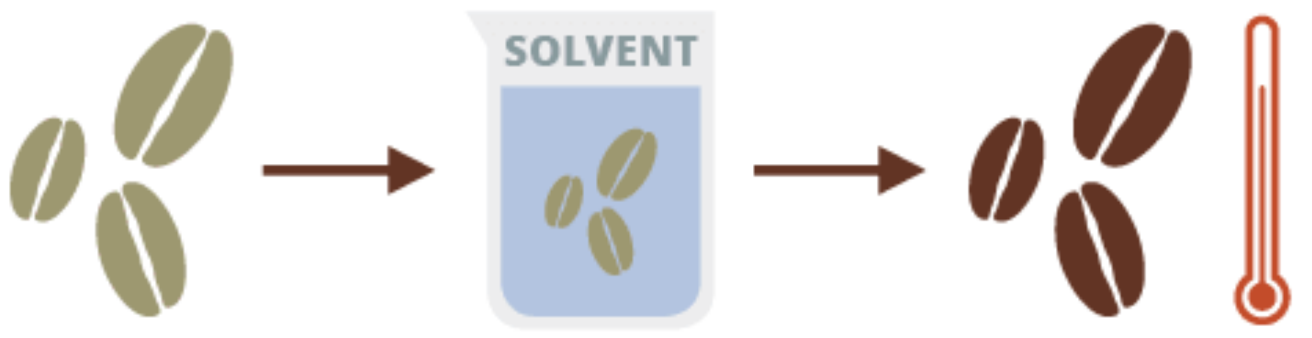

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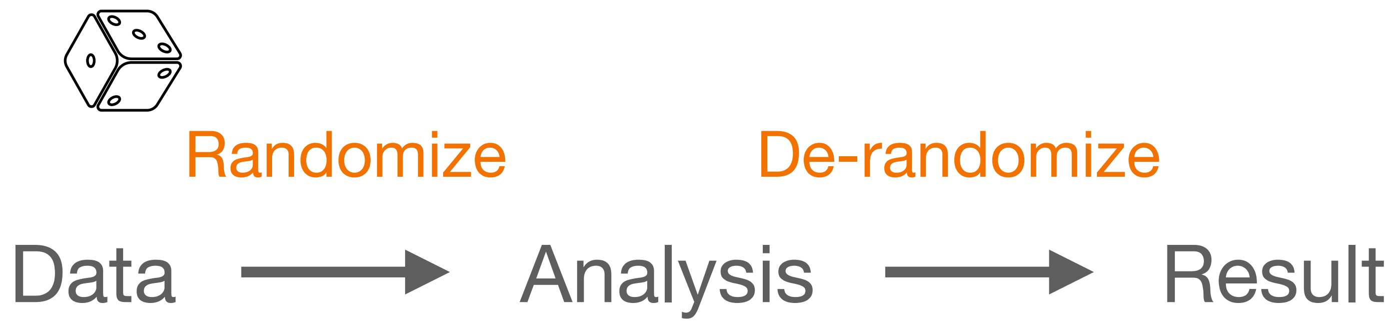

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🤔 How much power can we hope to extract?

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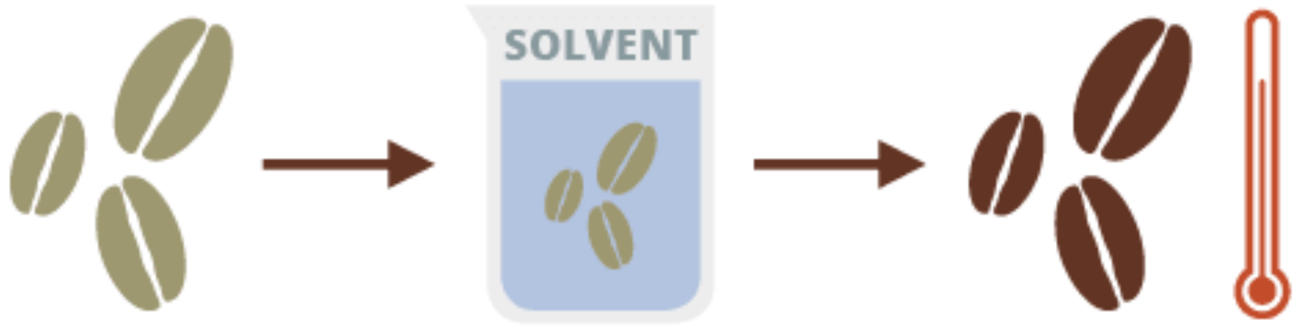

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🤔 How much power can we hope to extract?

🤔 Replicability: **computational** ➠ **statistical**

Multiple aggregations: Adaptive algorithm

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$T_n^{(1)}$	$T_n^{(2)}$	$T_n^{(3)}$	$T_n^{(4)}$	$\cdots$	$T_n^{(L)}$	🤔
*	**	.	*		*	$S = \text{avg}$ ✅
.			***			$S = \min$ ✅

Multiple aggregations: Adaptive algorithm

$T_n^{(1)}$	$T_n^{(2)}$	$T_n^{(3)}$	$T_n^{(4)}$	$\cdots$	$T_n^{(L)}$	🤔
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💡 Allow the user to specify $S^1, \ldots, S^W$

Multiple aggregations: Adaptive algorithm

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.			***			$S = \min$ ✅

$\widetilde{T}_m^{(1)}$	$\widetilde{T}_m^{(2)}$	$\ldots$	$\widetilde{T}_m^{(L)}$
1.6	-0.8		0.1
-1.1	-0.2		1.8
$\vdots$	$\vdots$		$\vdots$
2.7	0.2		2.8

Observed

$T_n^{(1)}$	$T_n^{(2)}$	$\ldots$	$T_n^{(L)}$
2.1	-1.2		0.3

💡 Allow the user to specify $S^1, \ldots, S^W$

Multiple aggregations: Adaptive algorithm

$T_n^{(1)}$	$T_n^{(2)}$	$T_n^{(3)}$	$T_n^{(4)}$	$\cdots$	$T_n^{(L)}$	🤔
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.			***			$S = \min$ ✅

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S^1

$\widetilde{T}_m^{(1)}$	$\widetilde{T}_m^{(2)}$	$\ldots$	$\widetilde{T}_m^{(L)}$	$\tilde{S}_n^1$
1.6	-0.8		0.1	0.5
-1.1	-0.2		1.8	-0.1
$\vdots$	$\vdots$		$\vdots$	$\vdots$
2.7	0.2		2.8	1.2

Observed

$T_n^{(1)}$	$T_n^{(2)}$	$\ldots$	$T_n^{(L)}$	S_n^1
2.1	-1.2		0.3	1.7

Multiple aggregations: Adaptive algorithm

$T_n^{(1)}$	$T_n^{(2)}$	$T_n^{(3)}$	$T_n^{(4)}$	$\cdots$	$T_n^{(L)}$	🤔
*	**	.	*		*	$S =$ avg ✅
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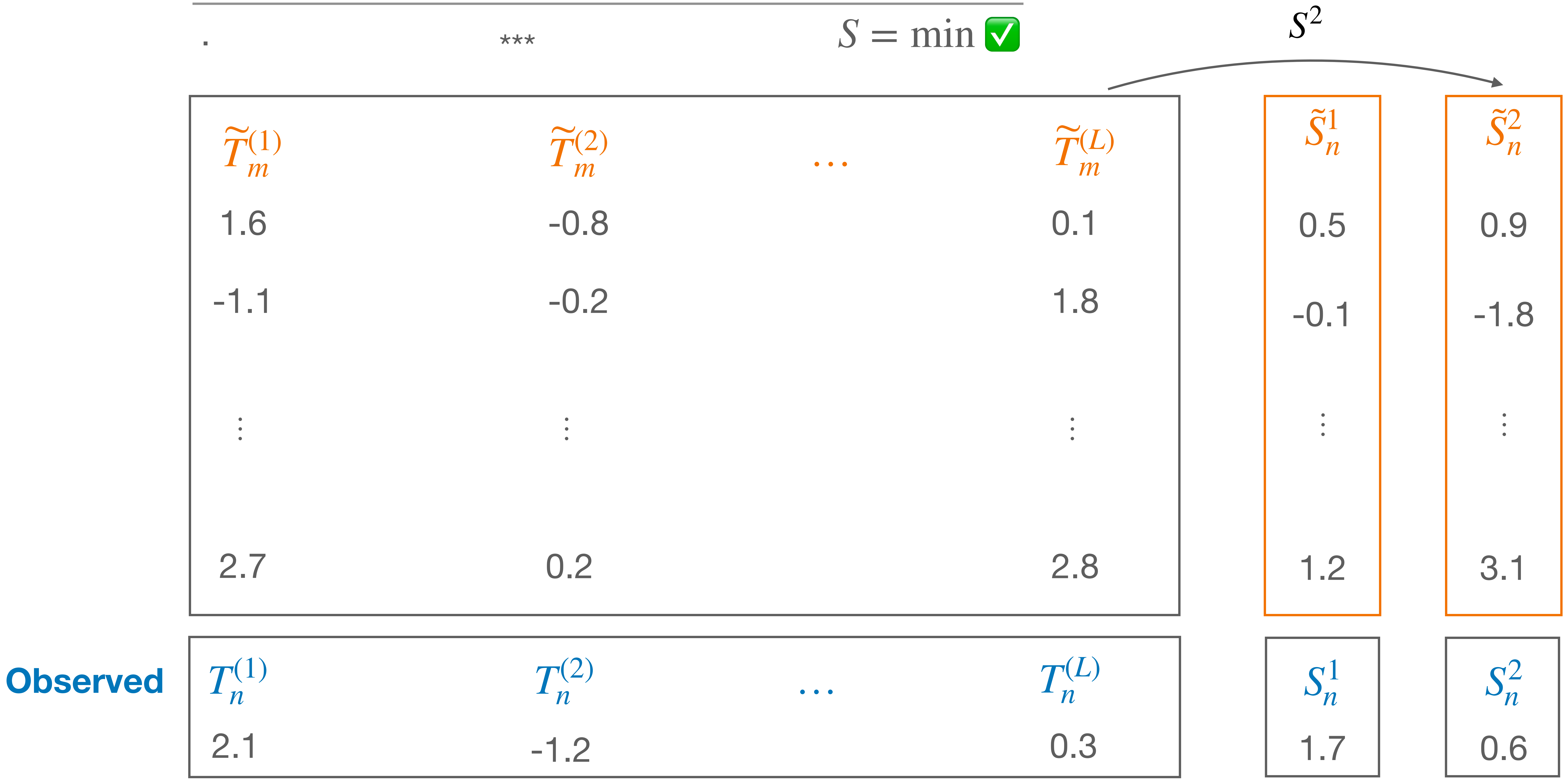
💡 Allow the user to specify $S^1, \ldots, S^W$



S^2

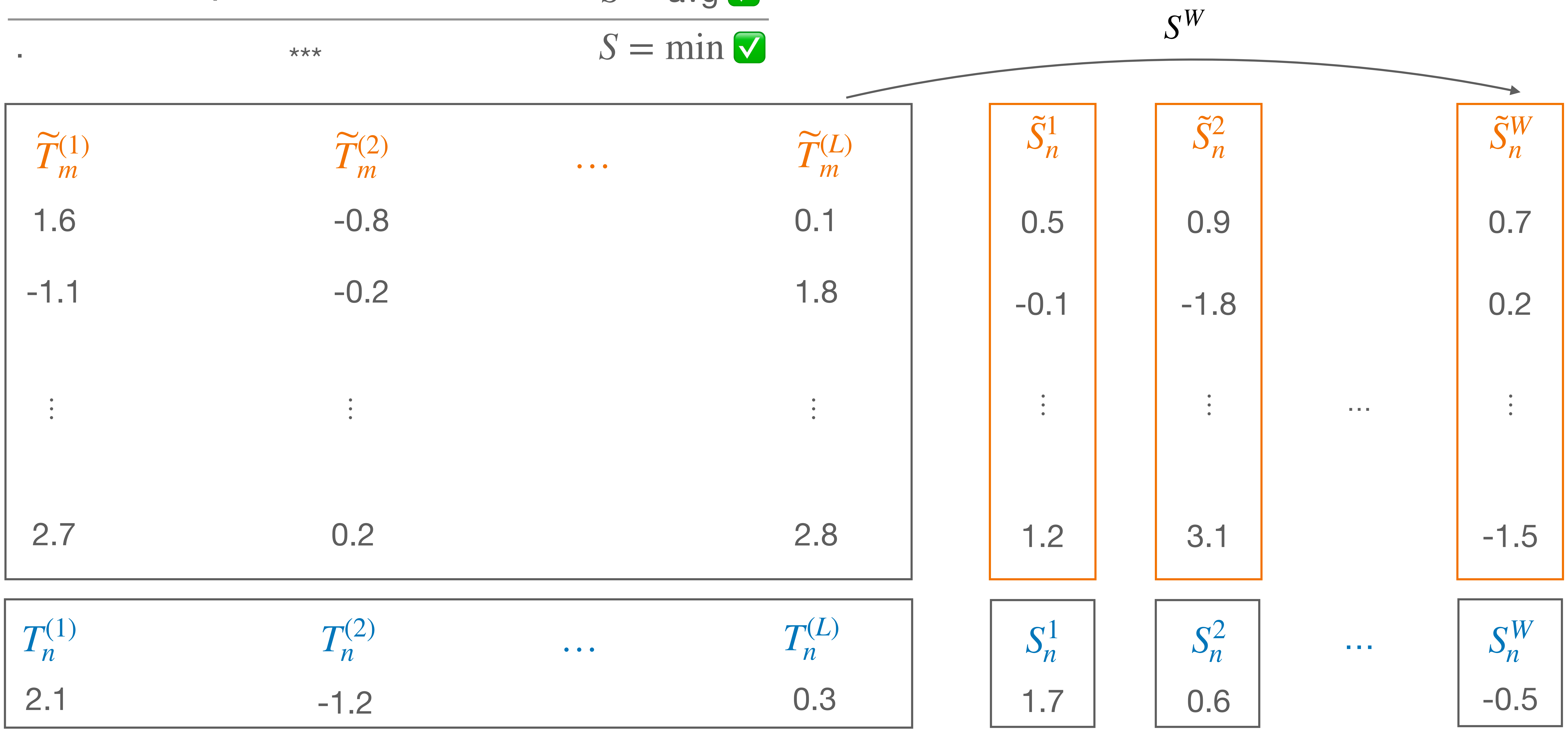
$\widetilde{T}_m^{(1)}$	$\widetilde{T}_m^{(2)}$	$\ldots$	$\widetilde{T}_m^{(L)}$	$\tilde{S}_n^1$	$\tilde{S}_n^2$
1.6	-0.8		0.1	0.5	0.9
-1.1	-0.2		1.8	-0.1	-1.8
$\vdots$	$\vdots$		$\vdots$	$\vdots$	$\vdots$
2.7	0.2		2.8	1.2	3.1

Observed	$T_n^{(1)}$	$T_n^{(2)}$	$\ldots$	$T_n^{(L)}$	S_n^1	S_n^2
	2.1	-1.2		0.3	1.7	0.6

Multiple aggregations: Adaptive algorithm

$T_n^{(1)}$	$T_n^{(2)}$	$T_n^{(3)}$	$T_n^{(4)}$	$\cdots$	$T_n^{(L)}$	🤔
*	**	.	*		*	$S = \text{avg}$ ✅
.			***			$S = \min$ ✅

💡 Allow the user to specify $S^1, \ldots, S^W$



$\widetilde{T}_m^{(1)}$	$\widetilde{T}_m^{(2)}$	$\ldots$	$\widetilde{T}_m^{(L)}$	$\tilde{S}_n^1$	$\tilde{S}_n^2$		$\tilde{S}_n^W$
1.6	-0.8		0.1	0.5	0.9		0.7
-1.1	-0.2		1.8	-0.1	-1.8		0.2
⋮	⋮		⋮	⋮	⋮	…	⋮
2.7	0.2		2.8	1.2	3.1		-1.5

	$T_n^{(1)}$	$T_n^{(2)}$	$\ldots$	$T_n^{(L)}$	S_n^1	S_n^2	…	S_n^W
Observed	2.1	-1.2		0.3	1.7	0.6		-0.5

Multiple aggregations: Adaptive algorithm

$T_n^{(1)}$	$T_n^{(2)}$	$T_n^{(3)}$	$T_n^{(4)}$	$\cdots$	$T_n^{(L)}$	🤔
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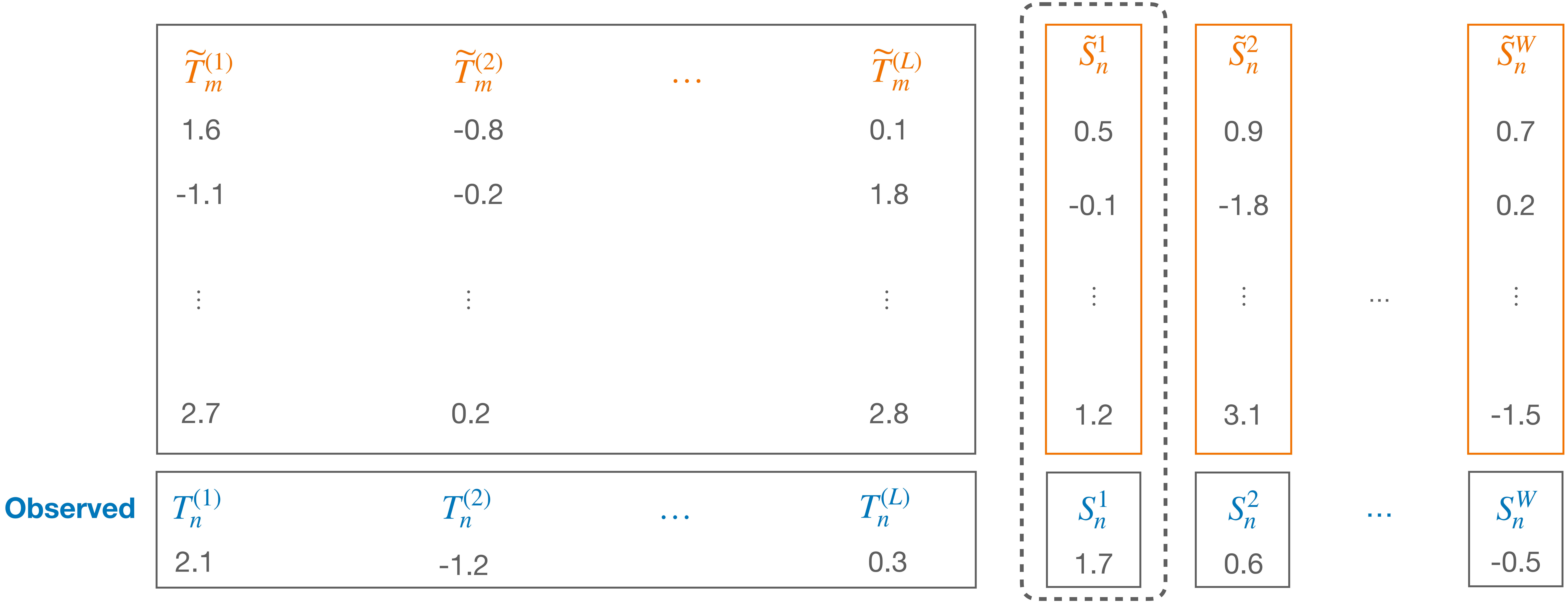
.			***			$S = \min$ ✅

💡 Allow the user to specify $S^1, \ldots, S^W$



	$\widetilde{T}_m^{(1)}$	$\widetilde{T}_m^{(2)}$	$\ldots$	$\widetilde{T}_m^{(L)}$	$\tilde{S}_n^1$	$\tilde{S}_n^2$		$\tilde{S}_n^W$
	1.6	-0.8		0.1	0.5	0.9		0.7
	-1.1	-0.2		1.8	-0.1	-1.8		0.2
	⋮	⋮		⋮	⋮	⋮	…	⋮
	2.7	0.2		2.8	1.2	3.1		-1.5
Observed	$T_n^{(1)}$	$T_n^{(2)}$	$\ldots$	$T_n^{(L)}$	S_n^1	S_n^2	…	S_n^W
	2.1	-1.2		0.3	1.7	0.6		-0.5

Multiple aggregations: Adaptive algorithm

$T_n^{(1)}$	$T_n^{(2)}$	$T_n^{(3)}$	$T_n^{(4)}$	$\cdots$	$T_n^{(L)}$	🤔
*	**	.	*		*	$S =$ avg ✅
.			***			$S = \min$ ✅

💡 Allow the user to specify $S^1, \ldots, S^W$

	$\widetilde{T}_m^{(1)}$	$\widetilde{T}_m^{(2)}$	$\ldots$	$\widetilde{T}_m^{(L)}$	$\tilde{S}_n^1$	$\tilde{S}_n^2$	$\cdots$	$\tilde{S}_n^W$
	1.6	-0.8		0.1	200	0.9		0.7
	-1.1	-0.2		1.8	77	-1.8		0.2
	$\vdots$	$\vdots$		$\vdots$	$\vdots$	$\vdots$	$\cdots$	$\vdots$
	2.7	0.2		2.8	431	3.1		-1.5
Observed	$T_n^{(1)}$	$T_n^{(2)}$	$\ldots$	$T_n^{(L)}$	S_n^1	S_n^2	$\cdots$	S_n^W
	2.1	-1.2		0.3	489	0.6		-0.5

Multiple aggregations: Adaptive algorithm

$T_n^{(1)}$	$T_n^{(2)}$	$T_n^{(3)}$	$T_n^{(4)}$	$\cdots$	$T_n^{(L)}$	🤔
*	**	.	*		*	$S =$ avg ✅
.			***			$S = \min$ ✅

💡 Allow the user to specify $S^1, \ldots, S^W$

$\widetilde{T}_m^{(1)}$	$\widetilde{T}_m^{(2)}$	$\ldots$	$\widetilde{T}_m^{(L)}$	$\tilde{S}_n^1$	$\tilde{S}_n^2$	$\cdots$	$\tilde{S}_n^W$
1.6	-0.8		0.1	200	142		289
-1.1	-0.2		1.8	77	33		260
$\vdots$	$\vdots$		$\vdots$	$\vdots$	$\vdots$		$\vdots$
2.7	0.2		2.8	431	460		12

Observed

$T_n^{(1)}$	$T_n^{(2)}$	$\ldots$	$T_n^{(L)}$	S_n^1	S_n^2	$\cdots$	S_n^W
2.1	-1.2		0.3	489	281		32

Multiple aggregations: Adaptive algorithm

$T_n^{(1)}$	$T_n^{(2)}$	$T_n^{(3)}$	$T_n^{(4)}$	$\cdots$	$T_n^{(L)}$	🤔
*	**	.	*		*	$S =$ avg ✅
.			***			$S = \min$ ✅

💡 Allow the user to specify $S^1, \ldots, S^W$

$\min$ ✅

	$\widetilde{T}_m^{(1)}$	$\widetilde{T}_m^{(2)}$	$\ldots$	$\widetilde{T}_m^{(L)}$	$\tilde{S}_n^1$	$\tilde{S}_n^2$	$\cdots$	$\tilde{S}_n^W$	$\tilde{R}_n$
	1.6	-0.8		0.1	200	142		289	**110**
	-1.1	-0.2		1.8	77	33		260	**25**
	⋮	⋮		⋮	⋮	⋮	$\cdots$	⋮	⋮
	2.7	0.2		2.8	431	460		12	**7**
Observed	$T_n^{(1)}$	$T_n^{(2)}$	$\ldots$	$T_n^{(L)}$	S_n^1	S_n^2	$\cdots$	S_n^W	R_n
	2.1	-1.2		0.3	489	281		32	**16**

Hunt and test: Flexible goodness-of-fit

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Linear model $Y \sim \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p$

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Consider introducing a new covariate $X_{p+1} := \xi(X)$ for as a non-linear $\xi(\,\cdot\,)$.

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Linear model $Y \sim \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p$

Consider introducing a new covariate $X_{p+1} := \xi(X)$ for as a non-linear $\xi(\,\cdot\,)$.

💡 If linear model is well-specified, then the should have $\beta_{p+1} = 0$ in

$$Y \sim \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p + \beta_{p+1} X_{p+1}.$$

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👉 Test $\cap_\xi \{H_0(\xi) : \beta_{p+1} = 0\}$.

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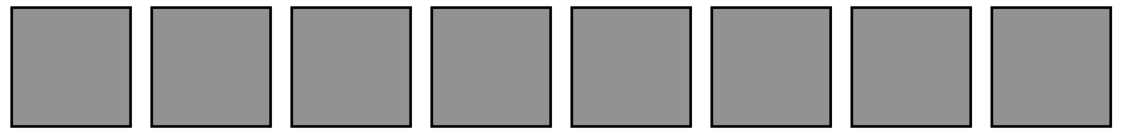

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🎲

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🟧🟦🟧🟦🟦🟧🟦🟧 (1) Use 🟦🟦🟦🟦 to find $\hat{\xi}$ such that $X_{p+1} = \xi(X)$ is likely to be “significant”.

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👆 Use any existing device for parameter inference.

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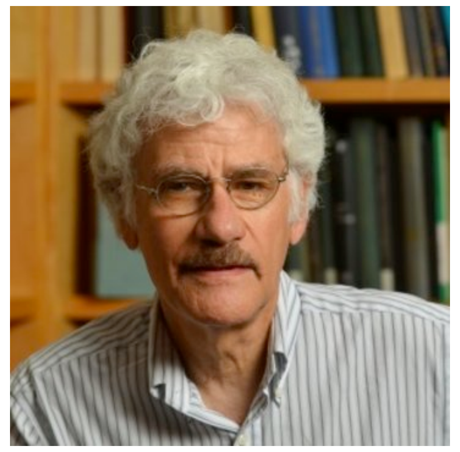
💡 **Gradient boosting!**

Jerome H. Friedman. Greedy function approximation: a gradient boosting machine. *Annals of Statistics* (2001).



Hunt and test: Flexible goodness-of-fit

Regression: $\min \mathbb{E} l(Y - \beta^\top X)$ for an **arbitrary** loss function $l(\,\cdot\,)$.

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Fitted $Y \sim \hat{\beta}^\top X$. With new covariate X_{p+1},

$$\sum_i l(Y_i - \hat{\beta}^\top X_i - \beta_{p+1} X_{i,p+1}) \approx \sum_i l(Y_i - \hat{\beta}^\top X_i) - \beta_i \sum_i l'(Y_i - \hat{\beta}^\top X_i)\, X_{i,p+1}$$

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(2) On 🟧🟧🟧🟧 : Compute statistic for testing $\beta_{p+1} = 0$ in $Y \sim \beta^\top X + \beta_{p+1}\, \hat{\xi}(X)$.

Hunt and test: Flexible goodness-of-fit

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Quantile regression

Hunt and test: Flexible goodness-of-fit

Quantile regression

1. Linear model is widely used.

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2. Developing goodness/lack-of-fit test is difficult.

   e.g., Zheng (1998), Horowitz & Spokoiny (2002), He & Zhu (2003),
   Escanciano and Velasco (2010), Escanciano & Goh (2014).

   (1) Asymptotic theory of certain residual statistics/processes.

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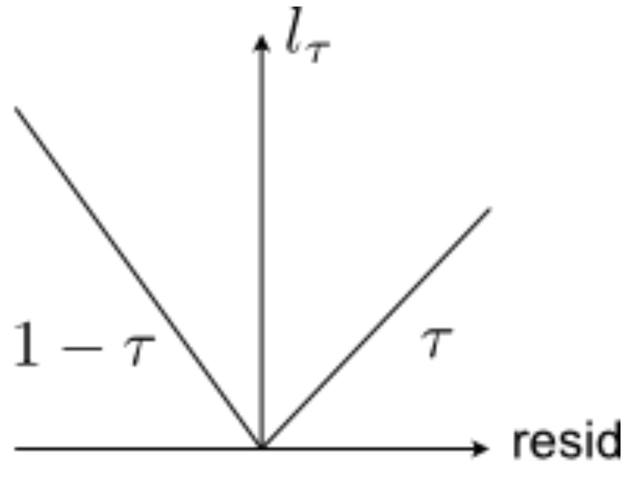

$\hat{\xi}$: random forest classifier sign(resid) $\sim X$.

T_n: standard "t-value" from `quantreg`.

Hunt and test: Flexible goodness-of-fit

Quantile regression

$\tau = 0.5$ (median)

$$Y = 1 + \beta_0^\top X + 4\, v\, n^{-1/2}\sqrt{X_1^2 + X_2^2} + (1 + X_2 + X_3)\,\varepsilon$$

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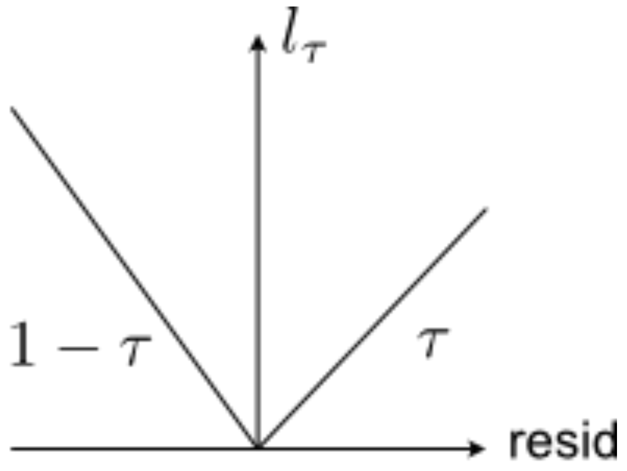

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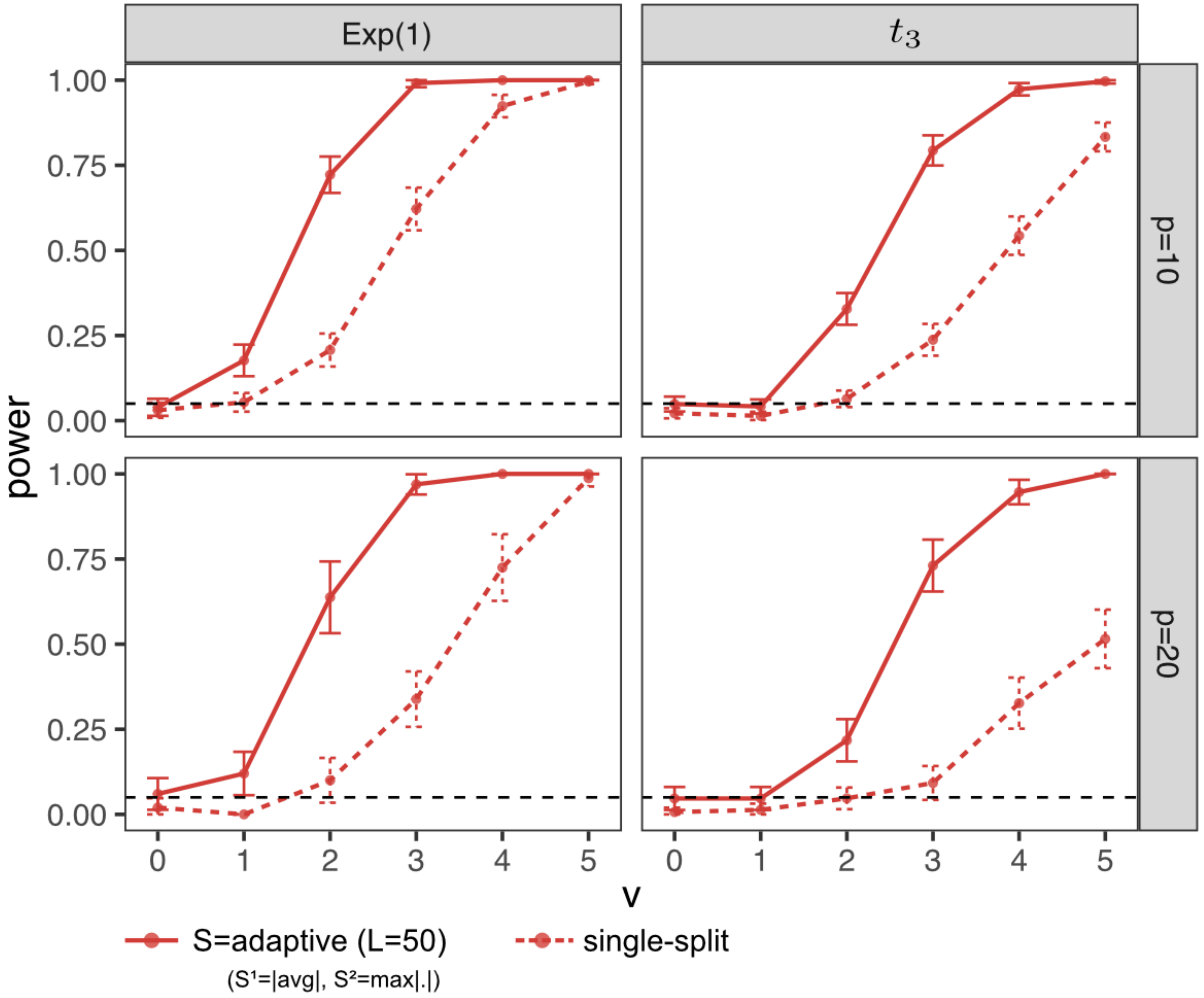

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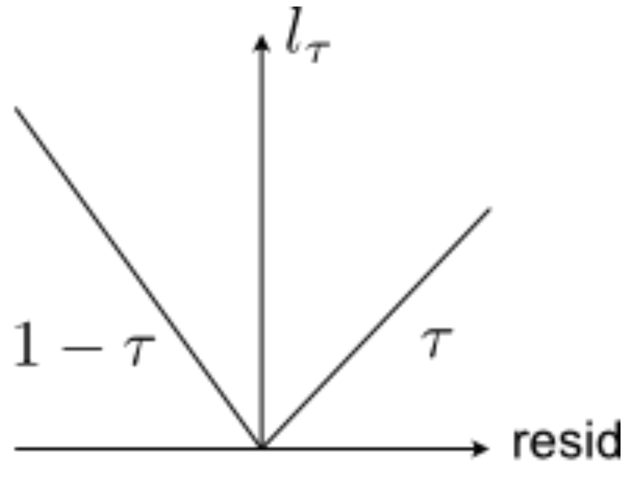

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Chen Dong, Guodong Li, and Xingdong Feng.
Lack-of-fit tests for quantile regression models.
Journal of the Royal Statistical Society: Series B (2019).

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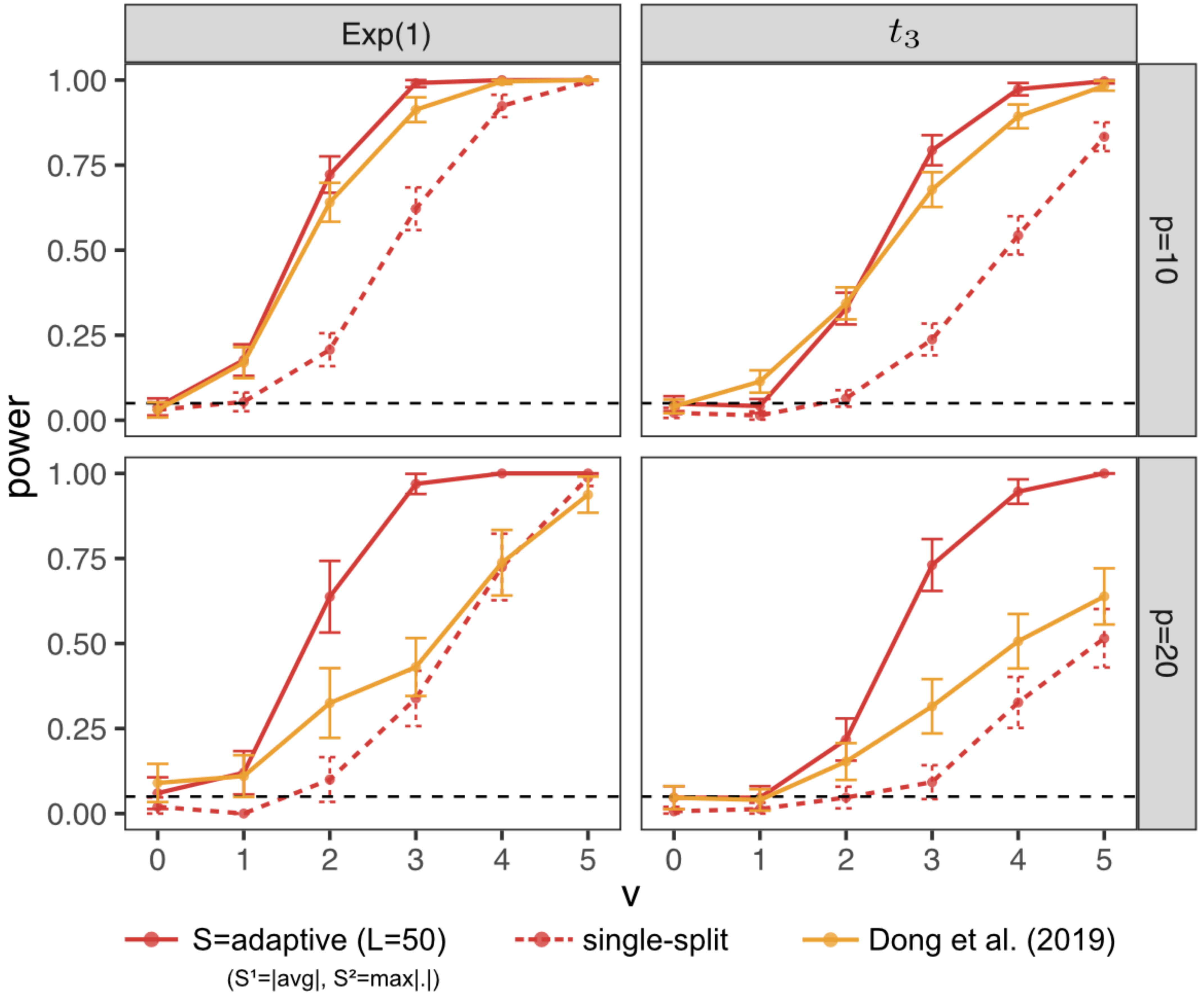
Exp(1)
t_3
p=10
p=20
power
1.00
0.75
0.50
0.25
0.00
0
1
2
3
4
5
v
S=adaptive (L=50)
(S^1=|avg|, S^2=max|.|)
single-split
Dong et al. (2019)