Sequential estimation of quantiles with applications to A/B testing and bandits

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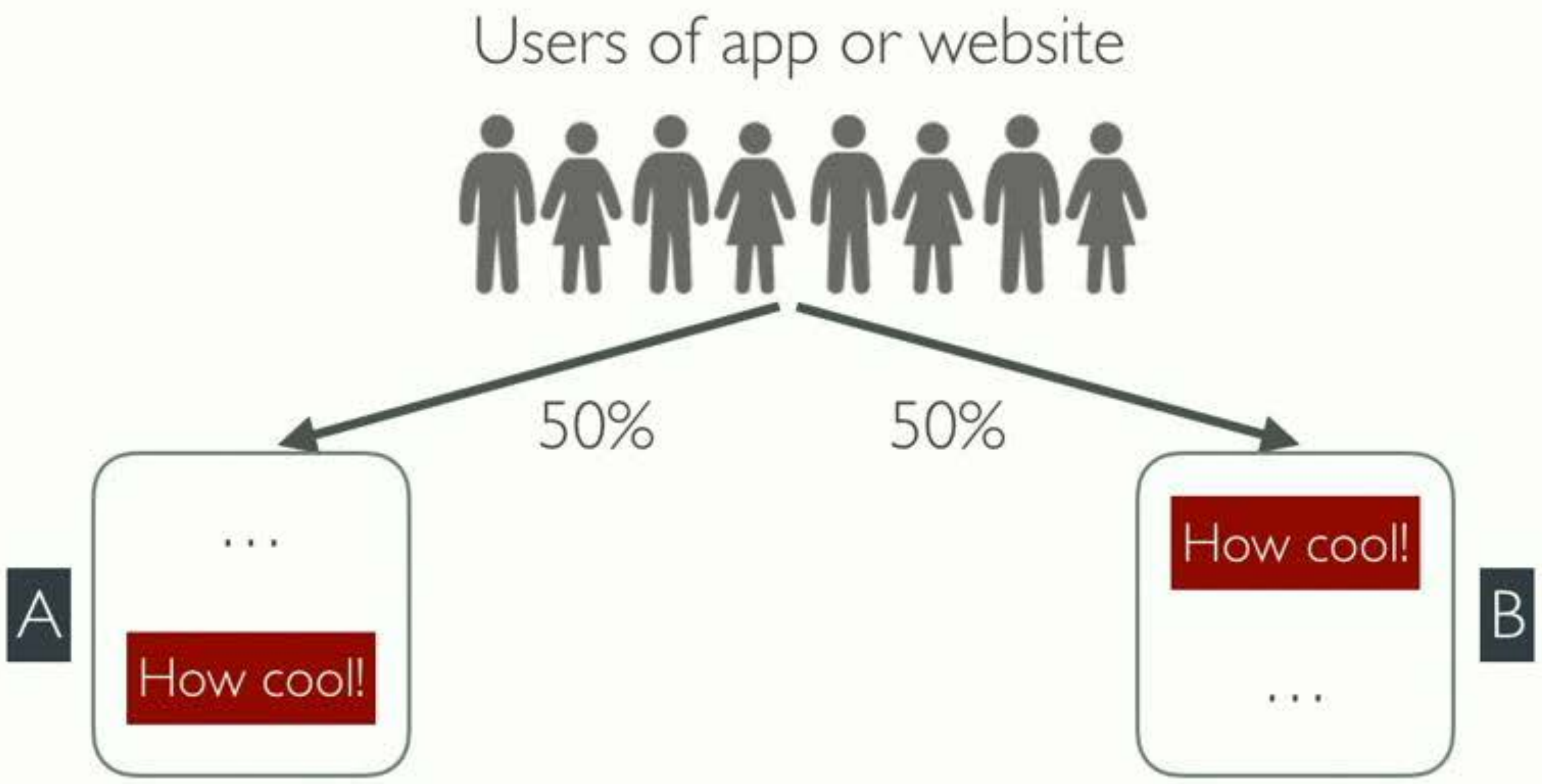
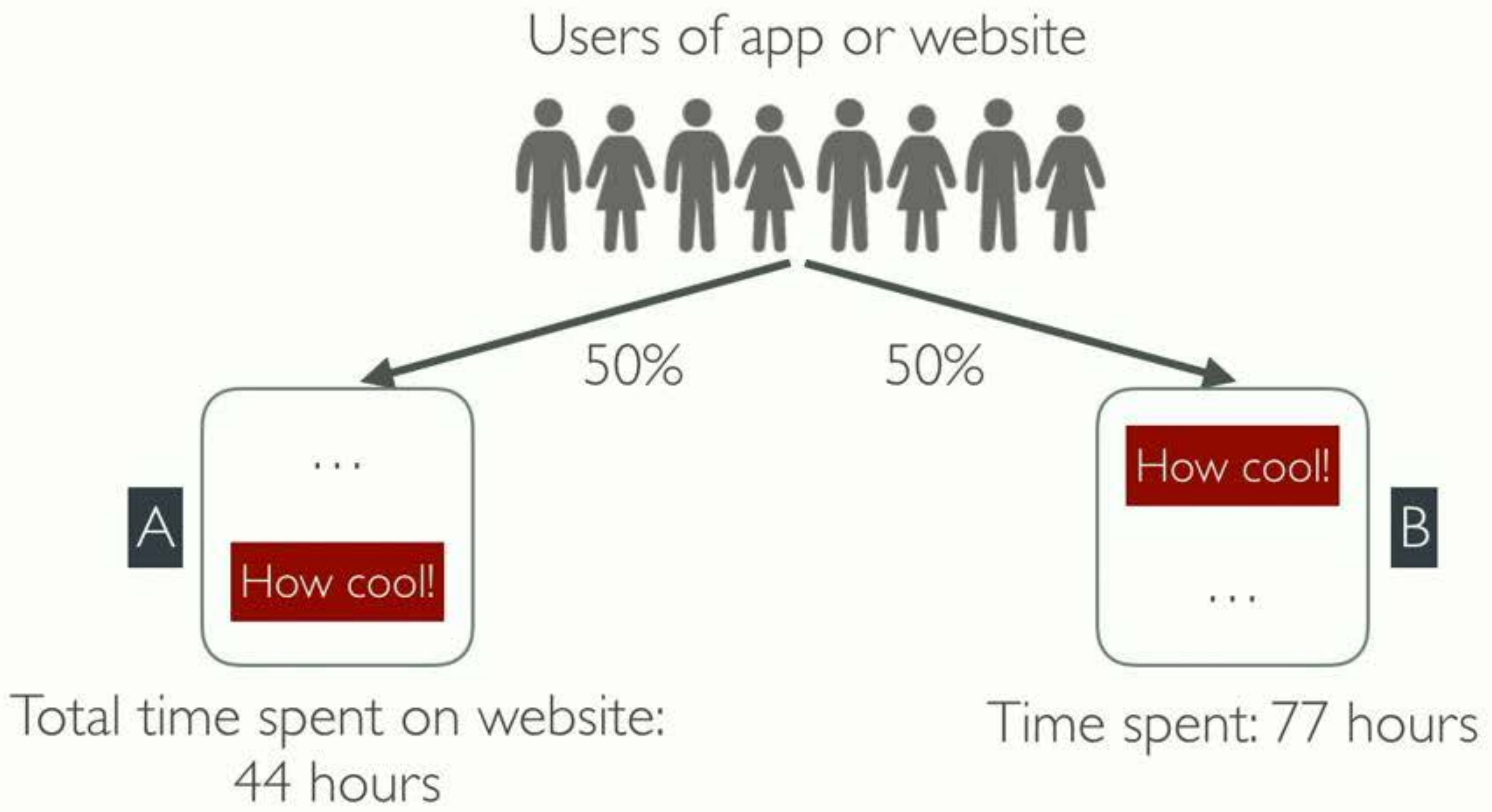

Users of app or website
50%
50%
A
...
How cool!
How cool!
B
...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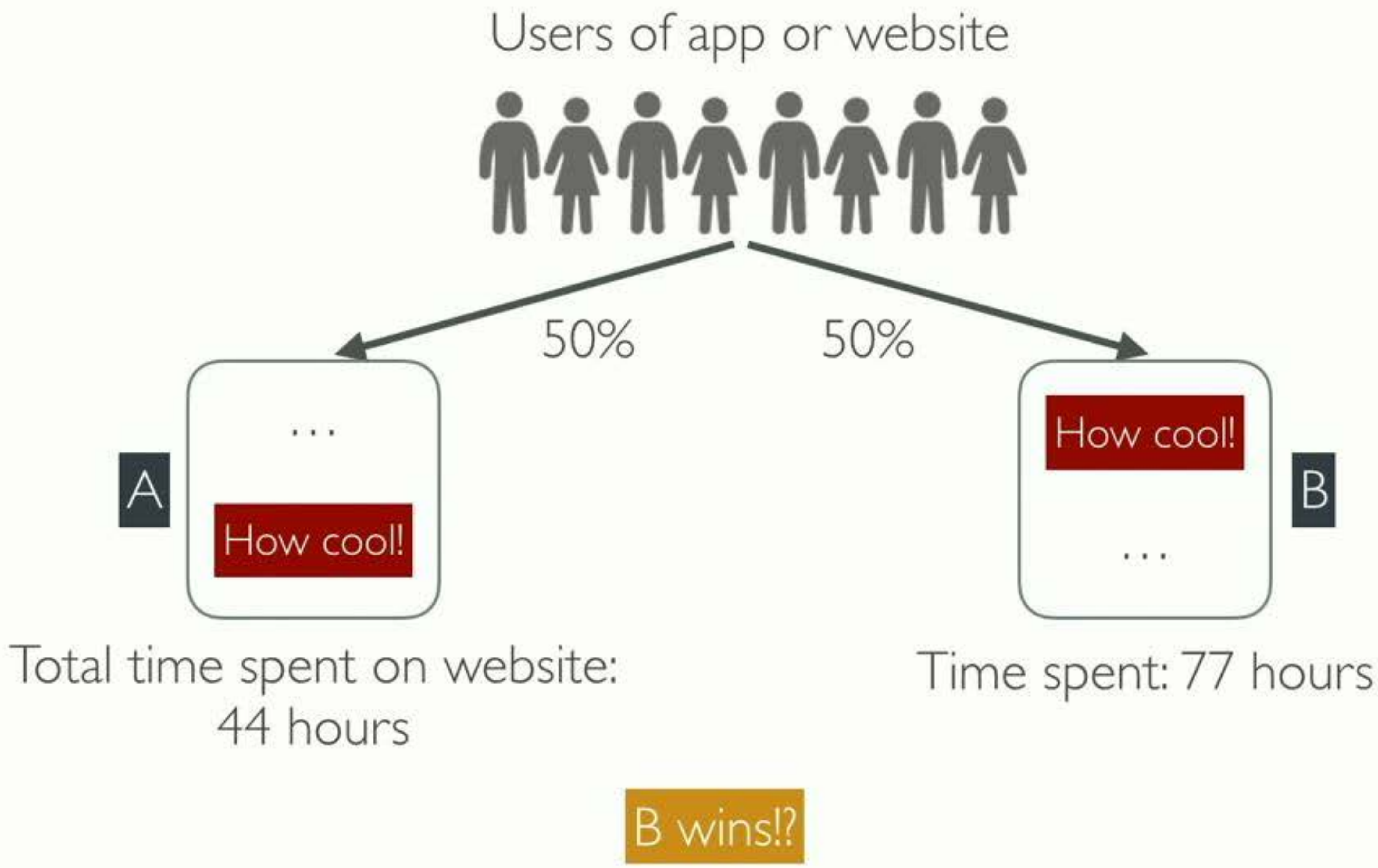
Total time spent on website:
44 hours
Time spent: 77 hours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B wins!?

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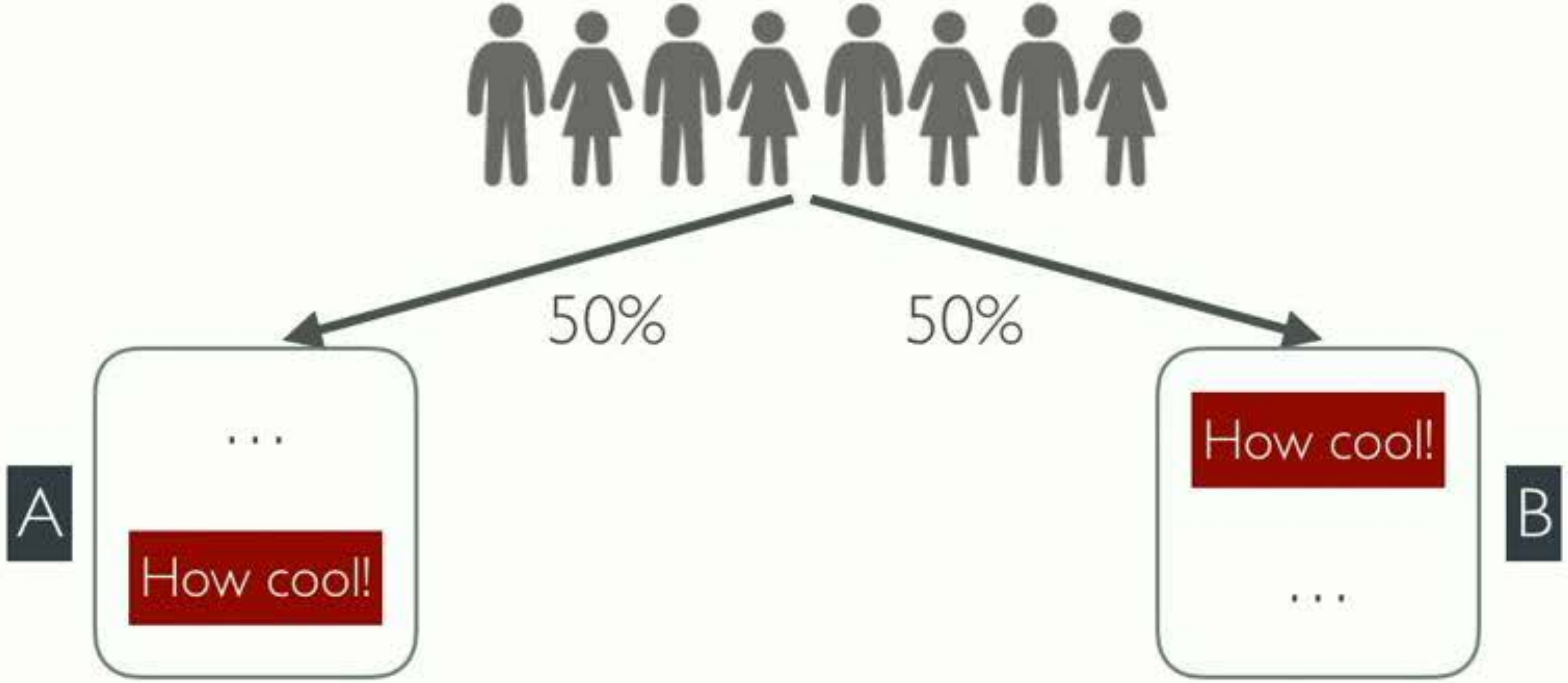

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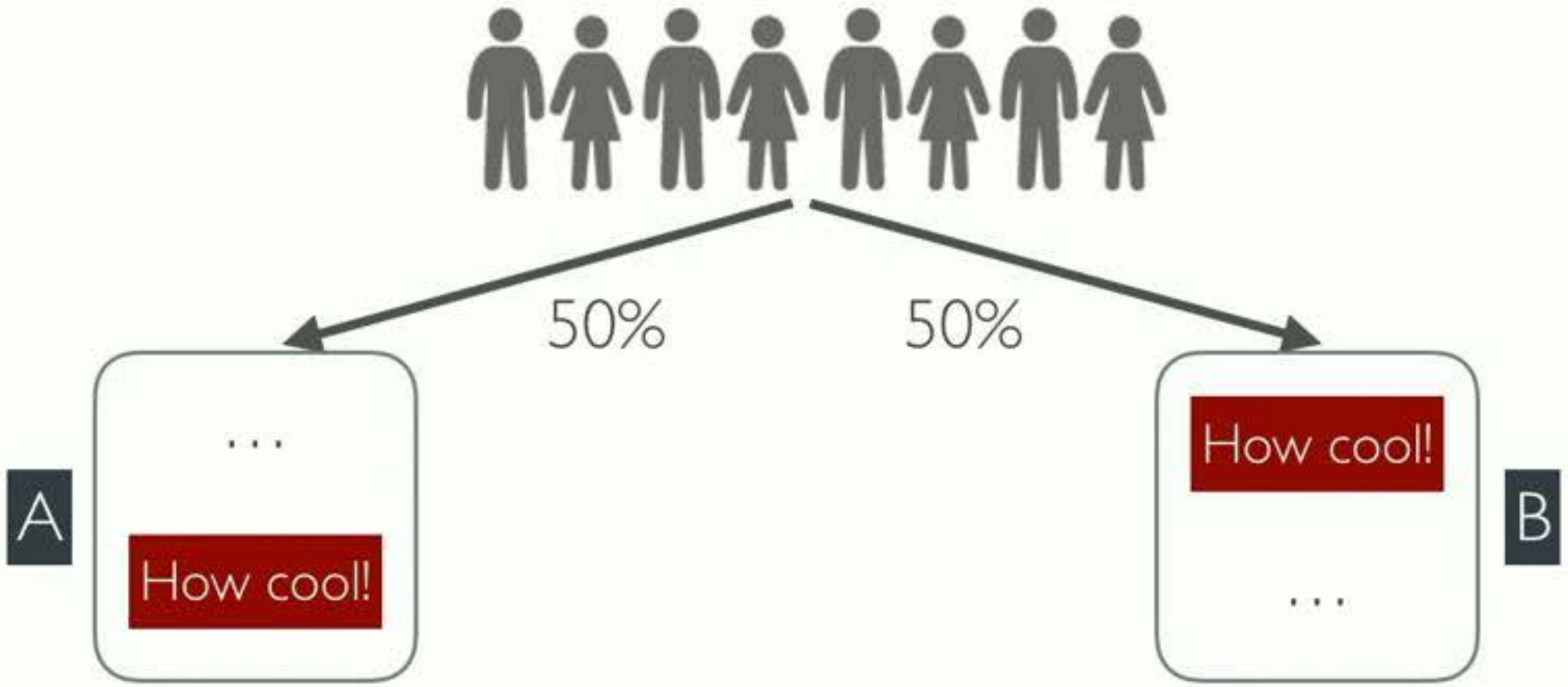
B wins!?

Summarize evidence as a p-value

Users of app or website



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B wins!?

Summarize evidence as a p-value

(Null hypothesis: A and B have equal means)

Calculate p-value

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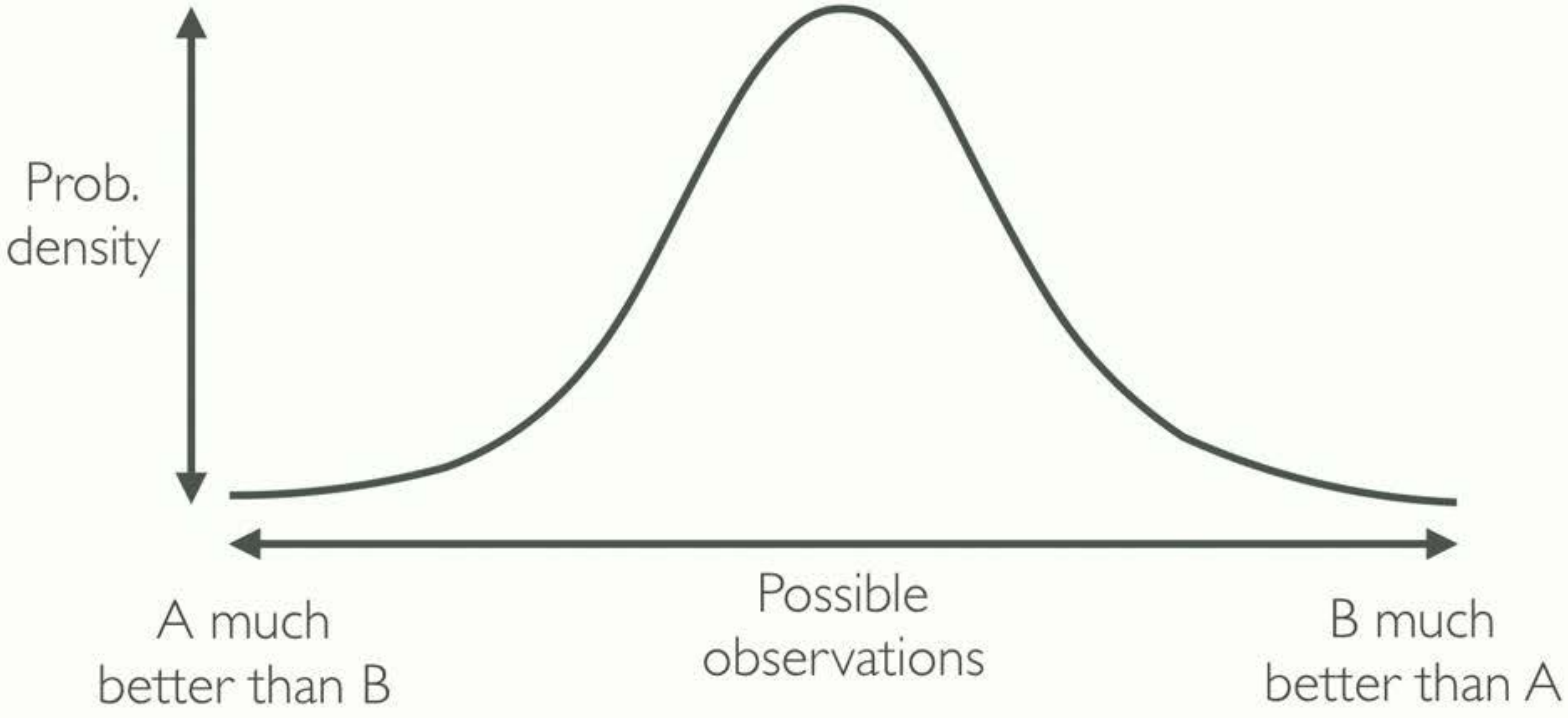

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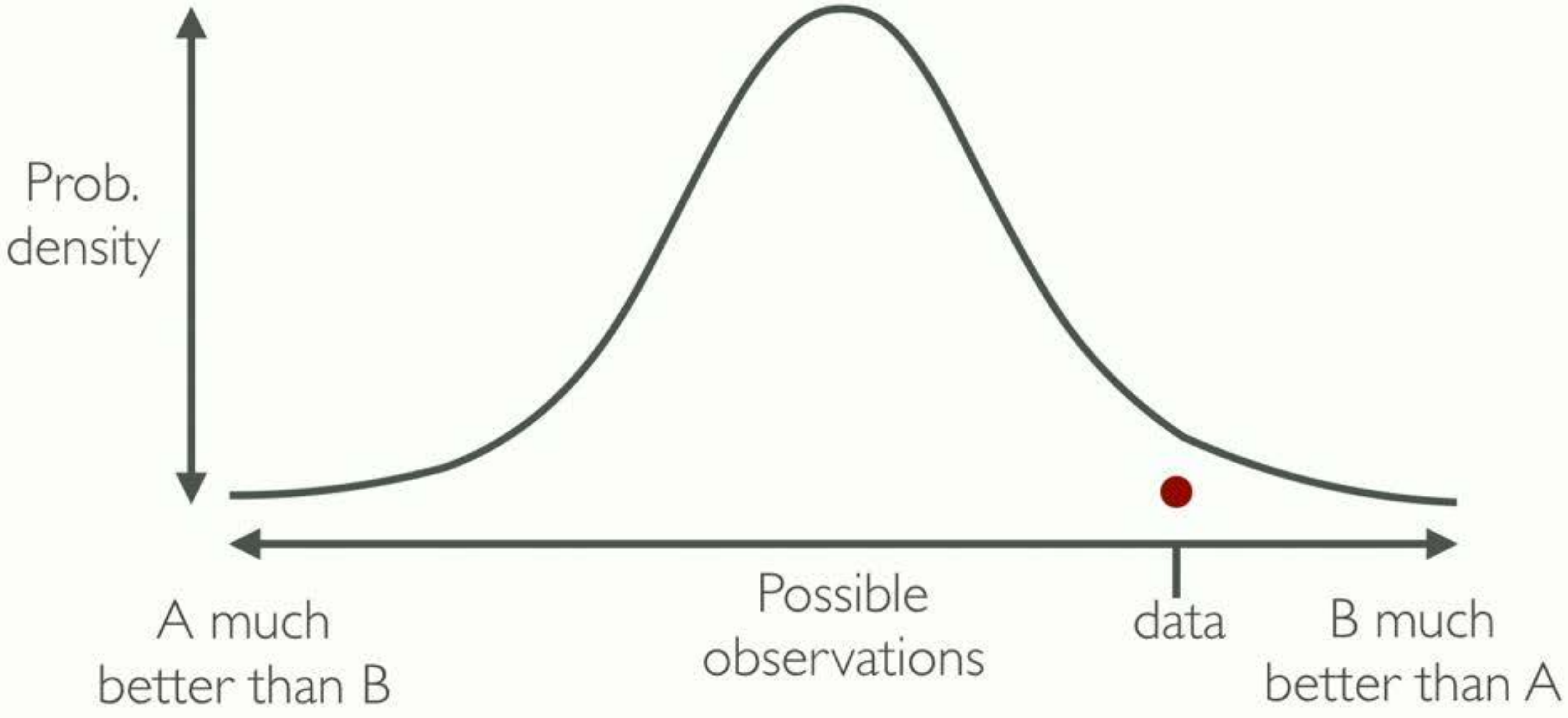

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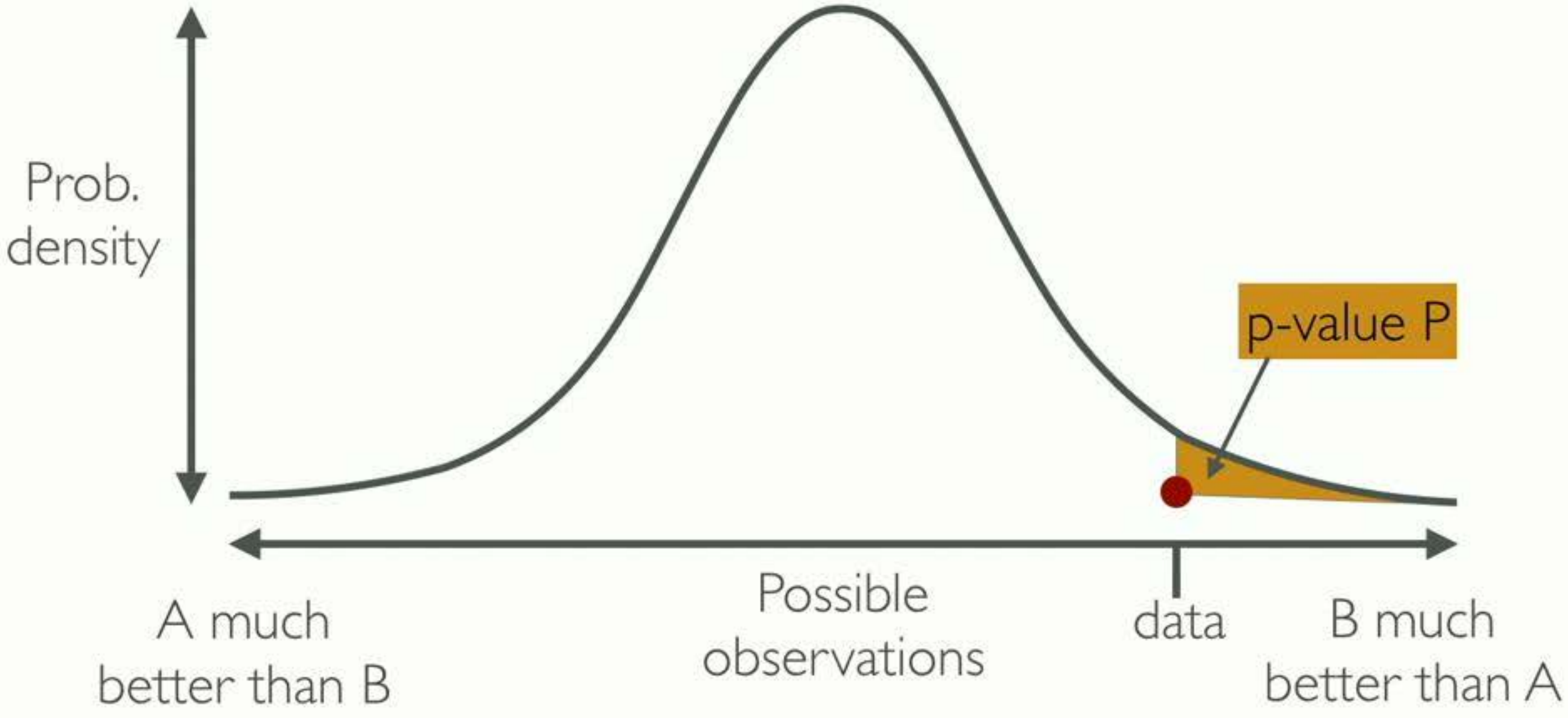

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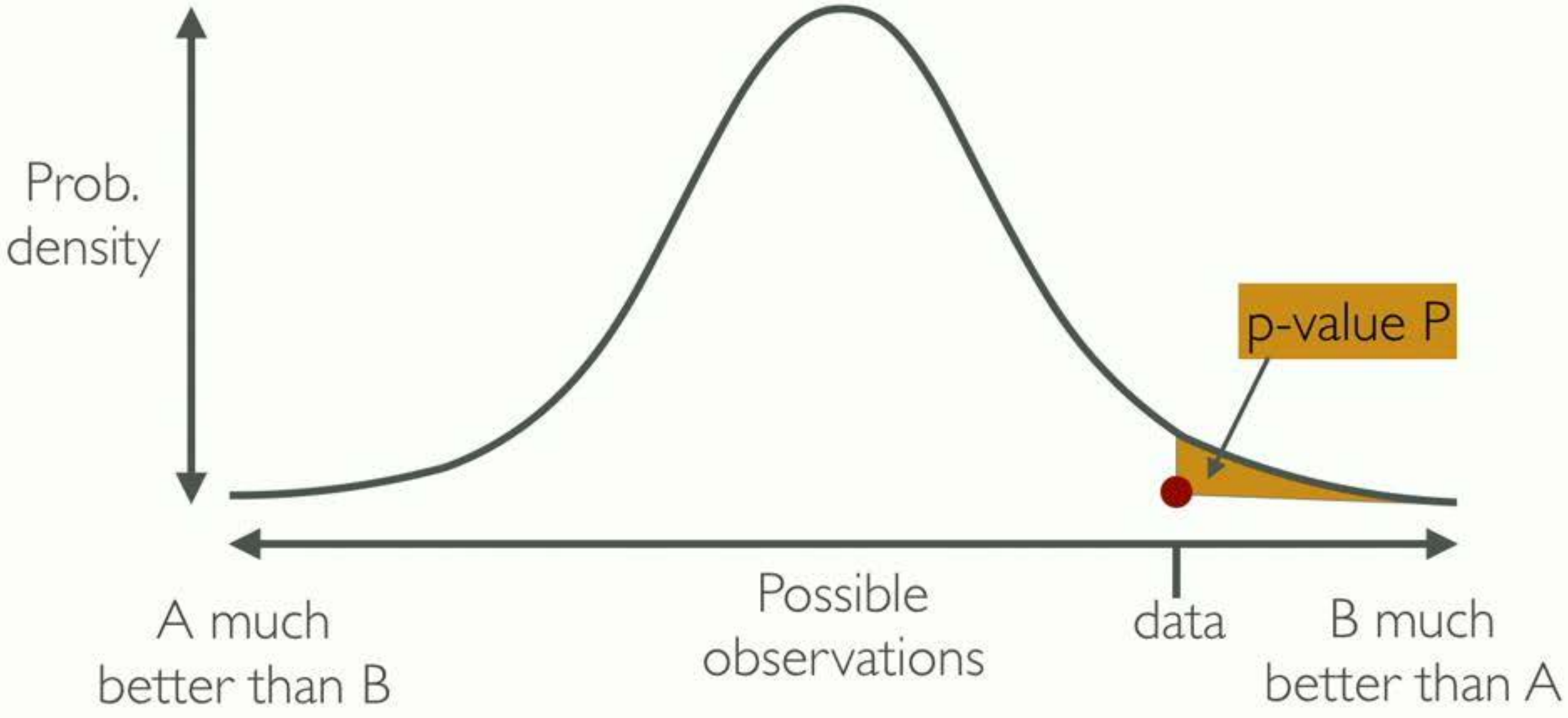
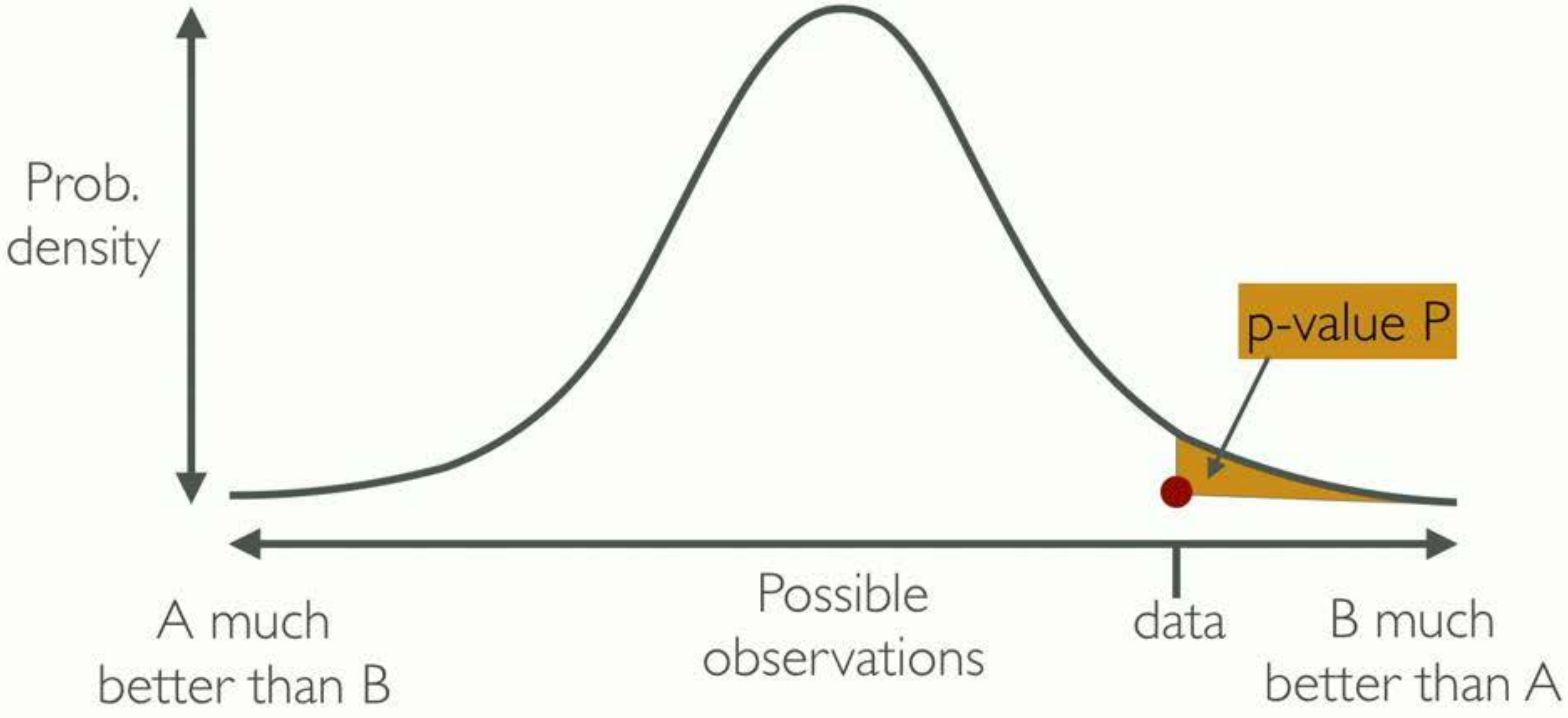


Reject null if $P \leq \alpha$

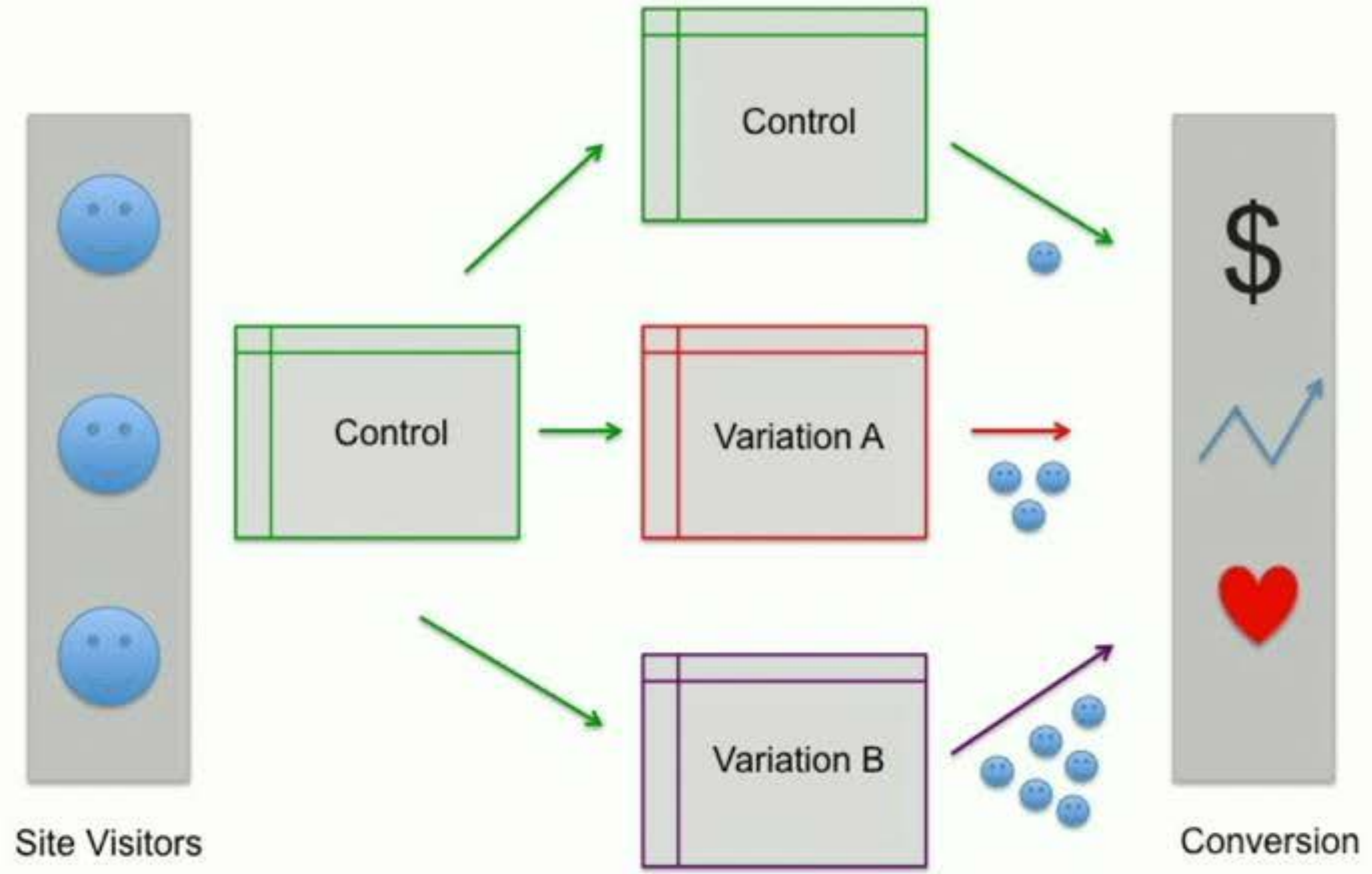
Calculate p-value



Reject null if $P \leq \alpha$

Then, $\mathbf{Pr}(\text{false positive}) \leq \alpha$.

What if we are testing more than one alternative?



Much more traffic needed by an A/B/n test

Multi-armed bandits

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$$H_0 : \mu_A \geq \max\{\mu_B, \mu_C\} \, .$$

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Or, maybe we want to identify the best arm with high probability.

Switch from estimating means to quantiles?

Let $X \sim F$. Define the p-quantile as $Q(p) := \sup\{x : F(x) \leq p\}$, and $Q^{-}(p) := \sup\{x : F(x) < p\}$ (hence $q_{1/2}$ is the median)

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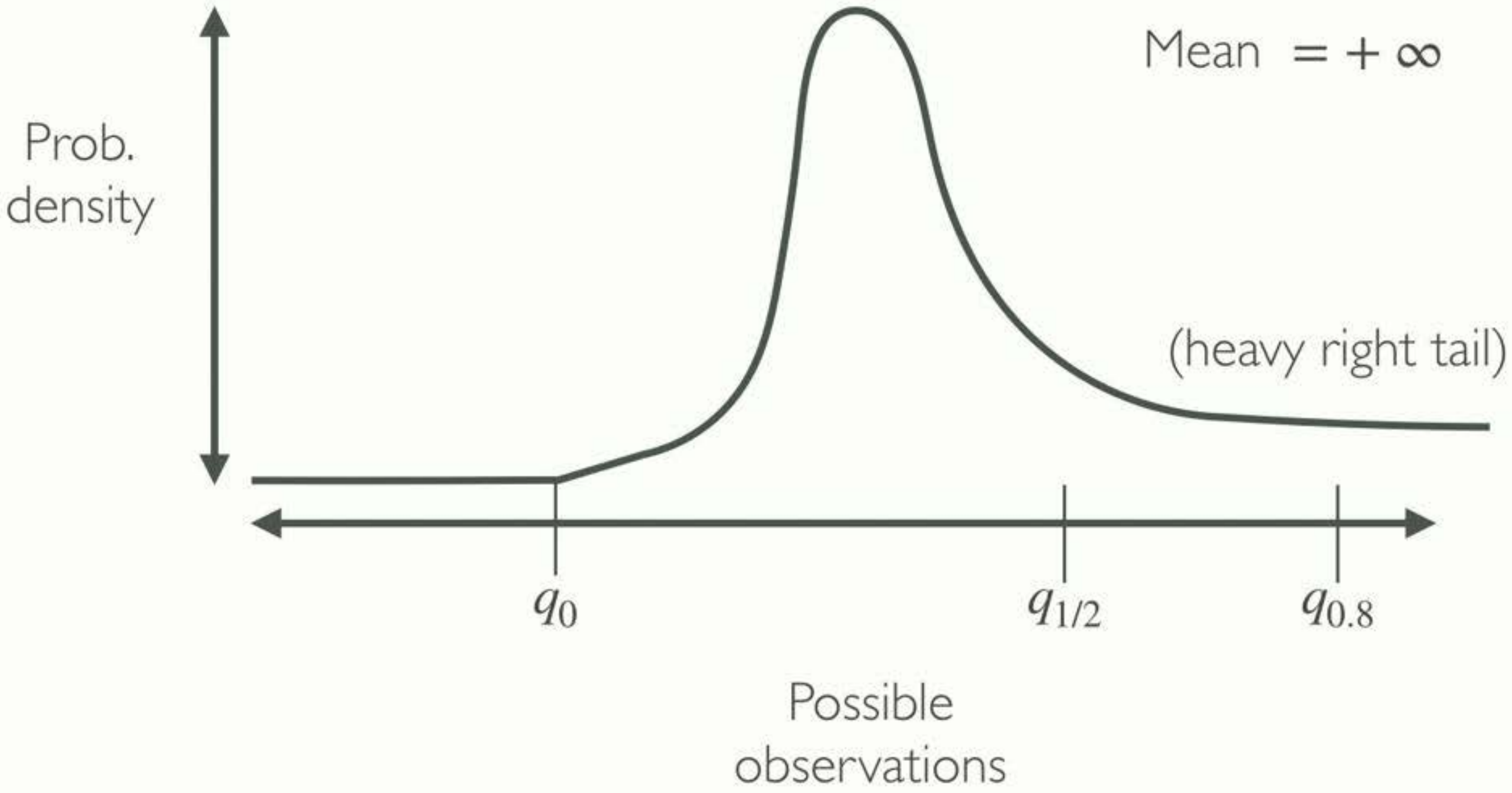
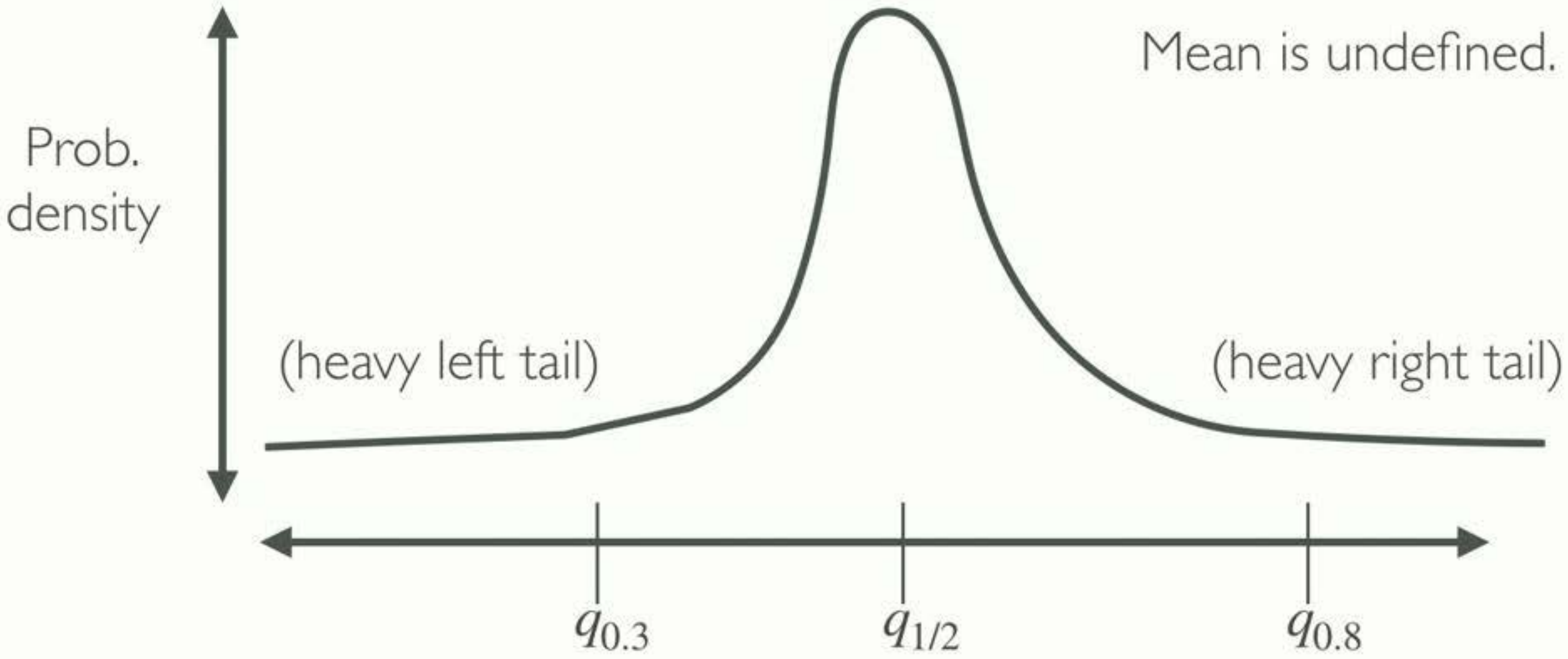
Can also estimate all quantiles simultaneously.

Quantiles are informative for heavy tails



Eg: amount of time spent on Reddit

The mean need not even exist (eg: Cauchy)



Eg: amount of money won/lost in a casino

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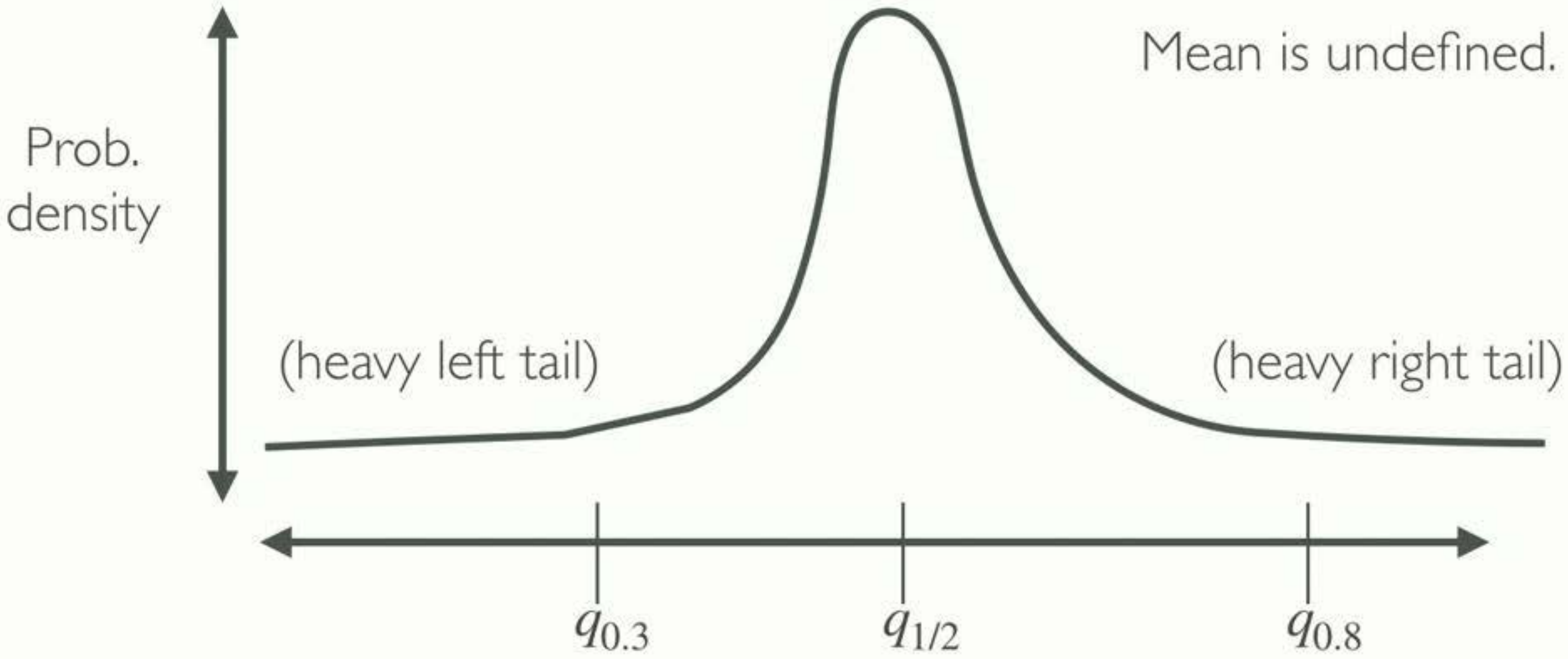
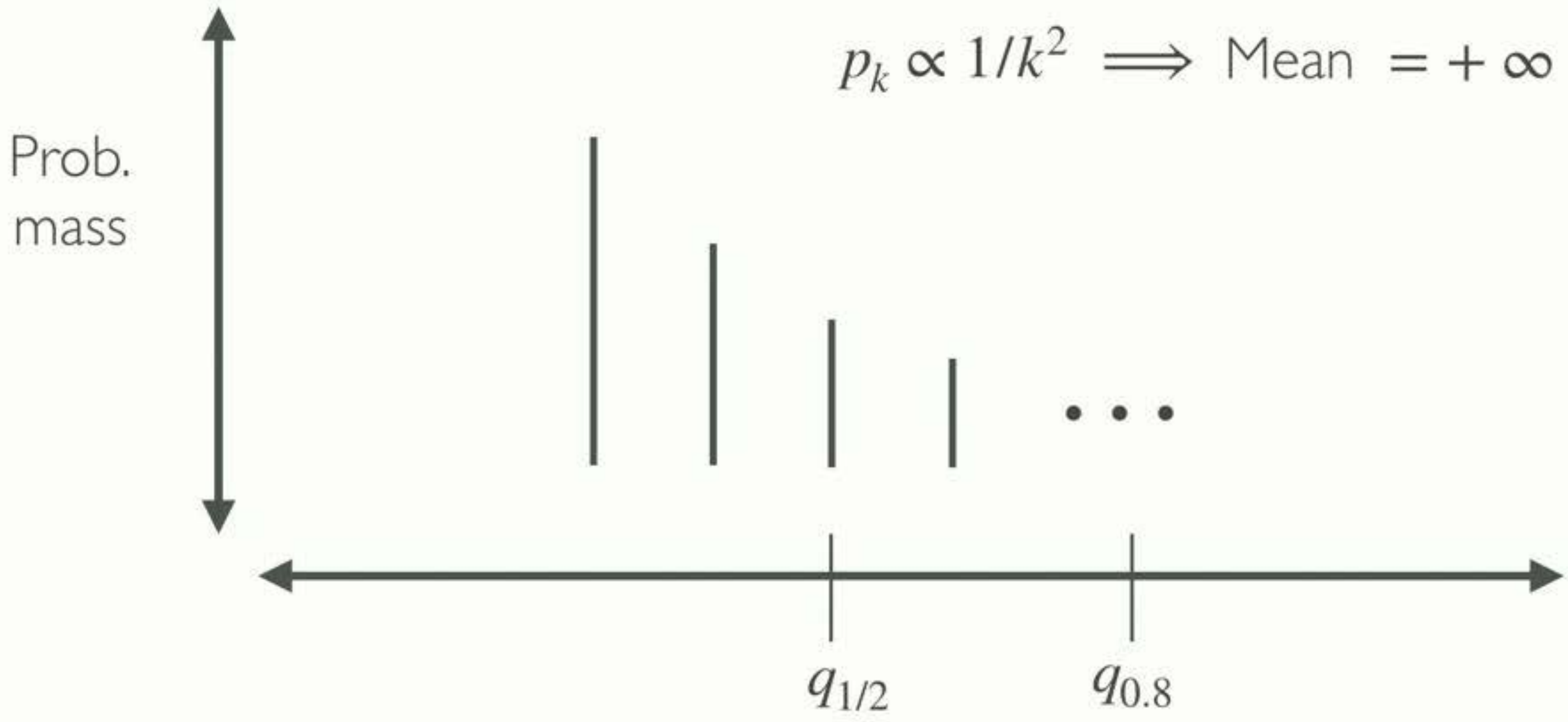


Eg: amount of money won/lost in a casino

Do not need to resort to trimming "outliers".
(How to pick threshold? Throw away or cap?)

The same could arise in discrete settings

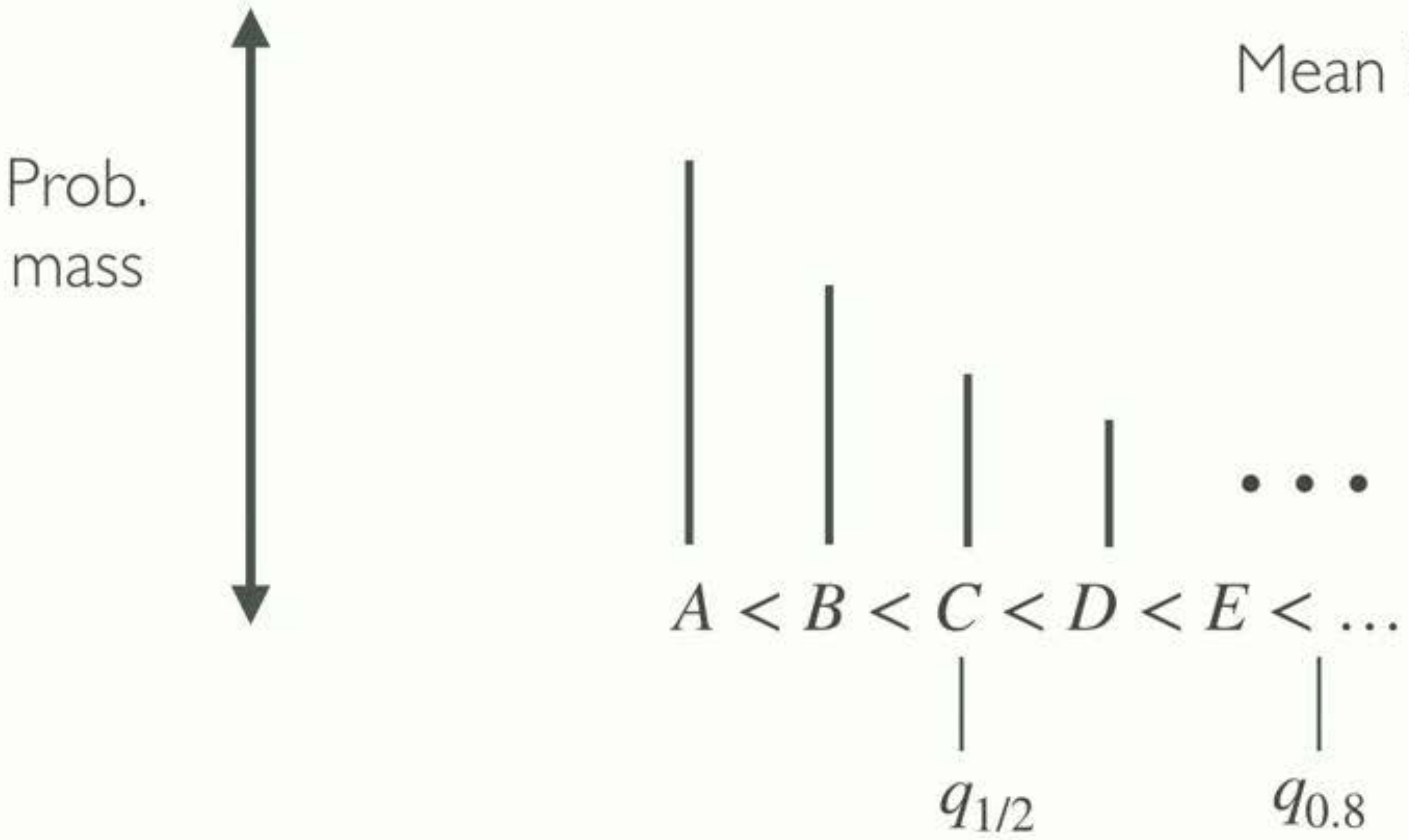
$p_k \propto 1/k^2 \implies \text{Mean} = +\infty$



Eg: number of links clicked

Quantile sensible in totally ordered settings

Mean is undefined.



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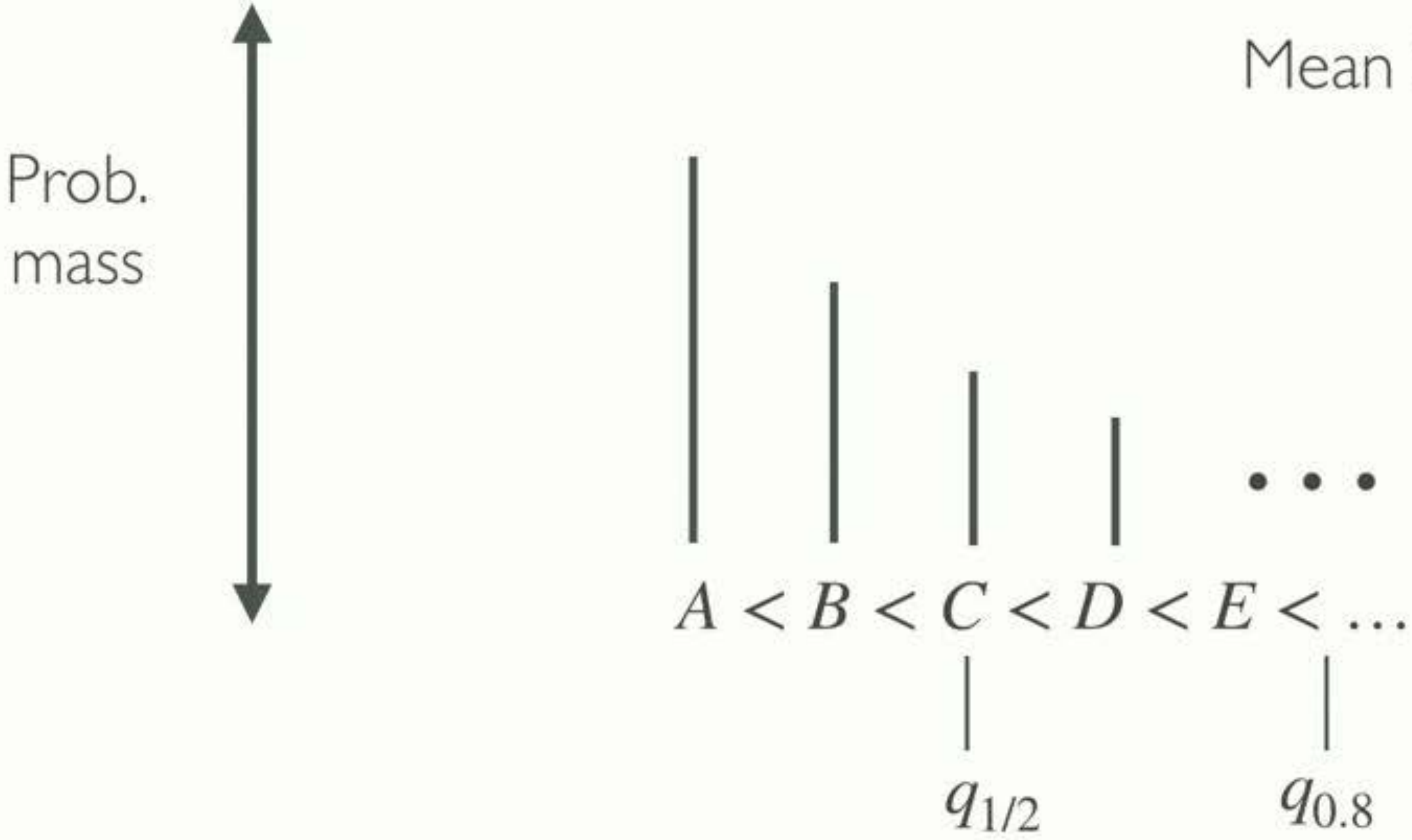

Eg: grades or non-numerical ratings

Do not need to artificially assign numerical values.
(Are they equally spaced? Spacing and start point matter.)

Q1. A/B testing with quantiles

First pick target quantile α (say 0.9).

$$H_0 : q_{0.9}(A) = q_{0.9}(B)$$

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Can we construct a p-value?

If numerical, can we get a confidence interval for $q_{0.9}(B) - q_{0.9}(A)$?

Q2. Best-arm identification with quantiles

Which arm has the highest 80% quantile?

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Can we design MAB algorithms to adaptively determine the "best" arm with a prescribed failure probability?

If the first arm is "special", can we design MAB algorithms to adaptively test the null hypothesis that A is best, and get a p-value?

Commonly taught confidence intervals
and p-values are only valid (correctly control error)
if the sample size is fixed in advance.

High-level caricature of an A/B-test

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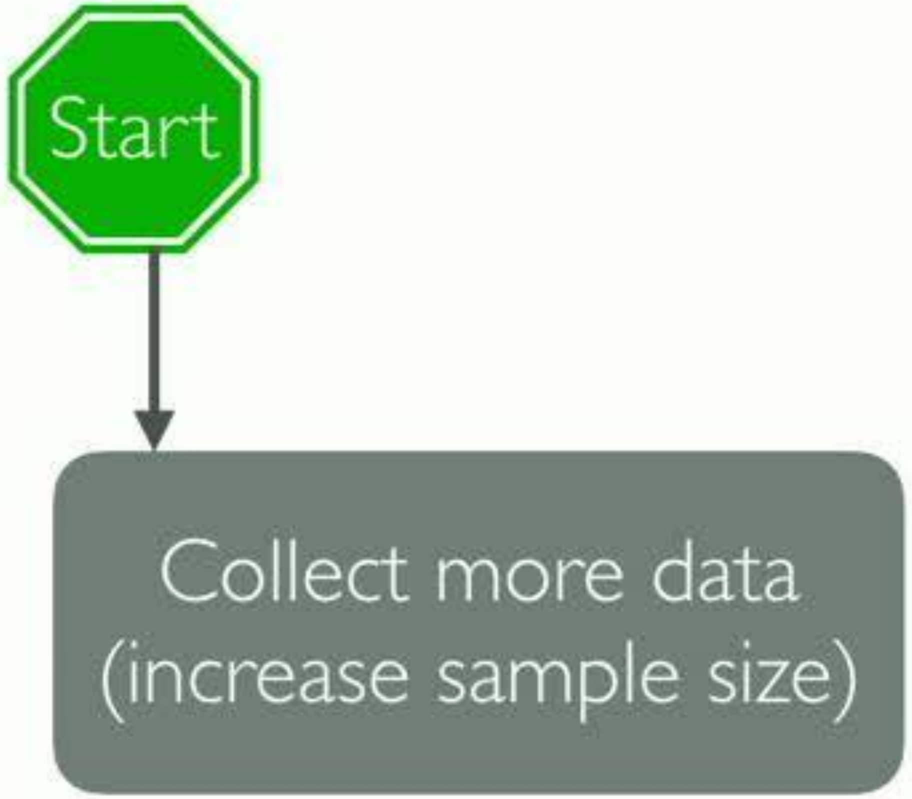
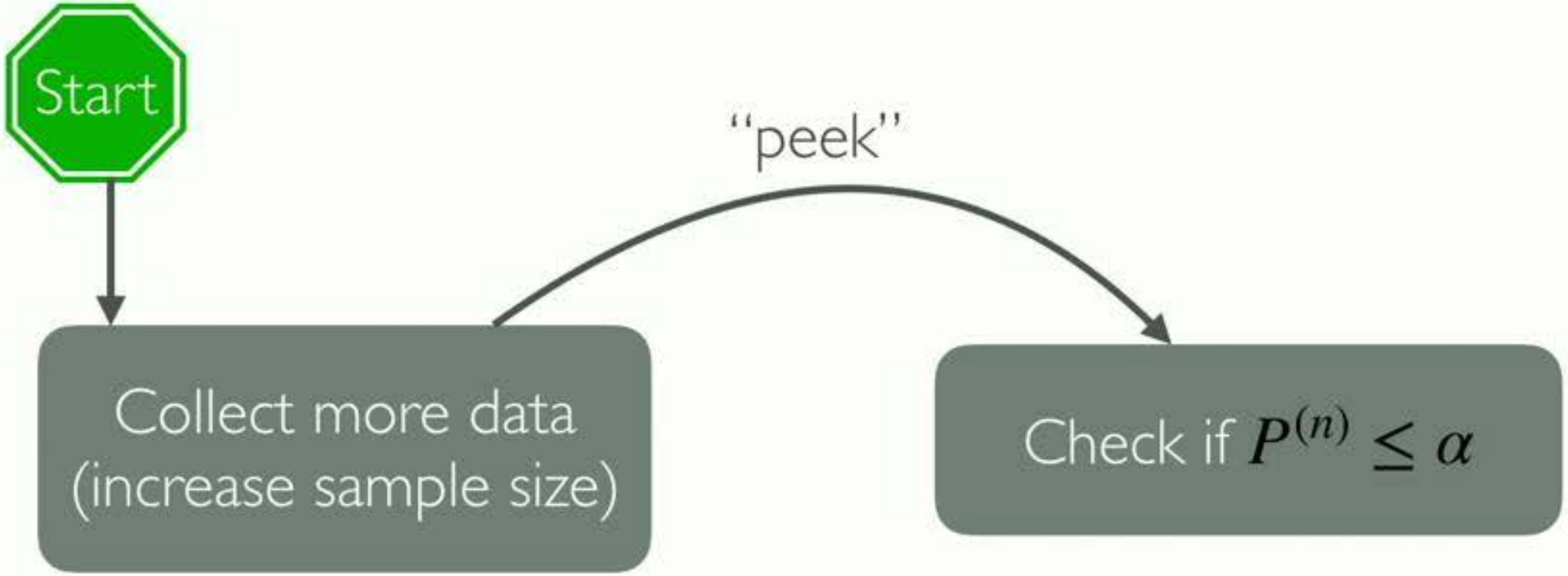


High-level caricature of an A/B-test



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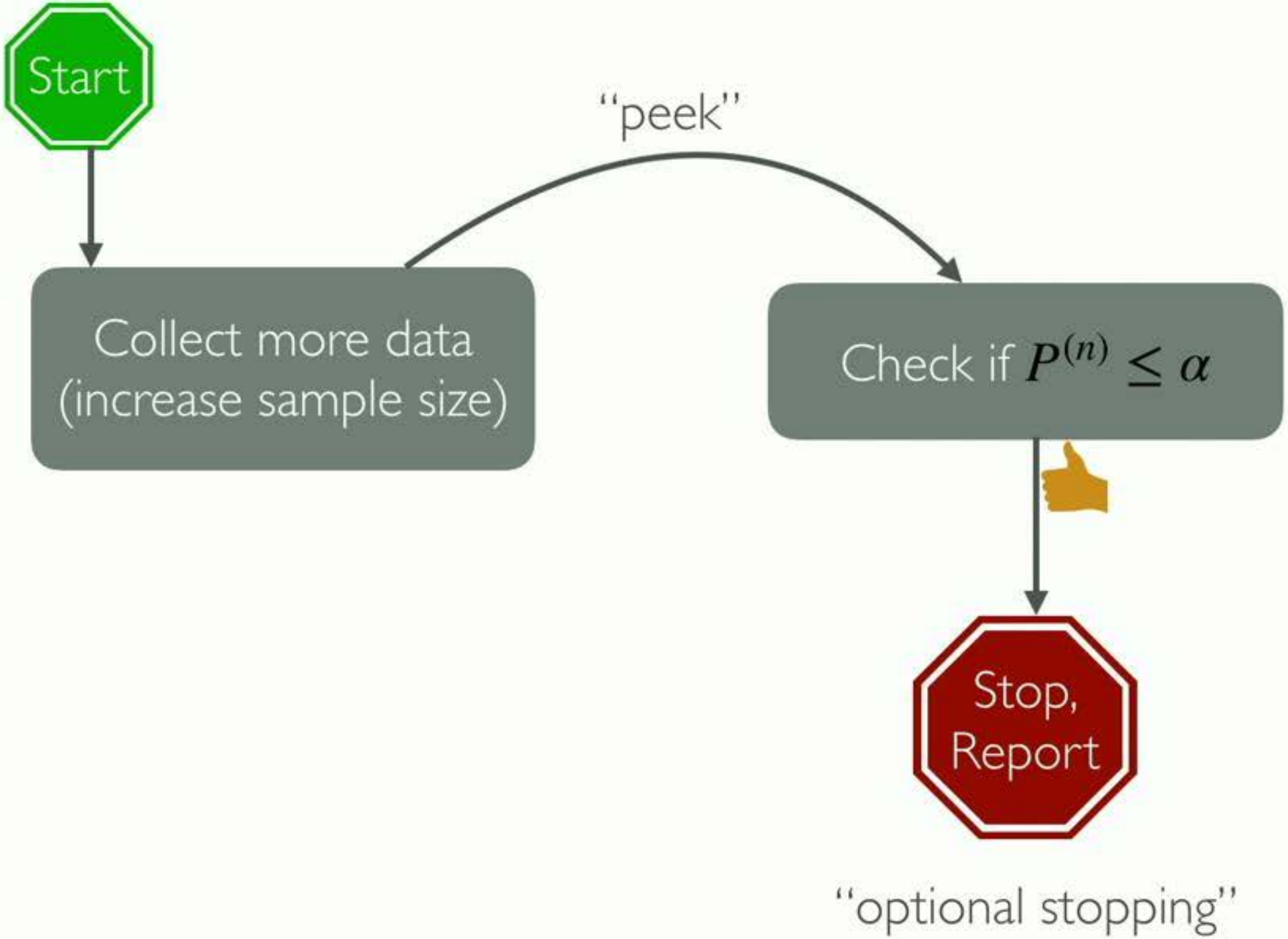

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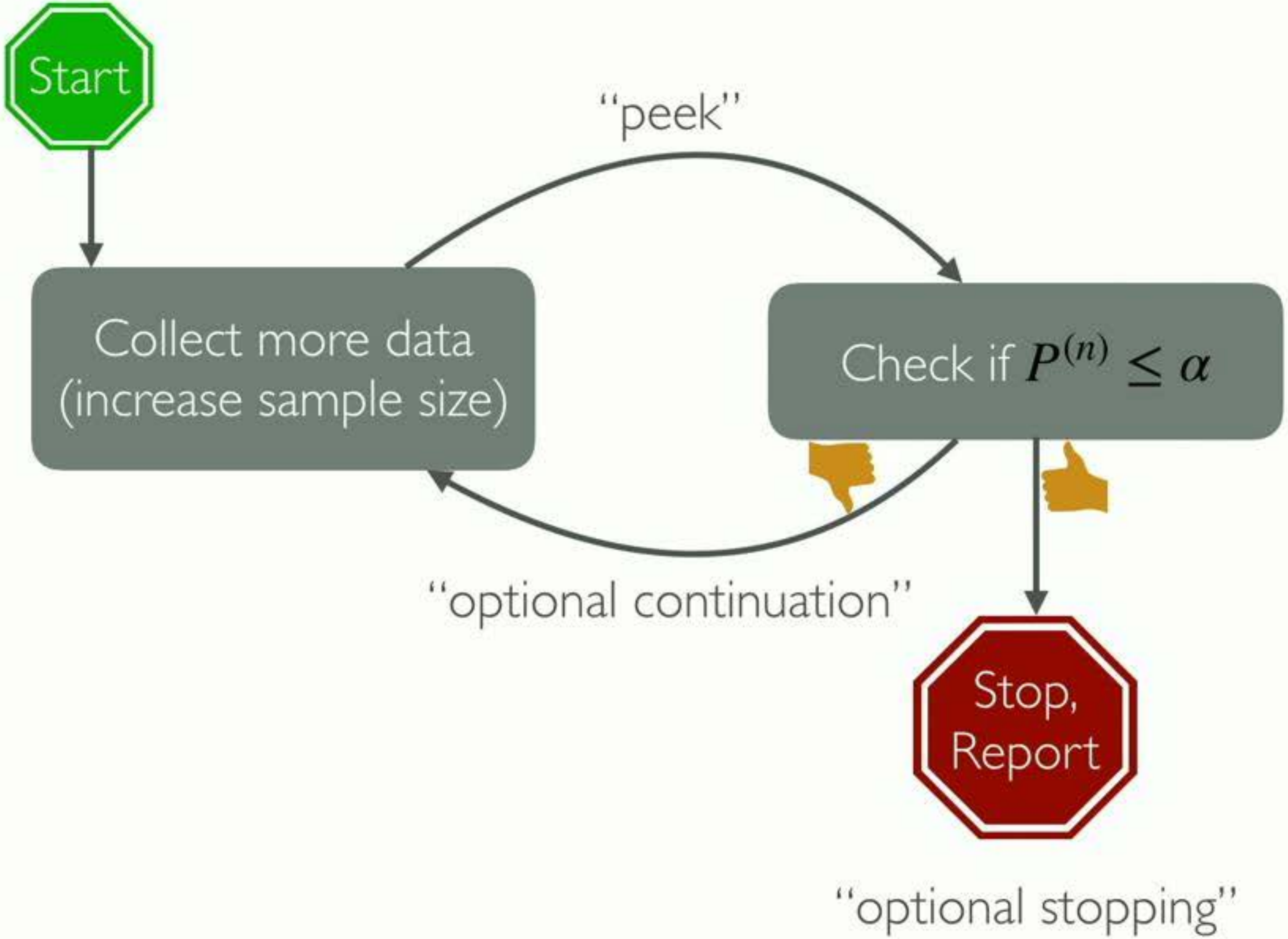

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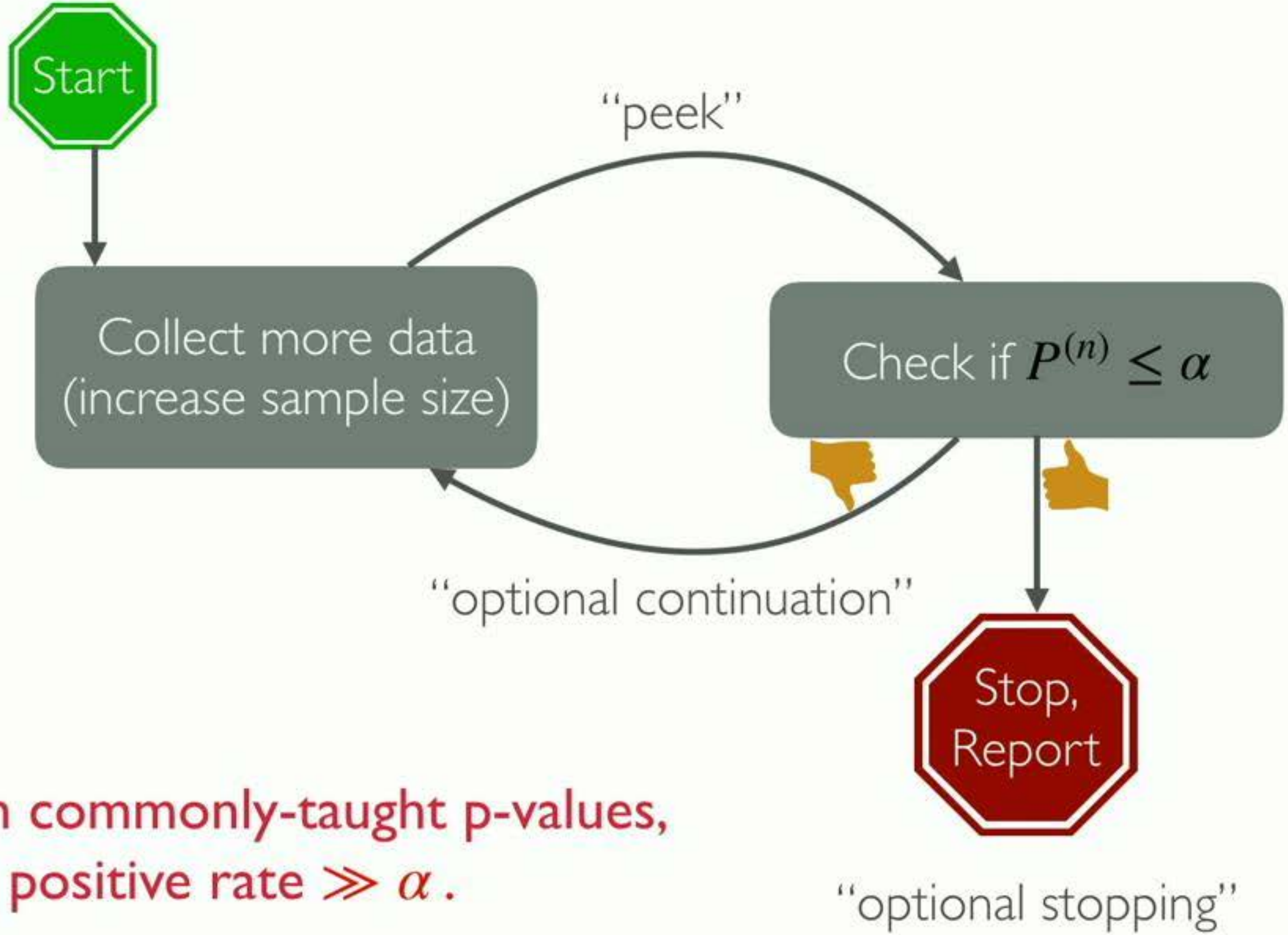

With commonly-taught p-values,
false positive rate $\gg \alpha$.


NOW
NOW
NOW
NOW
NOW
NOW
NOW
NOW

After 10 people

After 10 people

After 284 people

After 10 people

After 284 people

P < 0.05 — After 10 people

P < 0.05 — After 284 people

P < 0.05 — After 1214 people

After 2398 people

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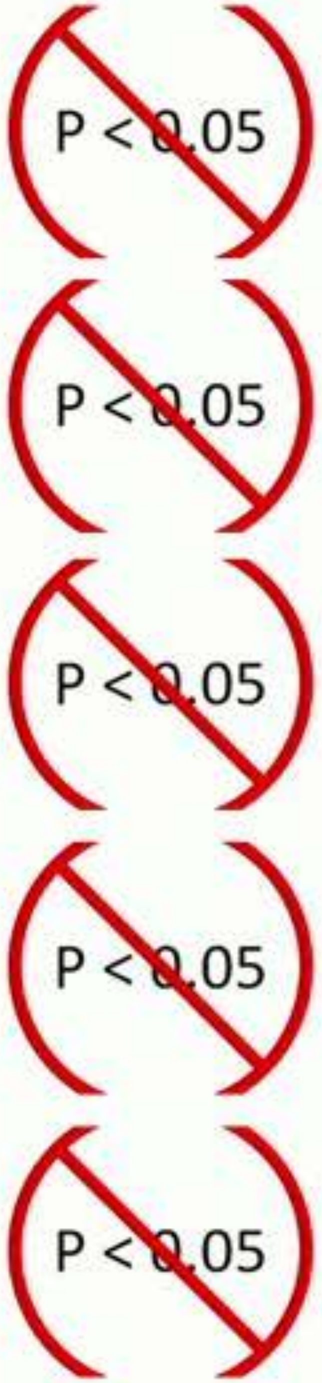
After 11,219 people, STOP!



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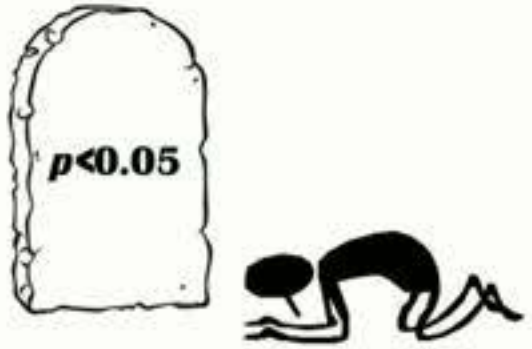

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Under the null hypothesis (no treatment effect),

$$\forall n \geq 1, \qquad \underbrace{\Pr(P^{(n)} \leq \alpha)}_{\text{prob. of false positive}} \qquad \leq \alpha\,.$$

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Let τ be the stopping time of the experiment.

Often, τ depends on data, eg: $\tau := \min\{n \in \mathbb{N} : P_n \leq \alpha\}$.

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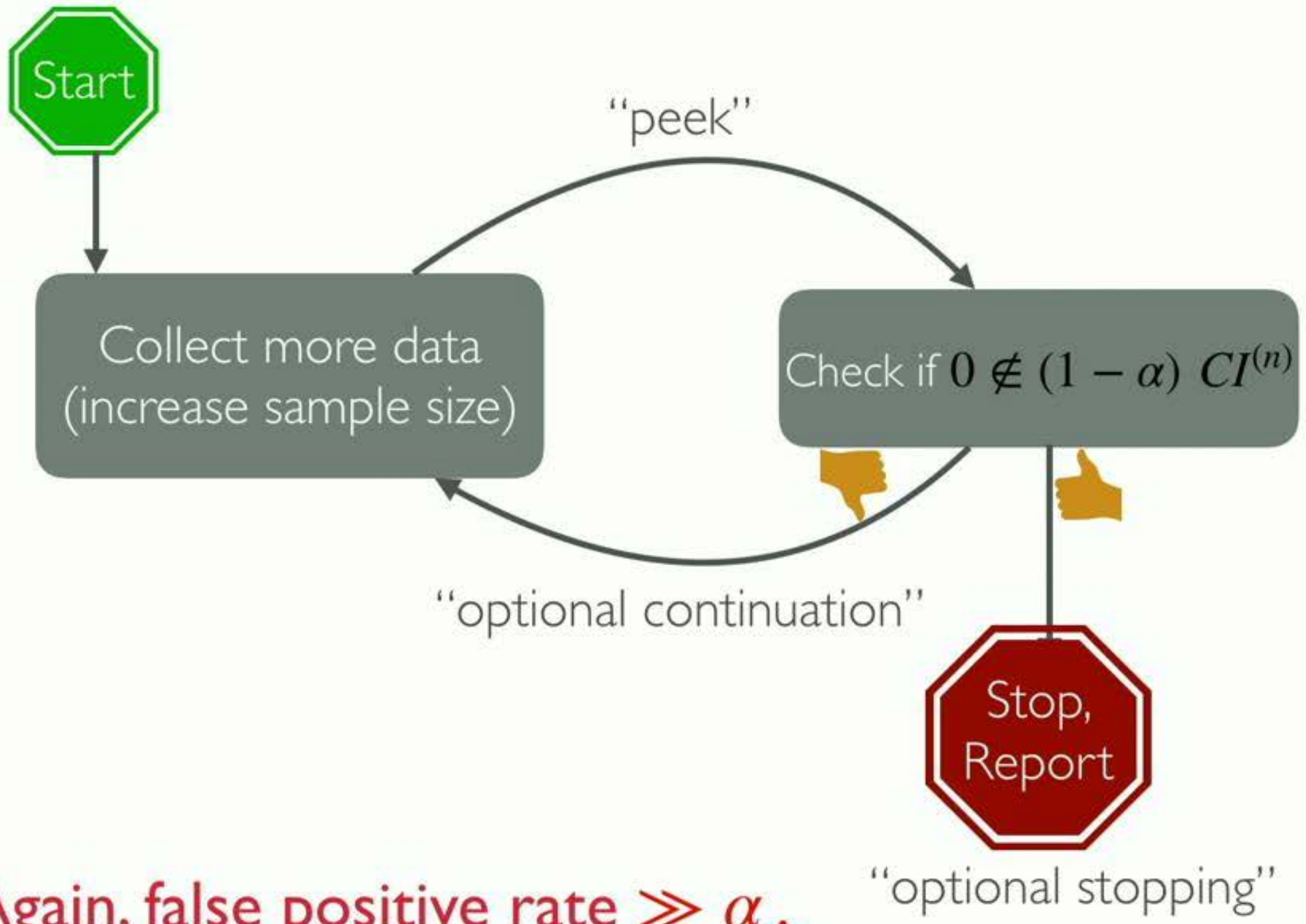
Unfortunately, under the null, $\Pr(P^{(\tau)} \leq \alpha) \nleq \alpha$.

In other words, $\Pr(\exists n \in \mathbb{N} : P^{(n)} \leq \alpha) \gg \alpha$.

Same problem with confidence interval (CI)



Again, false positive rate $\gg \alpha$.

Let $(L^{(n)}, U^{(n)})$ be any classical $(1 - \alpha)$ CI, calculated using the first n samples (eg: CLT).

Let $(L^{(n)}, U^{(n)})$ be any classical $(1-\alpha)$ CI, calculated using the first n samples (eg: CLT).

When trying to estimate the treatment effect θ,

$$\forall n \geq 1,\ \underbrace{\Pr(\theta \in (L^{(n)}, U^{(n)}))}_{\text{prob. of coverage}} \geq 1 - \alpha\,.$$

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In other words, $\Pr(\forall n \geq 1 : \theta \in (L^{(n)}, U^{(n)})) \ll 1 - \alpha\,.$

usually $= 0$.

Solution: “confidence sequence”
(aka “anytime confidence intervals”)

or “sequential p-values” for testing
(aka “always-valid p-values”)

A "confidence sequence" for a parameter θ is a sequence of confidence intervals (L_n, U_n) with a uniform (simultaneous) coverage guarantee.

$$\mathbb{P}(\forall n \geq 1 : \theta \in (L_n, U_n)) \geq 1 - \alpha \,.$$

Sample size

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Sample size

Darling, Robbins '67, '68
Lai '76, '84
Howard, Ramdas, McAuliffe, Sekhon '18

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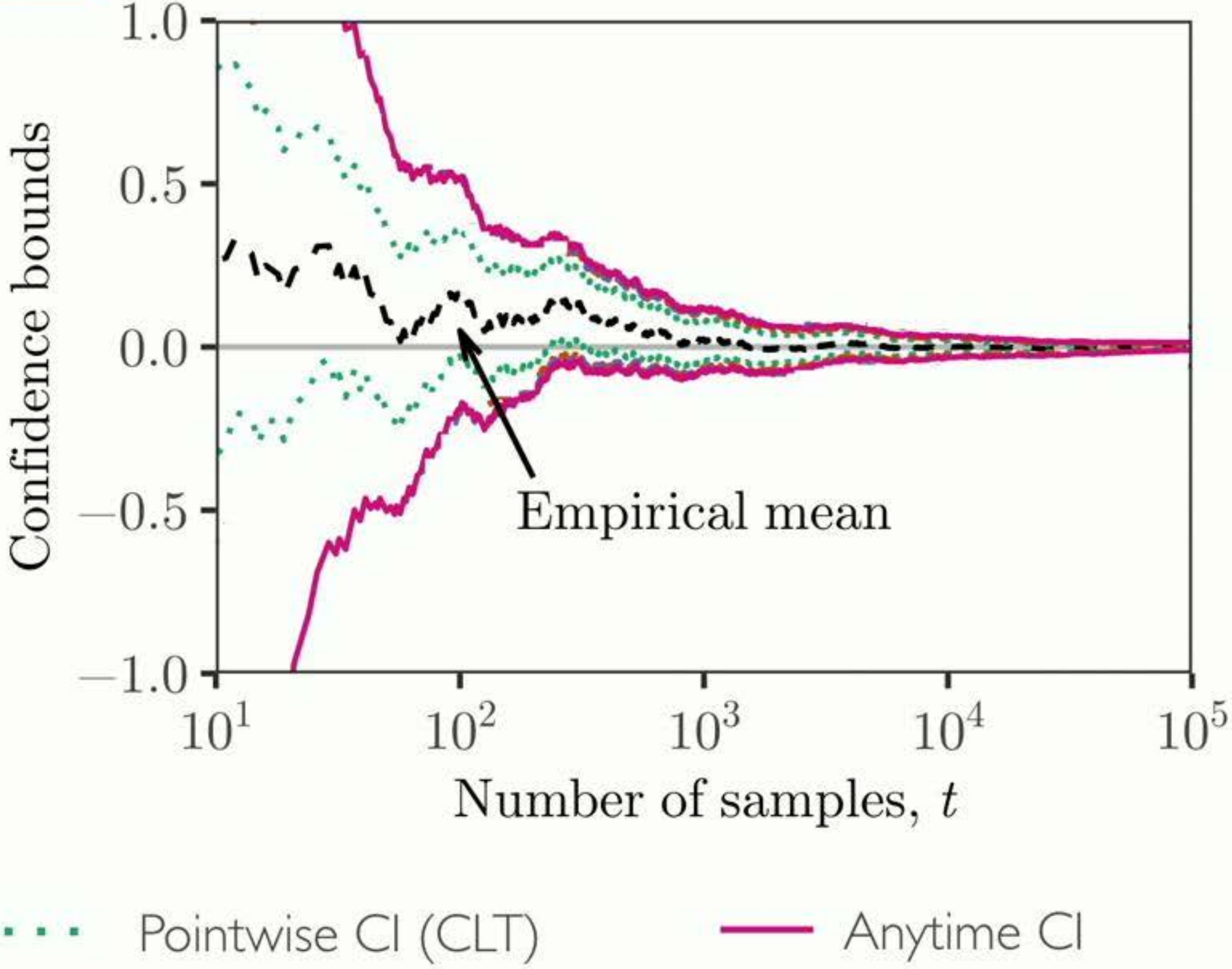
How do we produce a confidence sequence? (which is like a confidence band over time)

(Fair coin)



Confidence bounds
1.0
0.5
0.0
−0.5
−1.0
Empirical mean
10^1
10^2
10^3
10^4
10^5
Number of samples, t
Pointwise CI (CLT)
Anytime CI

Eg: If X_i is 1-subGaussian, then

$$\frac{\sum_{i=1}^{n} X_i}{n} \pm 1.71\sqrt{\frac{\log\log(2n) + 0.72\log(5.19/\alpha)}{n}}$$

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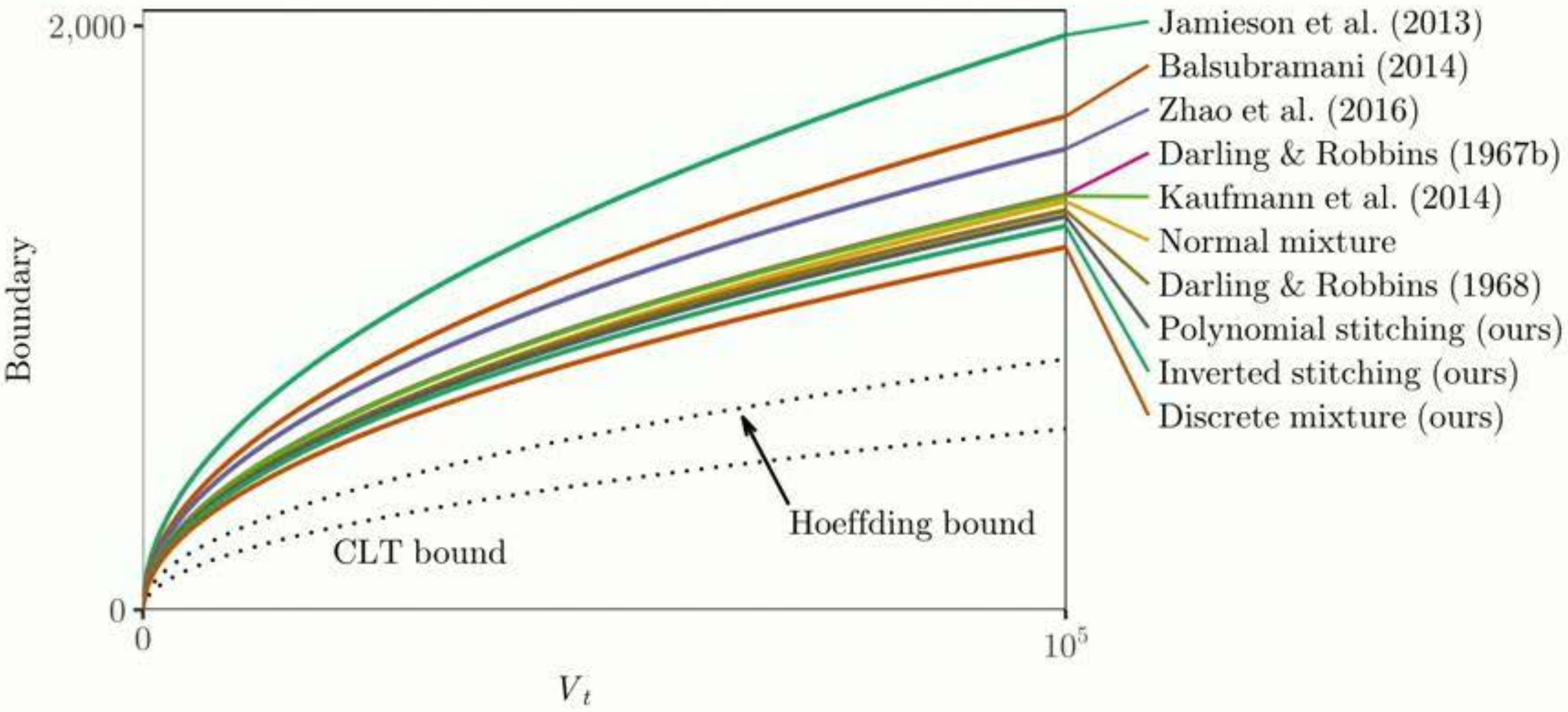

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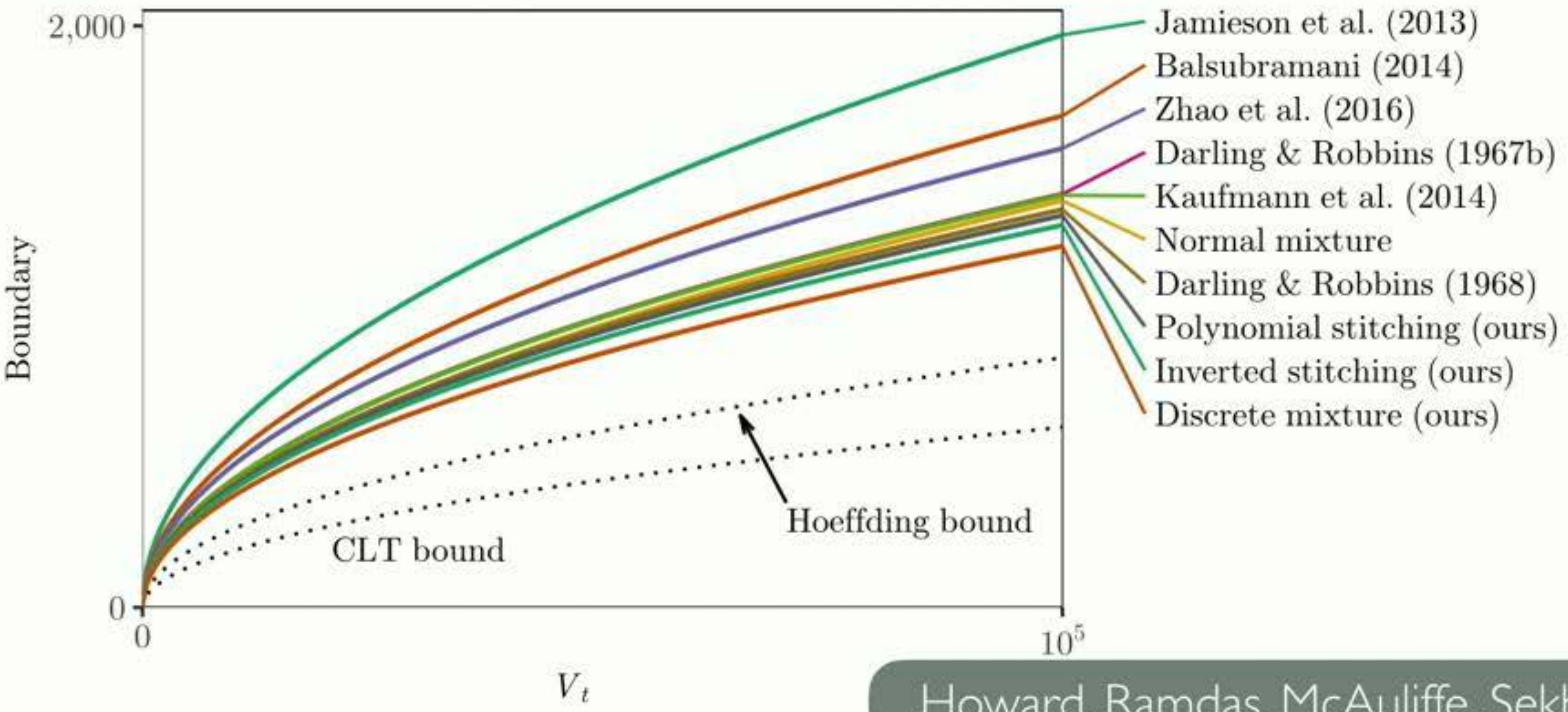

Howard, Ramdas, McAuliffe, Sekhon '18

$$\mathbb{P}\left(\bigcup_{n\in\mathbb{N}} \{\theta \notin (L_n, U_n)\}\right) \leq \alpha\,.$$

Some implications:

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$$\mathbb{P}\Big(\bigcup_{n\in\mathbb{N}} \{\theta \notin (L_n, U_n)\}\Big) \leq \alpha\,.$$

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2. Valid post-hoc inference (in hindsight):

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3. No pre-specified sample size:

   can extend or stop experiments adaptively.

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If $CI^{(n)}$ is an anytime CI then $P^{(n)}$ is an always-valid p-value.

$$\text{For all stopping times } \tau,\ \Pr(P^{(\tau)} \leq \alpha) \leq \alpha.$$

$$\text{For all data-dependent times } T,\ \Pr(P^{(T)} \leq \alpha) \leq \alpha.$$

Can construct confidence sequences
(and hence always valid p-values)
in a wide variety of *nonparametric* settings
(eg: random variables that are
bounded, or subGaussian, or subexponential)

Howard, Ramdas, McAuliffe, Sekhon '18

Confidence sequences for quantiles, and for all quantiles simultaneously

Howard, Ramdas'19

Confidence sequence for fixed quantiles

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for any $q \in [Q^-(p), Q(p)]$.

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(Also, a numerical "mixture" boundary that has better constants.)

Confidence sequence for all quantiles simultaneously

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Define $u_t := \sqrt{\dfrac{\log\log(et) + 0.75\log(34/\alpha)}{t}}$

$$\Pr(\forall t \in \mathbb{N}, p \in (0,1) : \widehat{Q}_t(p - u_t) \le Q(p) \le \widehat{Q}_t(p + u_t)) \ge 1 - \alpha .$$

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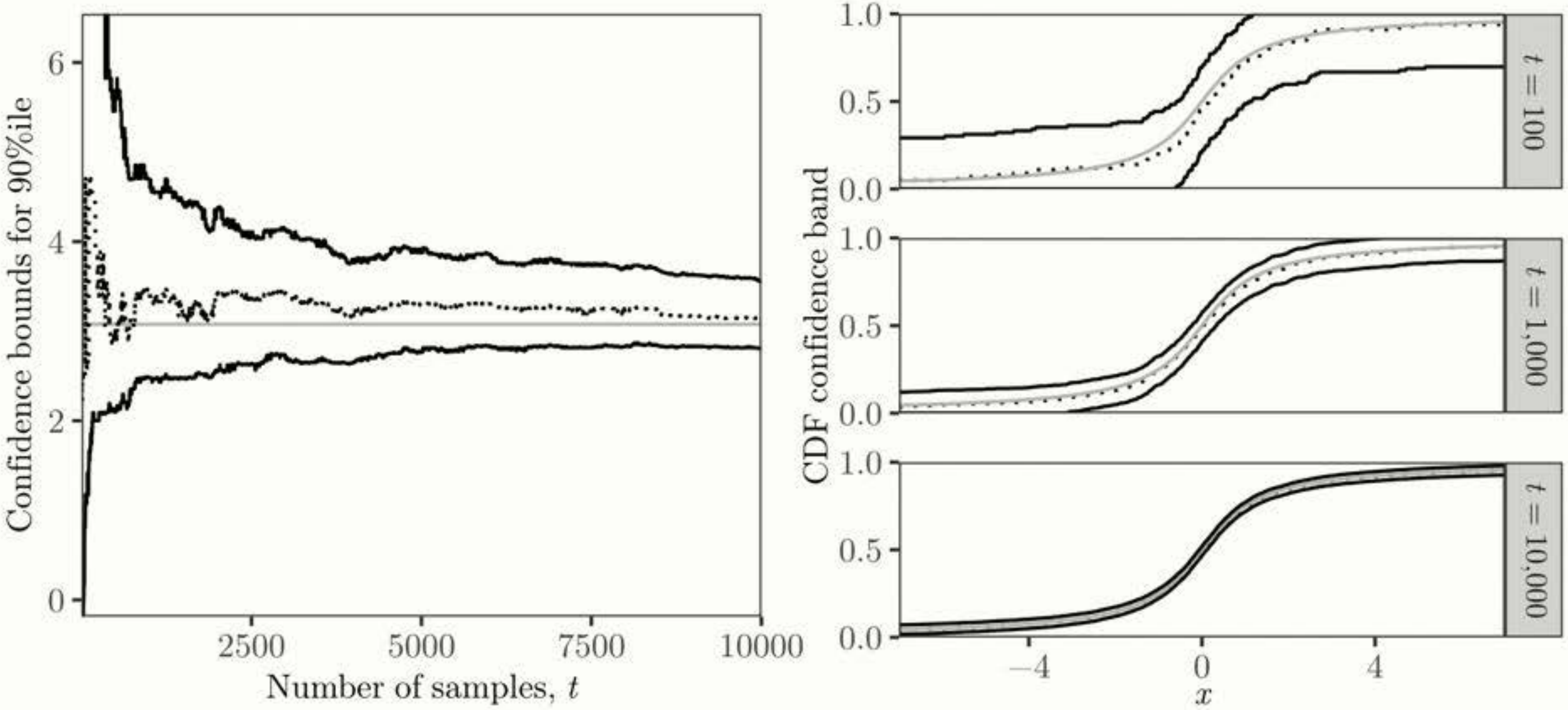
(also, a "practical" uniform DKW inequality, and numerical methods)


Confidence bounds for 90%ile
0
2
4
6
2500
5000
7500
10000
Number of samples, t
CDF confidence band
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0.5
0.0
t = 100
t = 1,000
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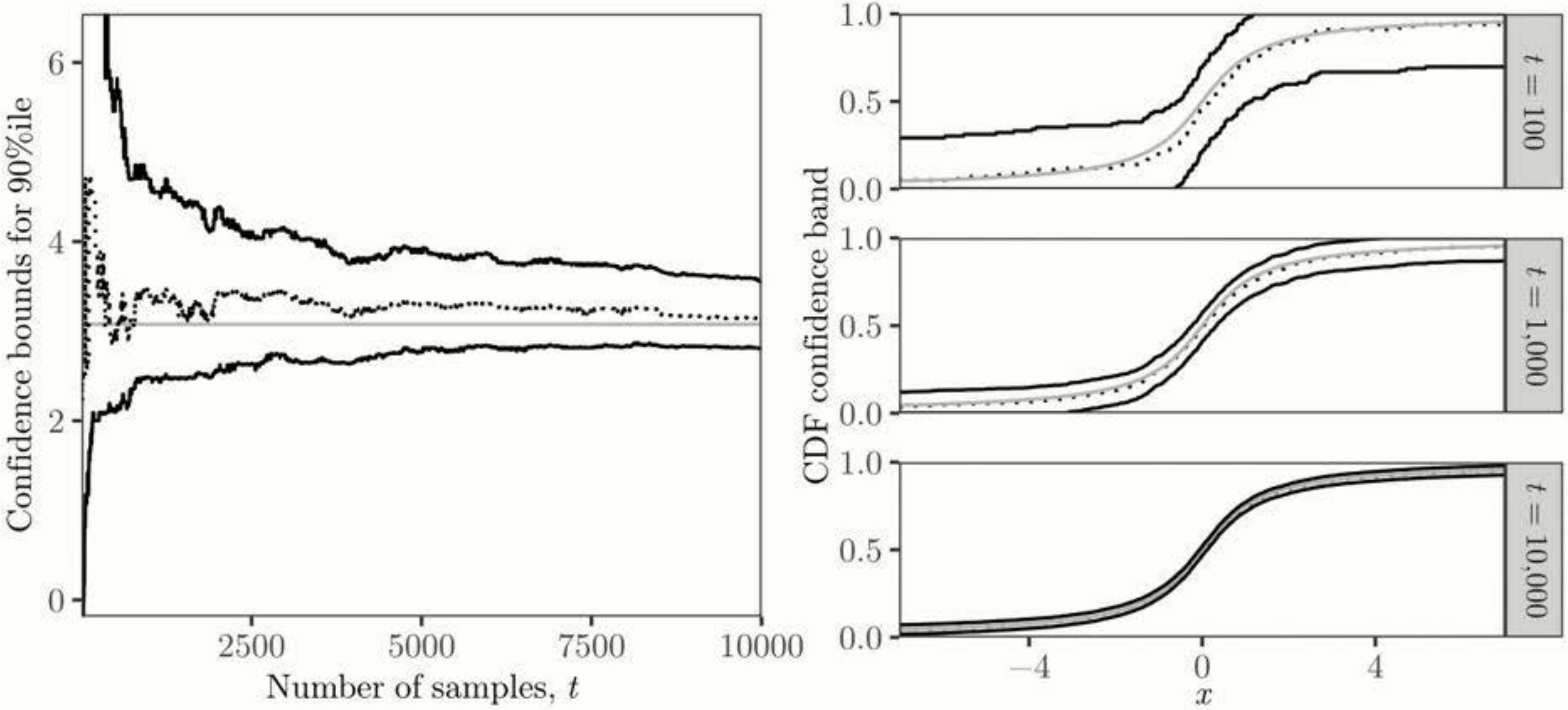
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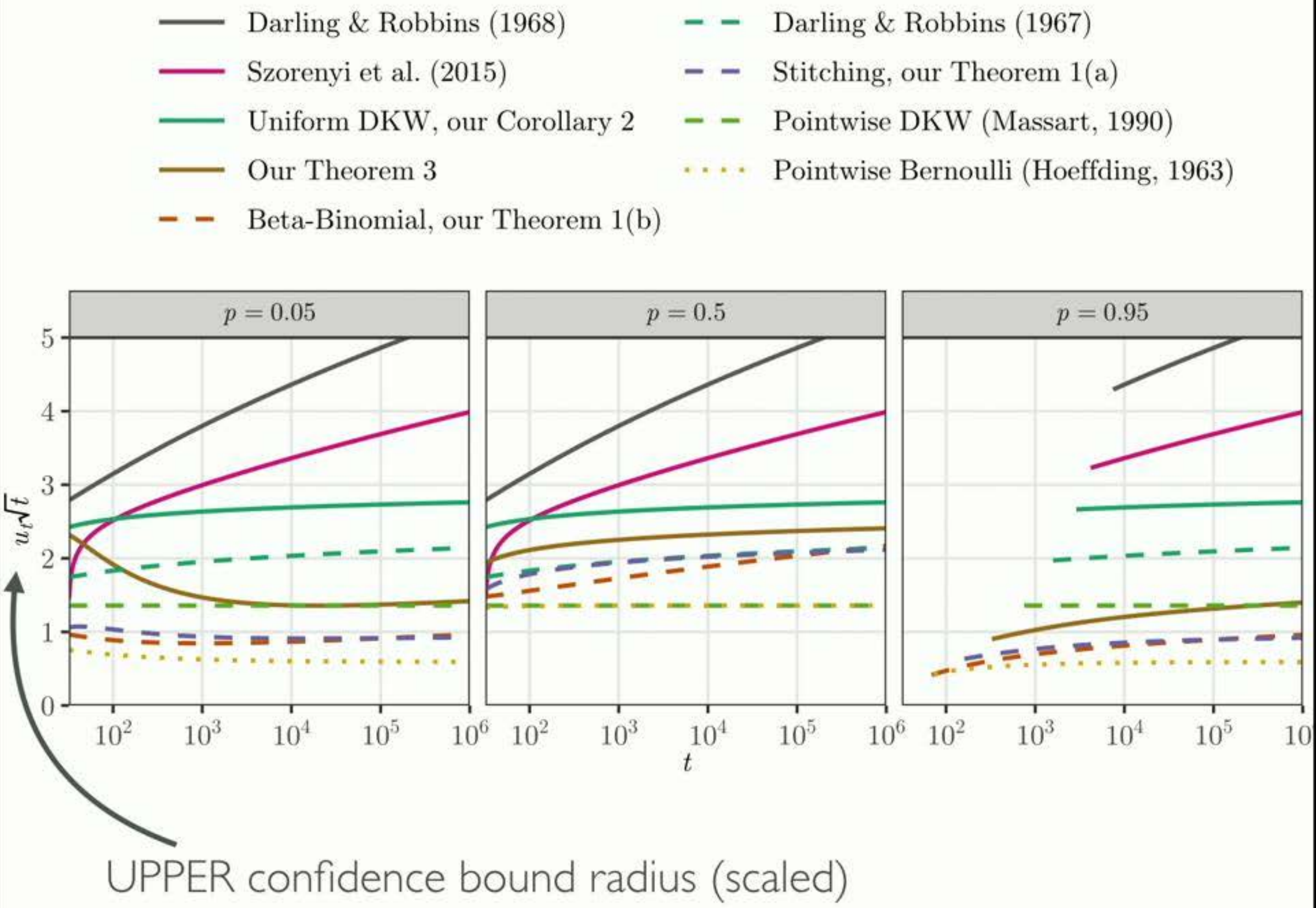


Darling & Robbins (1968)
Szorenyi et al. (2015)
Uniform DKW, our Corollary 2
Our Theorem 3
Beta-Binomial, our Theorem 1(b)
Darling & Robbins (1967)
Stitching, our Theorem 1(a)
Pointwise DKW (Massart, 1990)
Pointwise Bernoulli (Hoeffding, 1963)
p = 0.05
p = 0.5
p = 0.95
$u_t\sqrt{t}$
t
UPPER confidence bound radius (scaled)

Quantile ϵ-best arm identification

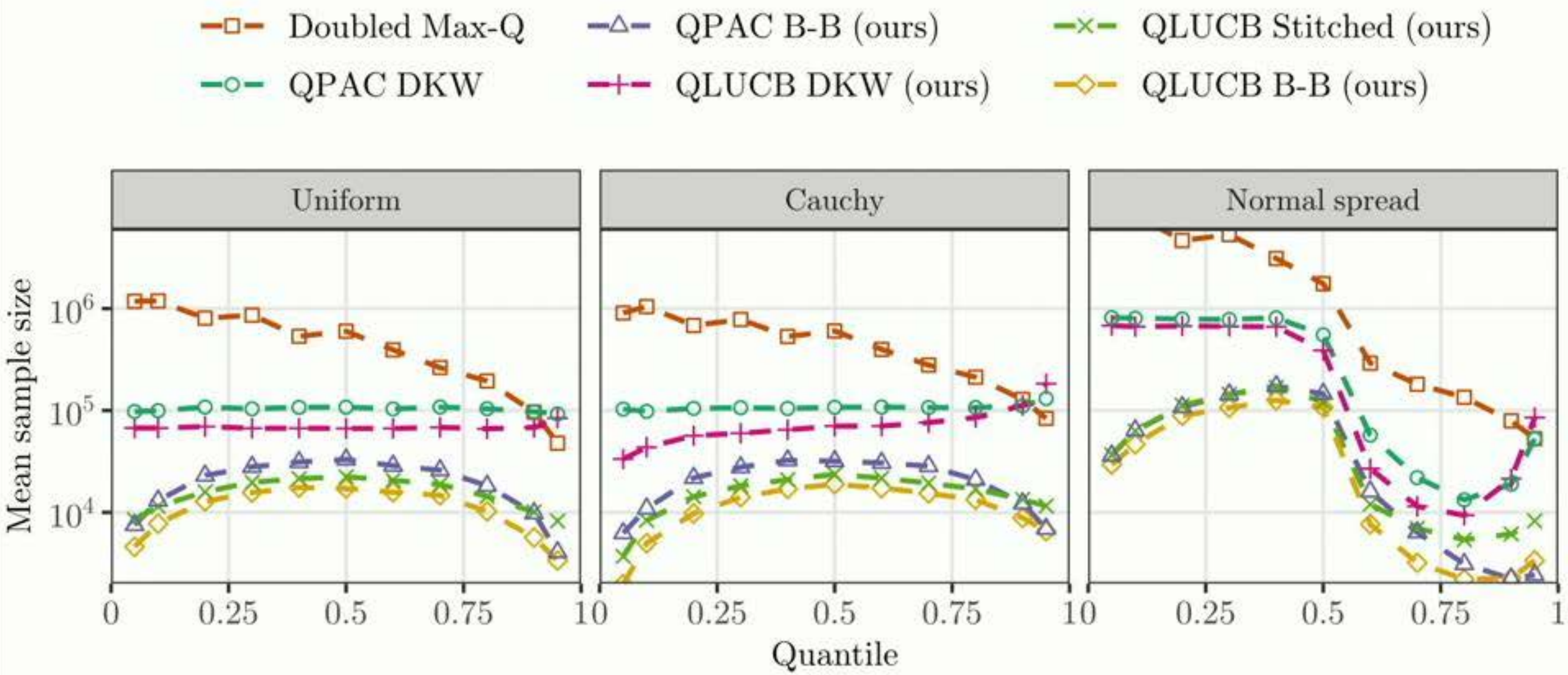
For a fixed $\pi \in (0,1)$ and $\epsilon \in (0,1-\pi)$, we call an arm ϵ-optimal

$$Q_{k^\star}(\pi+\epsilon) \geq Q_j(\pi) \text{ for all } j \neq k^\star .$$

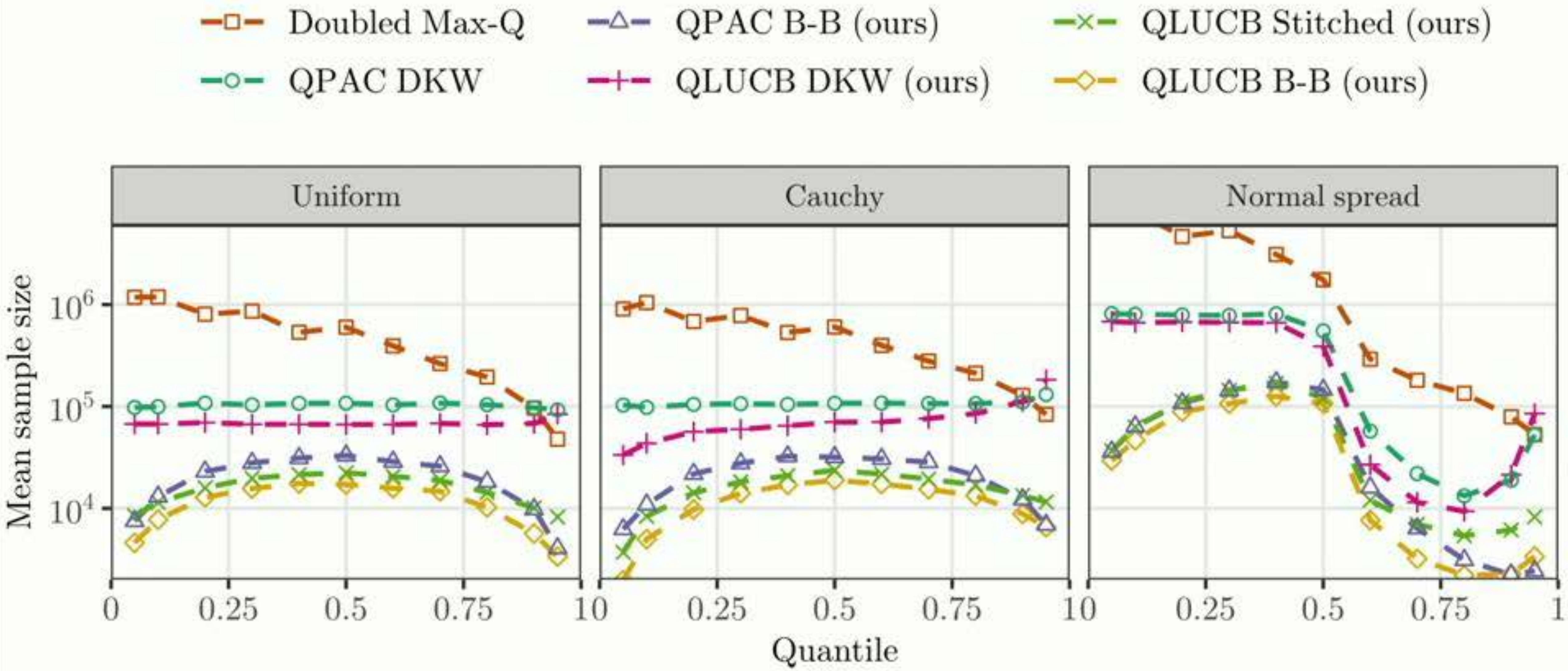
Task: identify any ϵ-optimal arm w.p. $1-\delta$, for given $\delta \in (0,1)$.

Input target quantile $\pi \in (0,1)$, approximation error $\epsilon \in (0,1-\pi)$, and error probability $\delta \in (0,1)$.
Sample each arm once, set $N_{k,1}=1$ for all $k \in [K]$ and set $t=1$.
while $L_{k,t}^{\pi+\epsilon} < \max_{j\neq k} U_{j,t}^{\pi}$ for all $k \in [K]$ **do**,
    Set $h_t \in \arg\max_{k\in[K]} L_{k,t}^{\pi+\epsilon}$ and $l_t \in \arg\max_{k\in[K]\setminus h_t} U_{k,t}^{\pi}$.
    Sample arms h_t and l_t.
    Set $N_{k,t+1}=N_{k,t}+1$ if $k=h_t$ or $k=l_t$, and $N_{k,t+1}=N_{k,t}$ otherwise.
    Increment $t \leftarrow t+1$.
end while
Output any element of $\arg\max_{k\in[K]} L_{k,t}^{\pi+\epsilon}$.

QLUCB (our variant of standard LUCB)

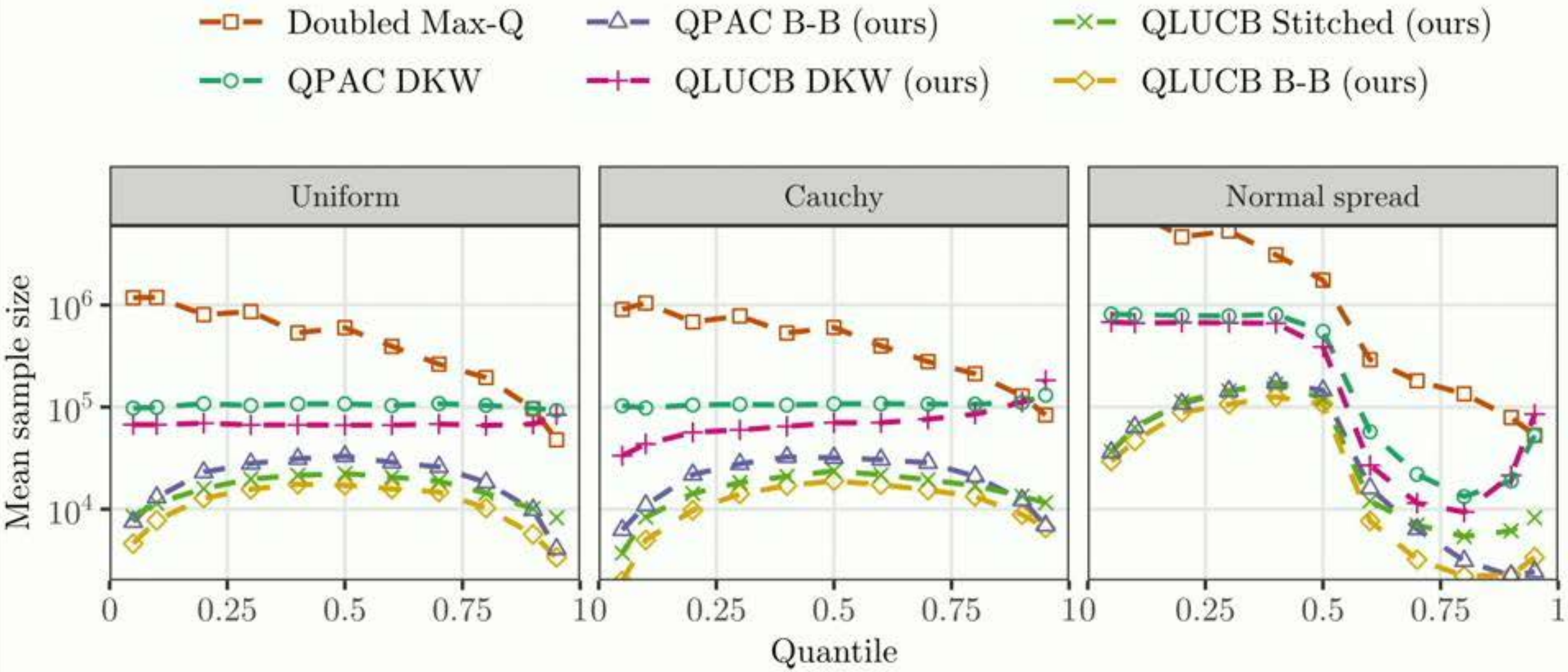


Doubled Max-Q
QPAC B-B (ours)
QLUCB Stitched (ours)
QPAC DKW
QLUCB DKW (ours)
QLUCB B-B (ours)
Uniform
Cauchy
Normal spread
Mean sample size
10^6
10^5
10^4
0
0.25
0.5
0.75
1
Quantile



Theorem: $$\Delta_k := \sup\left\{\Delta \geq 0 : Q_k(\pi + \Delta) < \max_{j \in [K]} Q_j(\pi)\right\}$$

QLUCB stops w.p. one, and w.p. $1 - \delta$, it picks an ϵ-optimal arm .



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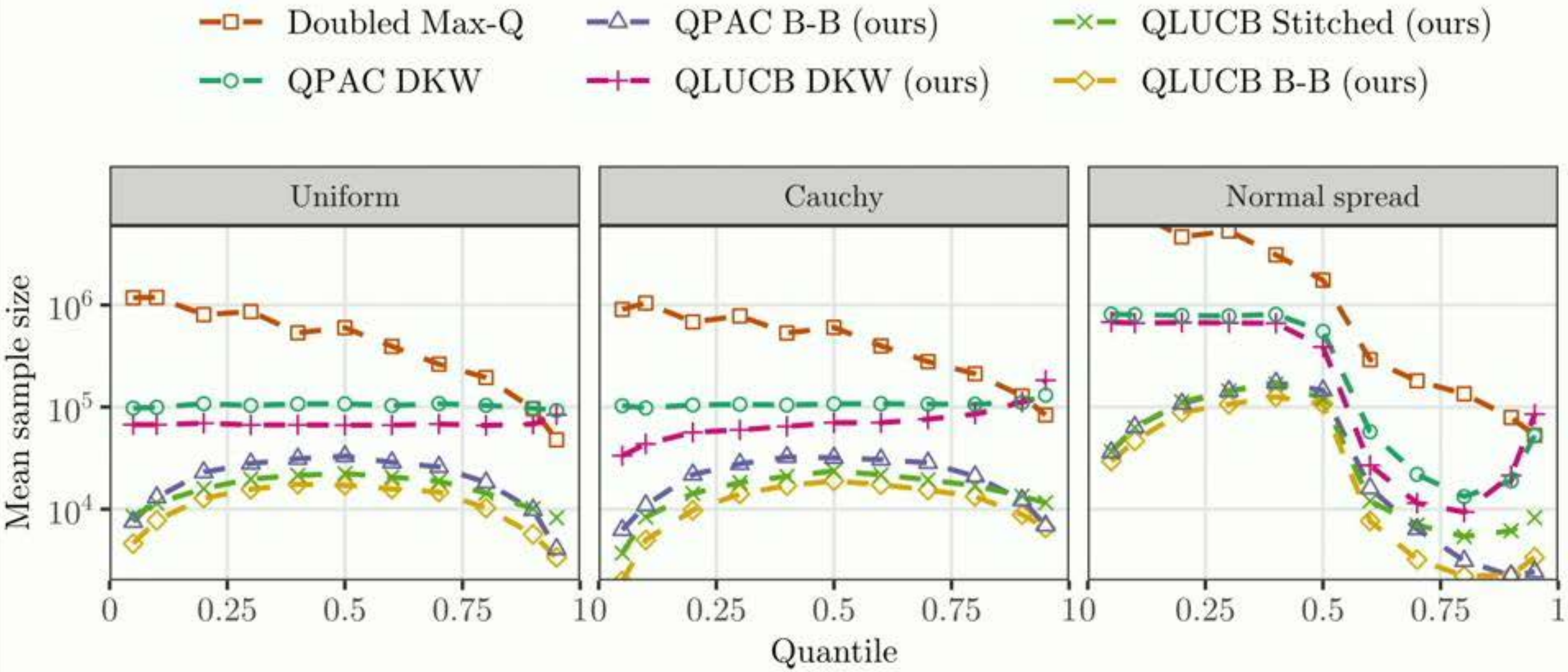

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$$T = \mathcal{O}\left(\sum_{k=1}^{K} (\epsilon \vee \Delta_k)^{-2} \log\left(\frac{K\left|\log\left(\epsilon \vee \Delta_k\right)\right|}{\delta}\right)\right).$$

Other applications in the paper

- A/B testing: how to derive an always valid p-value by inverting and combining confidence sequences
- Sequential Kolmogorov-Smirnov test (classical KS test)
- Sequential test for stochastic dominance

(all have controlled false positive rate, and power tending to one at the optimal rate)

Howard, Ramdas'19

SOFTWARE

Python package called "**confseq**"
Maintained by Steven R. Howard
Frequent updates + wrappers for months to come

Takeaway messages

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Reasons to use quantiles include:

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Open problems

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- Perhaps start with contextual bandits or MDPs.

Sequential estimation of quantiles with applications to A/B testing and bandits

Aaditya Ramdas

Assistant Professor
Dept. of Statistics and Data Science
Machine Learning Dept.
Carnegie Mellon University

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Thank you! Questions?