Log-Optimality & Multi-Armed Sequential Hypothesis Testing

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Outline

1. What is sequential hypothesis testing (by betting)?
2. How are sequential hypothesis tests derived?
3. Defining and deriving optimal sequential tests.
4. Multi-armed sequential hypothesis testing

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A motivating example to keep in mind: **treatment effect testing**.

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$$H_1 : \text{trt effect} \neq 0$$

$$\alpha := 0.01$$

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Recruit n patients and randomize (**trt** or **ctrl**).

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No! (This is "p-hacking".)

Alternatively, even if n was large enough to reject H_0, it is possible that $n' \ll n$ could have sufficed (time & money saved).

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Sequential testing addresses these unsettling scenarios.

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(Modern breakthroughs by Grünwald, Ramdas, and others in 2010's onwards)

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$$\textit{(e.g. } \mathcal{P} = \{P : \textit{trt effect} = 0\} \textit{ versus } \mathcal{Q} = \{P : \textit{trt effect} > 0\}\textit{)}$$

We are tasked with finding a test $\phi_n^{(\alpha)} \equiv \phi^{(\alpha)}(X_1, \ldots, X_n)$ that outputs 1 (rejects $\mathcal{P}$ in favour of $\mathcal{Q}$) with small probability under $\mathcal{P}$.

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Fixed-n test: $\quad \forall n \in \mathbb{N}, \ \sup_{\mathsf{P} \in \mathcal{P}} \mathsf{P}\left(\phi_n^{(\alpha)} \text{ rejects}\right) \leqslant \alpha.$

Sequential test: $\quad \sup_{\mathsf{P} \in \mathcal{P}} \mathsf{P}\left(\exists n \in \mathbb{N} : \phi_n^{(\alpha)} \text{ rejects}\right) \leqslant \alpha.$

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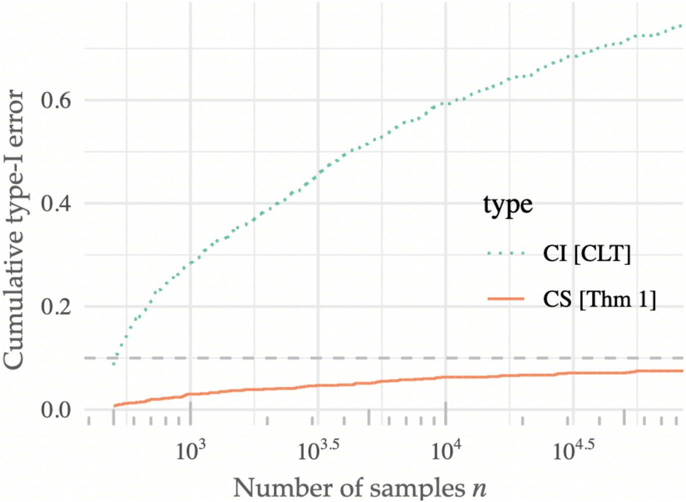
$$\iff \sup_{\mathsf{P} \in \mathcal{P}} \mathsf{P}\left(\phi_\tau^{(\alpha)} \text{ rejects}\right) \leqslant \alpha \quad \forall \tau.$$



$$\forall n,\ \mathsf{P}(\phi_n^{(\alpha)} = 1) \leqslant \alpha$$

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2. Set the test as $\phi_n^{(\alpha)} := \mathbb{1}\{W_n \geqslant 1/\alpha\}$.

This procedure works because of Ville's inequality which states that for a nonnegative $\mathcal{P}$-supermartingale $(W_n)_{n \in \mathbb{N}}$,

$$\forall x > 0, \quad \mathsf{P}\left(\exists n \in \mathbb{N} : W_n \geqslant x\right) \leqslant \frac{\mathbb{E}_{\mathsf{P}}[W_1]}{x}.$$

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$$\forall \alpha \in (0,1), \quad \mathsf{P}\left(\exists n \in \mathbb{N} : \phi_n^{(\alpha)} = 1\right) \leqslant \alpha.$$

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However, lots of progress has been made in recent years.

Example: Testing the mean of a bounded random variables.

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$$W_n := \prod_{i=1}^{n} (1 + \gamma_i \cdot (2X_i - 1))$$

forms a test martingale for any $[0,1]$-valued *predictable* $(\gamma_n)_{n \in \mathbb{N}}$.

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Therefore, $\phi_n^{(\alpha)} := \mathbb{1}\{W_n \geqslant 1/\alpha\}$ yields a sequential test for $\mathcal{P}$.

It is **not** obvious how to choose γ_i... more on that later.

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Definition: e-value. (See Shafer & Vovk, Grünwald et al., Vovk & Wang)

A nonnegative random variable $E \geqslant 0$ is said to be a $\mathcal{P}$-e-value if

$$\sup_{\mathsf{P} \in \mathcal{P}} \mathbb{E}_{\mathsf{P}}[E] \leqslant 1.$$

Example: For the testing-means-of-bounded-random-variables problem,

$$\prod_{i=1}^{n}(1 + \gamma_i(2X_i - 1))$$

is a special case of

$$\prod_{i=1}^{n} \lambda_i{}^{\top}\mathbf{E}_i$$

when taking $\mathbf{E}_i = (1, 2X_i)$ and $\lambda_i = (1 - \gamma_i, \gamma_i)$.

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$$\begin{aligned} &\mathbb{E}_{\mathsf{P}}\left[\prod_{i=1}^{n} \lambda_i^\top \mathbf{E}_i \mid \mathbf{E}_1, \ldots, \mathbf{E}_{n-1}\right] \\ = &\left(\prod_{i=1}^{n-1} \lambda_i^\top \mathbf{E}_i\right) \mathbb{E}_{\mathsf{P}}\left[\lambda_n^\top \mathbf{E}_n \mid \mathbf{E}_1, \ldots, \mathbf{E}_{n-1}\right] \\ \leqslant &\ W_{n-1}. \end{aligned}$$

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&\leqslant W_{n-1}.
\end{aligned}$$

Therefore, W_n forms a test supermartingale. □

Some other special cases found in the literature

One-sided bounded mean testing: Set $\mathbf{E}_i = (1, X_i/\mu_0)$.
Two-sided bounded mean testing: Set $\mathbf{E}_i = ((1 - X_i)/(1 - \mu_0), X_i/\mu_0)$.
Two-sample testing: Set $\mathbf{E}_i = (1, g^\star(X_i) - g^\star(Y_i))$ for a witness f'n $g^\star$.
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There has been one lingering question this entire discussion:

How should one choose $(\lambda_n)_{n\in\mathbb{N}}$?

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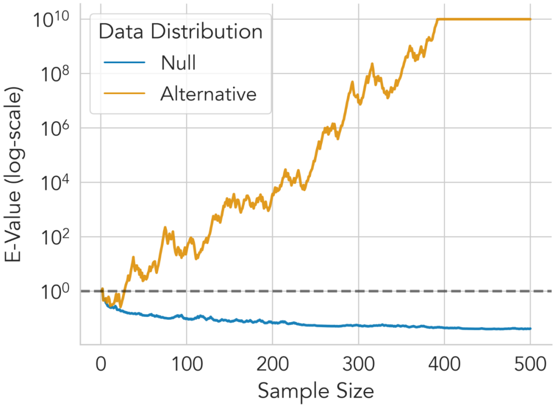
We show that these are optimized via the exact same criterion.

(i) Growth-rate-optimality.

(Kelly ['56], Long Jr. ['90], Grünwald et al. [2024], Larsson et al. [2024])



An e-process is expected to be small under the ***null****;*
we want it to grow large under the ***alternative****.*

Image credit: YJ Choe.

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$$\begin{aligned} W_n &= \exp\left\{ n \cdot \frac{1}{n} \sum_{i=1}^{n} \log\left(\lambda_i{}^\top \mathbf{E}_i \right) \right\} \\ &\approx \exp\left\{ n \cdot \mathbb{E}_{\mathsf{Q}} \left[\log\left(\lambda_i{}^\top \mathbf{E}_i \right) \right] + o(n) \right\} \end{aligned}$$

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So, if data comes from $\mathsf{Q} \in \mathcal{Q}$, it is reasonable to want to choose λ_i so as to maximize:

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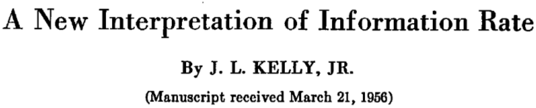
This is the "Kelly criterion" from gambling / information theory.


A New Interpretation of Information Rate

By J. L. KELLY, JR.

(Manuscript received March 21, 1956)

“Kelly bet”: $\lambda_{\mathsf{Q}} := \underset{\lambda \in \triangle_d}{\operatorname{argmax}} \, \mathbb{E}_{\mathsf{Q}} \left[\log(\lambda^\top \mathbf{E}_1) \right].$

(ii) Measuring optimality through expected rejection times

(Wald 1945, Breiman 1961, Kaufmann, Agrawal, Koolen, others from the bandit literature)

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Proposition: Lower bound on the expected stopping time

$$\mathbb{E}_{\mathsf{Q}}[\tau_\alpha] \geqslant \frac{\log(1/\alpha)}{\max_{\lambda \in \triangle_d} \mathbb{E}_{\mathsf{Q}}\left[\log\left(\lambda^\top \mathbf{E}_1\right)\right]}.$$

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Sequential testing as portfolio selection over $d+1$ stocks.

You start with $W_1 = \$1$.

For $n = 1, 2, \ldots$:

1. Choose portfolio $\lambda_n \in \triangle_d$.
2. Observe stock returns $\mathbf{E}_n = (E_n^{(0)}, \ldots, E_n^{(d)}) \in [0, \infty)^d$.
3. $W_n = W_{n-1} \lambda_n^\top \mathbf{E}_n$.

EndFor

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Then $W_n = \prod_{i=1}^n \lambda_i{}^\top \mathbf{E}_i$.

Given the form

$$W_n \approx \exp\left\{n\mathbb{E}_{\mathsf{Q}}\left[\log\left(\lambda^\top \mathbf{E}_1\right)\right] + o(1)\right\}$$

and the lower bound

$$\mathbb{E}_{\mathsf{Q}}[\tau_\alpha] \geqslant \frac{\log(1/\alpha)}{\max_{\lambda\in\triangle_d} \mathbb{E}_{\mathsf{Q}}\left[\log\left(\lambda^\top \mathbf{E}_1\right)\right]},$$

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$$\mathbb{E}_{\mathsf{Q}}[\tau_\alpha] \geqslant \frac{\log(1/\alpha)}{\max_{\lambda\in\triangle_d} \mathbb{E}_{\mathsf{Q}}\left[\log\left(\lambda^\top \mathbf{E}_1\right)\right]},$$

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However, λ_{Q} depends on the alternative Q. Can it be "learned"?

Yes; this motivates the definition of *portfolio regret*.

Definition: Portfolio regret.

Define the portfolio regret $\mathcal{R}_n$ of $(\lambda_n)_{n \in \mathbb{N}}$ to be

$$\mathcal{R}_n := \max_{\lambda \in \triangle_d} \sum_{i=1}^{n} \log\left(\lambda^\top \mathbf{E}_i\right) - \sum_{i=1}^{n} \log\left(\lambda_i{}^\top \mathbf{E}_i\right).$$

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This is *precisely* the notion of regret considered by Thomas Cover and Erik Ordentlich in their work on on universal portfolios circa 1990s.

Fortunately for us, Cover and Ordentlich derived an algorithm with *logarithmic* portfolio regret ("Universal Portfolio").

Theorem: Log-optimality via sublinear portfolio regret.

Suppose that $(\lambda_n)_{n \in \mathbb{N}}$ have sublinear portfolio regret. Then for $\mathsf{Q} \in \mathcal{Q}$,

$$\lim_{n \to \infty} \frac{1}{n} \log W_n = \max_{\lambda \in \triangle_d} \mathbb{E}_{\mathsf{Q}} \left[\log \left(\lambda^\top \mathbf{E}_1 \right) \right] \quad \mathsf{Q}\text{-almost surely.}$$

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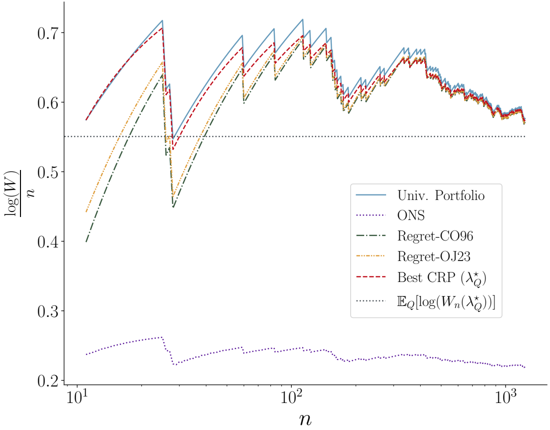
Moreover,

$$\lim_{\alpha\to 0^+} \frac{\mathbb{E}_{\mathsf{Q}}\left[\tau_\alpha\right]}{\log(1/\alpha)} = \frac{1}{\max_{\lambda\in\triangle_d} \mathbb{E}_{\mathsf{Q}}\left[\log\left(\lambda^\top \mathbf{E}_1\right)\right]}$$



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0.2
$\frac{\log(W)}{n}$
10^1
10^2
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n
Univ. Portfolio
ONS
Regret-CO96
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Best CRP ($\lambda_Q^\star$)
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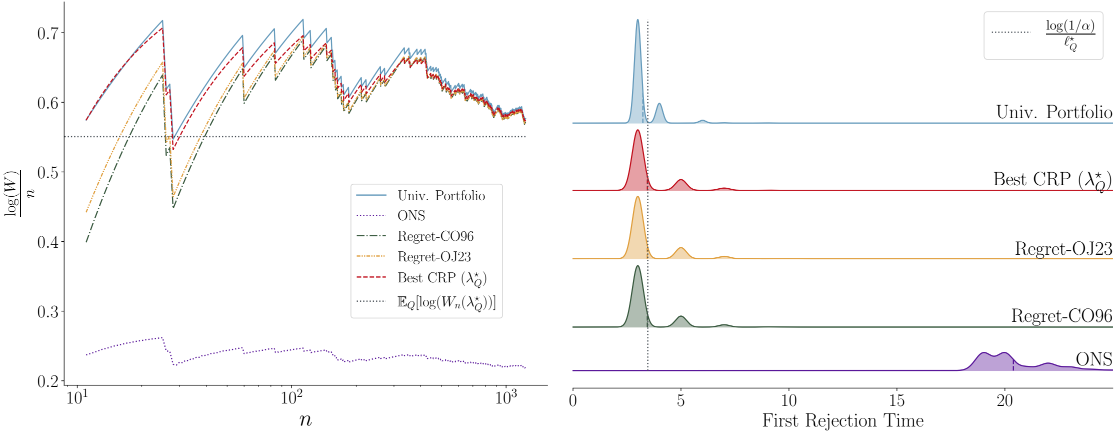

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Recap so far

1. **Q:** "What is sequential hypothesis testing?"
   A: For all stopping times τ, $\mathsf{P}(\phi_{\tau}^{(\alpha)} \text{ rejects}) \leqslant \alpha$.

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Recap so far

1. **Q:** "What is sequential hypothesis testing?"
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2. **Q:** "How to derive valid sequential tests?"
   A: $W_n \mapsto \mathbb{1}\{W_n \geqslant 1/\alpha\}$ for a test supermartingale $(W_n)_{n\in\mathbb{N}}$.

3. **Q:** "How to derive a powerful supermartingale $(W_n)_{n\in\mathbb{N}}$?"
   A: Sublinear portfolio regret (e.g. Universal Portfolio algorithms).

Outline

1. What is sequential hypothesis testing (by betting)?

2. How are sequential hypothesis tests derived?

3. Defining and deriving optimal sequential tests.

4. Multi-armed sequential hypothesis testing

0mg 0.2mg 0.4mg 0.6mg 0.8mg 1mg

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How does this complicate type-I error control under $\mathcal{P}$ and/or log-optimality under $\mathcal{Q}$?

Let $\mathcal{A} = \{1, \ldots, K\}$ be the arm set.

Multi-armed sequential testing.

Start with $W_1 = \$1$.

For $n = 1, 2, \ldots$:

1. **Choose arm $A_n \in \mathcal{A}$.**
2. Choose portfolio $\lambda_n \in \triangle_d$.
3. Observe $\mathbf{E}_n(A_n) \sim \mathsf{P}(A_n)$.
4. $W_n = W_{n-1} {\lambda_n}^\top \mathbf{E}_n(A_n)$.

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EndFor

Next: Type-I error control is preserved under *arbitrary* arm selection.

Proposition Type-I error control under $\mathcal{P}$

Suppose that λ_n and $A_n \in \mathcal{A}$ depend only on

$$\mathbf{E}_1(A_1), \ldots, \mathbf{E}_{n-1}(A_{n-1}).$$

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$$W_n = \prod_{i=1}^{n} \lambda_i^\top \mathbf{E}_i(A_i)$$

forms a test supermartingale and hence

$$\phi_n^{(\alpha)} := \mathbb{1}\{W_n \geqslant 1/\alpha\}$$

forms a sequential hypothesis test for the global null $\mathcal{P}$.

The proof proceeds almost identically to before.

Takeaway: type-I error control in the multi-armed setting is easy.

Optimality is a different story.

$$\max_{\lambda \in \triangle_d} \mathbb{E}_{\mathsf{Q}} \left[\log \left(\lambda^\top \mathbf{E}_1 \right) \right].$$

$$\max_{(a,\lambda)\in\mathcal{A}\times\triangle_d} \mathbb{E}_{\mathsf{Q}}\left[\log\left(\lambda^\top \mathbf{E}_1(a)\right)\right].$$

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Let us now see how $\frac{1}{n}\sum_{i=1}^n \log\left(\lambda_i{}^\top \mathbf{E}_i(A_i)\right)$ might concentrate around the above.

$$
\max_{(a,\lambda)\in\mathcal{A}\times\triangle_d} n\mathbb{E}_{\mathsf{Q}}\left[\log\left(\lambda^\top \mathbf{E}_1(a)\right)\right] - \sum_{i=1}^{n} \log\left({\lambda_i}^\top \mathbf{E}_i(A_i)\right)
$$

$$
= \underbrace{\max_{(a,\lambda)\in\mathcal{A}\times\triangle_d} n\mathbb{E}_{\mathsf{Q}}\left[\log\left(\lambda^\top \mathbf{E}_1(a)\right)\right] - \sum_{i=1}^{n} \mathbb{E}_{\mathsf{Q}}\left[\log(\lambda_{\mathsf{Q}}(A_i)^\top \mathbf{E}(A_i))\right]}_{\textbf{Allocation (multi-armed bandit) regret}}
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+ \underbrace{\sum_{i=1}^{n} \mathbb{E}_{\mathsf{Q}}\left[\log(\lambda_{\mathsf{Q}}(A_i)^\top \mathbf{E}_i(A_i))\right] - \sum_{i=1}^{n} \log\left(\lambda_{\mathsf{Q}}(A_i)^\top \mathbf{E}_i(A_i)\right)}_{\approx 0 \ \mathsf{Q}\text{-a.s. by the strong law of large numbers.}}
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This is *almost exactly* the type of regret considered in stochastic multi-armed bandits.

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Illustration (credits: Adrien Prevost, INRIA)

</detour>

"Nice" confidence intervals $\implies$ allocation regret minimization.

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These are *neither* sub-Gaussian *nor* observed iid from any distribution.

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Define the upper confidence bound

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This turns out to have all the "nice" properties needed for UCB-style analyses. In particular, it suffices for

$$\text{Allocation regret}_n = O\left(\log(n)\right).$$

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Theorem: Multi-armed log-optimality

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$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} \log\left(\lambda_i(a)^\top \mathbf{E}_i(A_i)\right) = \max_{(a,\lambda)\in\mathcal{A}\times\triangle_d} \mathbb{E}_{\mathsf{Q}}\left[\log\left(\lambda^\top \mathbf{E}_1(a)\right)\right]$$

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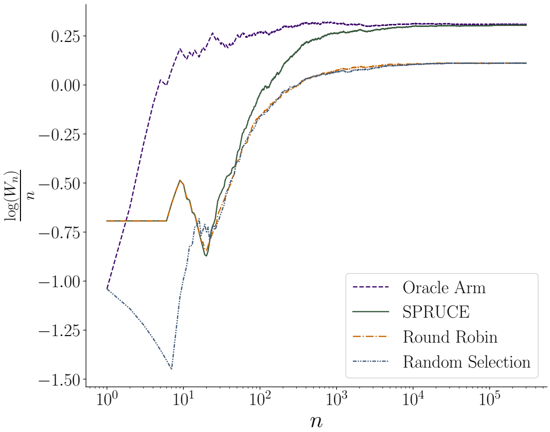
$$\lim_{\alpha \to 0^+} \frac{\mathbb{E}_{\mathsf{Q}}[\tau_\alpha]}{\log(1/\alpha)} = \left(\max_{(a,\lambda) \in \mathcal{A} \times \triangle_d} \mathbb{E}_{\mathsf{Q}}\left[\log\left(\lambda^\top \mathbf{E}_1(a)\right)\right]\right)^{-1}$$


0.25
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$\frac{\log(W_n)}{n}$
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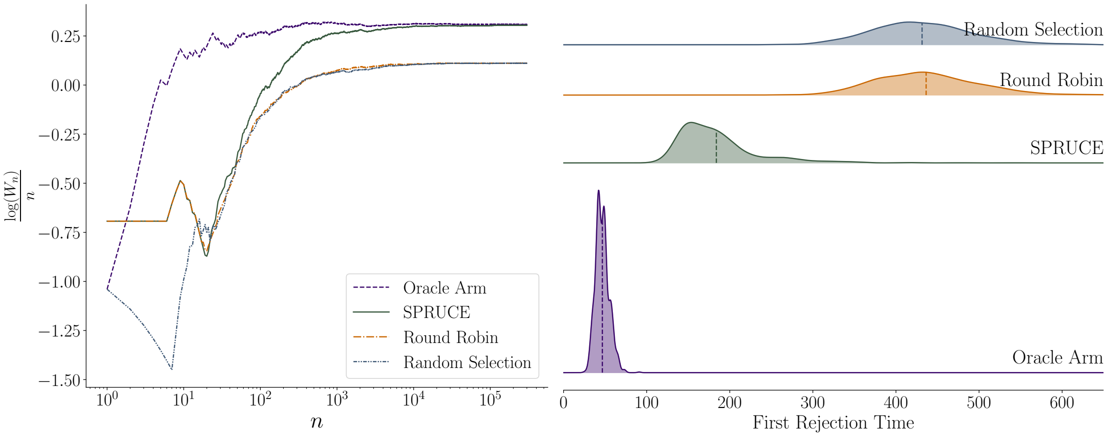
Oracle Arm
SPRUCE
Round Robin
Random Selection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4. **Q:** "How to do the same when multiple arms are present?"
   A: Bespoke upper-confidence-bound algorithms.

Thank you

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