

# An Efficient Algorithm for PAC Mode Estimation

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Denil Mehta <sup>1</sup>   Inderjeet Nair <sup>1</sup>   Jian Vora <sup>2</sup>   Sushil Khyalia <sup>1</sup>  
Sourav Das <sup>3</sup>   Vinay J. Ribeiro <sup>1</sup>   Shivaram Kalyanakrishnan <sup>1</sup>

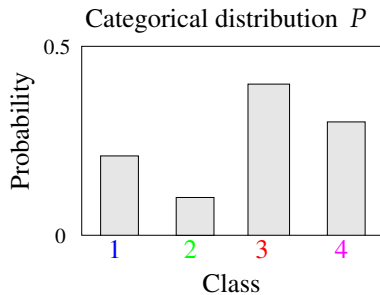
<sup>1</sup>Indian Institute of Technology Bombay

<sup>2</sup>Stanford University

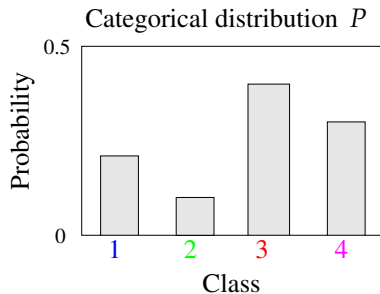
<sup>3</sup>University of Illinois Urbana-Champaign

August 2023

# Mode Estimation

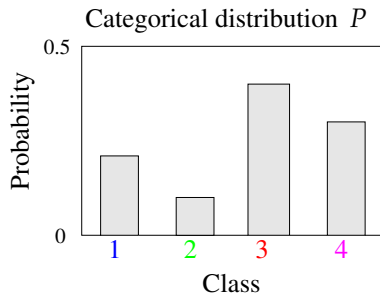


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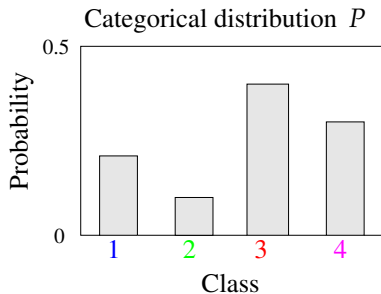
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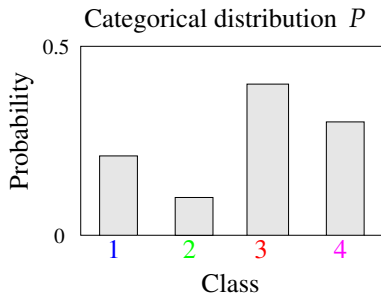
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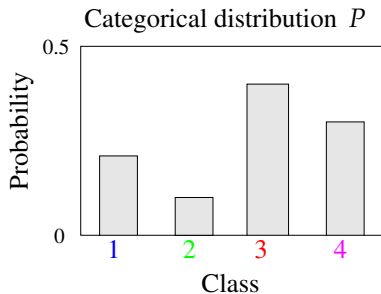
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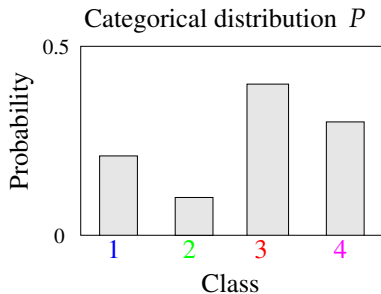
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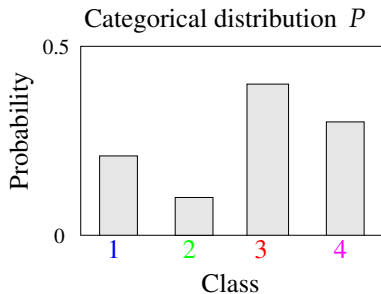


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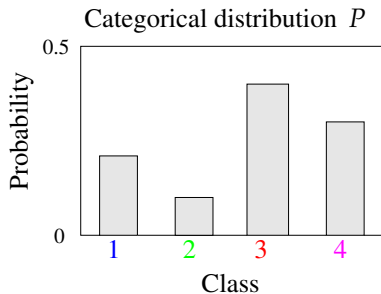
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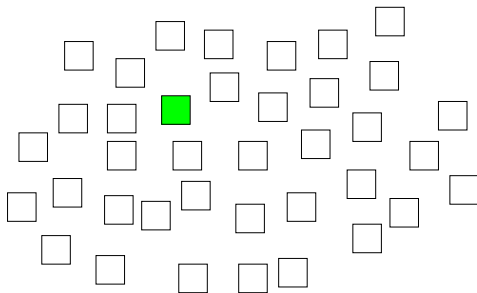
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When can we confidently stop sampling and declare the mode?

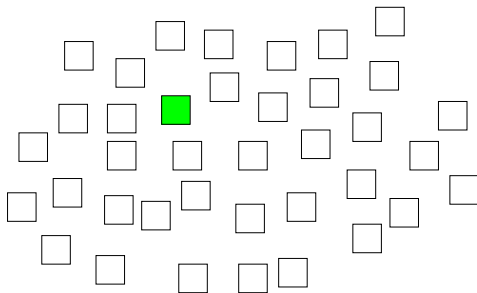
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- Ask a node for the result of a hard computation.
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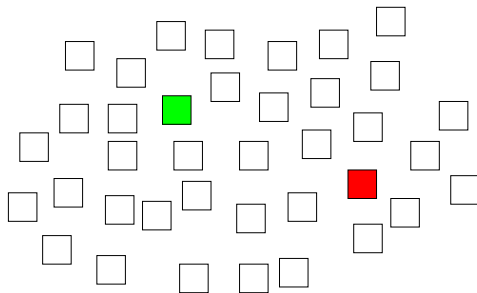
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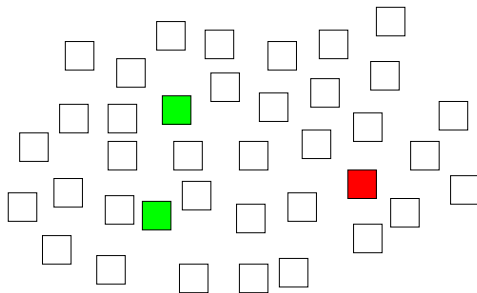
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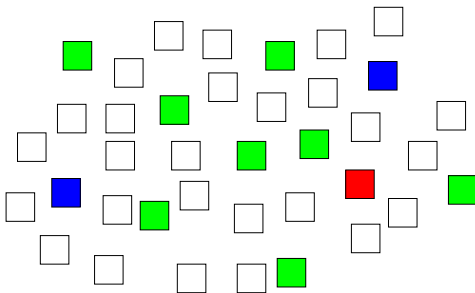
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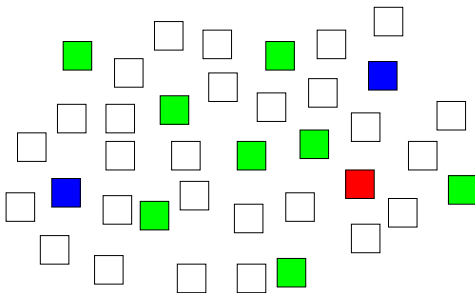
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- Assume that most frequently returned result is correct.
- Determine most frequently returned result with sufficient confidence, while minimising number of queries.



















# Election Forecasting


Seat	Vote share	Winner
1		
2		
3		
4		
5		
6		
7		
⋮	⋮	⋮
543		

Majority party:



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Majority party: 

- Confidently identify winner of each seat by [sampling](#).
- Aggregate wins to predict overall winner.

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1. PAC Formulation
2. Solutions for  $K = 2$  classes
3. Generalising to  $K \geq 2$  classes
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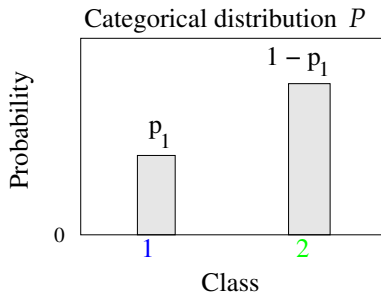
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- **Prefer**  $\delta$ -correct algorithm with low sample complexity.



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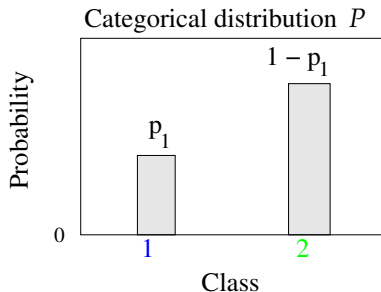
# Solving the $K = 2$ Special Case



- Have to ascertain whether  $p_1 > 0.5$  or  $p_1 < 0.5$  based on samples

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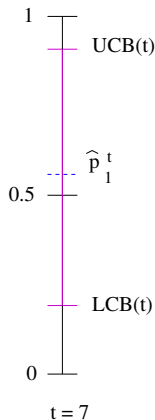
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2, 1, 2, 1, 1, 2, 2, 1, 2, 1, 1 ...
- Maintain lower confidence bound LCB and upper confidence bound UCB on  $p_1$ , stop if  $LCB > 0.5$  or  $UCB < 0.5$ .

# Using Confidence Bounds

- After  $t$  samples, let  $\hat{p}_1^t$  be the empirical fraction of class 1.

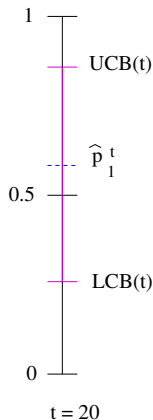
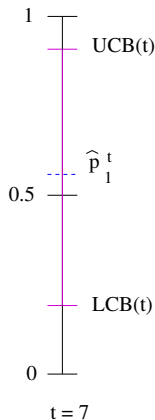
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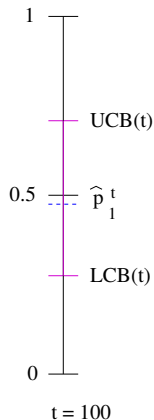
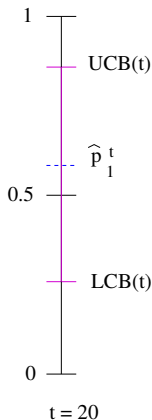
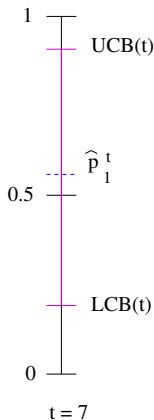
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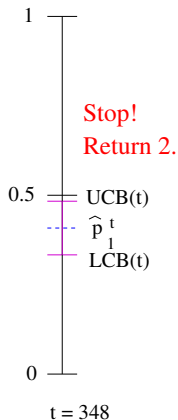
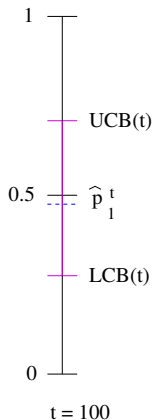
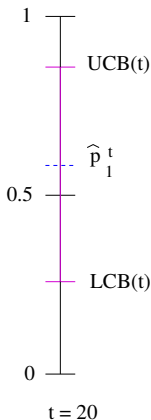
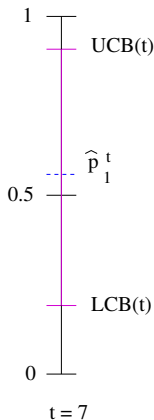
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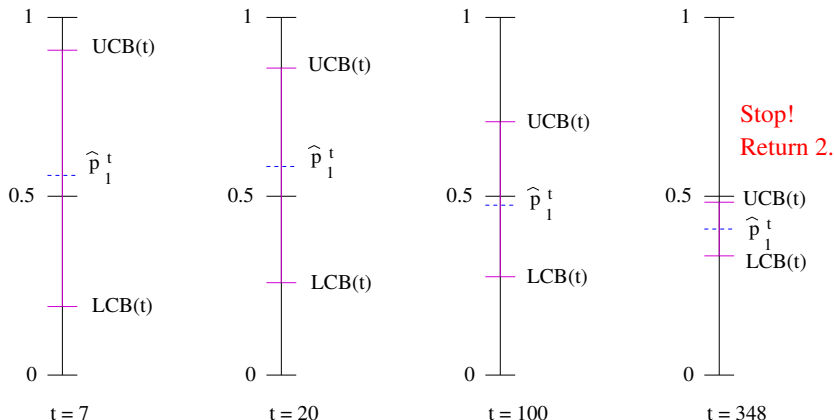
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- Note that the stopping time is **random**.

# Some Baselines

- Using [Hoeffding's Inequality](#).

$$LCB(t), UCB(t) = \hat{p}_1^t \pm \beta(t, \delta),$$

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- [“Self-normalised” inequality](#) to avoid naïve union bound over  $t$ .  
KL-SN, Garivier (2013).

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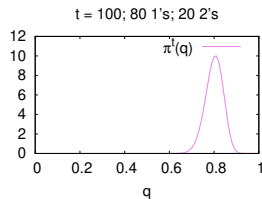
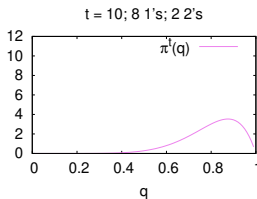
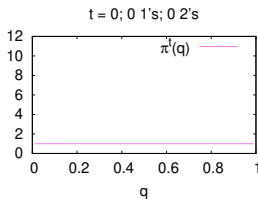
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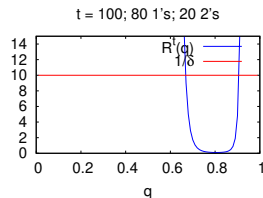
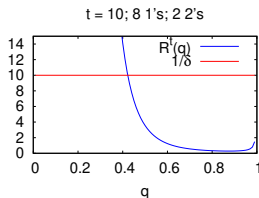
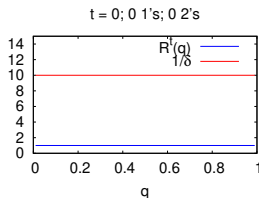
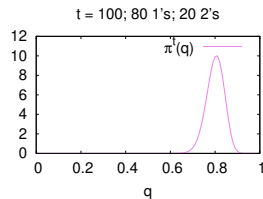
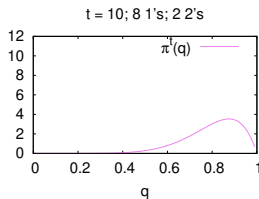
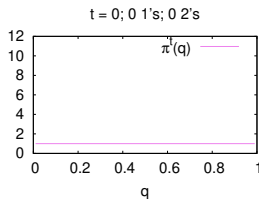
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- Proof by establishing that  $R^t(p_1)$  is a martingale, then applying Ville’s inequality on nonnegative supermartingales.
- Method more generally applicable, even for estimating multiple parameters simultaneously.

# PPR Martingale Confidence Sequences: Illustration



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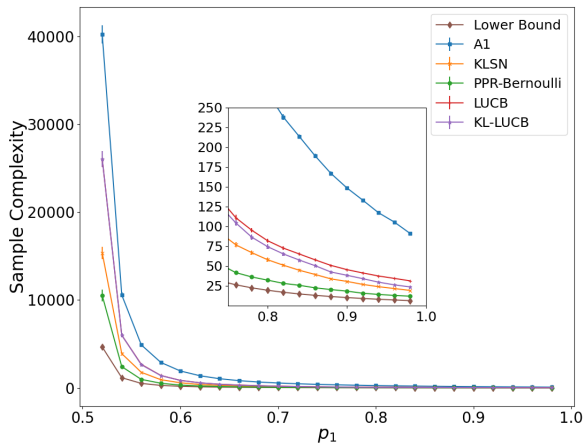
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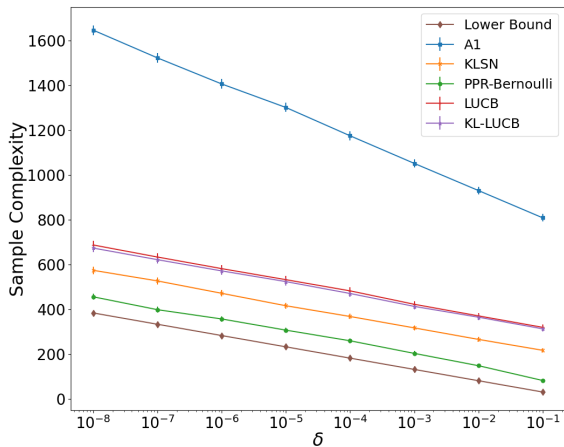
**PPR-Bernoulli:** Stop, declare  $\text{first}(t)$  as mode iff

$$\text{Beta}\left(\frac{1}{2}; s_{\text{first}(t)}^t + 1, s_{\text{second}(t)}^t + 1\right) \leq \delta.$$

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$$p_1 = 0.65$$

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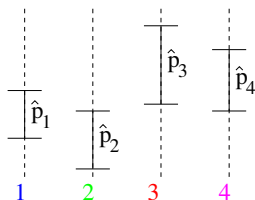
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## 1-versus-rest approach

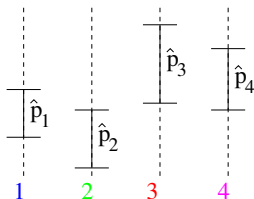


- For each class  $i$ , estimate underlying probability  $p_i$ .
- Stop and declare  $i$  as mode if LCB on  $p_i$  exceeds UCB on  $p_j$  for all  $j \neq i$ .

# Two Approaches to Generalise

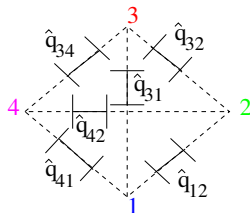
3, 1, 3, 4, 2, 1, 3, 2, 4, 3, 3, 1, 2, 3, ...

## 1-versus-rest approach



- For each class  $i$ , estimate underlying probability  $p_i$ .
- Stop and declare  $i$  as mode if LCB on  $p_i$  exceeds UCB on  $p_j$  for all  $j \neq i$ .

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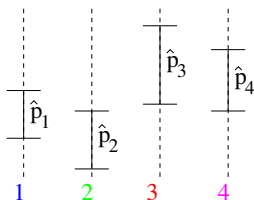


- For each pair of classes  $(i, j)$ , estimate  $q_{ij} = \frac{p_i}{p_i + p_j}$ .
- Stop and declare  $i$  as mode if for all  $j \neq i$ ,  $q_{ij}$  confidently exceeds 0.5.

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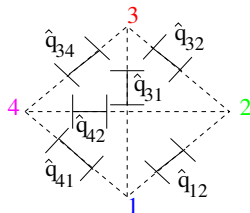
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1-versus-1 appears to waste samples, but ...



# Empirical Comparison: 1vr and 1v1

Sample complexity

Distribution	K	Type	$\mathcal{A}_1$	KL-SN	PPR
$\mathcal{P}_1: .5, .25 \times 2$	3	1vr	$1344 \pm 20$	$418 \pm 14$	$262 \pm 12$
		1v1	$1158 \pm 19$	$346 \pm 13$	<b><math>218 \pm 11</math></b>
$\mathcal{P}_2: .4, .2 \times 3$	4	1vr	$1919 \pm 29$	$632 \pm 18$	$397 \pm 15$
		1v1	$1516 \pm 24$	$468 \pm 15$	<b><math>298 \pm 13</math></b>
$\mathcal{P}_3: .2, .1 \times 8$	9	1vr	$5082 \pm 51$	$1900 \pm 42$	$1201 \pm 29$
		1v1	$3340 \pm 43$	$1138 \pm 31$	<b><math>789 \pm 28</math></b>
$\mathcal{P}_4: .1, .05 \times 18$	19	1vr	$12015 \pm 129$	$4686 \pm 81$	$2850 \pm 55$
		1v1	$7352 \pm 88$	$2554 \pm 57$	<b><math>1840 \pm 53</math></b>
$\mathcal{P}_5: .35, .33, .12, .1 \times 2$	5	1vr	$155277 \pm 2356$	$63739 \pm 2238$	$38001 \pm 1311$
		1v1	$117988 \pm 2078$	$47205 \pm 1291$	<b><math>33660 \pm 1125</math></b>
$\mathcal{P}_6: .35, .33, .04 \times 8$	10	1vr	$158254 \pm 2442$	$66939 \pm 2241$	$41963 \pm 1330$
		1v1	$121150 \pm 2183$	$49576 \pm 1341$	<b><math>36693 \pm 1185</math></b>

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**PPR-1v1:** Stop and declare  $\text{first}(t)$  as mode iff

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- **Computationally light** compared to PPR-1vr, and other KL-divergence-based rules (which have to perform a numerical computation at each step).

# Overview of Talk

1. PAC Formulation
2. Solutions for  $K = 2$  classes
3. Generalising to  $K \geq 2$  classes
4. Theoretical guarantees
5. Summary and outlook



# Asymptotic Optimality

- **Lower bound** [Shah *et al.*, 2020]: Any  $\delta$ -correct algorithm requires at least  $\text{LB}(\mathcal{P}, \delta)$  samples in expectation, where

$$\text{LB}(\mathcal{P}, \delta) \stackrel{\text{def}}{=} \sup_{\mathcal{P}': \text{mode}(\mathcal{P}') \neq \text{mode}(\mathcal{P})} \frac{1}{\text{KL}(\mathcal{P} || \mathcal{P}')} \ln \left( \frac{1}{2.4\delta} \right).$$

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- **PPR-1v1 upper bound**: Let  $\tau(\mathcal{P}, \delta)$  be the expected stopping time of PPR-1v1 on  $\mathcal{P}$  when run with mistake probability  $\delta$ . Then,

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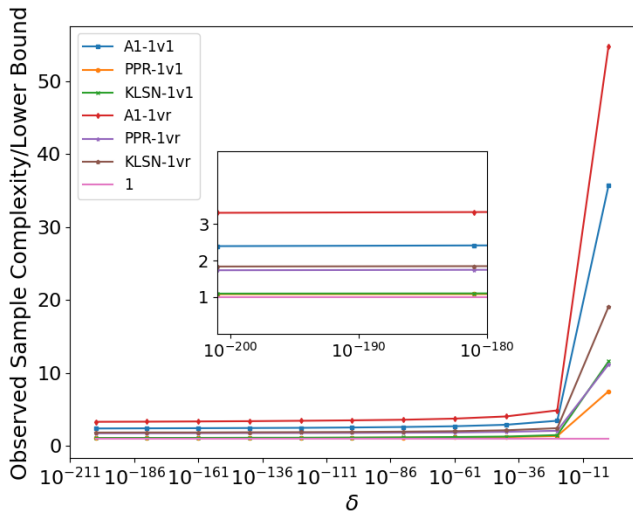
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- Proof uses probability, functions, some results from Garivier and Kaufmann (2016) (who obtain similar result for PAC bandits).

# Asymptotic Optimality (continued)



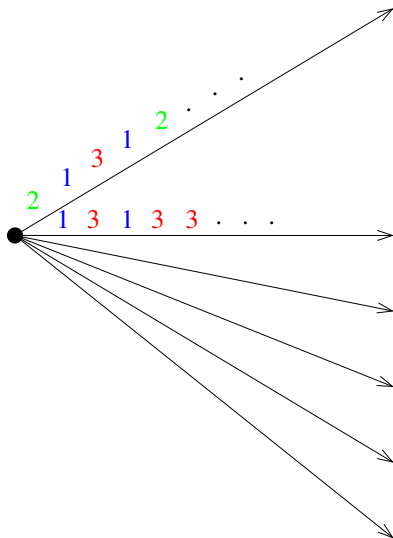
Result from  $\mathcal{P}_3$

# Uniform Domination

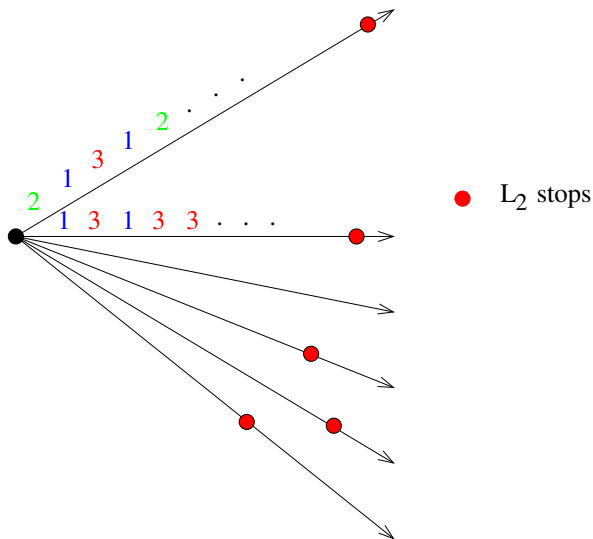
- Let  $X = x^1, x^2, \dots$  be an infinite sequence of samples from  $\mathcal{P}$ .
- For algorithm  $L$ , let  $T(L, X)$  denote the stopping time of  $L$  on  $X$ .
- Define algorithm  $L_1$  to **uniformly dominate** algorithm  $L_2$  if for every sequence  $X$ ,  $\delta \in (0, 1)$ ,

$$T(L_2, X) < \infty \implies T(L_1, X) \leq T(L_2, X).$$

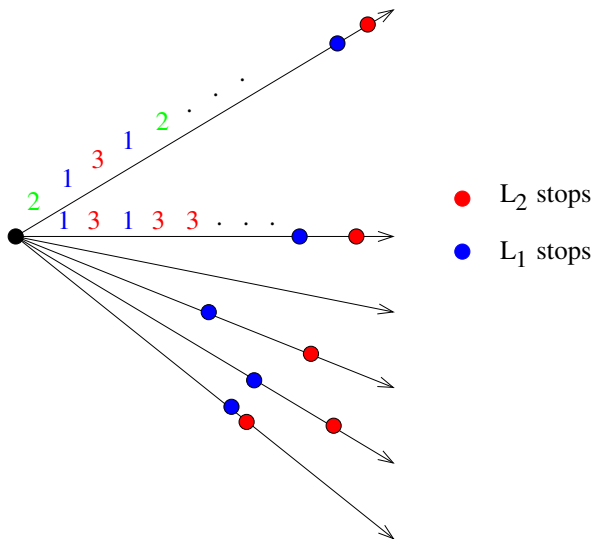
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- These proofs done by showing

$L_2$  terminates on  $X \implies L_1$  terminates on  $X$ .

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# Concluding Notes

- Have addressed **PAC mode estimation** problem.
- **PPR** an elegant approach to handle random stopping time.
- **1v1 outperforms 1vr** to generalise to  $K \geq 2$  classes.
- PPR-1v1 simple, asymptotically optimal, efficient in practice.
- Flexible to apply in practice, validated on two distinct applications.
- Code base released along with AISTATS 2022 paper.
- **Conjecture** on PPR-1v1 termination preceding PPR-1vr termination remains unresolved.
- Can PPR help in bandits, too?
- Do you have a practical application of mode estimation?