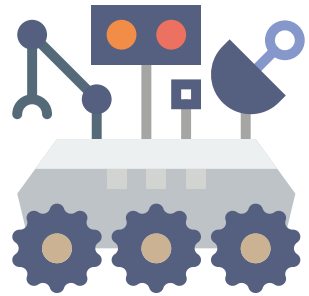
Reinforcement Learning 2021
Guest Lecture on Pure Exploration



Wouter M. Koolen

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- Pure Exploration:
  - PAC Learning
  - Best Arm Identification
  - Minimax Strategies in Noisy Games (Zero-Sum, Extensive Form)

Introduction and Motivation

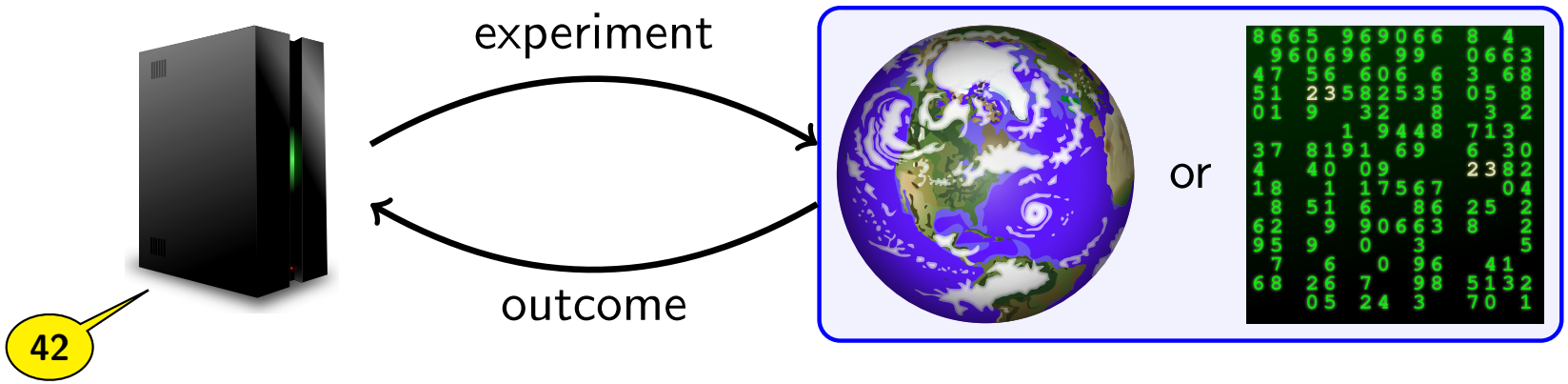
Grand Goal: Interactive Machine Learning

Query:

most effective drug dose?

most appealing website layout?

safest next robot action?



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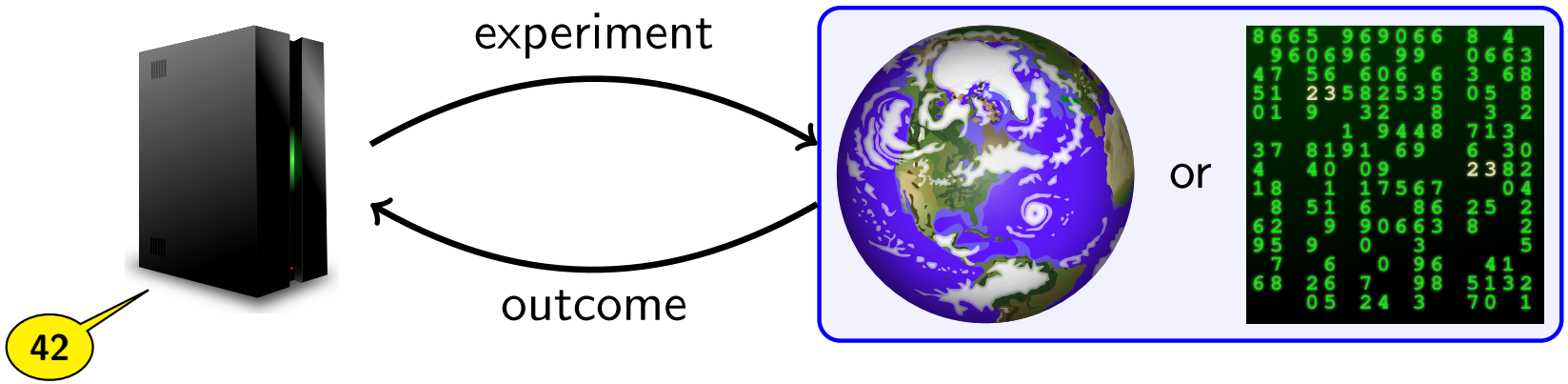

Main scientific questions

- *Efficient* systems
- **Sample complexity** as function of query and environment

Pure Exploration and Reinforcement Learning

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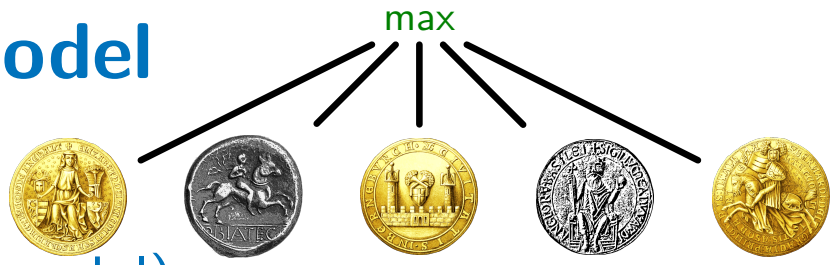
Some problems approached with RL are in fact **better modelled** as pure exploration problems. Most notably MCTS for playing games.

Best Arm Identification

Formal model



Environment (Multi-armed bandit model)

K distributions parameterised by their means $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_K)$.

The *best arm* is

$$i^* = \operatorname*{argmax}_{i \in [K]} \mu_i$$

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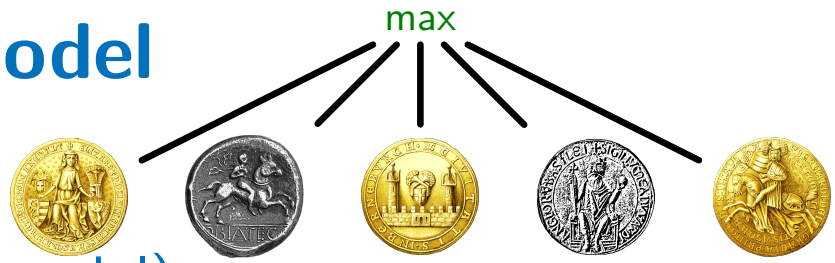

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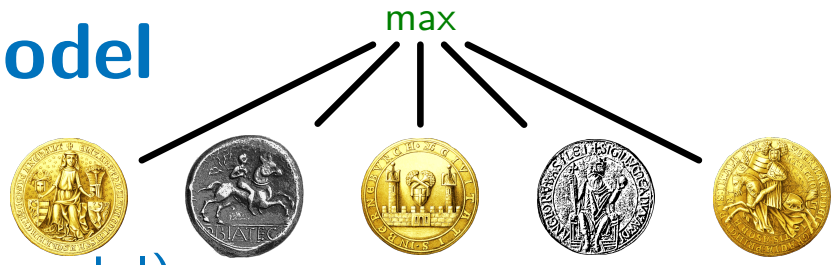
Strategy

- *Stopping rule* $\tau \in \mathbb{N}$
- In round $t \leq \tau$ *sampling rule* picks $I_t \in [K]$. See $X_t \sim \mu_{I_t}$.
- *Recommendation rule* $\hat{I} \in [K]$.

Formal model



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Realisation of interaction: $(I_1, X_1), \ldots, (I_\tau, X_\tau), \hat{I}$.

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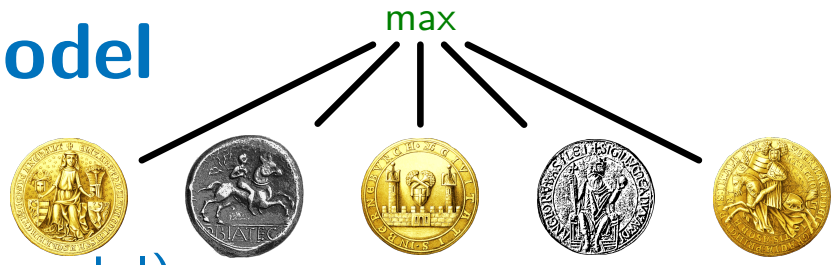

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Realisation of interaction: $(I_1, X_1), \ldots, (I_\tau, X_\tau), \hat{I}$.

Two objectives: *sample efficiency* τ and *correctness* $\hat{I} = i^*$.

Objective

On bandit $\boldsymbol{\mu}$, strategy $(\tau, (I_t)_t, \hat{I})$ has

- *error probability* $\mathbb{P}_{\boldsymbol{\mu}}\big(\hat{I} \neq i^*(\boldsymbol{\mu})\big)$, and
- *sample complexity* $\mathbb{E}_{\boldsymbol{\mu}}[\tau]$.

Idea: constrain one, optimise the other.

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Fix small confidence $\delta \in (0,1)$. A strategy is δ-*correct* (aka δ-*PAC*) if

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(Generalisation: output ϵ-best arm)

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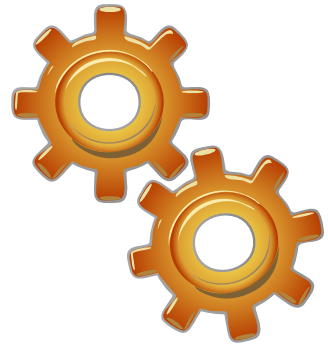
Goal: minimise $\mathbb{E}_{\boldsymbol{\mu}}[\tau]$ over **all δ-correct strategies**.

Algorithms



- Sampling rule I_t?
- Stopping rule τ?
- Recommendation rule $\hat{I}$?

$$\hat{I} = \underset{i \in [K]}{\text{argmax}} \ \hat{\mu}_i(\tau)$$

where $\hat{\boldsymbol{\mu}}(t)$ is *empirical mean*.

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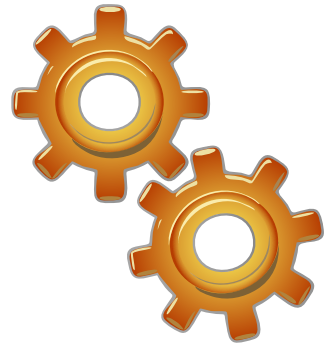

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Approach: start investigating **lower bounds**

Instance-Dependent Sample Complexity Lower bound

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Fix a δ-correct strategy. Then for every bandit model $\boldsymbol{\mu}$

$$\mathop{\mathbb{E}}_{\boldsymbol{\mu}}[\tau] \;\geq\; T^*(\boldsymbol{\mu}) \ln \frac{1}{\delta}$$

where the characteristic time $T^*(\boldsymbol{\mu})$ is given by

$$\frac{1}{T^*(\boldsymbol{\mu})} \;=\; \max_{\boldsymbol{w} \in \triangle_K} \min_{\boldsymbol{\lambda} \in \mathsf{Alt}(\boldsymbol{\mu})} \sum_{i=1}^{K} w_i \, \mathsf{KL}(\mu_i \| \lambda_i).$$

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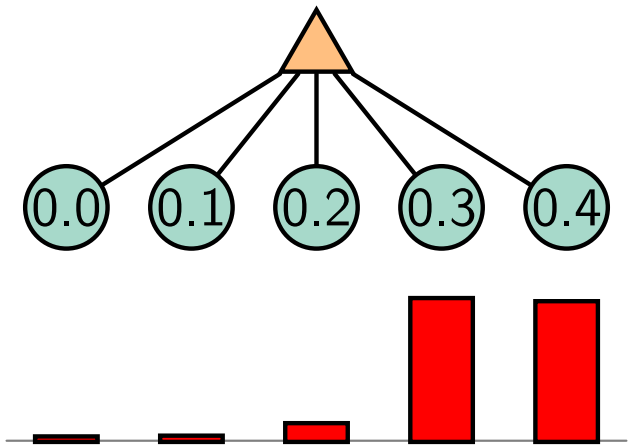
Intuition (going back to Lai and Robbins [1985]): if observations are likely under both $\boldsymbol{\mu}$ and $\boldsymbol{\lambda}$, yet $i^*(\boldsymbol{\mu}) \neq i^*(\boldsymbol{\lambda})$, then learner cannot stop and be correct in both.

Instance-Dependent Sample Complexity Lower bound

Blackboard proof

Example



$K = 5$ arms, Bernoulli $\boldsymbol{\mu} = (0.0, 0.1, 0.2, 0.3, 0.4)$.

$$T^*(\boldsymbol{\mu}) \;=\; 200.4 \qquad \boldsymbol{w}^*(\boldsymbol{\mu}) \;=\; (0.01, 0.02, 0.06, 0.46, 0.45)$$

At $\delta = 0.05$, the time gets multiplied by $\ln \frac{1}{\delta} = 3.0$.

Sampling Rule

Look at the lower bound again. Any good algorithm **must** sample with optimal (*oracle*) proportions

$$\boldsymbol{w}^*(\boldsymbol{\mu}) \;=\; \operatorname*{argmax}_{\boldsymbol{w}\in\triangle_K} \; \min_{\boldsymbol{\lambda}\in \mathsf{Alt}(\boldsymbol{\mu})} \; \sum_{i=1}^{K} w_i \,\mathsf{KL}(\mu_i \| \lambda_i)$$

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Track-and-Stop

Idea: draw $I_t \sim \boldsymbol{w}^*(\hat{\boldsymbol{\mu}}(t-1))$.

- Ensure $\hat{\boldsymbol{\mu}}(t) \to \boldsymbol{\mu}$ hence $N_i(t)/t \to w_i^*$ by "forced exploration"
- Draw arm with $N_i(t)/t$ below w_i^* (tracking)
- Computation of $\boldsymbol{w}^*$ (reduction to 1d line search)

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Definition

Generalized Likelihood Ratio (GLR) measure of evidence

$$\mathrm{GLR}_n(\hat{\imath}) \;:=\; \ln \frac{\sup_{\boldsymbol{\mu}:\hat{\imath}\in i^*(\boldsymbol{\mu})} P\left(X^n|A^n,\boldsymbol{\mu}\right)}{\sup_{\boldsymbol{\lambda}:\hat{\imath}\notin i^*(\boldsymbol{\lambda})} P\left(X^n|A^n,\boldsymbol{\lambda}\right)}$$

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Idea: stop when $\mathrm{GLR}_n(\hat{\imath})$ is big for some answer $\hat{\imath}$.

GLR Stopping

For any plausible answer $\hat{\imath} \in i^*(\hat{\boldsymbol{\mu}}(n))$, the GLR_n simplifies to

$$\mathrm{GLR}_n(\hat{\imath}) \;=\; \inf_{\boldsymbol{\lambda}:\hat{\imath}\notin i^*(\boldsymbol{\lambda})} \sum_{a=1}^{K} N_a(n)\,\mathrm{KL}(\hat{\mu}_a(n), \lambda_a)$$

where $\mathrm{KL}(x, y)$ is the Kullback-Leibler divergence in the exponential family.

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Good **anytime deviation inequalities** exist for that upper bound.

Theorem (Kaufmann and Koolen, 2018)

$$\mathbb{P}\left(\exists n : \boxed{\sum_{a=1}^{K} N_a(n)\,\mathrm{KL}(\hat{\mu}_a(n), \mu_a)} - \sum_{n} \ln\ln N_a(n) \geq C(K,\delta)\right) \leq \delta$$

for $C(K,\delta) \approx \ln\frac{1}{\delta} + K\ln\ln\frac{1}{\delta}$.

All in all

Final result: lower and upper bound meet on **every problem instance**.

Theorem (Garivier and Kaufmann 2016)

For the Track-and-Stop algorithm, for any bandit $\boldsymbol{\mu}$

$$\limsup_{\delta \to 0} \frac{\mathbb{E}_{\boldsymbol{\mu}}[\tau]}{\ln \frac{1}{\delta}} = T^*(\boldsymbol{\mu})$$

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Very similar optimality result for *Top Two Thompson Sampling* by Russo (2016). Here $N_i(t)/t \to w_i^*$ result of posterior sampling.

Problem Variations and Algorithms

Variations

- Prior knowledge about μ
  - Shape constraints: linear, convex, unimodal, etc. bandits
  - Non-parametric (and heavy-tailed) reward distributions (Agrawal, Koolen, and Juneja, 2021)
  - ...
- Questions beyond Best Arm
  - A/B/n testing (Russac et al., 2021)
  - Robust best arm (part 2 today)
  - Thresholding
  - Best VaR, CVaR and other tail risk measures (Agrawal, Koolen, and Juneja, 2021)
  - ...
- Multiple correct answers
  - ϵ-best arm
  - In general (Degenne and Koolen, 2019)
    (Requires a change in lower bound and upper bound)

Lazy Iterative Optimisation of w^*

Instead of computing at every round the plug-in oracle weights

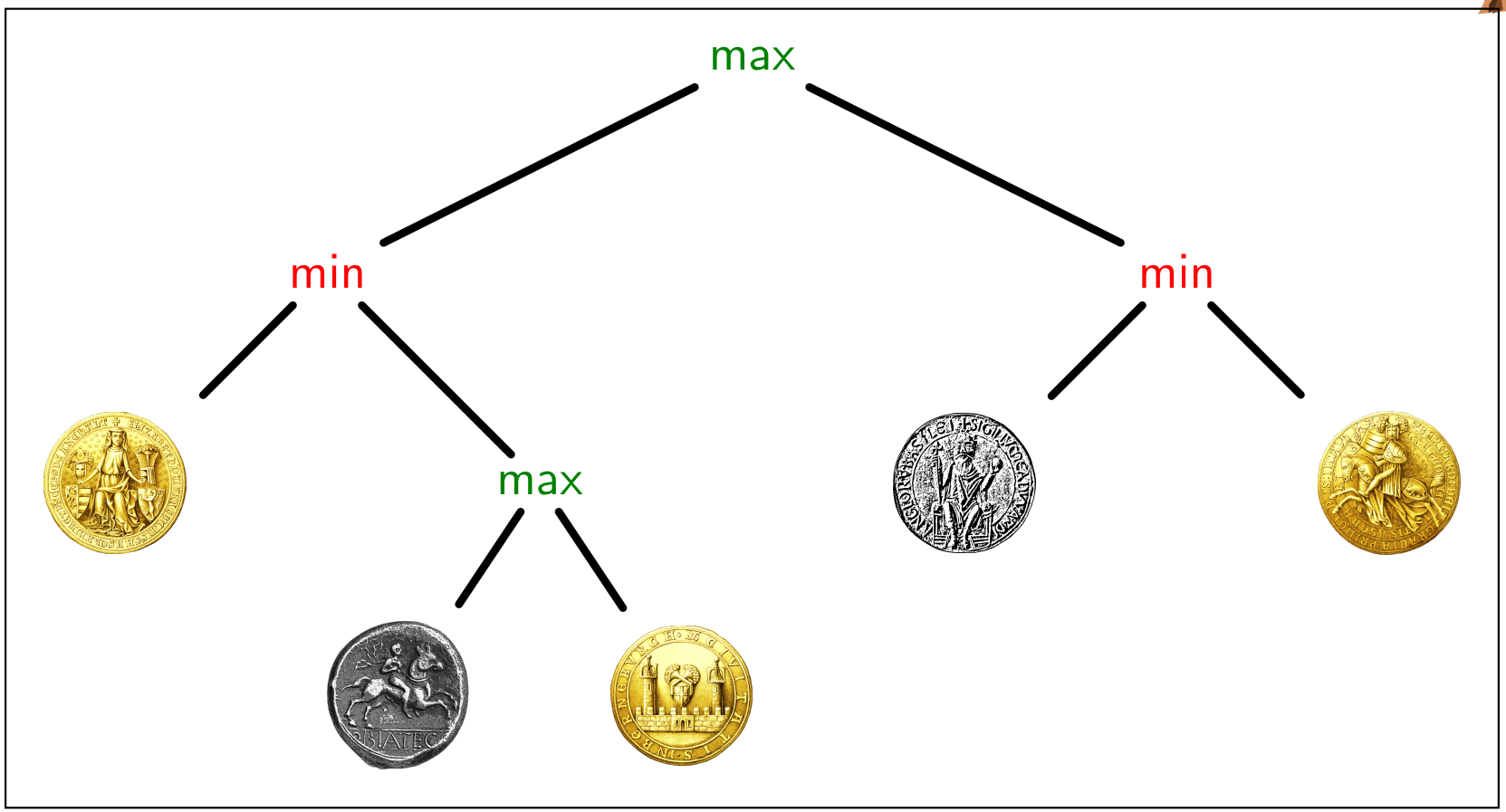
$$\boldsymbol{w}^*(\hat{\boldsymbol{\mu}}) \;=\; \operatorname*{argmax}_{\boldsymbol{w}\in\triangle_K} \underbrace{\min_{\boldsymbol{\lambda}\in \mathrm{Alt}(\hat{\boldsymbol{\mu}})} \sum_{i=1}^{K} w_i \,\mathrm{KL}(\hat{\mu}_i \| \lambda_i)}_{\text{concave in } \boldsymbol{w}}$$

We may work as follows

- The inner problem is concave in $\boldsymbol{w}$.
- It can be maximised iteratively, i.e. with gradient descent.
- We may **interleave sampling** and **gradient** steps.
- A **single** gradient step per sample is enough (Degenne, Koolen, and Ménard, 2019)

Minimax Action Identification

Model (Teraoka, Hatano, and Takimoto, 20



Maximin Action Identification Problem

Find **best move at root** from samples of **leaves**.

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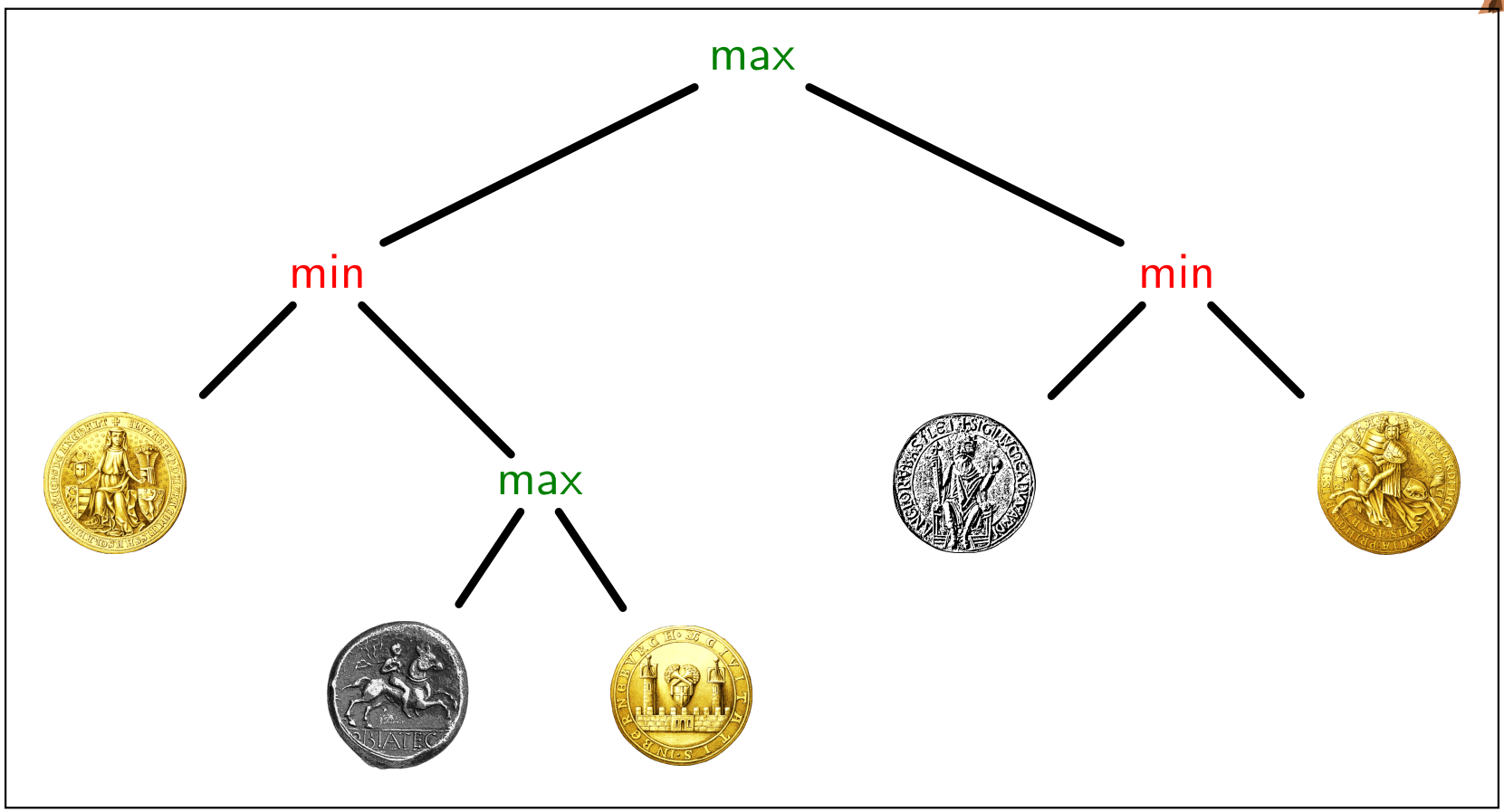

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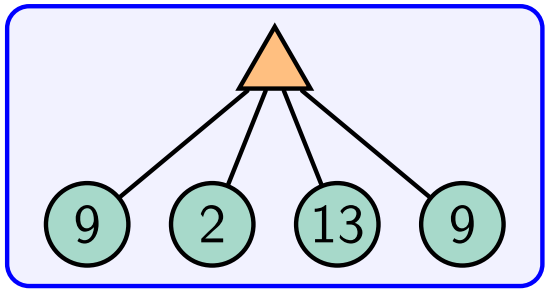
guarantee?

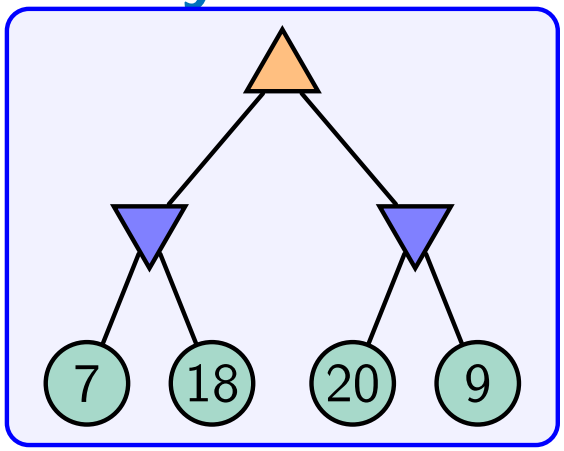
My Brief History



Best Arm Identification

(Garivier and Kaufmann, 2016)

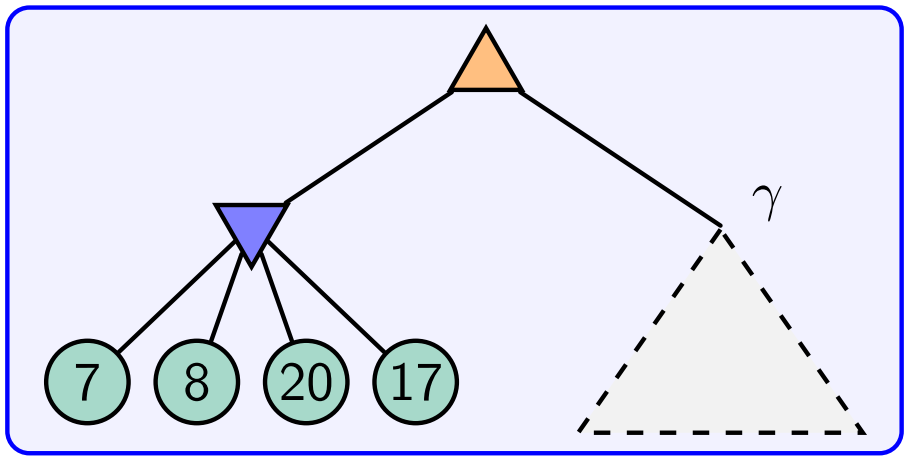
Solved, continuous



Depth 2 Game

(Garivier, Kaufmann, and Koolen, 2016)

Open, continuous?



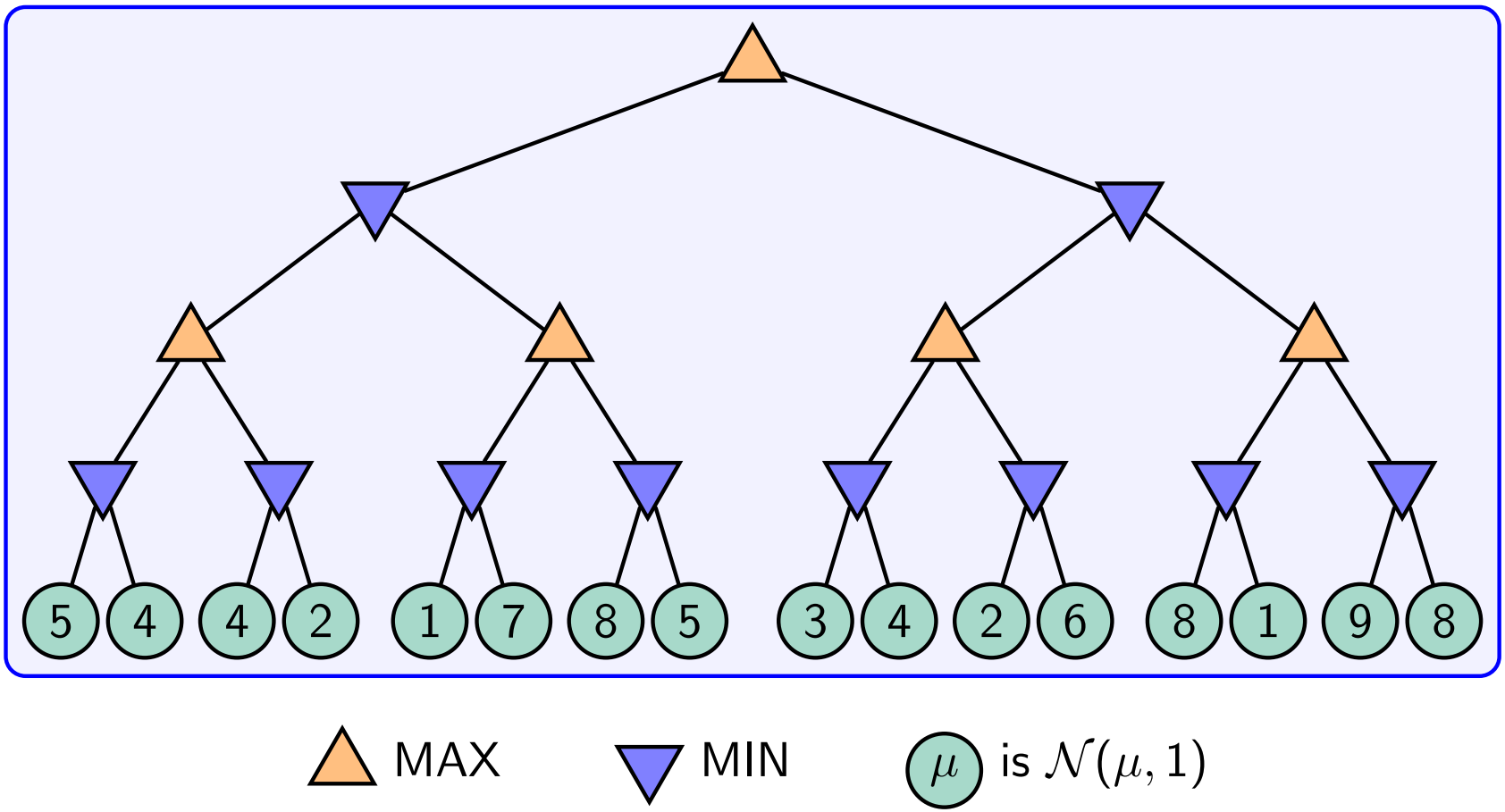
Depth 1.5 Game

(Kaufmann, Koolen, and Garivier, 2018)

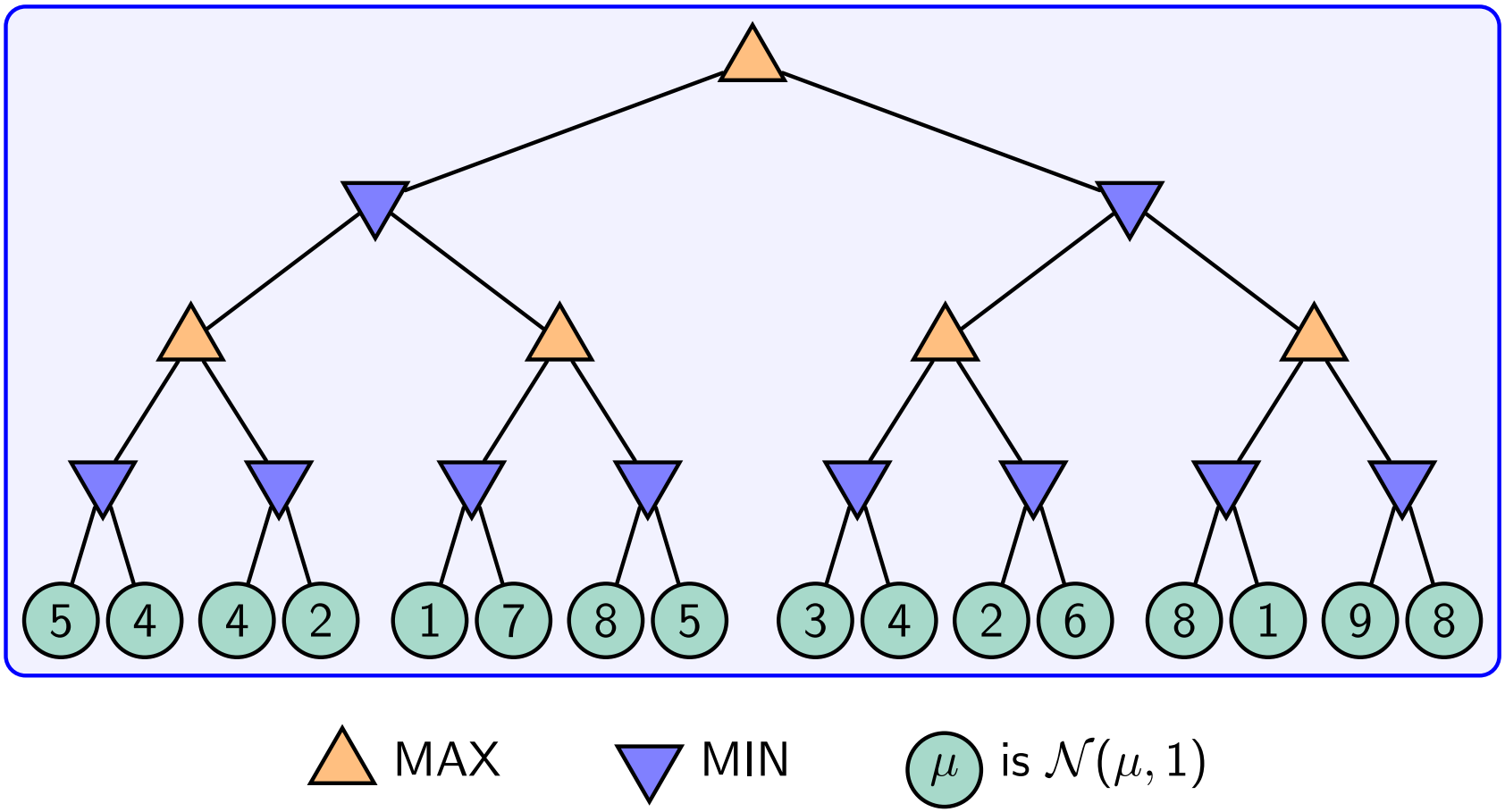
Solved, discontinuous

What we are able to solve today

Noisy games of any depth



Example Backward Induction Computation



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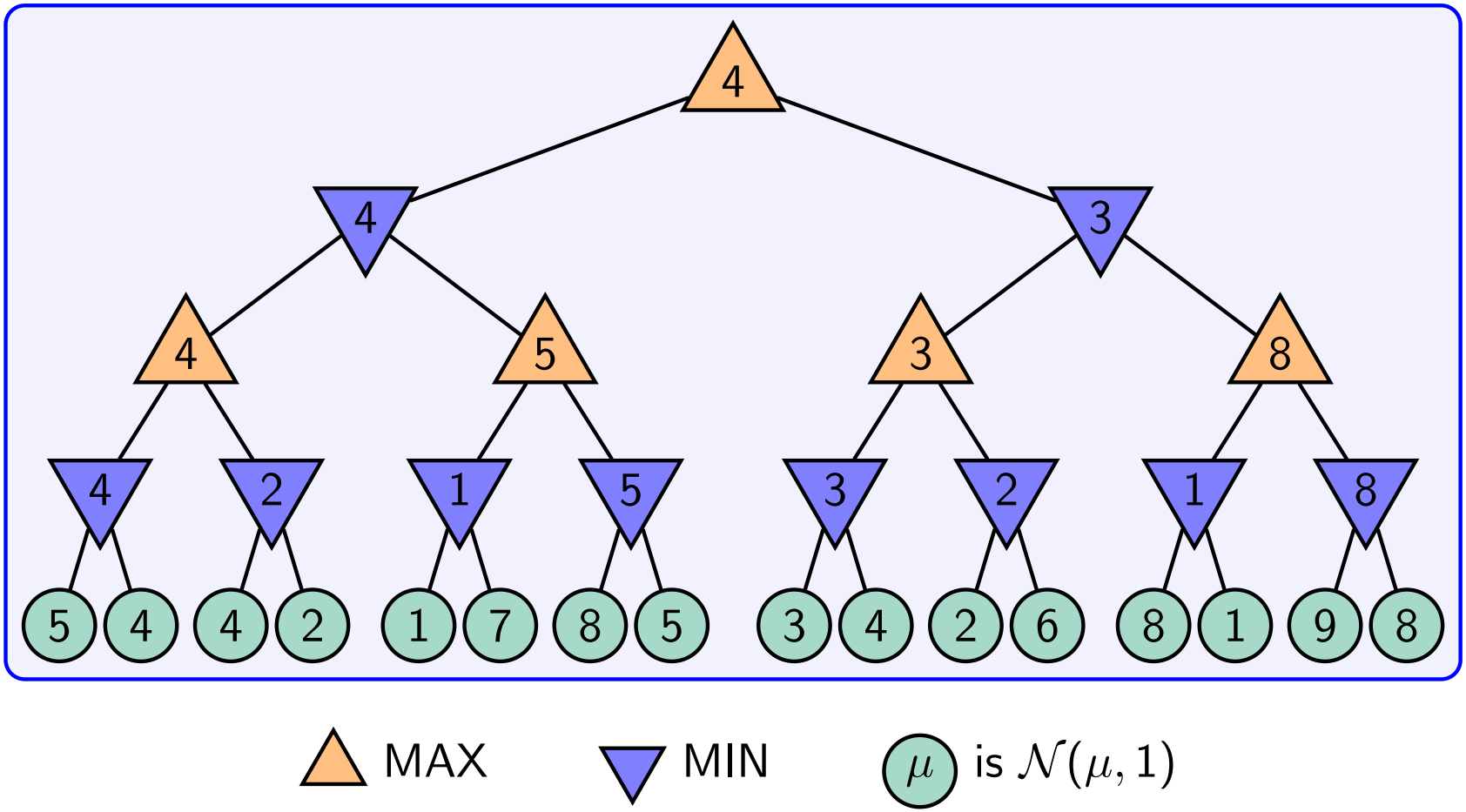

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Learner is δ-PAC if

$$\forall \boldsymbol{\mu} : \mathop{\mathbb{P}}_{\boldsymbol{\mu}} \left(\tau < \infty \wedge \hat{I} \neq i^*(\boldsymbol{\mu}) \right) \leq \delta$$

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$$\mathop{\mathbb{E}}_{\boldsymbol{\mu}}[\tau] \;\geq\; T^*(\boldsymbol{\mu}) \ln \frac{1}{\delta}$$

where the characteristic time $T^*(\boldsymbol{\mu})$ is given by

$$\frac{1}{T^*(\boldsymbol{\mu})} \;=\; \max_{\boldsymbol{w} \in \triangle_K} \min_{\boldsymbol{\lambda} \in \mathsf{Alt}(\boldsymbol{\mu})} \sum_{i=1}^{K} w_i \, \mathsf{KL}(\mu_i \| \lambda_i).$$

Main Theorem II: Algorithm

Idea is still to consider the oracle weight map

$$\boldsymbol{w}^*(\boldsymbol{\mu}) \coloneqq \operatorname*{argmax}_{\boldsymbol{w}\in\triangle_K} \min_{\boldsymbol{\lambda}\in\mathsf{Alt}(\boldsymbol{\mu})} \sum_{i=1}^{K} w_i \,\mathsf{KL}(\mu_i\|\lambda_i)$$

and track the plug-in estimate: $L_t \sim \boldsymbol{w}^*(\hat{\boldsymbol{\mu}}(t-1))$.

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But $\boldsymbol{w}^*$ is **not continuous**. Even at depth "1.5" with 2 arms.

Main Theorem II: Algorithm

Idea is still to consider the oracle weight map

$$w^*(\mu) := \operatorname*{argmax}_{w \in \triangle_K} \min_{\lambda \in \mathrm{Alt}(\mu)} \sum_{i=1}^{K} w_i \, \mathrm{KL}(\mu_i \| \lambda_i)$$

and track the plug-in estimate: $L_t \sim w^*(\hat{\mu}(t-1))$.

But what about **continuity**? Does $\hat{\mu}(t) \to \mu$ imply $w^*(\mu(t)) \to w^*(\mu)$?

But w^* is **not continuous**. Even at depth "1.5" with 2 arms.

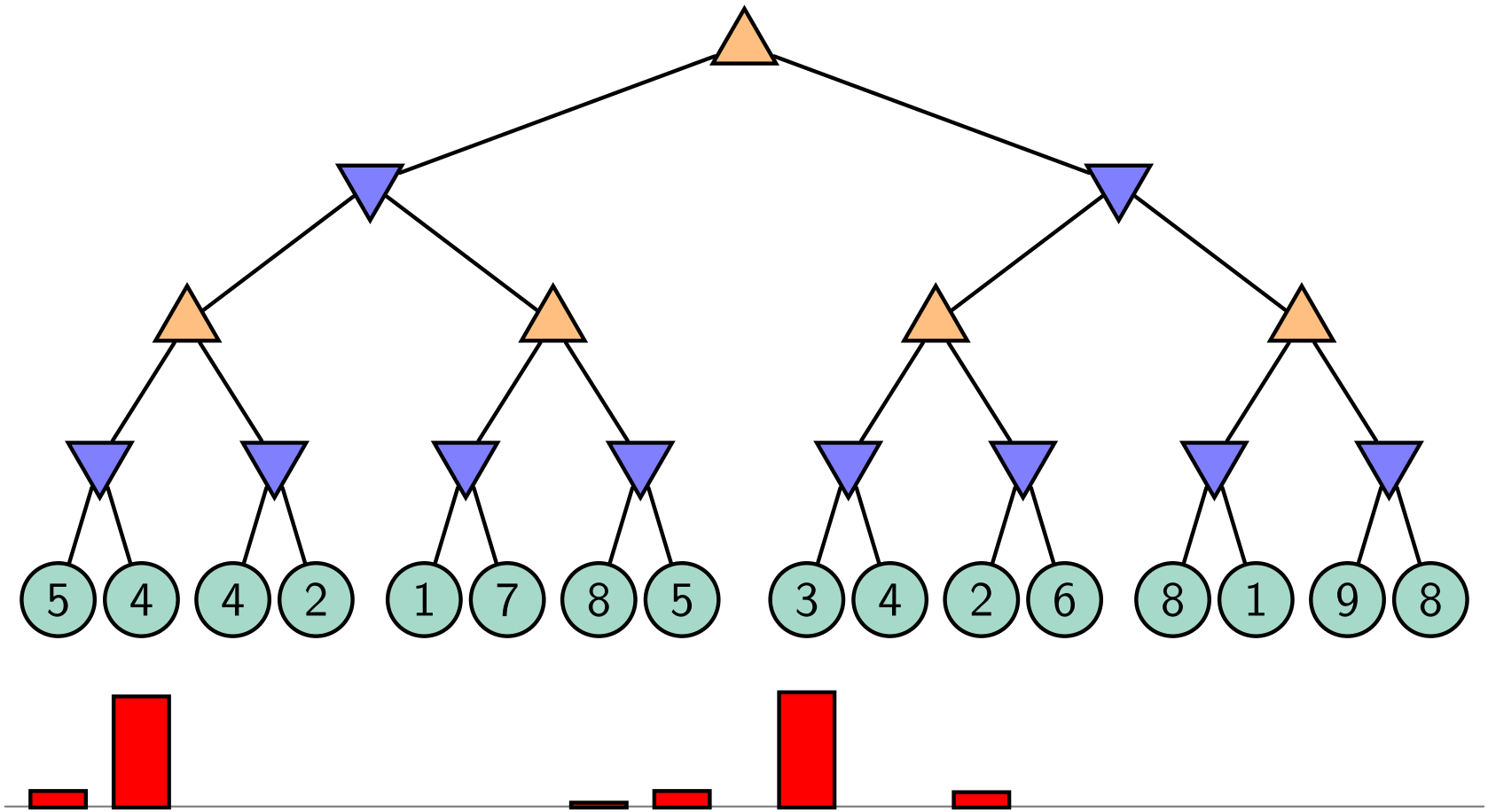
Theorem (Degenne and Koolen, 2019)

Take set-valued interpretation of argmax *defining* w^*. *Then* $\mu \mapsto w^*(\mu)$ *is upper-hemicontinuous and convex-valued. Suitable tracking ensures that as* $\hat{\mu}(t) \to \mu$, *any* $w_t \in w^*(\hat{\mu}(t-1))$ *have*

$$\min_{w \in w^*(\mu)} \|w_t - w\|_\infty \to 0$$

Track-and-Stop is asymptotically optimal.

Example



On Computation

To compute a gradient (in $\boldsymbol{w}$) we need to differentiate

$$\boldsymbol{w} \;\mapsto\; \min_{\boldsymbol{\lambda} \in \mathrm{Alt}(\boldsymbol{\mu})} \; \sum_{i=1}^{K} w_i \, \mathrm{KL}(\mu_i \| \lambda_i)$$

An optimal $\boldsymbol{\lambda} \in \mathrm{Alt}(\boldsymbol{\mu})$ can be found by binary search for common value plus tree reasoning in $O(|\mathcal{L}|)$ (board).

Conclusion

Conclusion

This concludes the guest lecture.

- It has been a pleasure
- Good luck for the exam
- If you have an idea that you want to work on ...

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