Exploration-Exploitation Tradeoffs: a Gentle Introduction

Nicolas Gast

Inria

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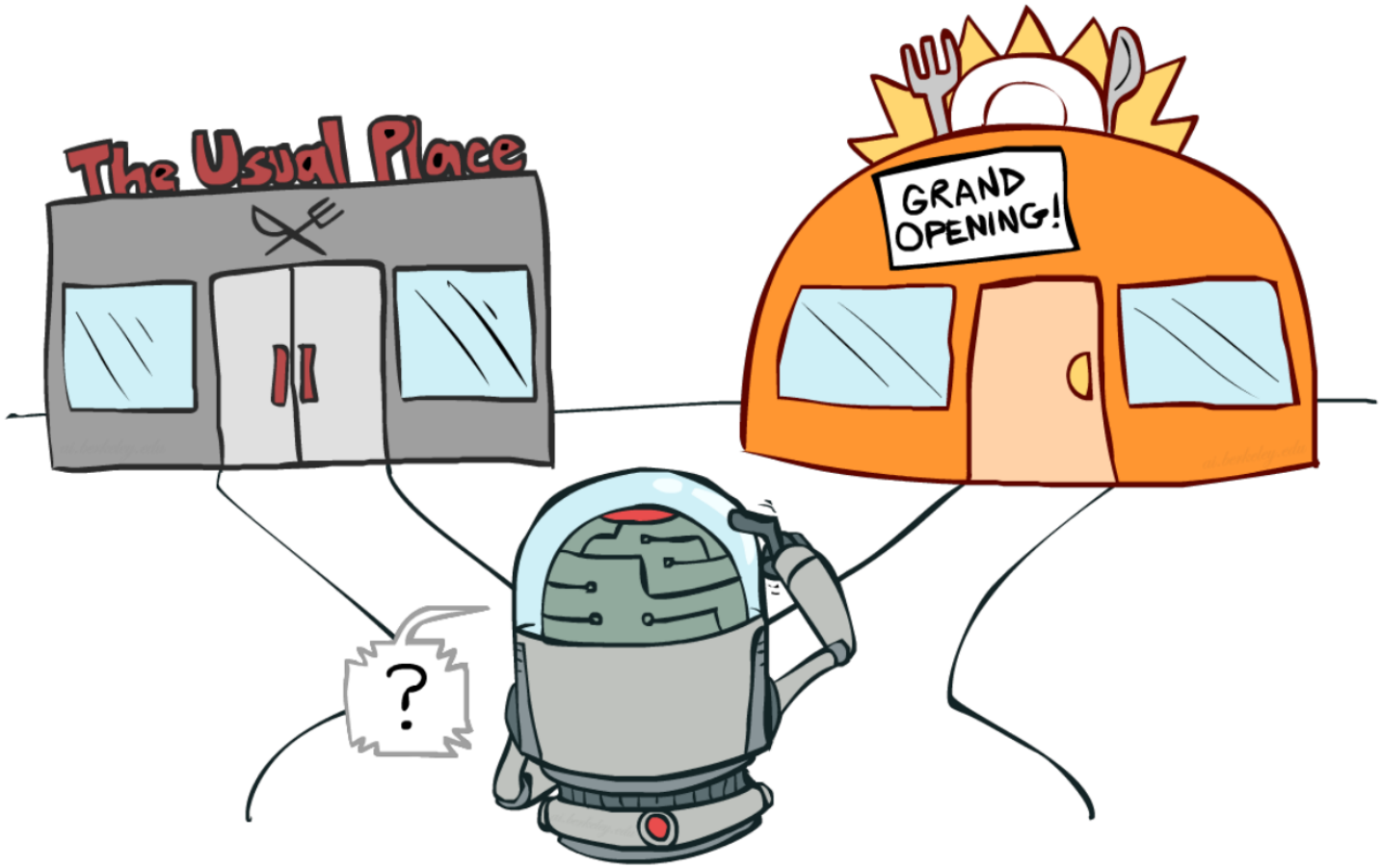
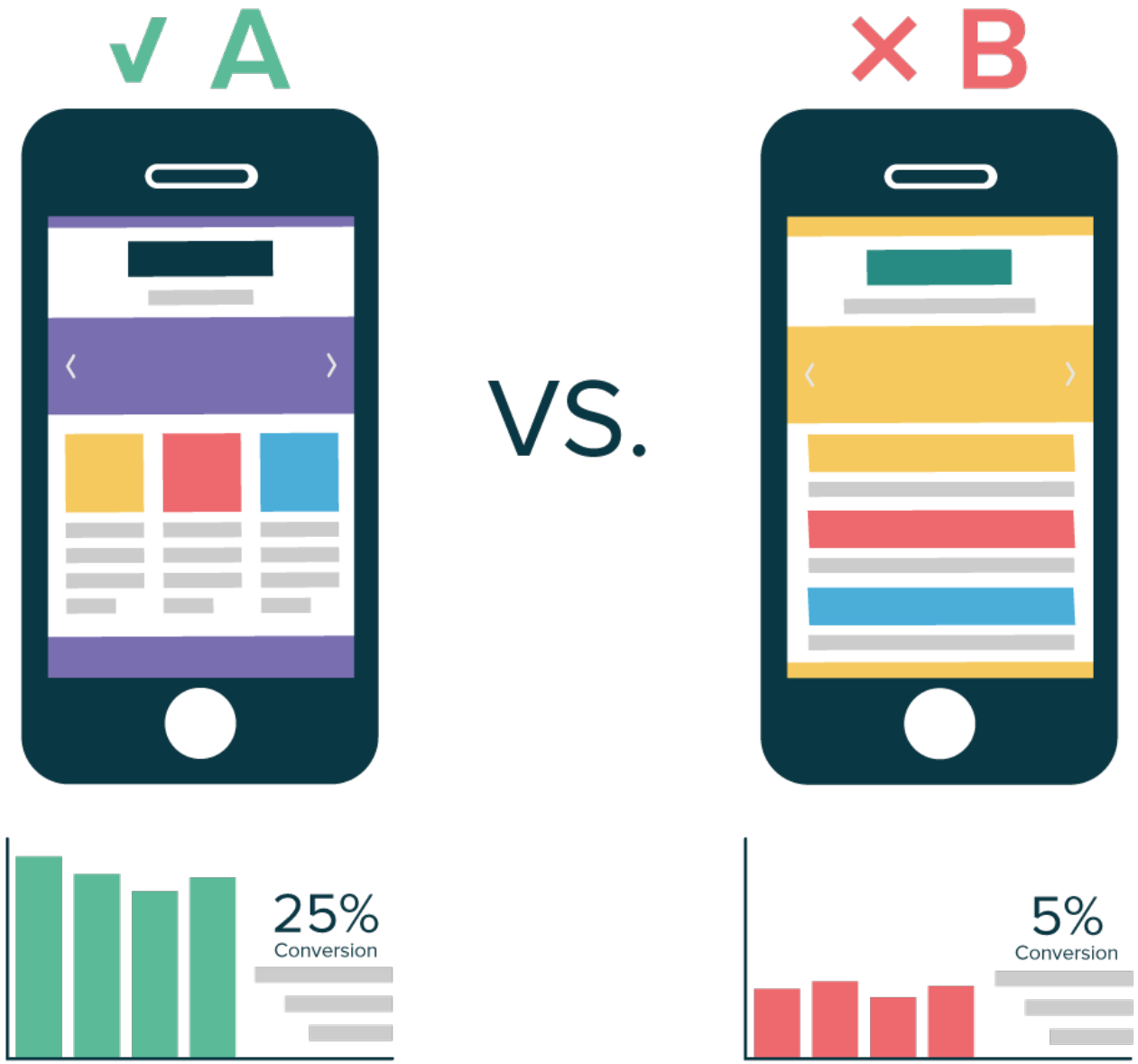
The exploration-exploitation dilemma



Example: AB-testing



How to decide when and what to explore?

We need models

- To think of the tradeoff.
- To design new algorithms.

Outline

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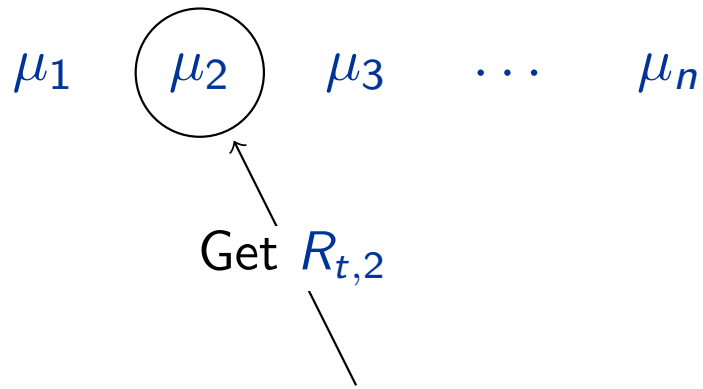
The Bernoulli multi-armed bandit

At each time step, you make a choice $A_t \in \{1 \dots n\}$.



The average reward of a is $\mathbb{E}[R_{t,a}] = \mu_a$ but you do not know the μ_as.

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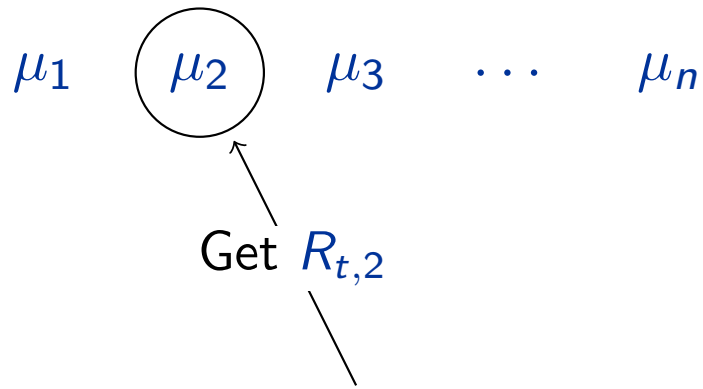

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Assumption: The rewards are independent and Bernoulli.

This is called stochastic Bernoulli bandit.

Motivation

- **Maximize clicks**, e.g., the choice of a title of a news article :

Title	Click proba.
"Murder victim found in adult entertainment venue"	μ_1
"Headless Body found in Topless Bar"	μ_2

  - Choose which title to display. Observe (click or no click).

This is close to **A-B testing**.

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- **Clinical trial**

μ_1 μ_2 μ_3 μ_4




  - Choose treatment A_t for patient t. Observe healed / not healed.

Our metric is the regret

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We define the regret of a sequence of action $\mathcal{A} = (A_1, A_2 \dots)$ as

$$\text{Regret}(\mathcal{A}, T) = \underbrace{(T \max_a \mu_a)}_{\text{reward of an oracle}} - \underbrace{\mathbb{E}\left[\sum_{t=1}^{T} R_{t,A_t}\right]}_{\text{your reward}}.$$

- Goal : design strategies that have a small regret (regardless of μ).

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$$A_{t+1} = \underset{a \in \{1 \dots n\}}{\arg\max}\, \hat{\mu}_a(t)$$

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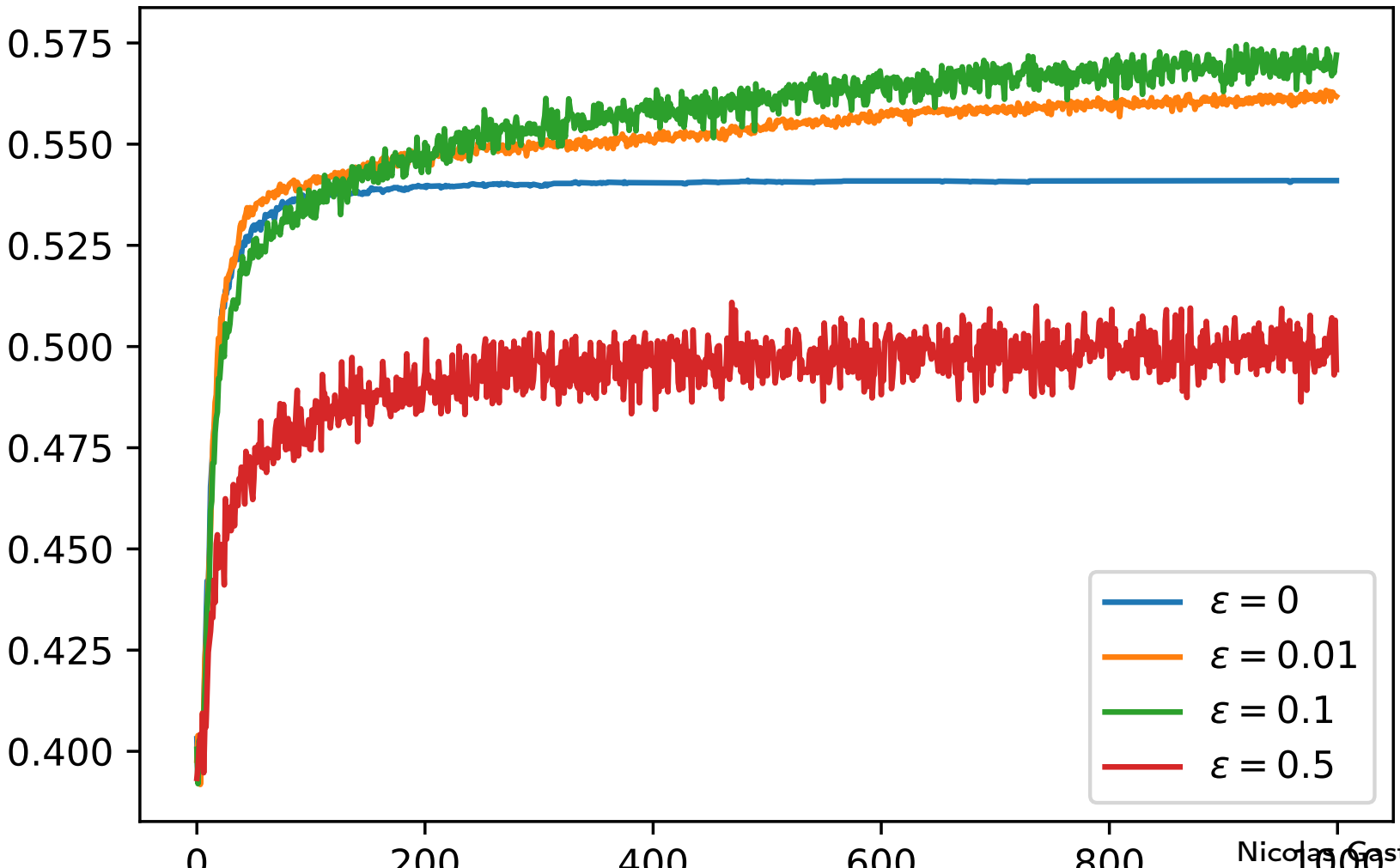
ε-greedy : Smaller or larger ϵ are not necessarily better

$$\text{Regret}(\varepsilon\text{-greedy}, T) = T(\sum_{a=1}^{n}(\mu_* - \mu_a))\frac{\varepsilon}{n} + o(T) \text{ if } \varepsilon > 0.$$



Asymptotically optimal regret

ε-greedy policies have $O(T)$ **regret** (this is called linear regret).

Can we do better?

[1] Meaning Regret$(\mathcal{I}, T) = o(T^{\alpha})$ for all μ and α.

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Theorem (Lai and Robbins, 1985. (Asymptotically Efficient Adaptive Allocation Rules))
There exists a constant c (that depends on μ) such that any uniformly efficient[1] *strategy satisfies :*

$$Regret(\mathcal{A}, T) \geq c \log T$$

[1] Meaning $\text{Regret}(\mathcal{I}, T) = o(T^{\alpha})$ for all μ and α.

UCB builds on Confidence Intervals

Consider a coin that gives "Head" with probability μ. Suppose that you draw a coin N times and observe K times "head". The natural estimator of μ is:

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Hoeffding inequality gives us

$$\mathbb{P}\left(\hat{\mu} - \sqrt{\frac{\alpha}{2N}} \leq \underbrace{\mu}_{\text{real } \mu} \leq \underbrace{\hat{\mu} + \sqrt{\frac{\alpha}{2N}})}_{\text{upper confidence bound}} \right) \geq 1 - 2e^{-\alpha}.$$

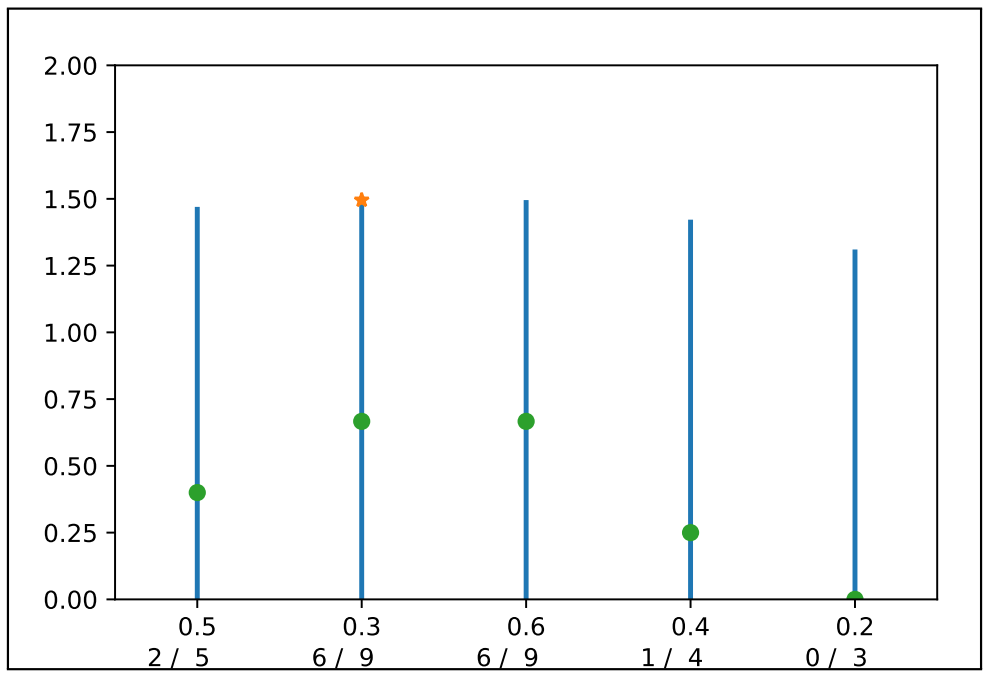
The idea of UCB is to use the above bound with a growing α.

The UCB algorithm

UCB computes a confidence bound $UCB_a(t)$ such that $\mu_a(t) \leq UCB_a(t)$ with high probability. Example : $UCB1$ [Auer et al. 02] uses

$$UCB_a(t) = \hat{\mu}_a(t) + \sqrt{\frac{\alpha \log t}{2N_a(t)}}.$$

- Choose $A_{t+1} \in \arg\max_{a \in \{1 \dots n\}} UCB_a(t)$ (optimism principle).



UCB has logarithmic regret

Theorem. $Regret(UCB) \leq c \log(T)$.

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Idea of optimism. Let $\tilde{\mu}_a = \hat{\mu}_{t,a} + bonus_{t,a}$. Note that $\tilde{\mu}_{A_t} = \max_a \tilde{\mu}_a$.

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$$
\begin{aligned}
Regret &= \sum_t \max_a \mu_a - \mu_{A_t} \\
&= \sum_t \underbrace{\max_a \mu_a - \max_a \tilde{\mu}_a}_{\text{Optimism}} + \underbrace{\tilde{\mu}_{A_t} - \mu_{A_t}}_{\text{Concentration.}}
\end{aligned}
$$

≤ 0 if bonus large.

small if bonus small.

More on regret

- Bayesian approach (Thompson sampling 1933, analyzed in Kauffman et al 2012)
- What about MDPs?
  - UCRL2, UCBVI,... (see next slide)
- Adversarial aspects, games (see second part of the course)

Can we use optimism for MDPs?

Observe the empirical means $\hat{R}(s,a)$ and $\hat{P}(s' \mid s,a)$.

What bonus should one use?

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Observe the empirical means $\hat{R}(s,a)$ and $\hat{P}(s' \mid s,a)$.

What bonus should one use?

- UCRL2 (Jaksch 2010) or variant: use bonus on R and P. Let $\delta(s,a) = C\sqrt{t/N_t(s,a)}$ where $N_t(s,a)$ is the number of time that you took action a in state s before time t.

$$\mathcal{R} = \{\text{vector } r \text{ such that for all } s,a\text{: } |r(s,a) - \hat{r}(s,a)| \leq \delta(s,a)\}$$

$$\mathcal{P} = \{\text{trans. matrix } P \text{ s.t. for all } s,a,a' \left|P(s,a,a') - \hat{P}(s,a,a')\right| \leq \delta(s,a)$$

Optimism:

  - Apply π that maximizes $V^{\pi}_{r,P\in\mathcal{R},\mathcal{P}}$ (by using extended value iteration) and re-update the policy periodically.

Outline

Tree search

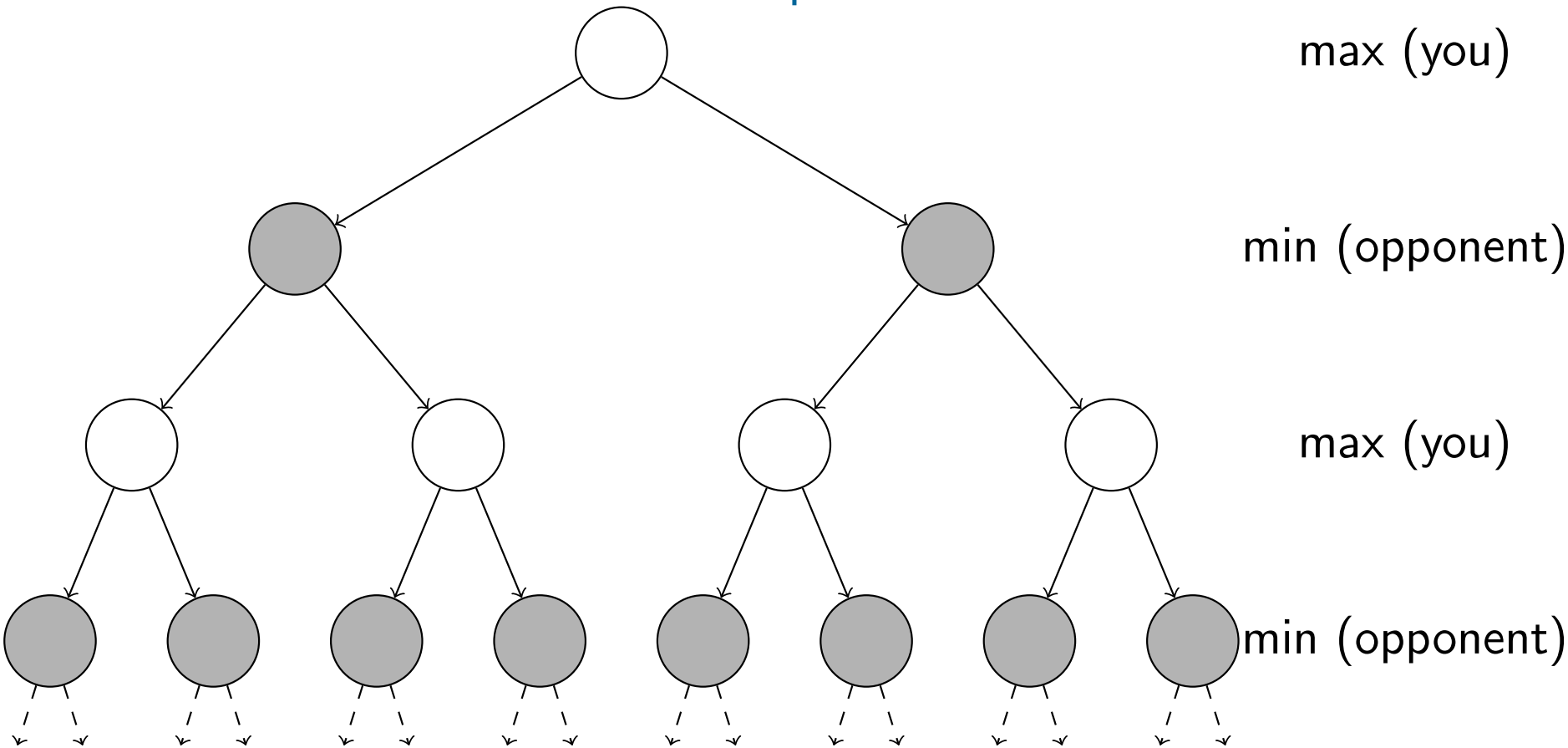
For turn-based two players zero sum games

From a given position, takes the best decision.

- Generate a tree of possibilities.
- Explore this tree.

What if the tree is too big?

You can construct the tree of possibilities



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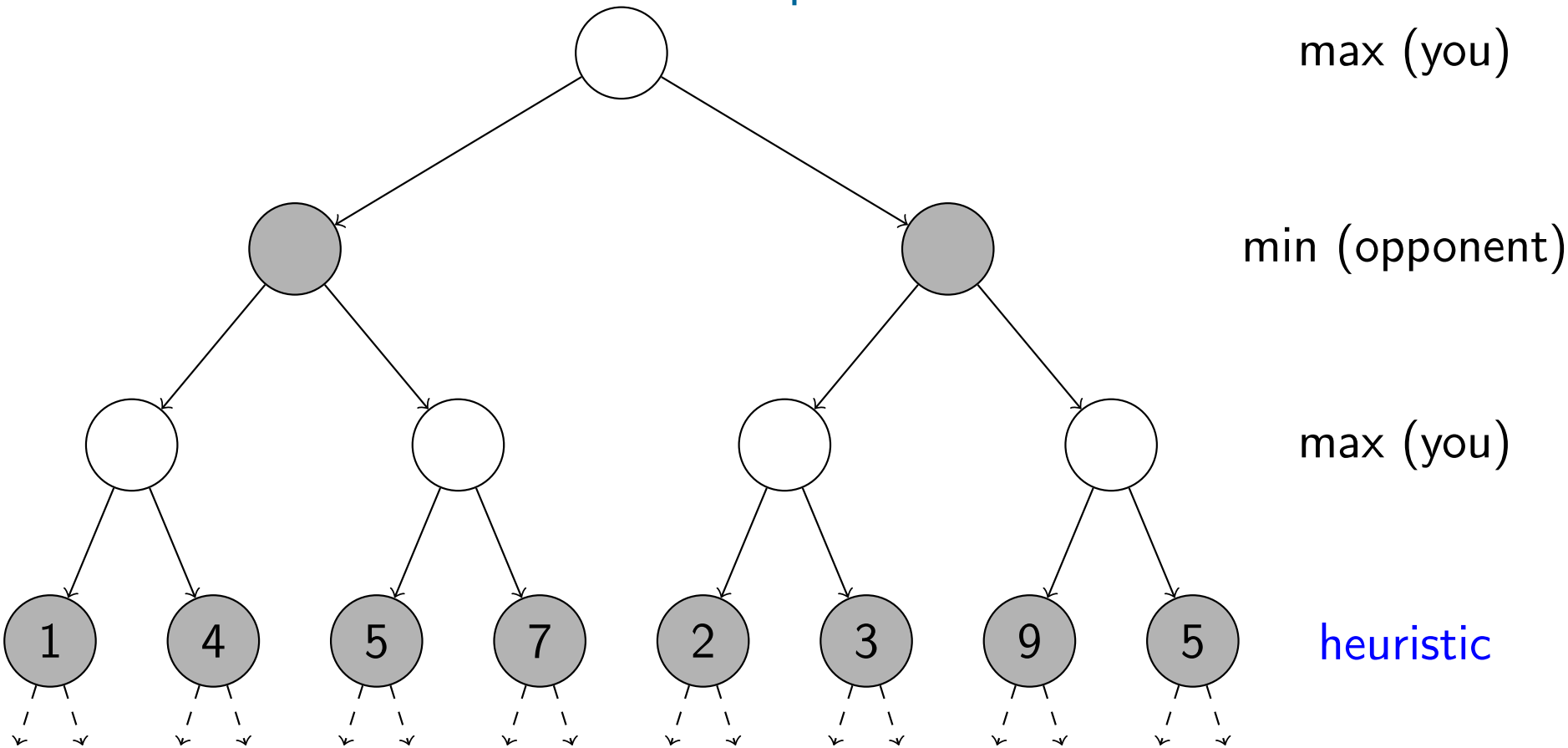

If the tree is too big, you stop at depth D and use a heuristic.

- You can backtrack with the min-max algorithm.

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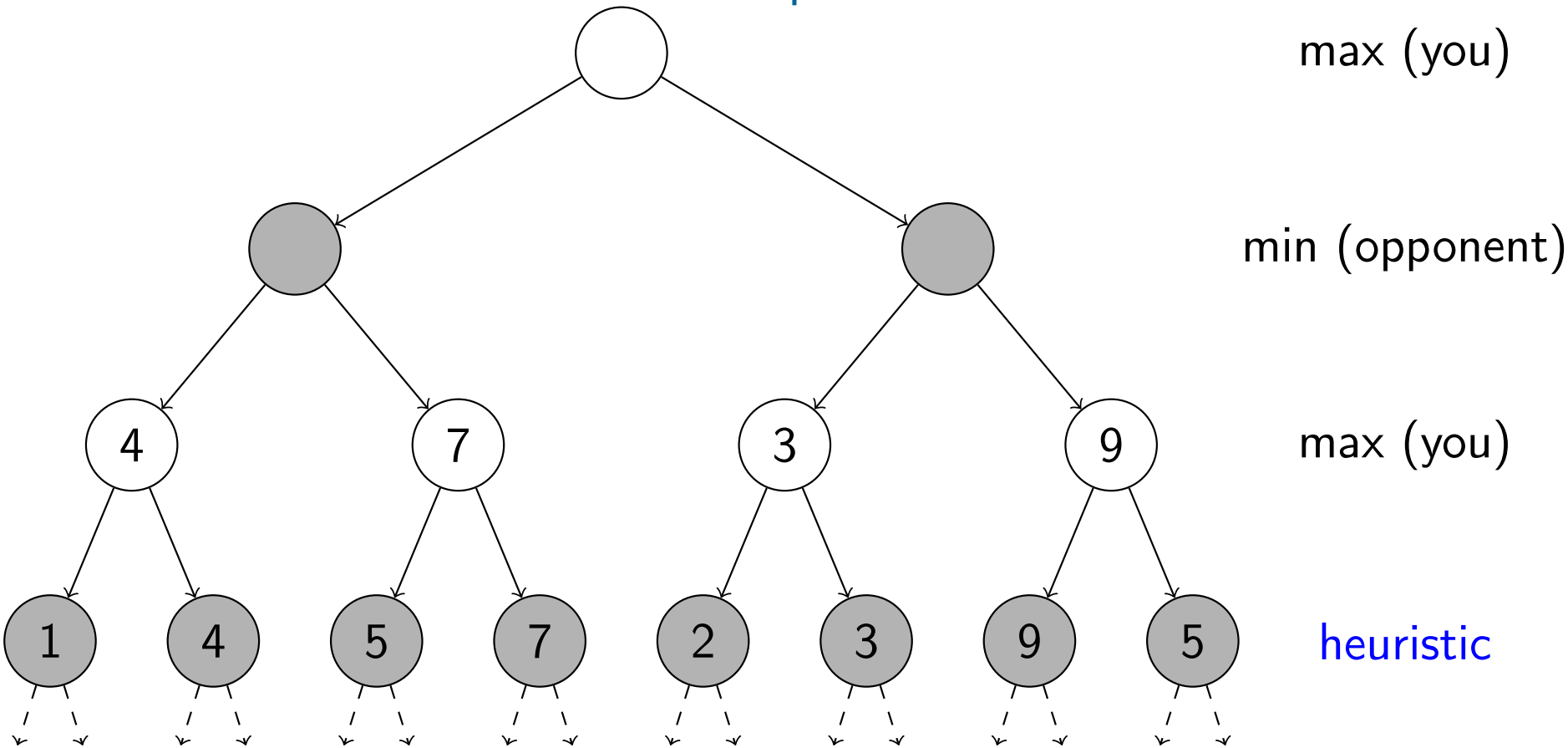

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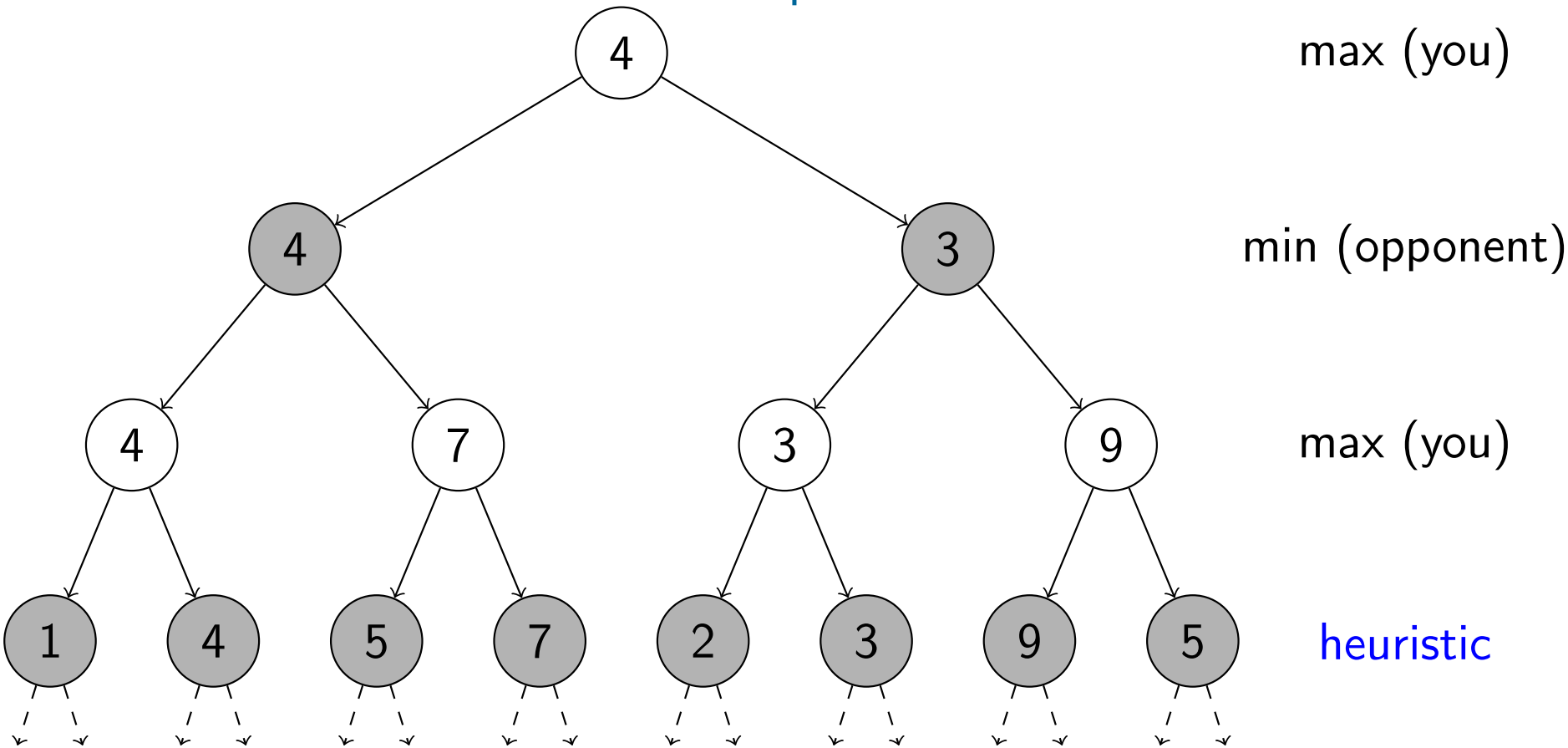

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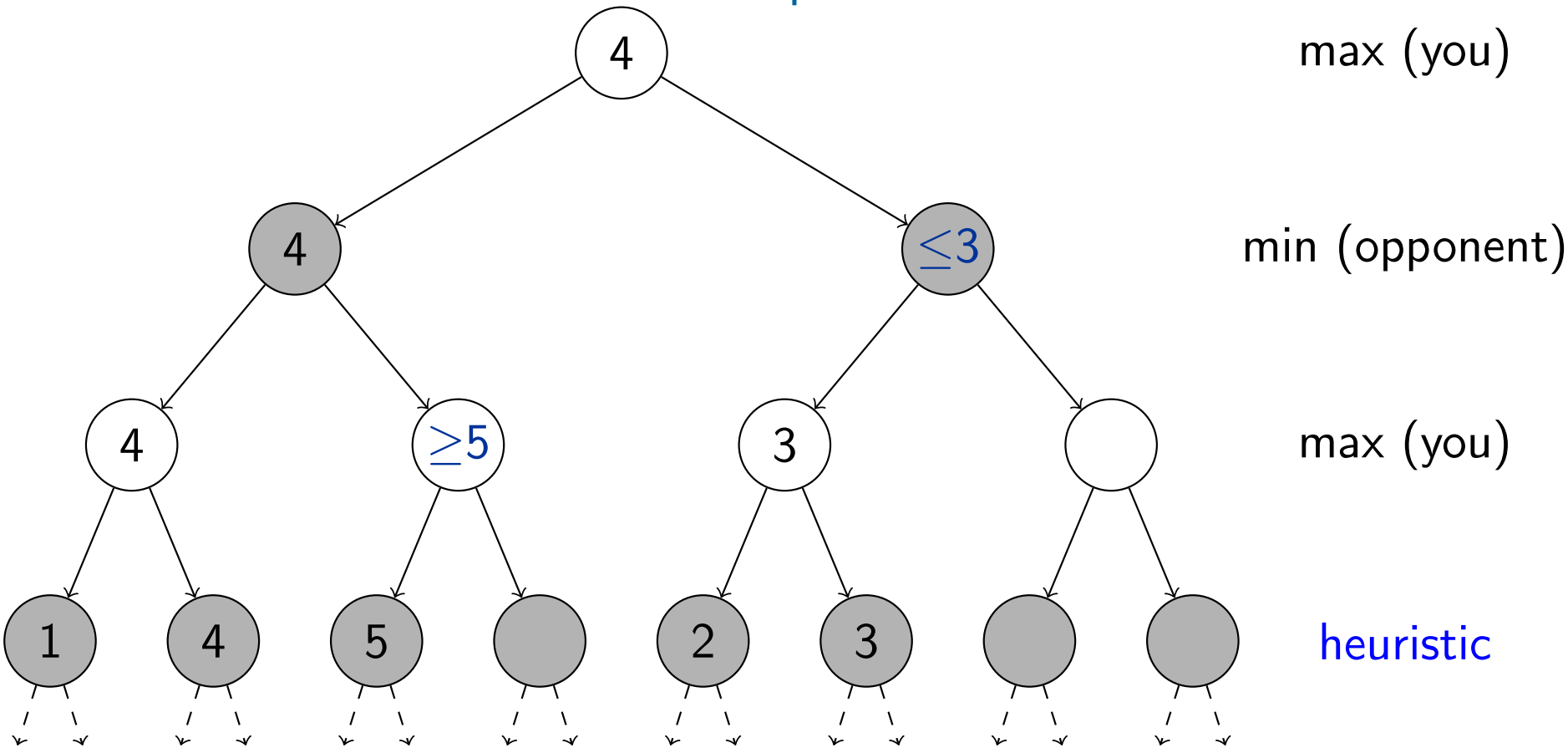

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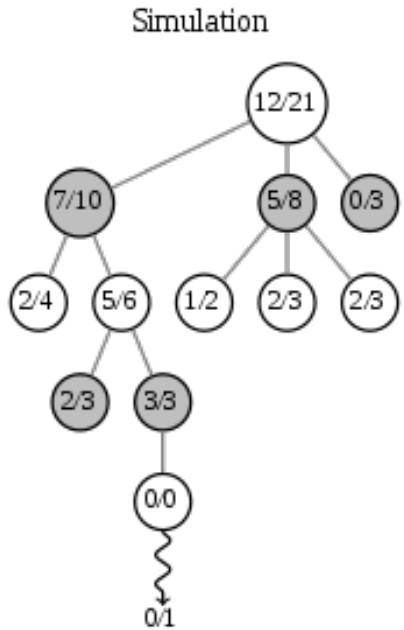
- You can backtrack with the min-max algorithm.
- For optimization, you can use alpha-beta pruning.

Min-max and alpha-beta perform well (ex: Chess)...

...but can be limited (ex: go)

- Tree can still be very big (A^D)
- You need a good heuristic.
  - Result is only available at the end
- You might want to avoid the exploration of not promising parts.
  - For that you need a good heuristic.

MCTS (Monte Carlo Tree Search) uses simulation to conduct the tree search



- Simulate many games and compute how many were won.
- Explore carefully which actions were best.

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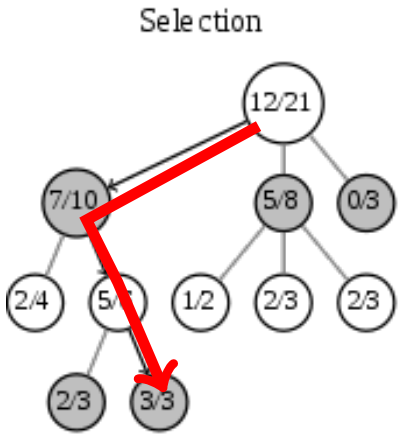

For each child, let $S(c)$ be the number of success and $N(c)$ be the number of time you played c, and $t = \sum_{c'} N(c')$.

- Explore $\arg\max_c \frac{S(c)}{N(c)} + 2\sqrt{\frac{\log t}{N(c)}}$.

Open question: no guarantee with $\sqrt{\log t / N(c)}$. Is $\sqrt{t}/N(c)$ better?

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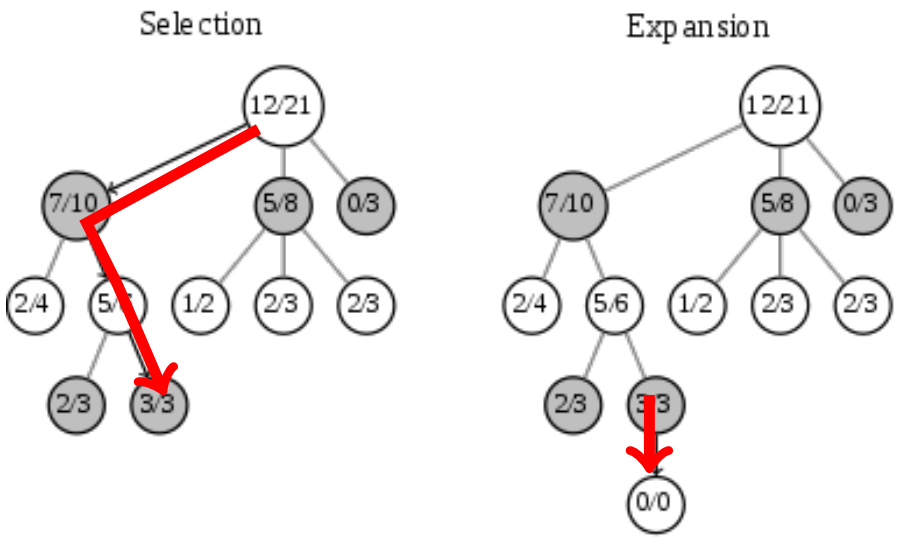

- Create one or multiple children of the leaf.

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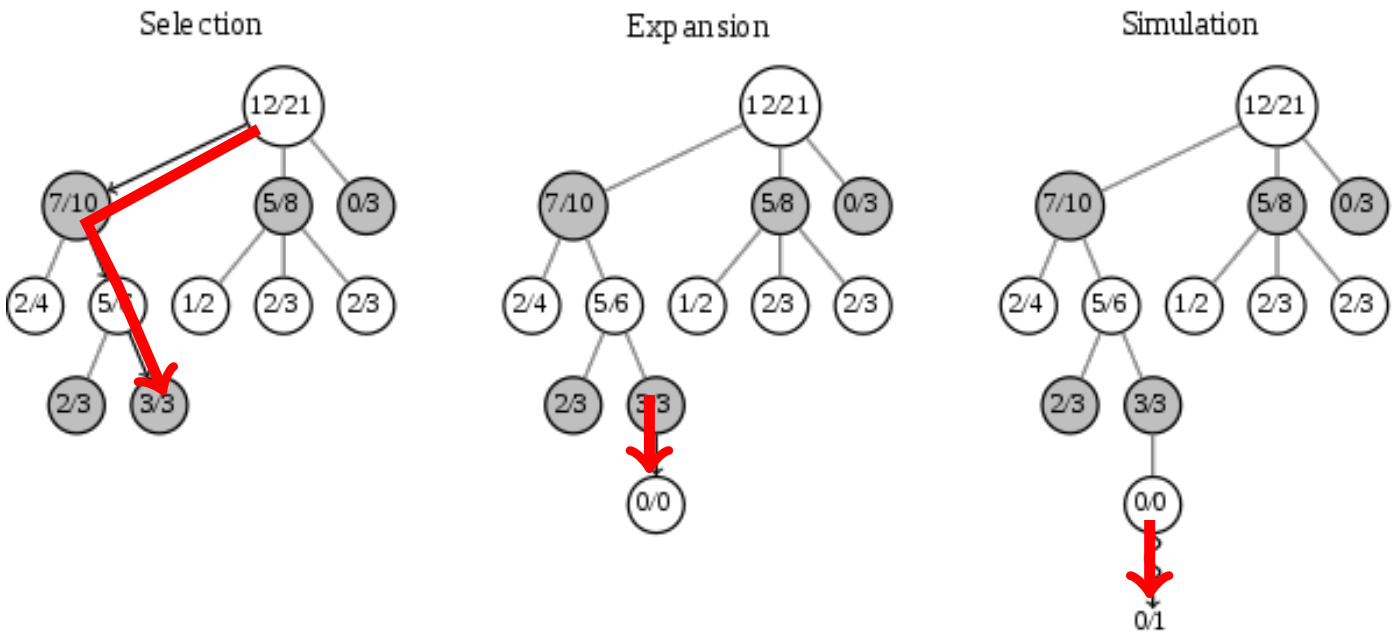

- Obtain a value of the node (e.g. rollout)

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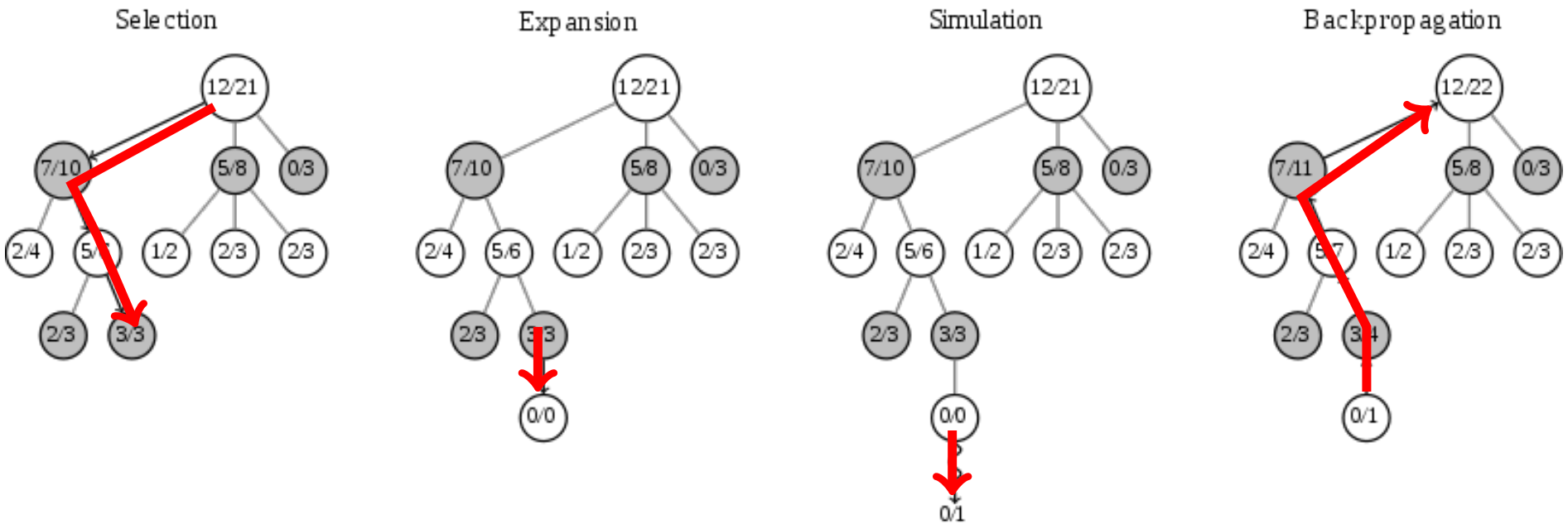

Rollout policy
(ex: random)

- Backpropagate to the root

MCTS algorithm

MCTS

1: **while** Some time is left **do**
2: Select a leaf node *#UCB-like*
3: Expand a leaf
4: Use rollout (or equivalent) to estimate the leaf *#random sampling*
5: Backpropagate to the root
6: **end while**
7: Return $\arg\max_{c \in \text{children(root)}} N(c)$ *#or* $S(c)/N(c)$.

Outline

Conclusion

Exploration v.s. exploitation is central in RL

- Bandits and regret help formalizing this idea.
- One important notion is the use of optimism to force exploration.
  - Bayesian sampling can also be used
- Theoretical tools guide practical implementations.

In the team

- Kimang: PSRL-like algorithms for Markovian bandits.
- Chen: optimization Markovian bandits.
- Romain (Cravic): learning in stochastic games.
- (and many others)