Monte Carlo Tree Search in **continuous spaces** using Voronoi optimistic optimization with **regret bounds**

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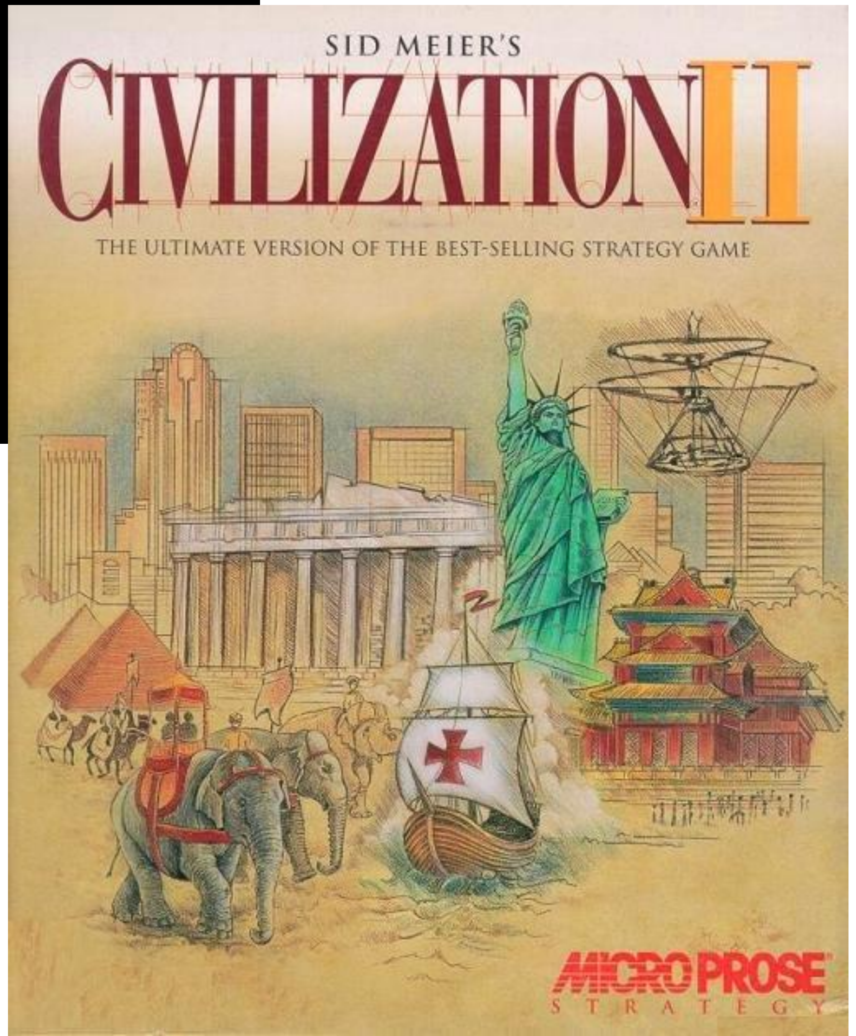
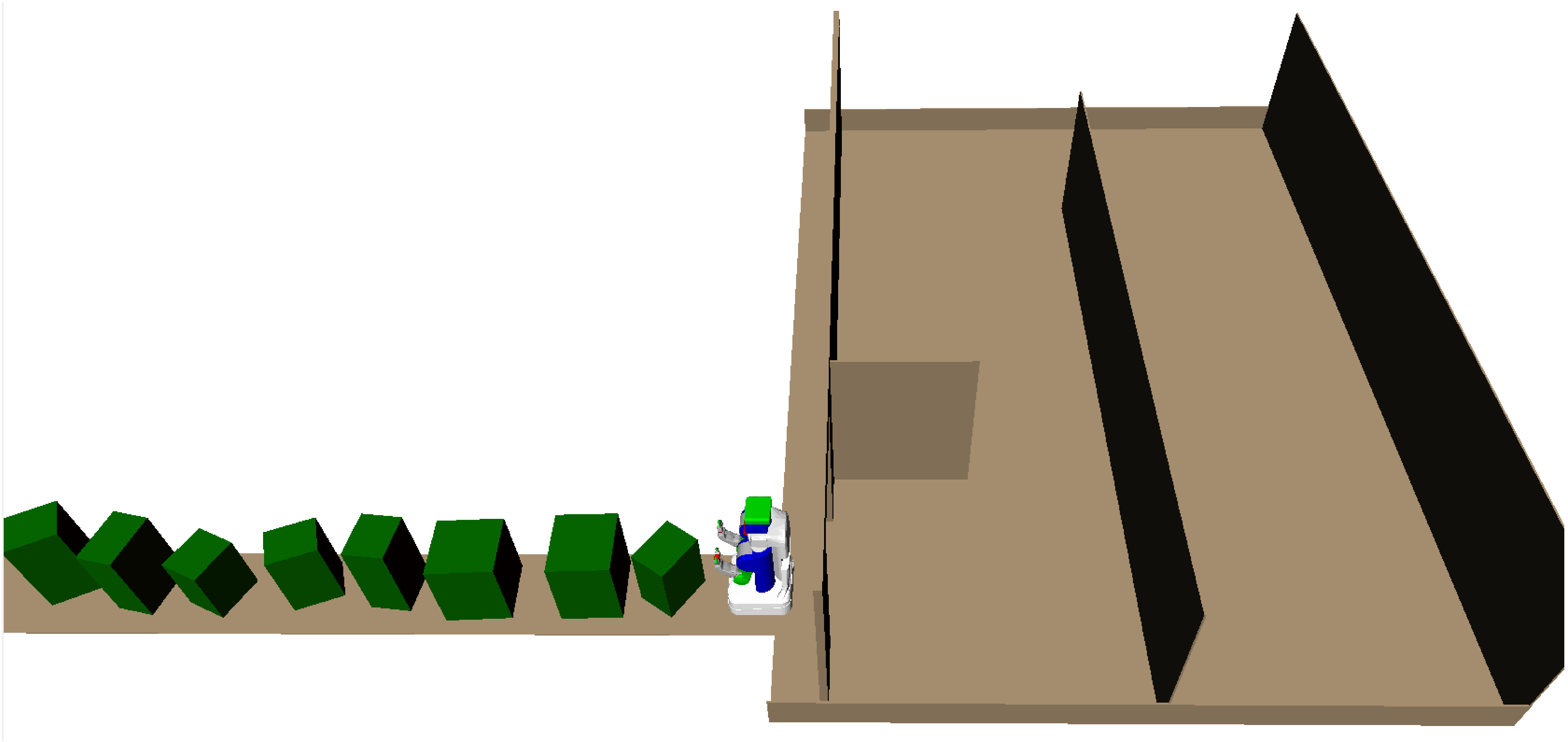
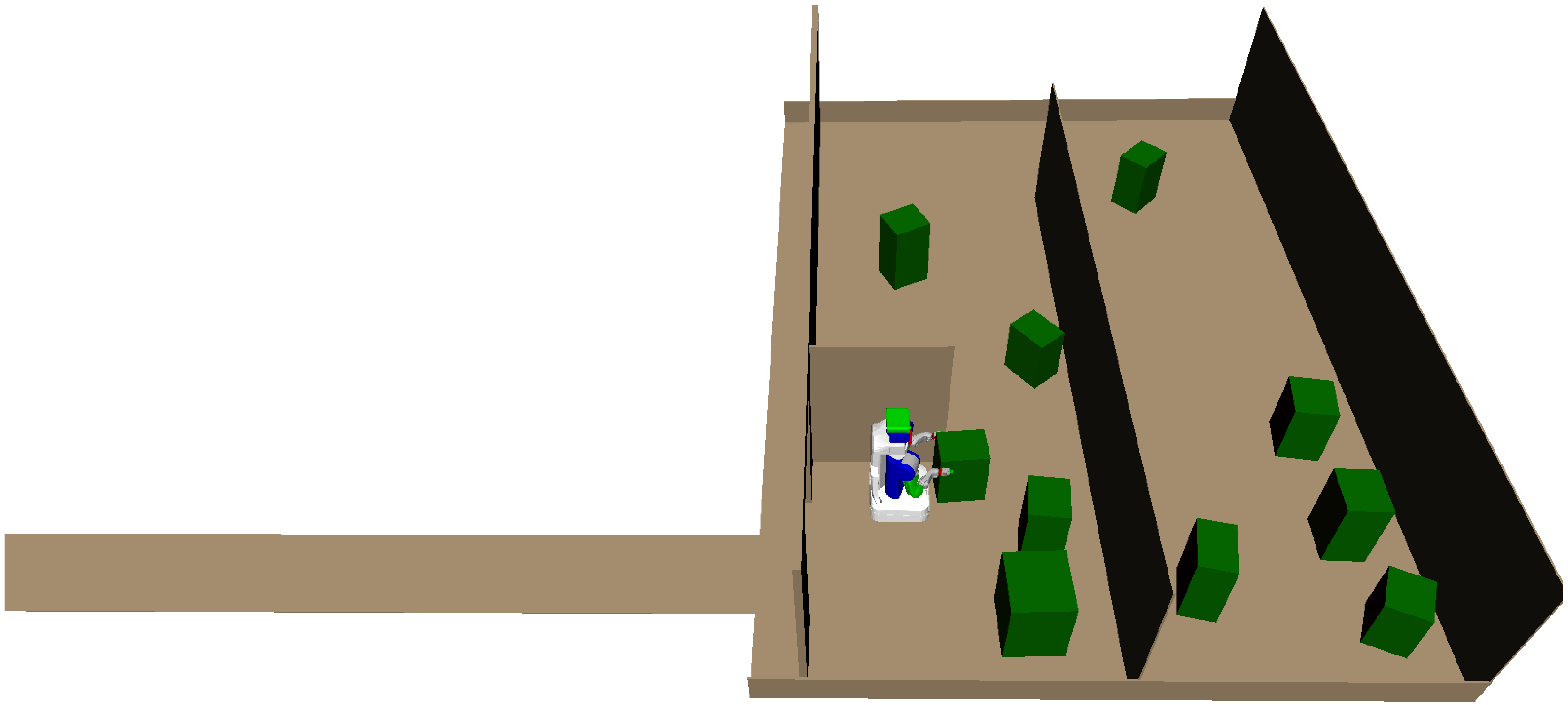
(with Kyungjae Lee, Sungbin Lim, Leslie Pack Kaelbling, Tomas Lozano-Perez)

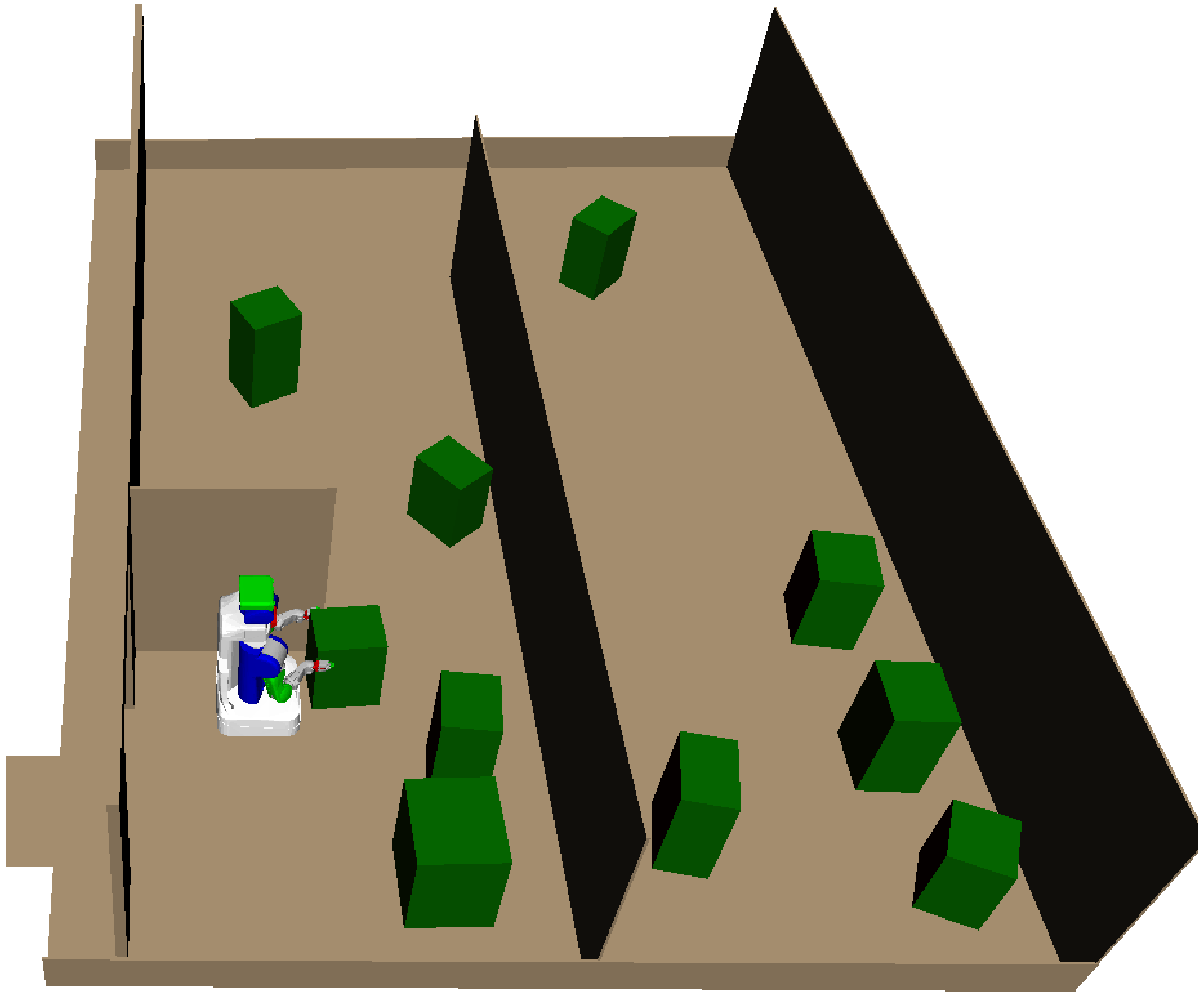
Monte Carlo Tree Search in **discrete** action spaces







Characteristics of **robotics** problems



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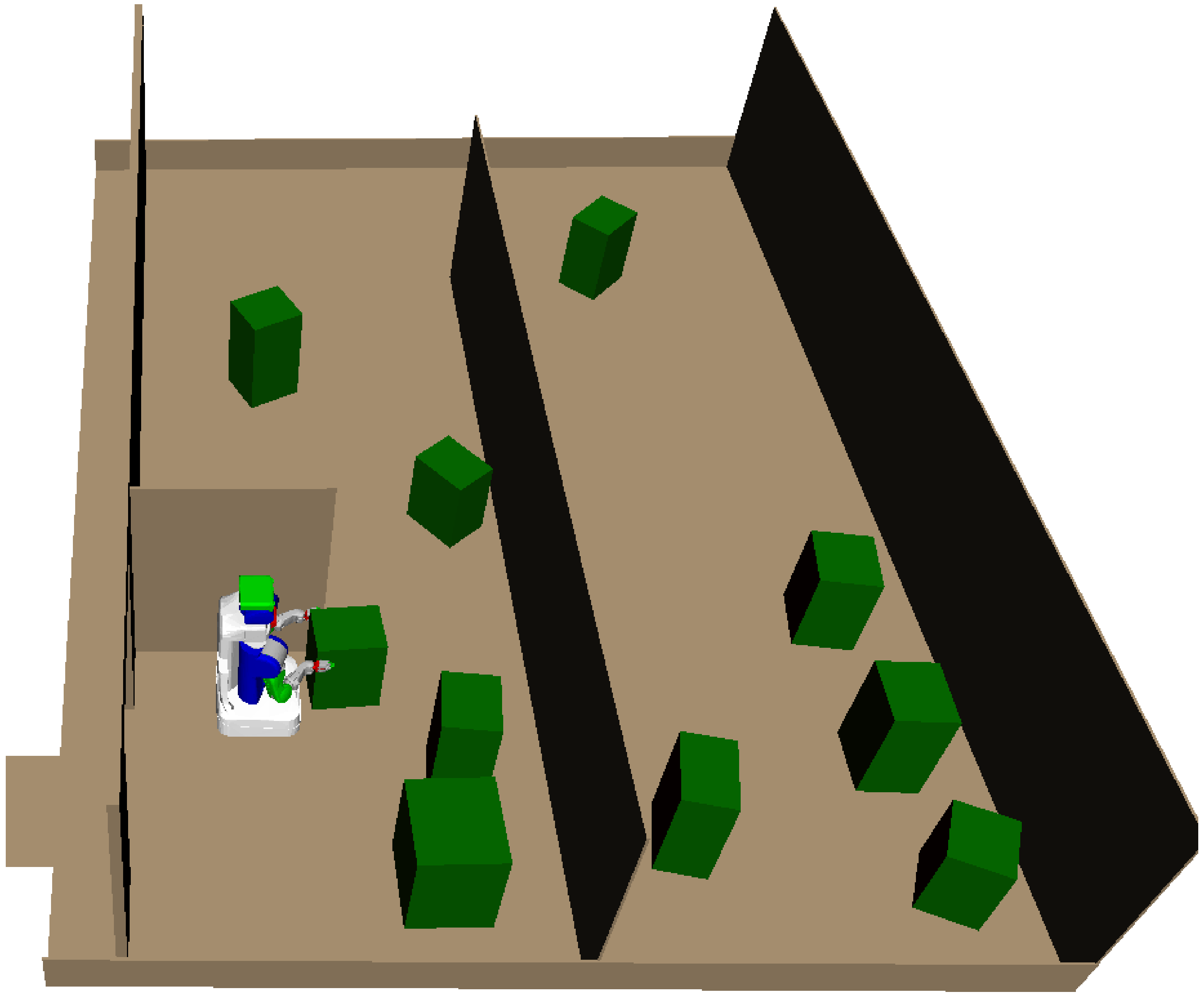

Continuous and high-dimensional action spaces

Main question addressed in our paper

How can we extend MCTS to **high-dimensional continuous action space** problems?

First, consider the easier problem

- Assume **planning horizon is 1**

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- The problem is reduced to a **budgeted-black-box-function optimization** (BBFO) problem

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$$\max_{a \in \mathcal{A}} R(a)$$

First, consider the easier problem

- Assume **planning horizon is 1**
- The problem is reduced to a **budgeted-black-box-function optimization** (BBFO) problem

$\max_{a \in \mathcal{A}} R(a)$ within **n number of evaluations**

BBFO: general problem formulation

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- Given:
  - Budget n
  - Bounded search space $\mathcal{X}$
  - Objective function f

BBFO problem formulation

- Goal: minimize the ***simple regret***

$$f(x_\star) - \max_{t \in [n]} f(x_t)$$

A class of BBFO methods

Bayesian Optimization (BO)

EI (Mockus, 1974)
PI (Kushner, 1964)
GP-UCB (Srinivas et al., 2010)
ES (Hennig & Schuler, 2012)
PES (Hernandez-Lobato et al., 2014)
EST (Wang et al., 2016)

Drawback in high-dimensional search spaces

Bayesian Optimization (BO)

Requires global optimization of the acquisition function

- EI (Mockus, 1974)
- PI (Kushner, 1964)
- GP-UCB(Auer, 2002; Srinivas et al., 2010)
- ES (Hennig & Schuler, 2012)
- PES (Hernandez-Lobato et al., 2014)
- EST (Wang et al., 2016)

Another class of BBFO methods

Bayesian Optimization (BO)

Requires global optimization of the acquisition function

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- PI (Kushner, 1964)
- GP-UCB(Auer, 2002; Srinivas et al., 2010)
- ES (Hennig & Schuler, 2012)
- PES (Hernandez-Lobato et al., 2014)
- EST (Wang et al., 2016)

Hierarchical Partitioning (HP)

DOO (Munos, 2011)
SOO (Valko et al., 2013)
HOO (Bubeck et al., 2010)

How hierarchical partitioning methods work

- Consecutively partitioning the search space

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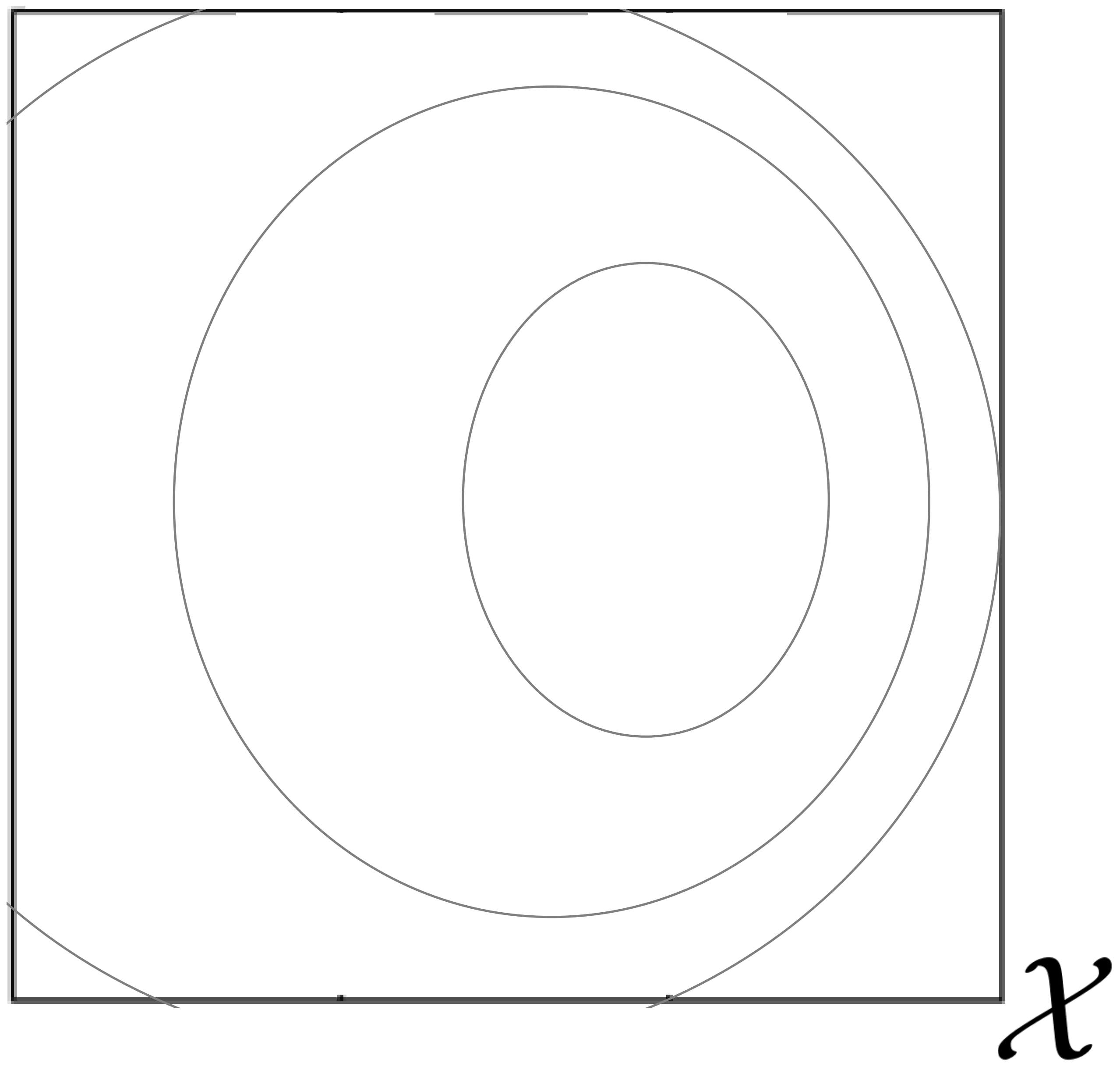
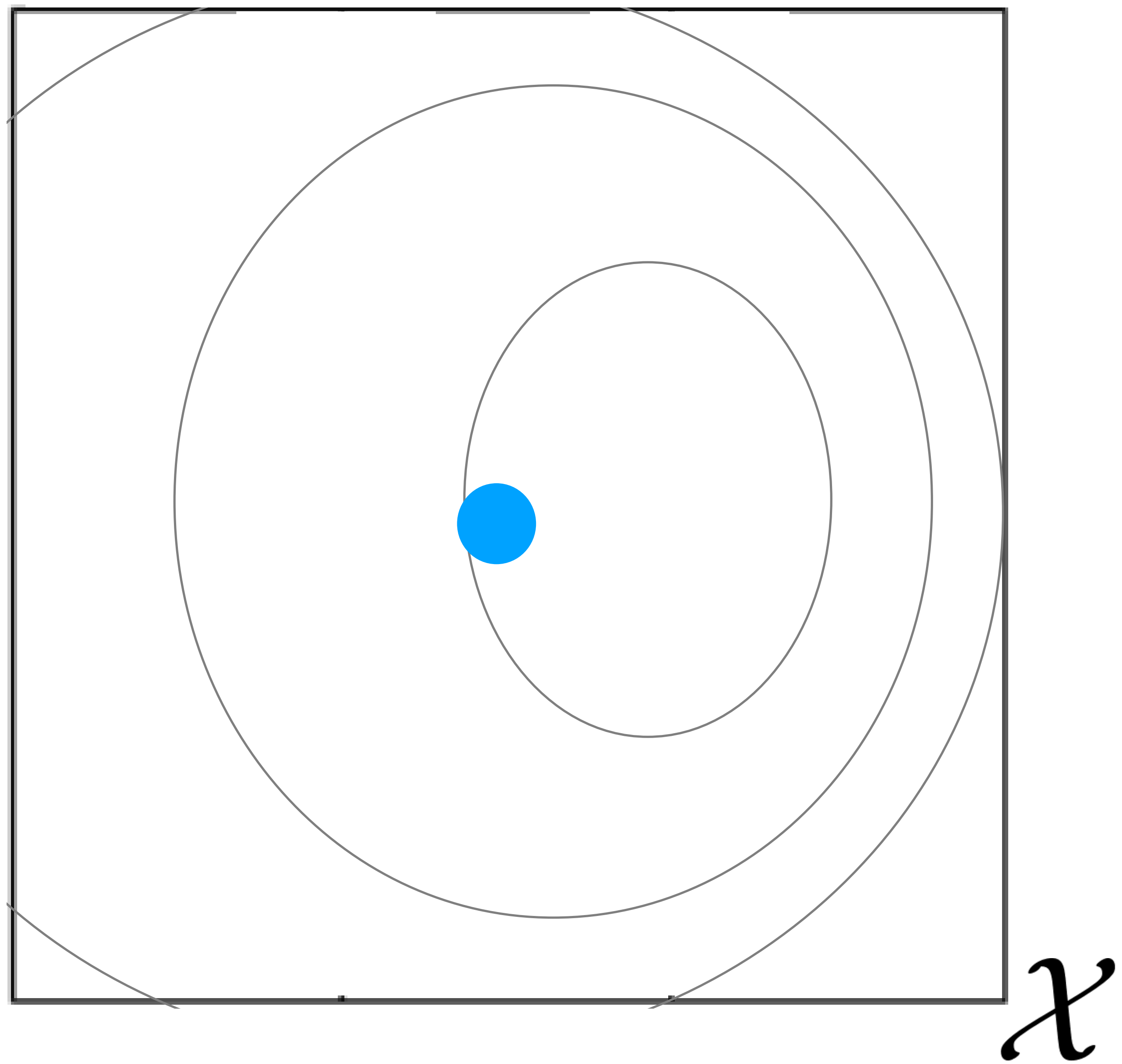


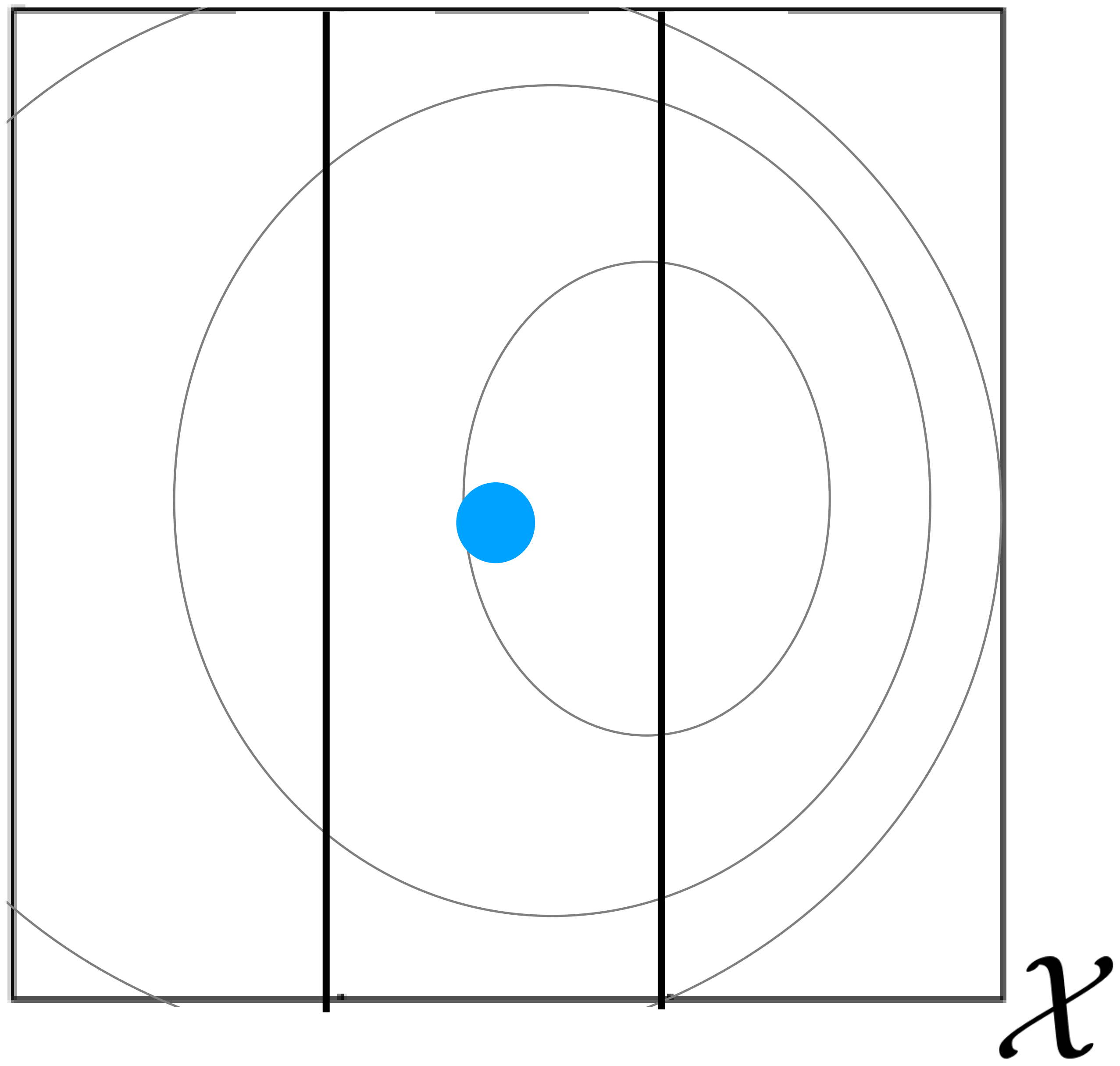
How hierarchical partitioning methods work

- First evaluated point



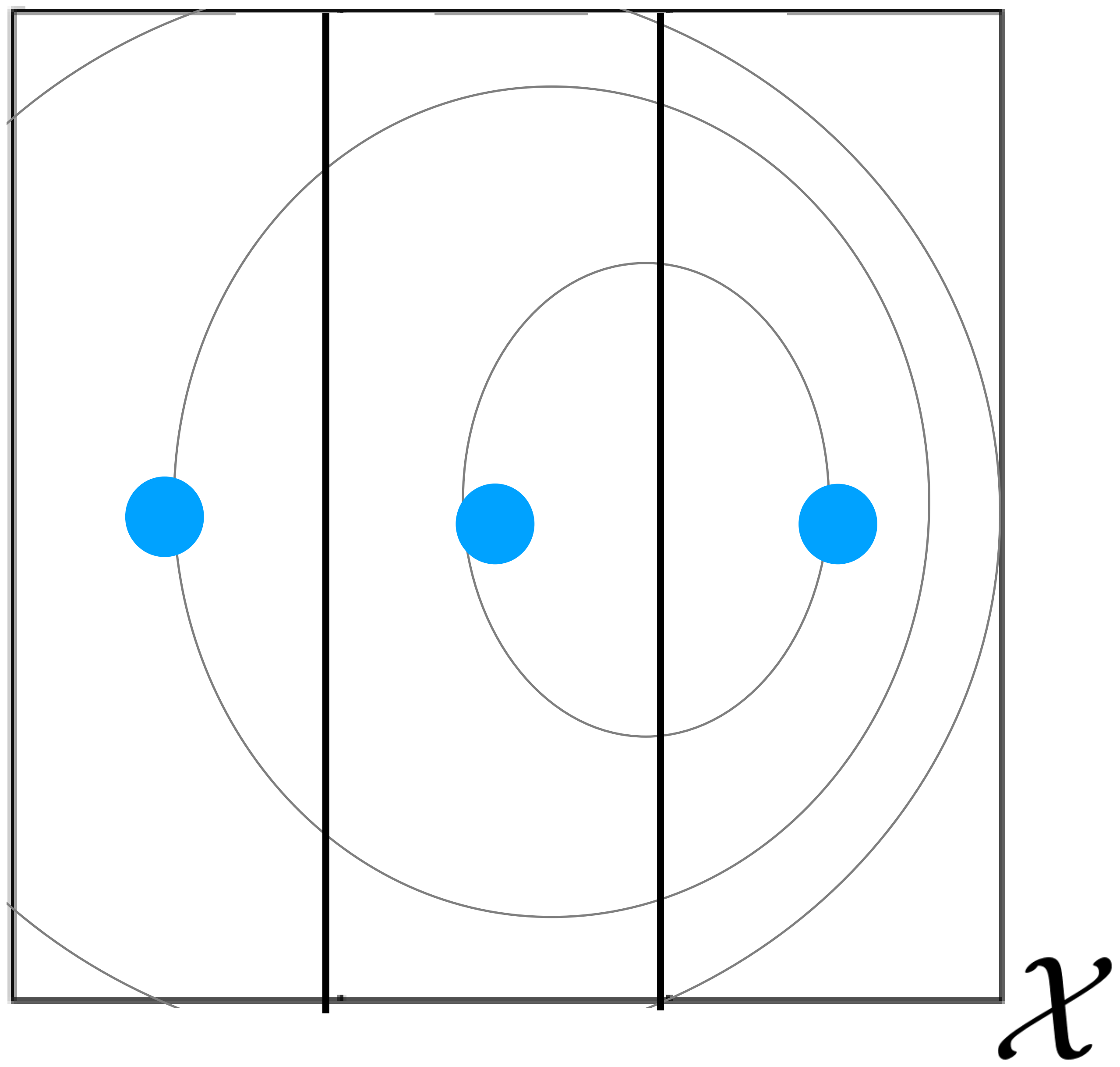
How hierarchical partitioning methods work

- Partition space by constructing K cells. Let's say K = 3



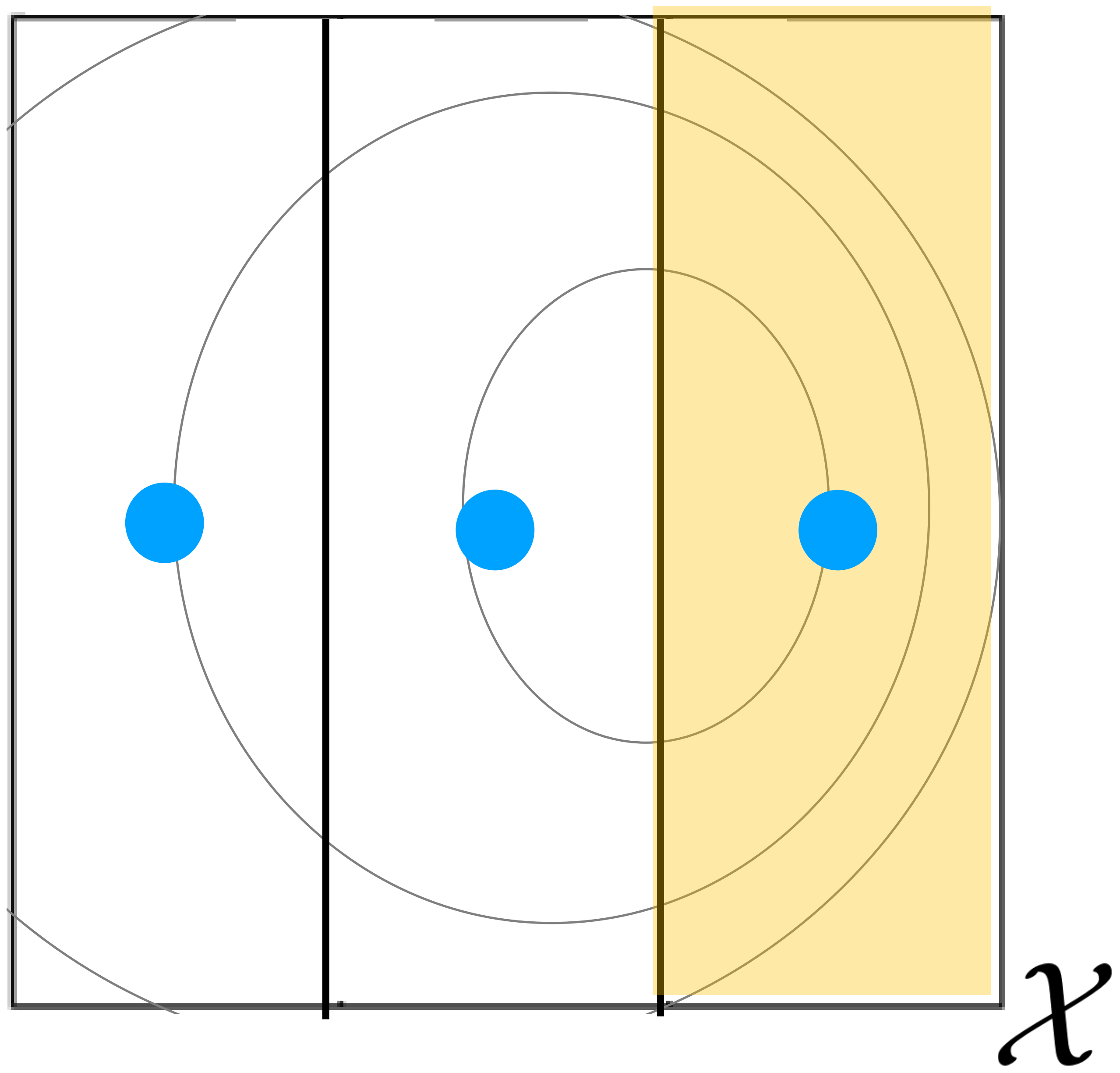
How hierarchical partitioning methods work

- Evaluate points in the new cells



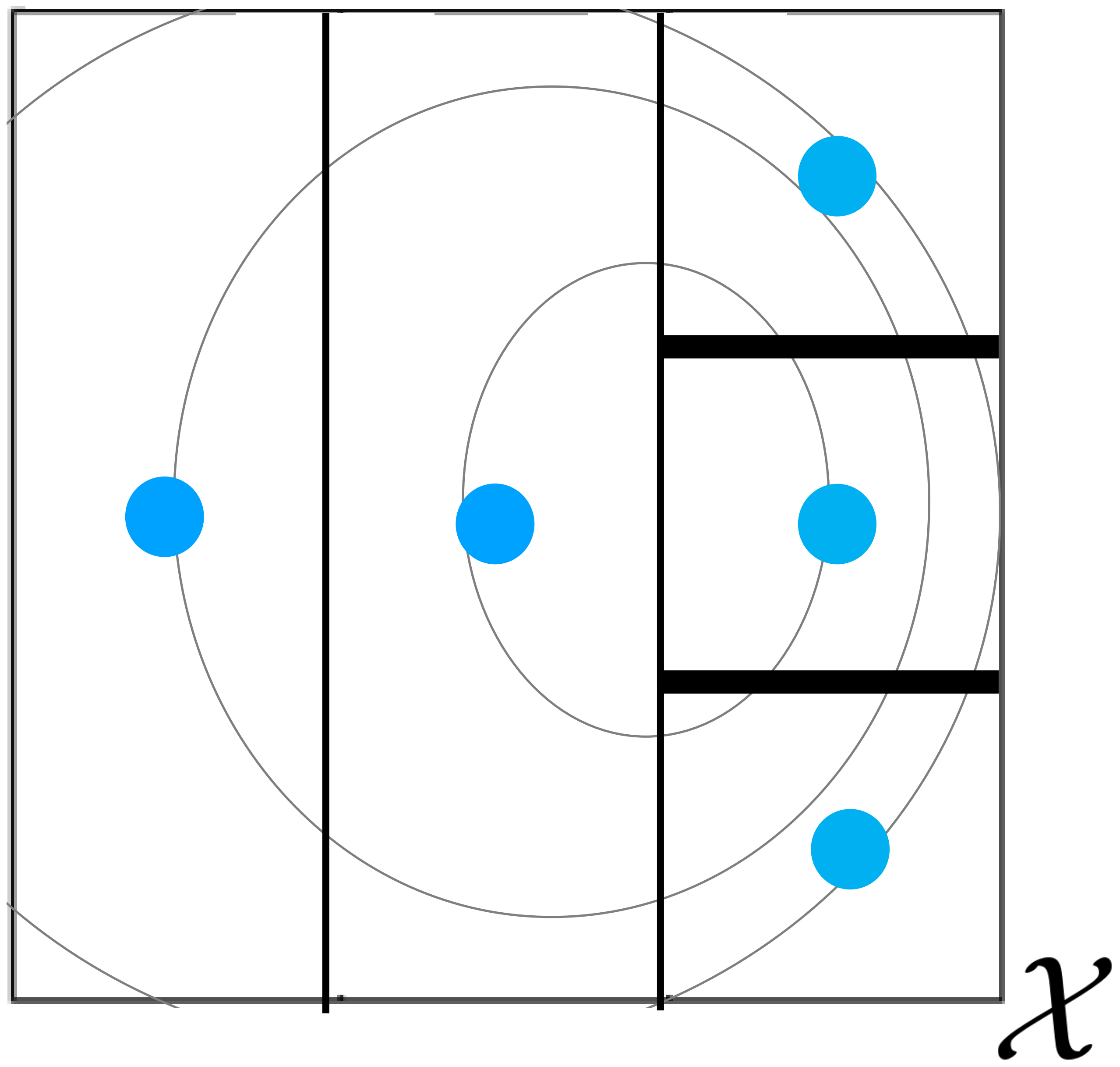
How hierarchical partitioning methods work

- Choose the most promising cell



How hierarchical partitioning methods work

- Construct a new partition, and evaluate points



How to select the **most promising cell?**

Selecting the **most promising cell**

- **Deterministic Optimistic Optimization** [Munos 2011]

Selecting the **most promising cell**

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- Compute the b-value of each cell, where

$$b(x_i)$$

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$$b(x_i) = f(x_i)$$

Selecting the **most promising cell**

- **Deterministic Optimistic Optimization** [Munos 2011]
- Compute the b-value of each cell, where

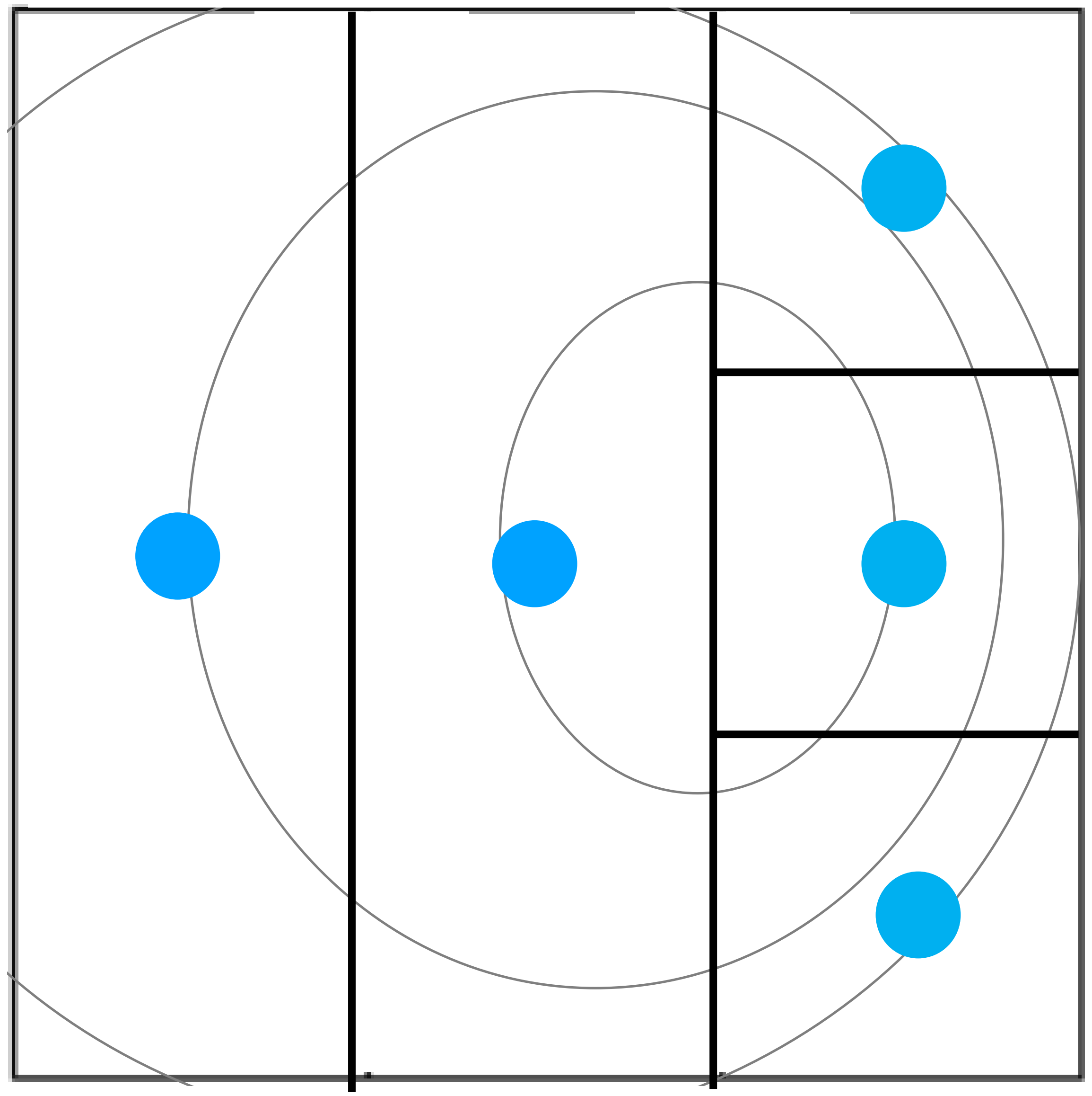
Exploration bonus

$$b(x_i) = f(x_i) + \boxed{\delta(i)}$$

Prefers larger cells

Diameter of a cell

$$b(x_i) = f(x_i) + \delta(i)$$



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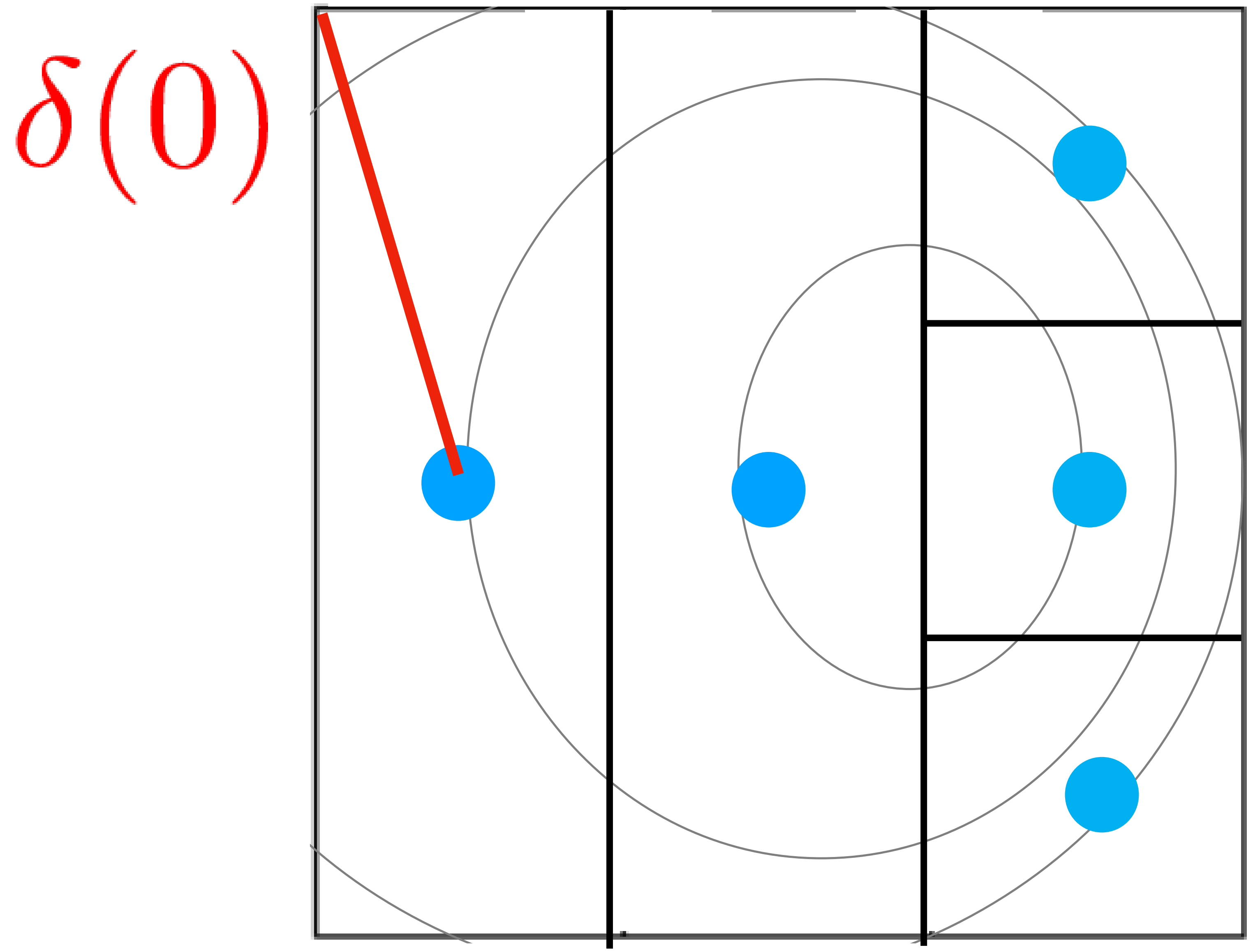

Diameter of a cell

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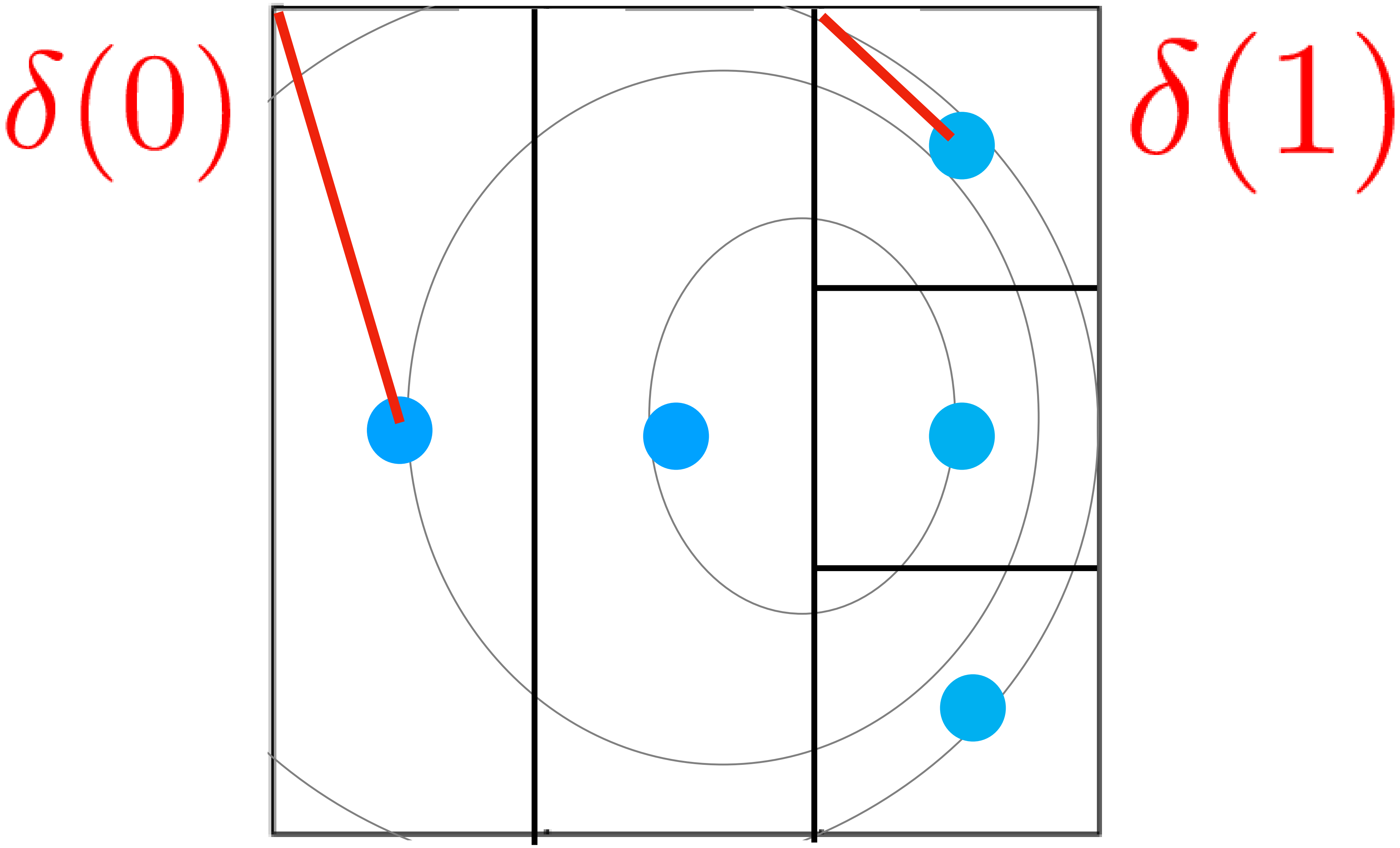

DOO: **Choose the cell with the highest b-value**

$$\arg\max_i f(x_i) + \delta(i)$$

DOO: **exploration vs. exploitation**

$$\arg\max_i f(x_i) + \delta(i)$$

DOO: **exploration vs. exploitation**

Exploitation of current function knowledge

prefer cells that have high function values

$$\arg\max_i \boxed{f(x_i)} + \delta(i)$$

DOO: **exploration vs. exploitation**

Exploitation of current function knowledge

prefer cells that have high function values

$$\arg\max_i f(x_i) + \delta(i)$$

Exploration of the search space

prefer cells with large diameters

BUT: it requires **deciding which dimension to cut**

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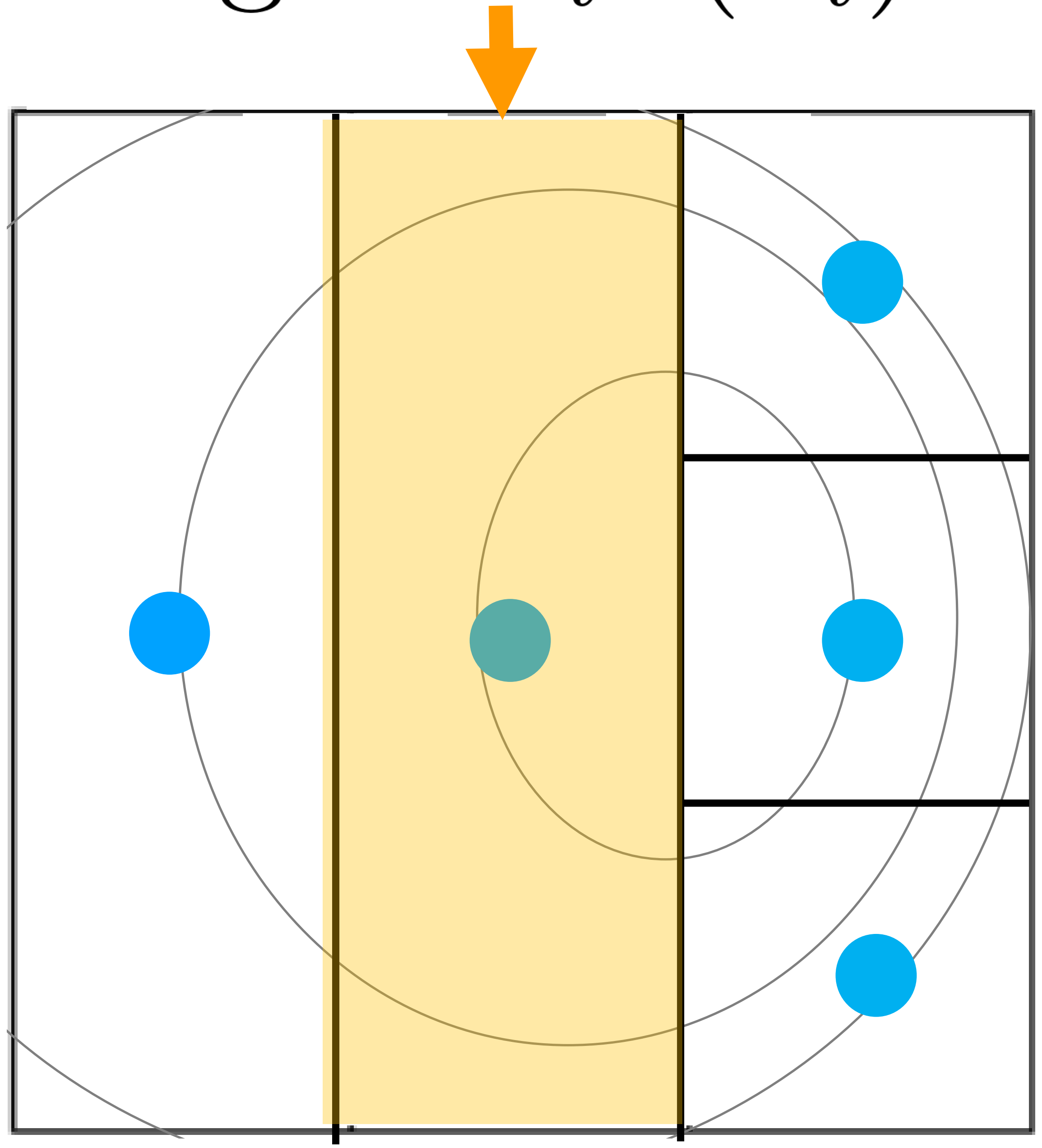
$$\arg\max_i b(x_i)$$



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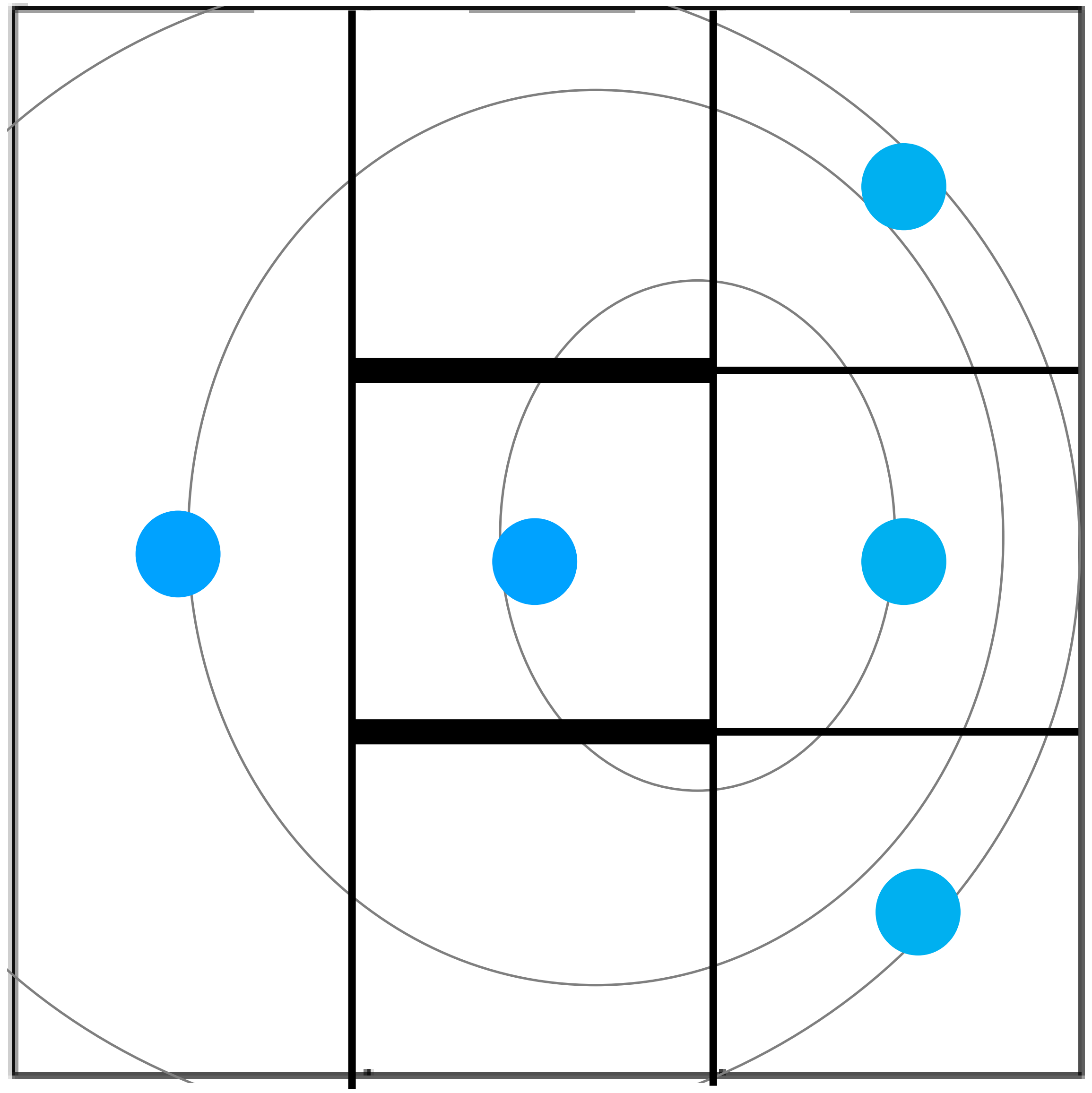

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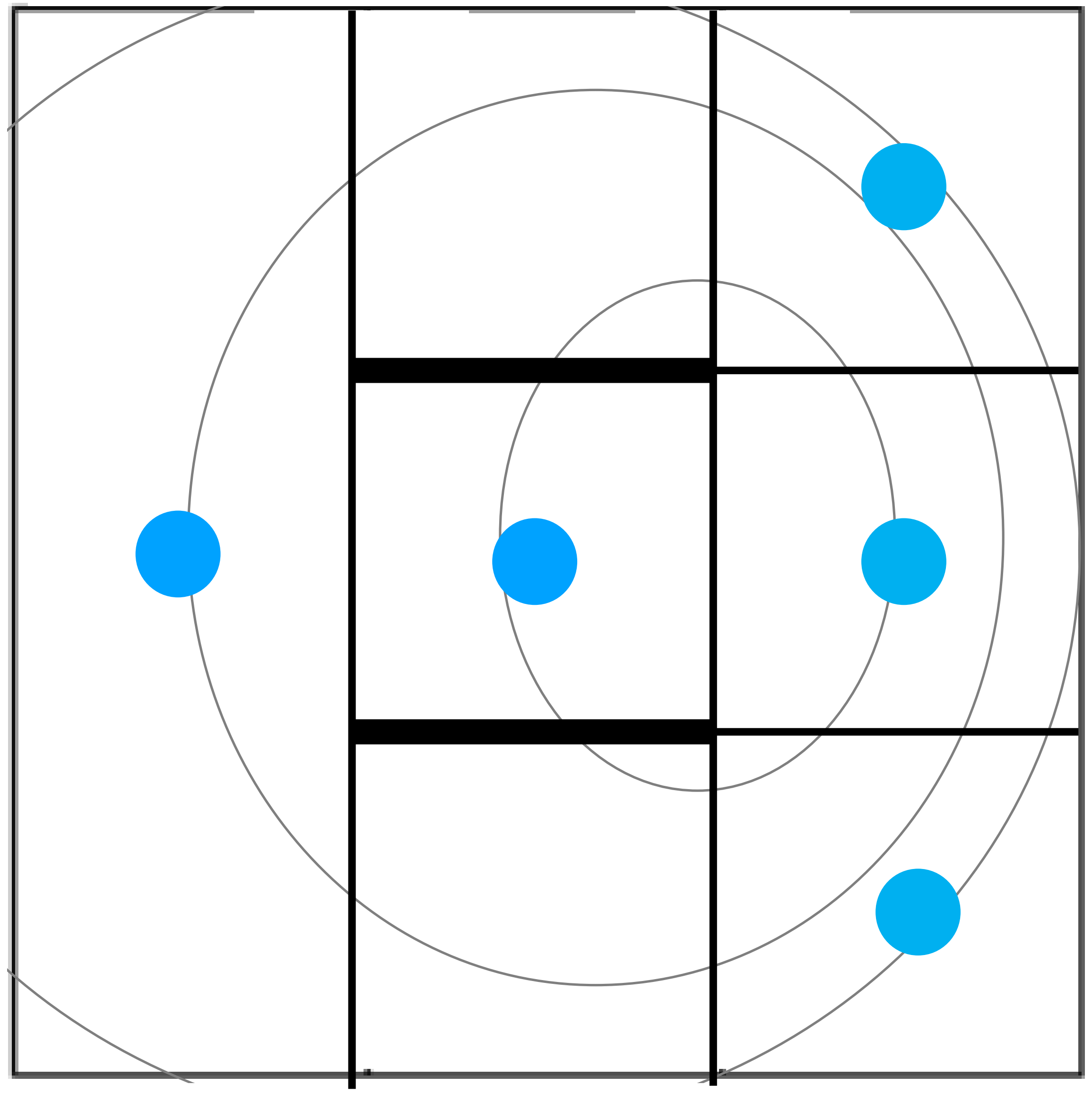
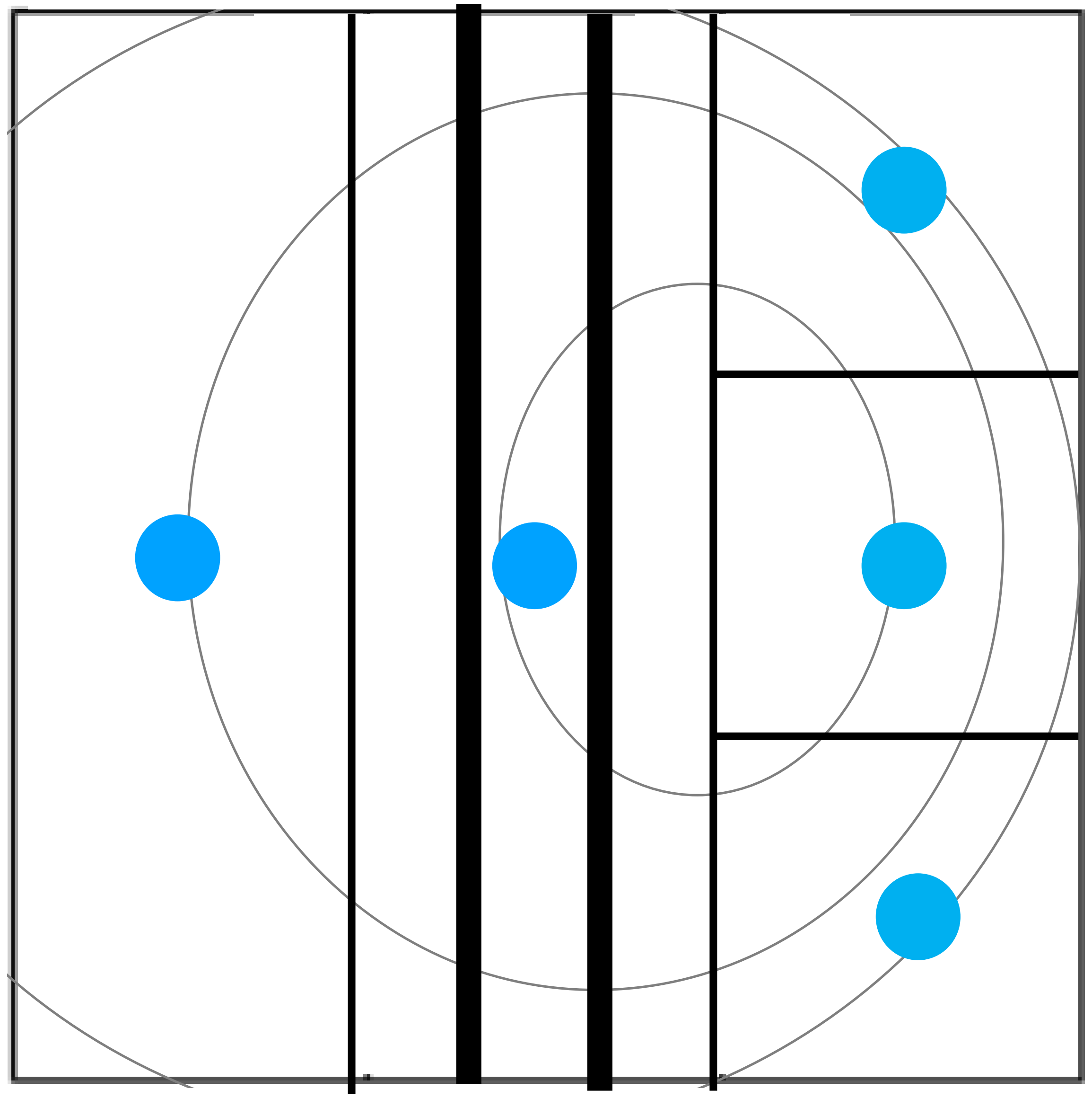


VS.



BUT: it requires **deciding which dimension to cut**

In D-dimensional search space, you have D^n number of choices

BUT: it requires **deciding which dimension to cut**

In D-dimensional search space, you have D^n number of choices

Finding the ***optimal sequence of dimensions*** to cut is not trivial

DOO's intuitive idea

- DOO idea:
  - The **larger the cell**, the more the **exploration** bonus
  - The **larger the value of the cell**, the more the **exploitation** bonus

Our main question

DOO idea:

How can we use this idea **without cell constructions**?

The larger the cell, the more the exploration bonus

The larger the value of the cell, the more the exploitation bonus

Our method: **Implicitly** construct **cells**

Our method: **Implicitly** construct **Voronoi cells**

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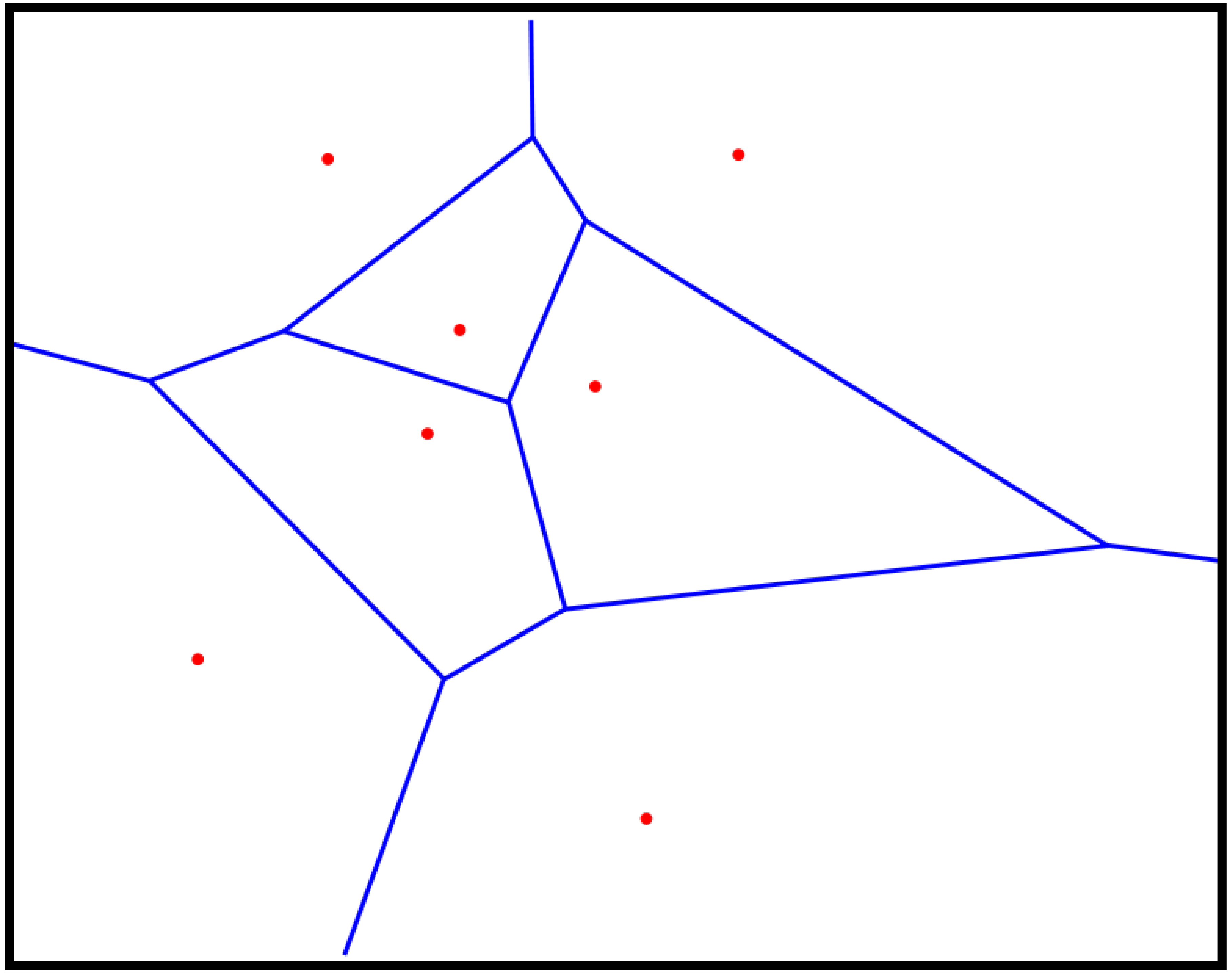
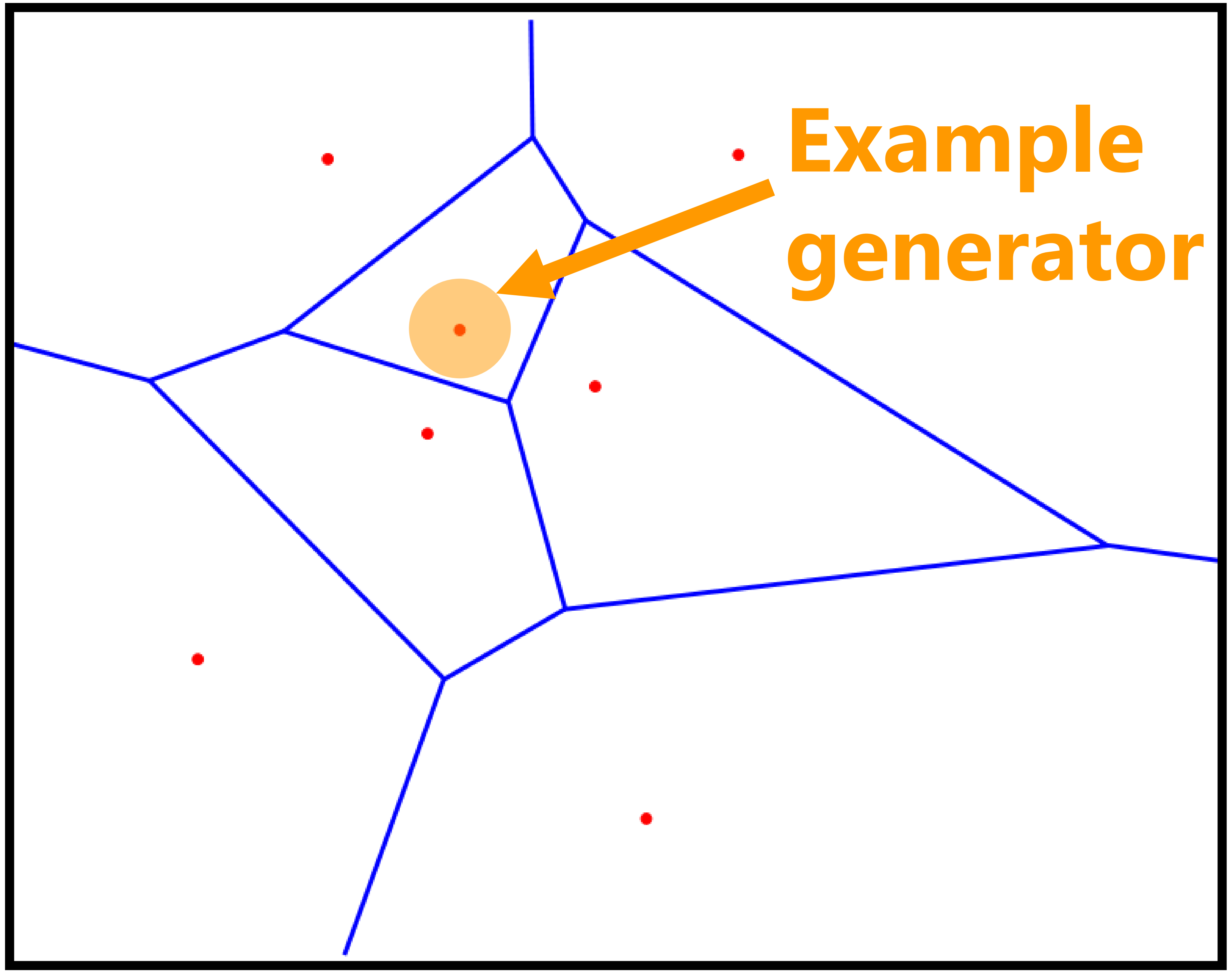


Voronoi cell:

A set of points closer to its generator than all the other generators

Our method: **Implicitly** construct **Voronoi cells**



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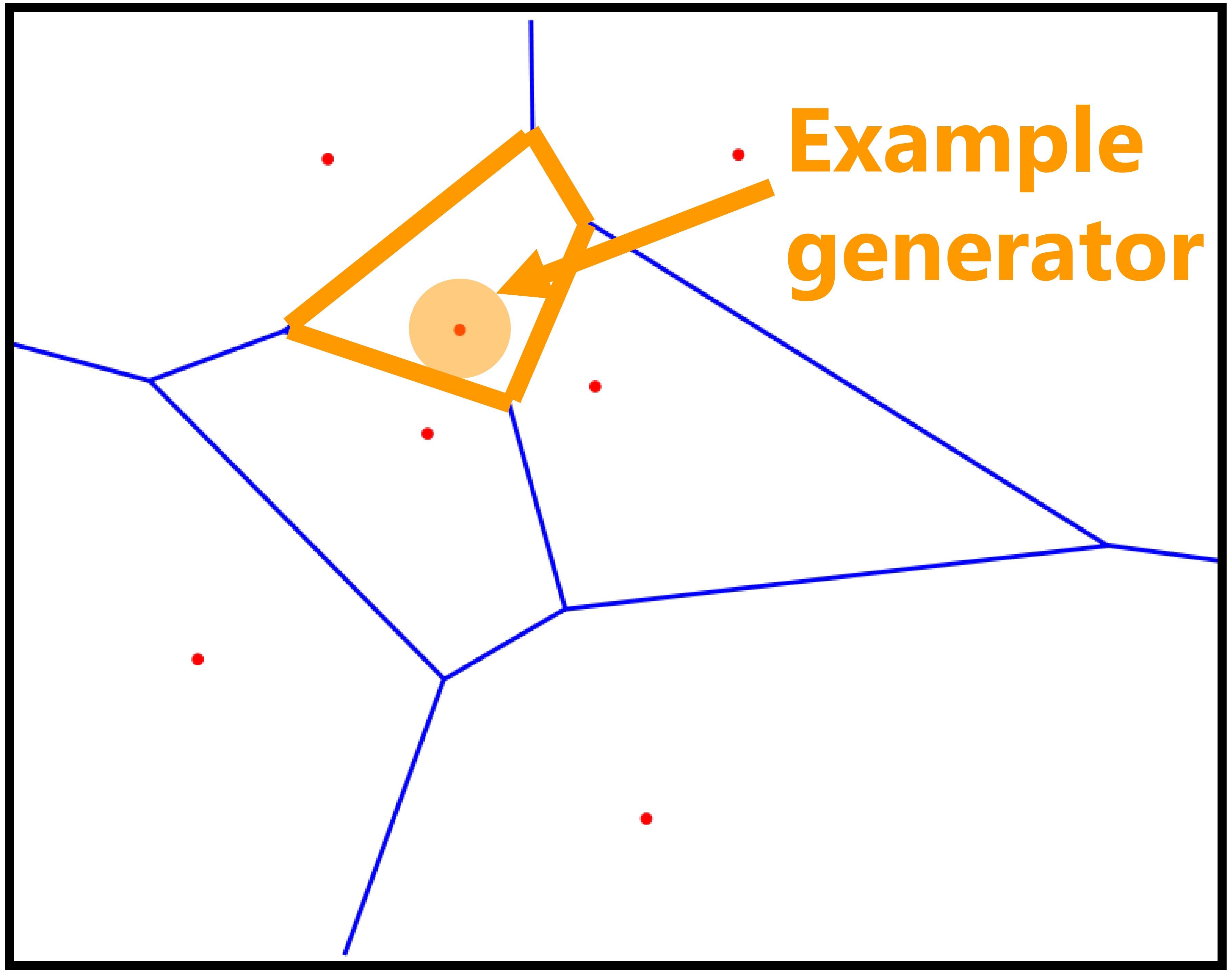

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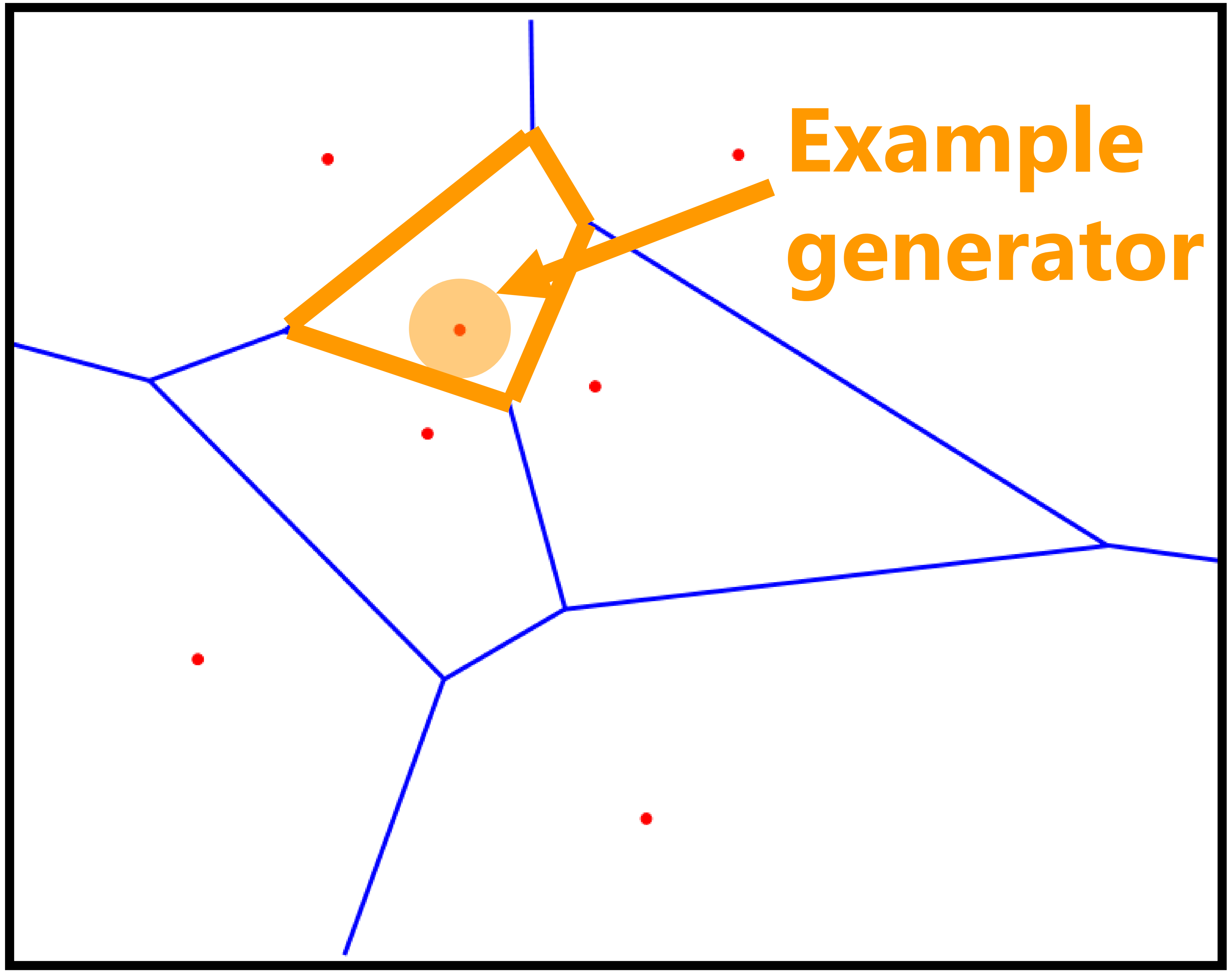

Voronoi cell:

A set of points closer to its generator than all the other generators

Evaluated points represent generators

Exploration

How do you prefer the larger cells
without constructing Voronoi cells?

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without constructing Voronoi cells?

Use **Voronoi bias**

Exploration: Don't construct Vcells, use **Voronoi bias**

$$x_{t+1} \sim \mathrm{Unif}(\mathcal{X}) \Longrightarrow P(x_{t+1} \in C) = \frac{\mu(C)}{\mu(\mathcal{X})}$$

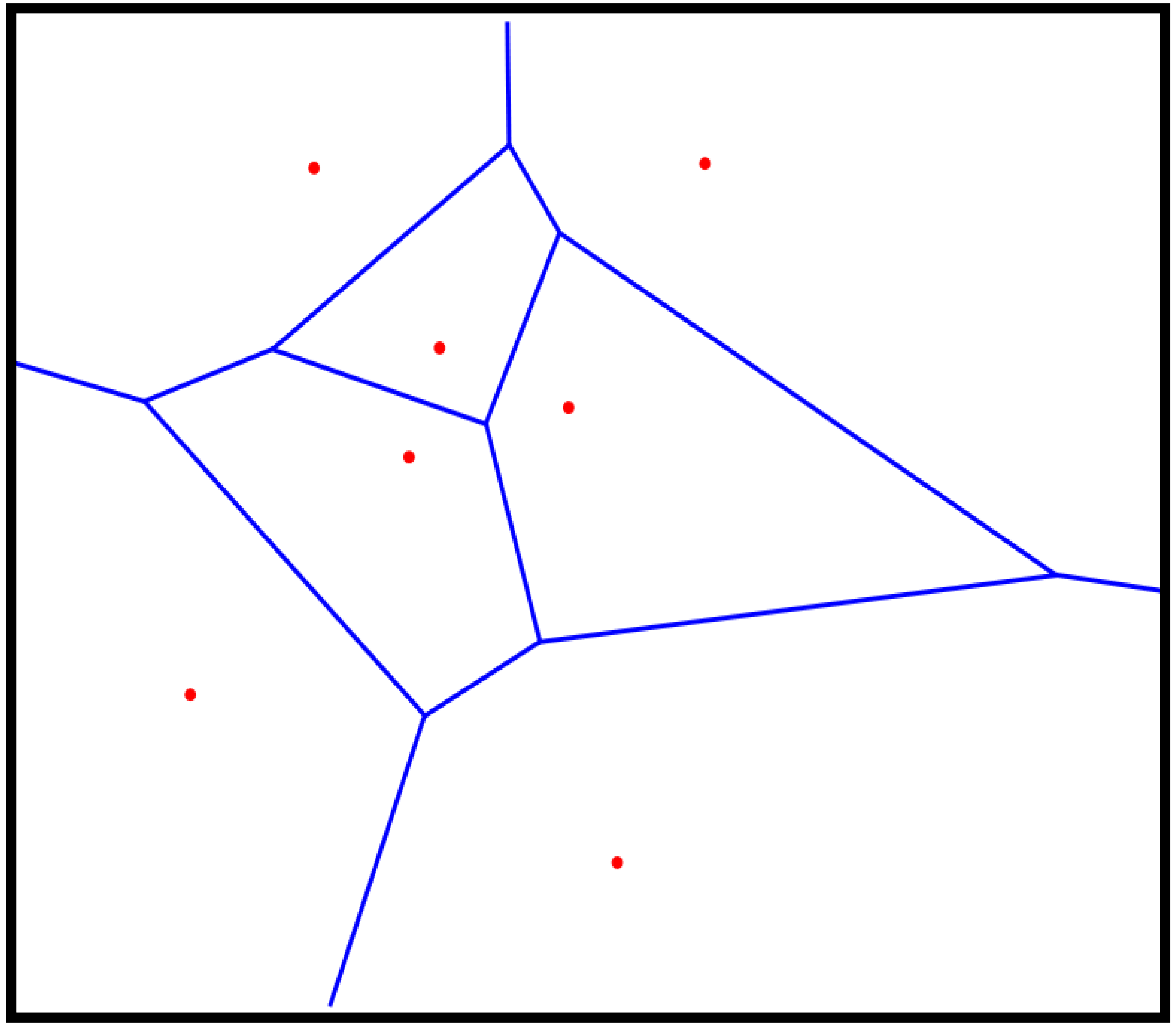
Exploration: Don't construct Vcells, use **Voronoi bias**

Volume of **a cell**

$$x_{t+1} \sim \mathrm{Unif}(\mathcal{X}) \Longrightarrow P(x_{t+1} \in C) = \frac{\mu(C)}{\mu(\mathcal{X})}$$

Volume of **the search space**

Exploration: Don't construct Vcells, use **Voronoi bias**



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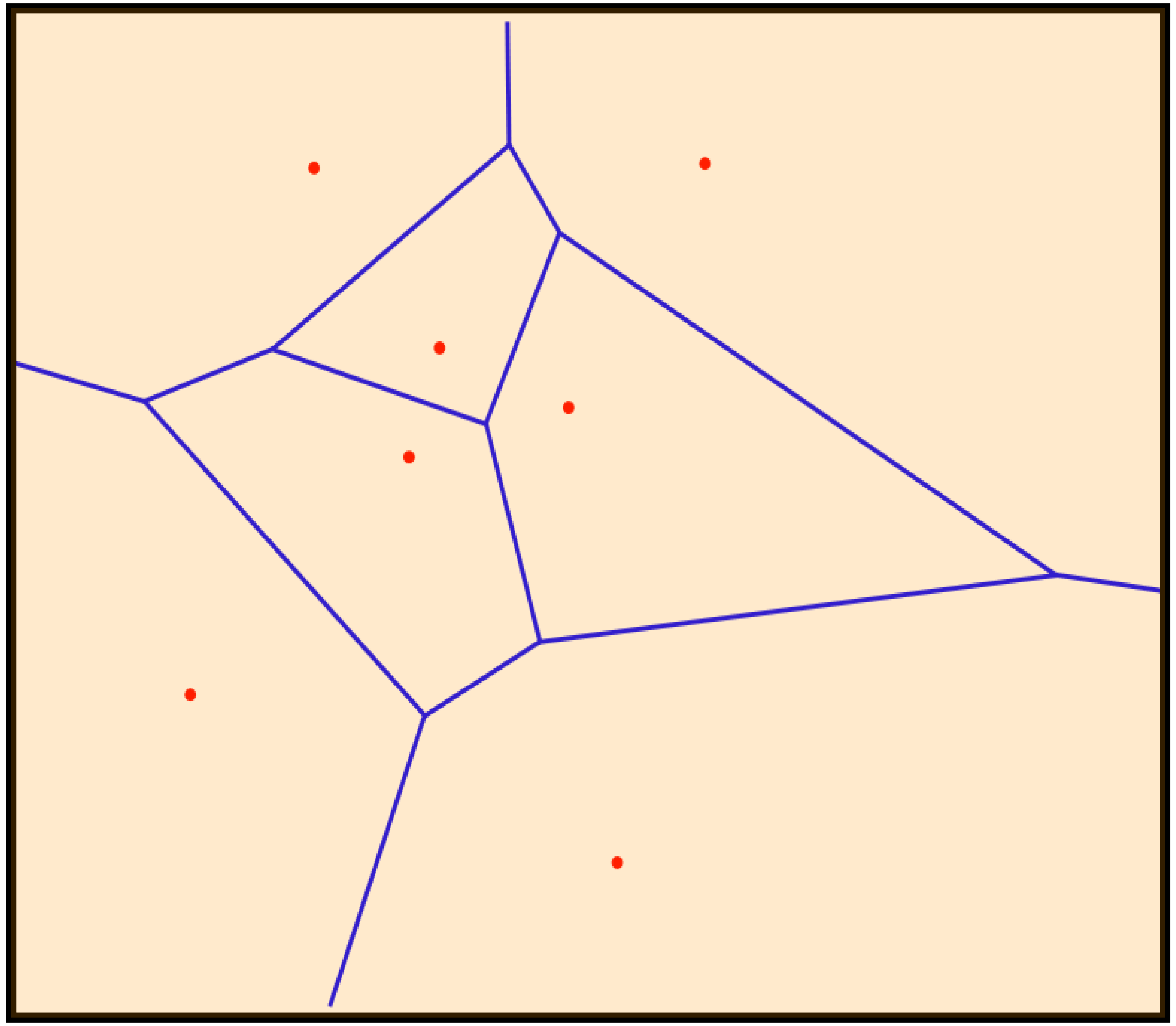
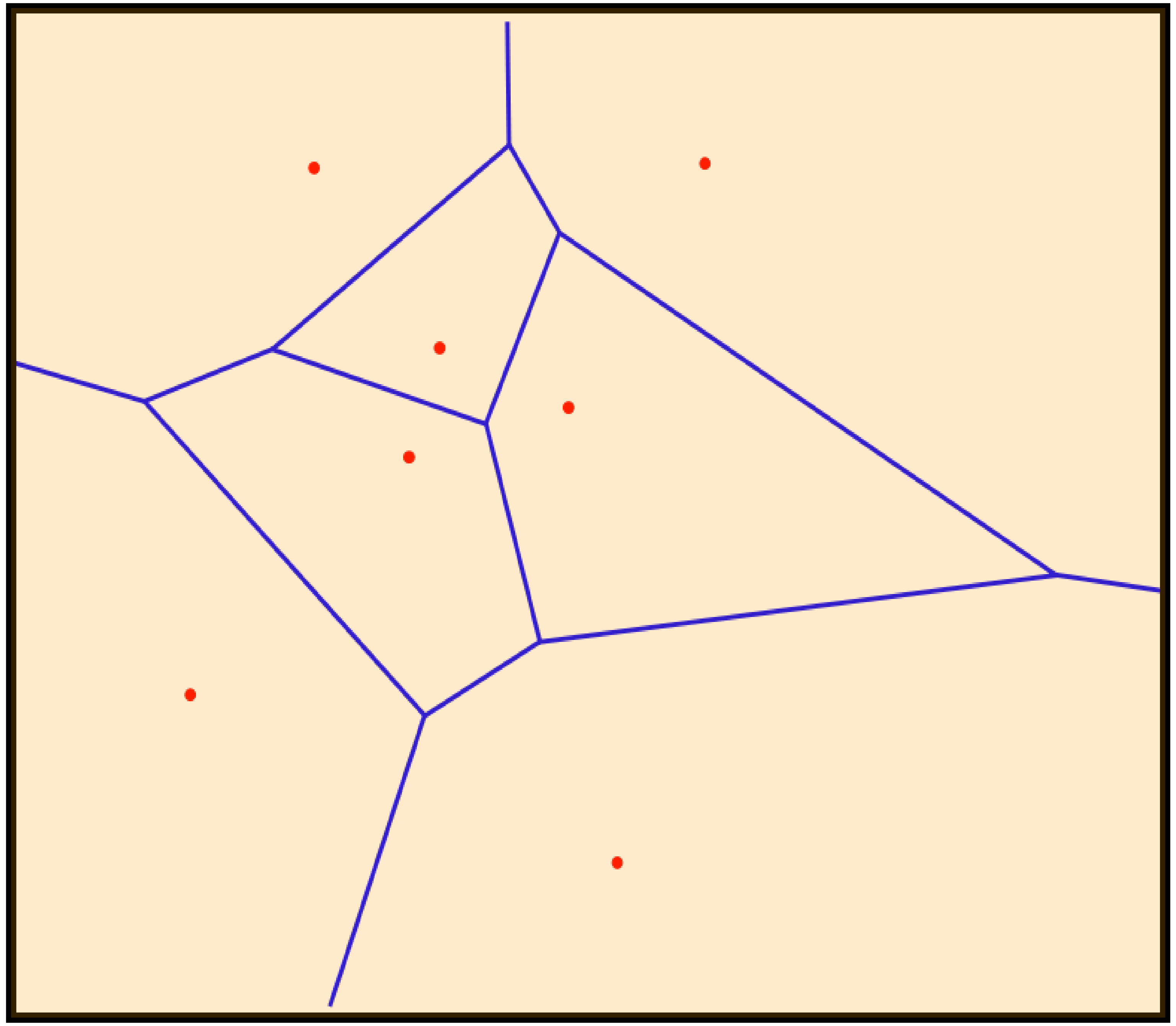


$$\mathrm{Unif}(\mathcal{X})$$

Exploration: Don't construct Vcells, use **Voronoi bias**



$$x_{t+1} \sim \mathrm{Unif}(\mathcal{X})$$

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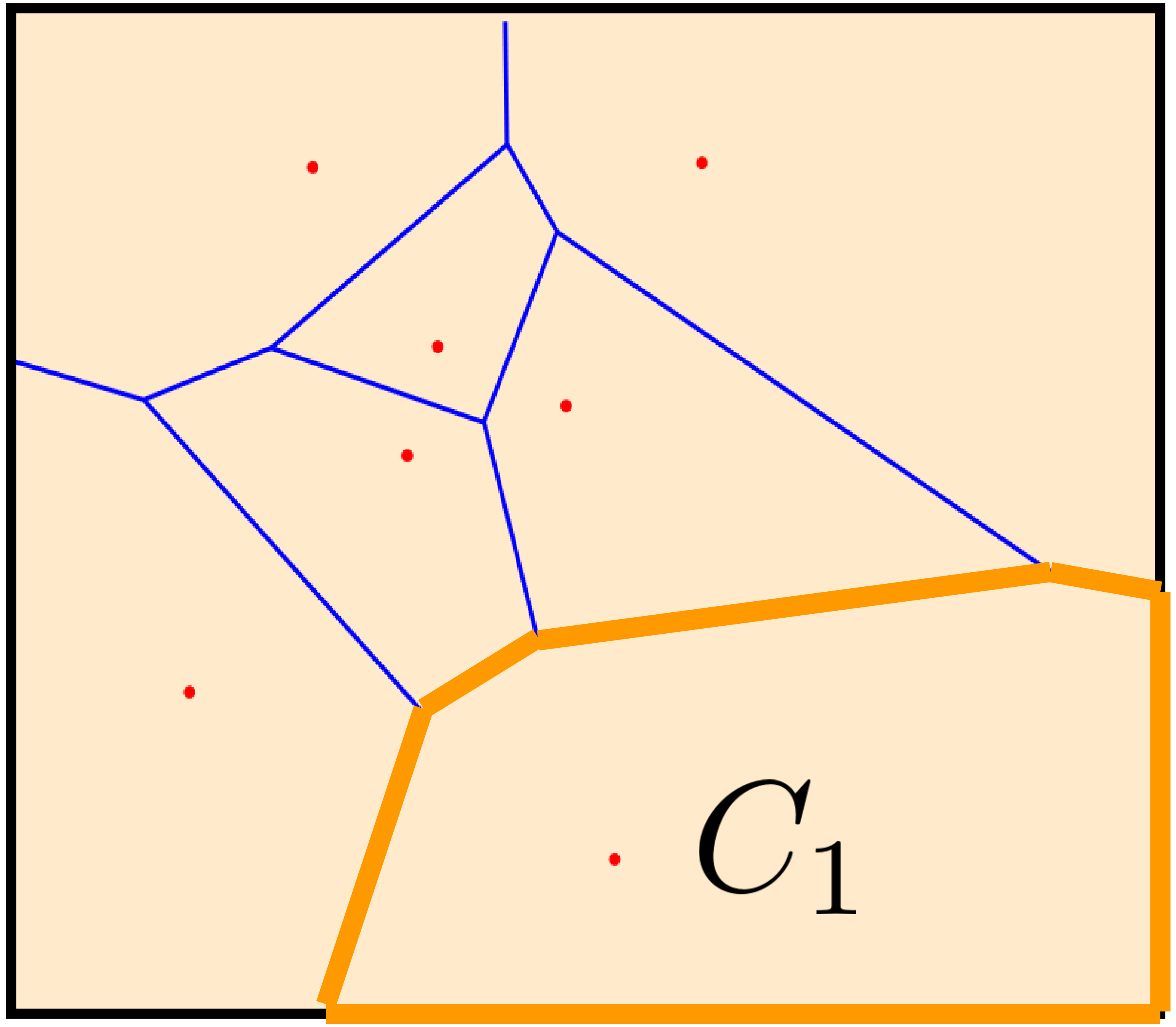

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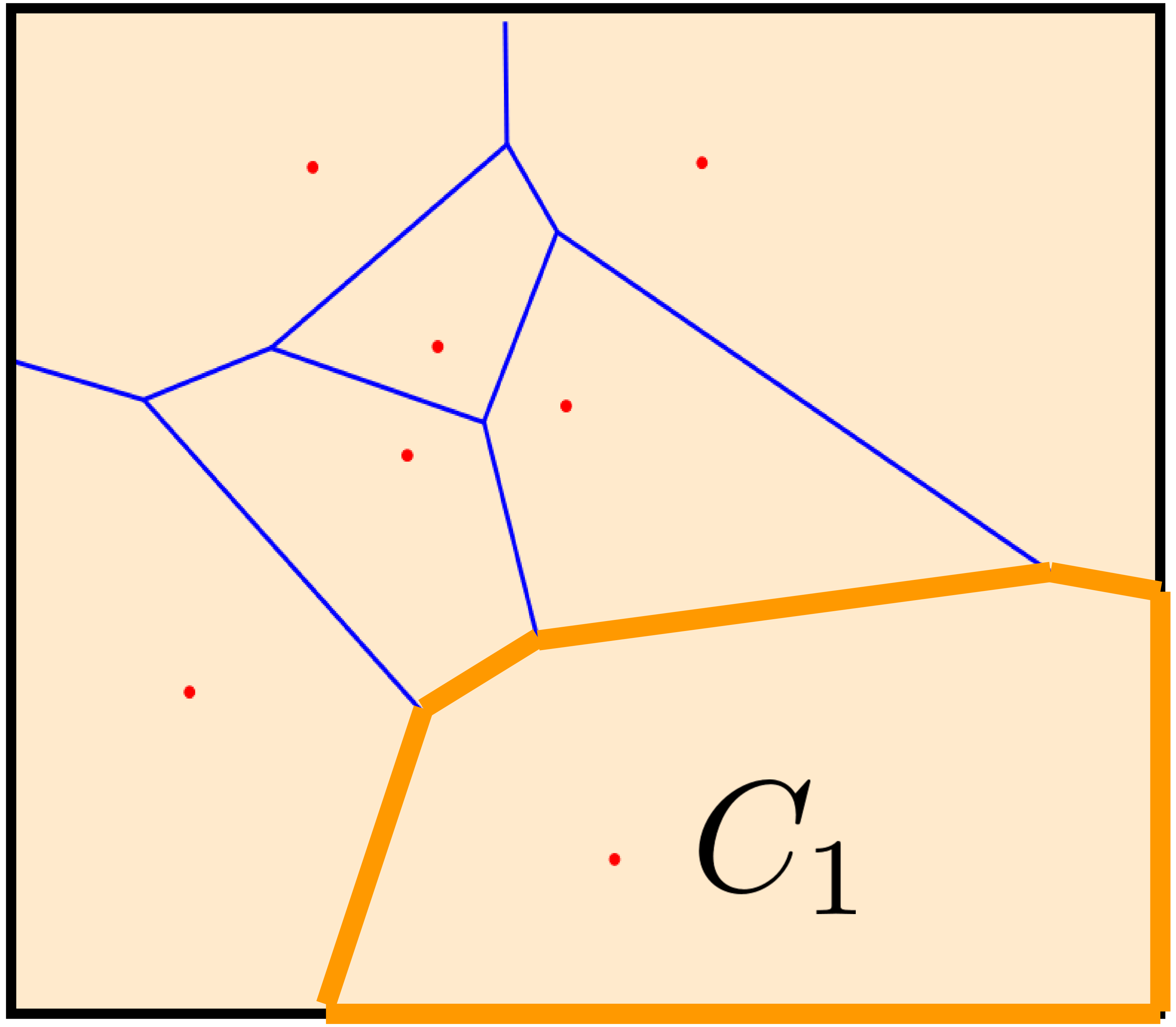

$$x_{t+1} \sim \mathrm{Unif}(\mathcal{X})$$

$$P(x_{t+1} \in C_1) = \frac{\mathrm{Area}(C_1)}{\mathrm{Area}(\mathcal{X})}$$

Exploitation

How do you select the cell with the highest value **without constructing Voronoi cells?**

Exploitation

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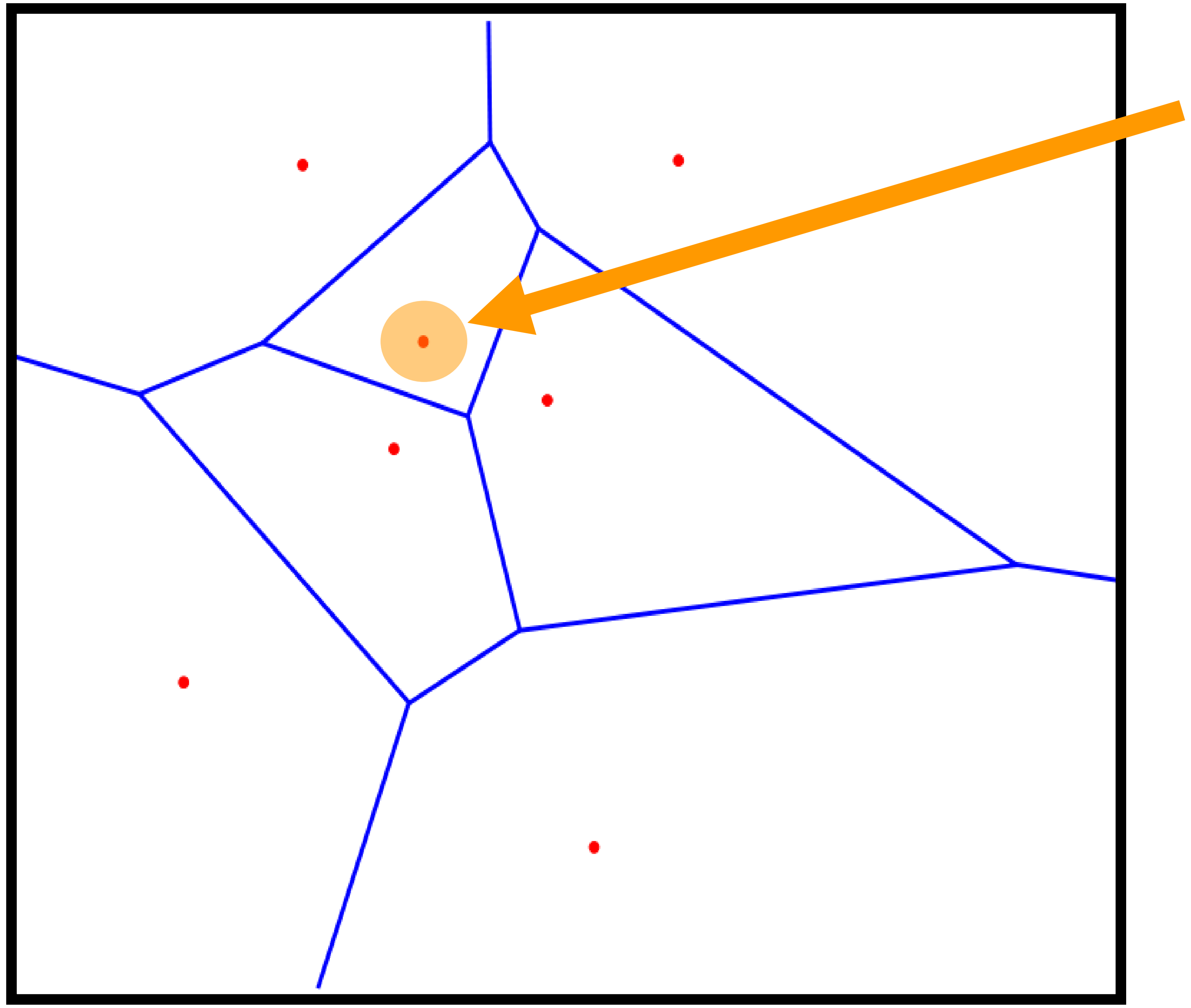
without constructing Voronoi cells?

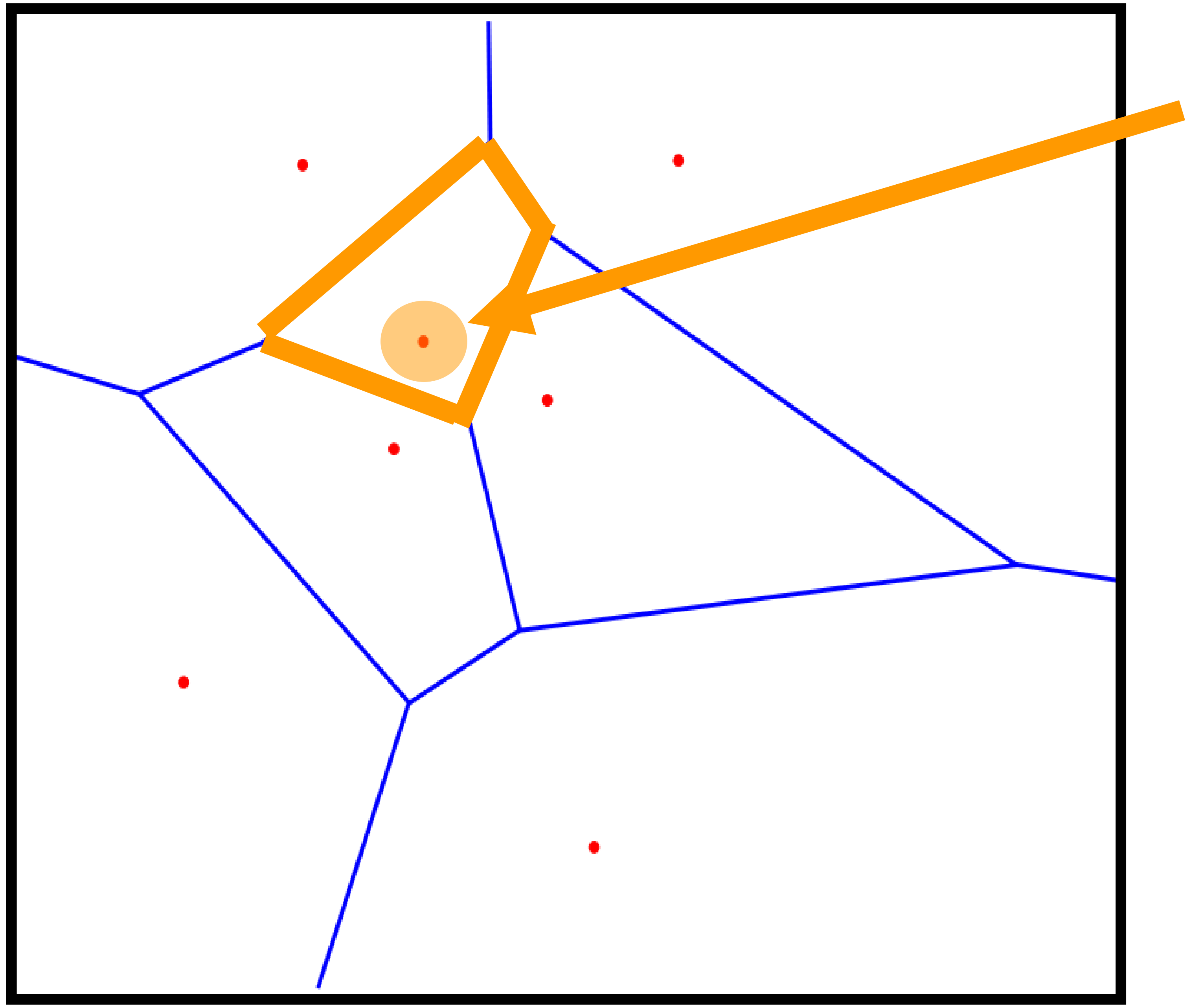
Use **rejection sampling**

Use **rejection sampling** to do exploitation



Assume best point found so far

Use **rejection sampling** to do exploitation



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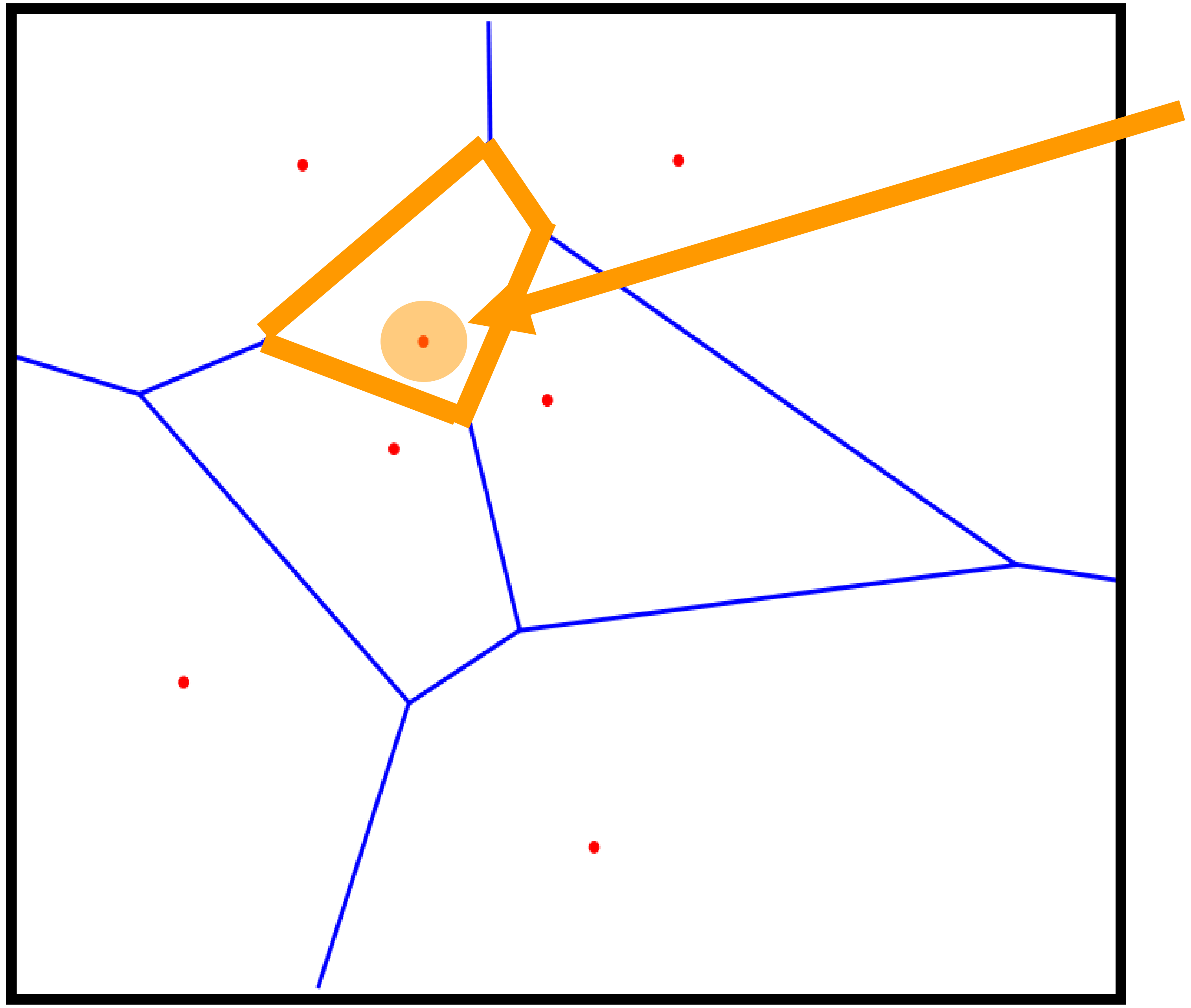
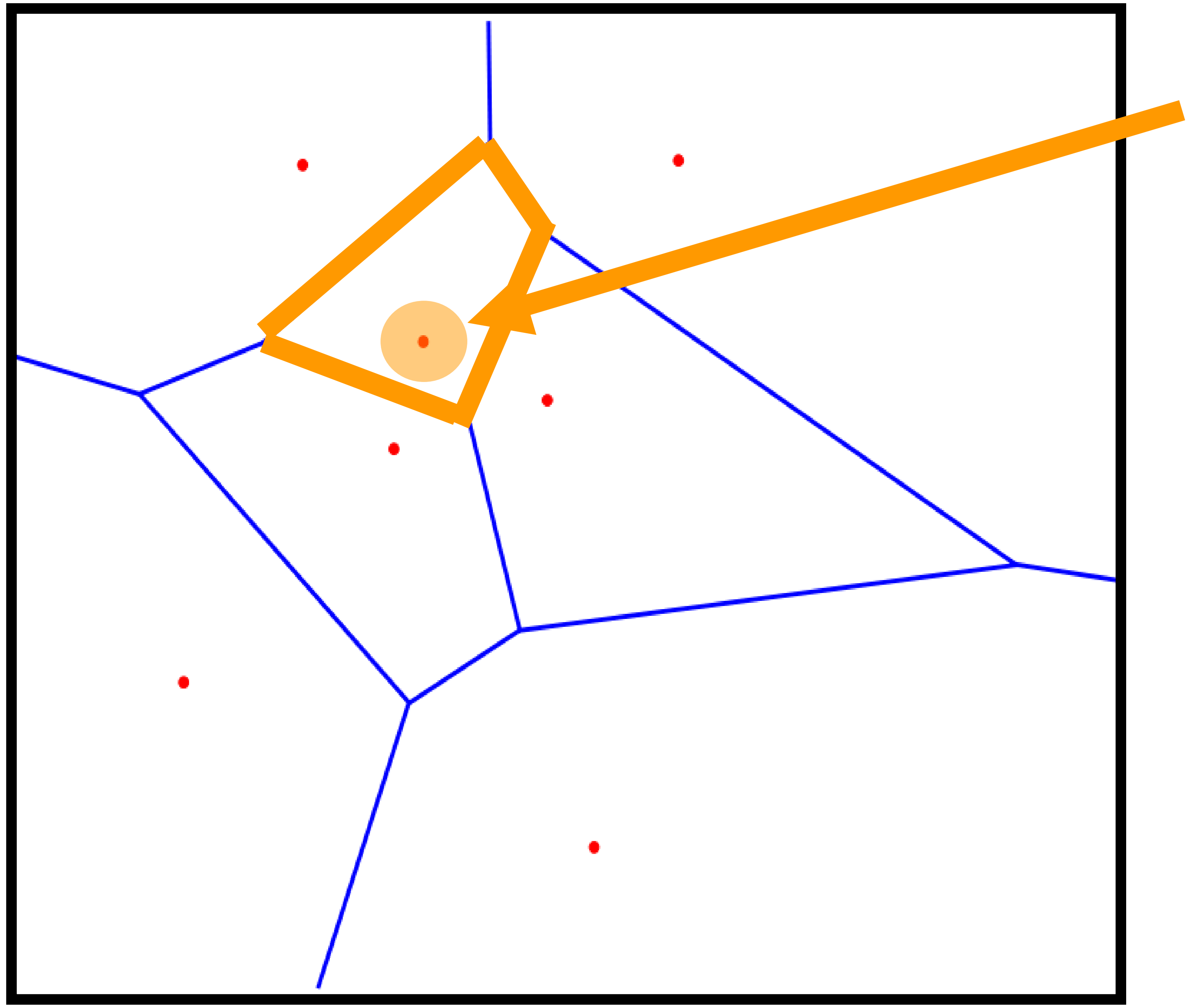


Assume best point found so far

Randomly Sample:

$$x_{t+1} \sim P(\mathcal{X})$$

Use **rejection sampling** to do exploitation



Assume best point found so far

Randomly Sample:

$$x_{t+1} \sim P(\mathcal{X})$$

Reject until the **sampled point is closest to the best point**

VOO: Voronoi optimistic optimization

$$\mathrm{VOO}(\mathcal{X}, \omega, d(\cdot,\cdot), n)$$

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Search space

VOO: Voronoi optimistic optimization

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Search space

Exploration parameter

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Search space

Exploration parameter

Distance metric

VOO: Voronoi optimistic optimization

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Search space

Exploration parameter

Distance metric

Budget

VOO: Voronoi optimistic optimization

$$\mathrm{VOO}(\mathcal{X}, \omega, d(\cdot,\cdot), n)$$

With probability ω

$$x_{t+1} \sim \mathrm{UniformRandomlySample}(\mathcal{X})$$

VOO: Voronoi optimistic optimization

$$\mathrm{VOO}(\mathcal{X}, \omega, d(\cdot,\cdot), n)$$

With probability ω **Exploration**

$$x_{t+1} \sim \mathrm{UniformRandomlySample}(\mathcal{X})$$

VOO: Voronoi optimistic optimization

$$\mathrm{VOO}(\mathcal{X}, \omega, d(\cdot,\cdot), n)$$

With probability ω **Exploration**

$$x_{t+1} \sim \mathrm{UniformRandomlySample}(\mathcal{X})$$

With probability $1-\omega$

$$x_{t+1} \sim \mathrm{SampleBestVCell}(d(\cdot,\cdot), x_{1:t})$$

VOO: Voronoi optimistic optimization

$$\mathrm{VOO}(\mathcal{X}, \omega, d(\cdot,\cdot), n)$$

With probability ω

Exploration

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Exploitation

VOO: Voronoi optimistic optimization

$$\mathrm{VOO}(\mathcal{X}, \omega, d(\cdot,\cdot), n)$$

With probability ω

Exploration

$$x_{t+1} \sim \mathrm{UniformRandomlySample}(\mathcal{X})$$

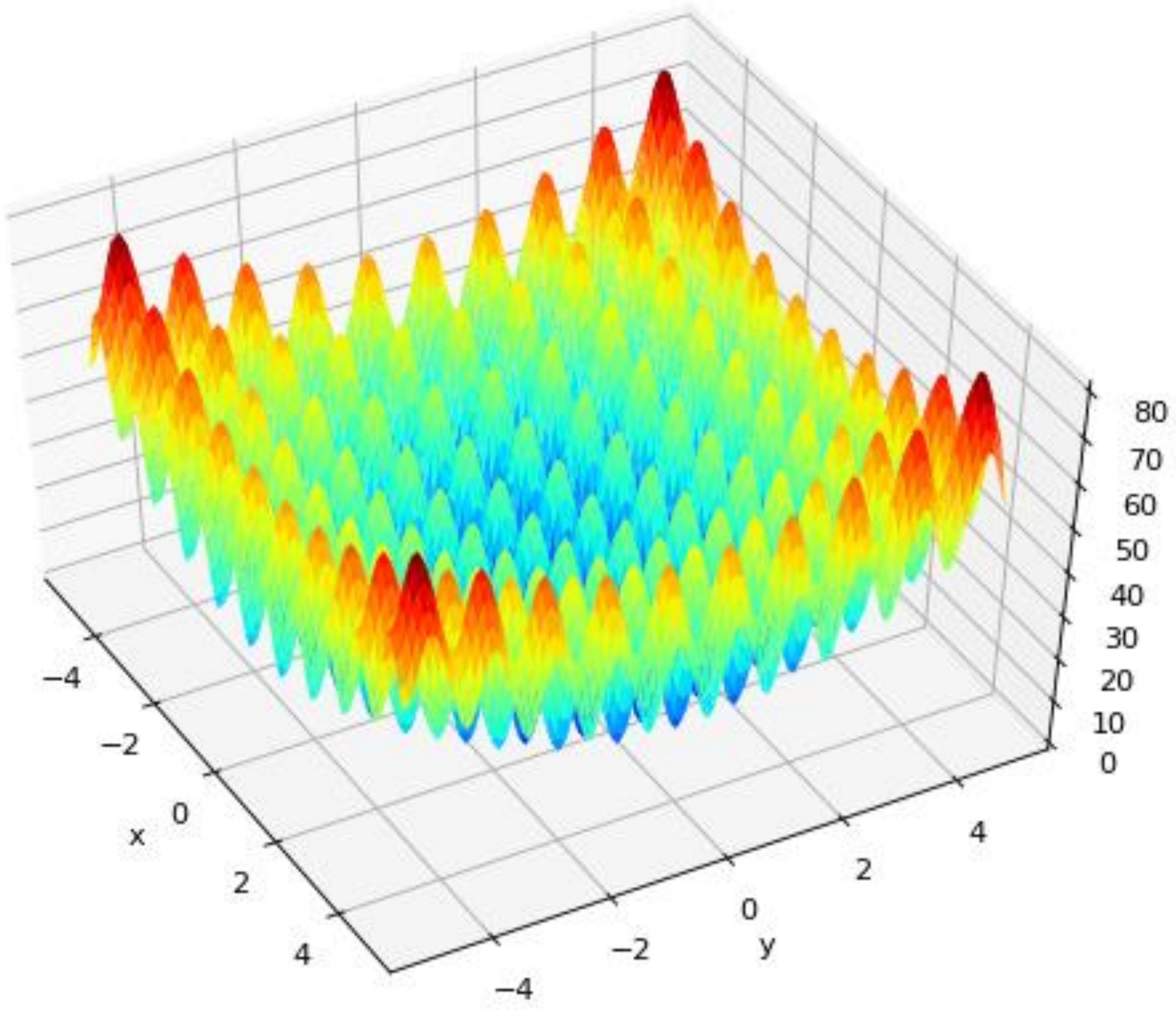
With probability $1 - \omega$

$$x_{t+1} \sim \mathrm{SampleBestVCell}(d(\cdot,\cdot), x_{1:t})$$

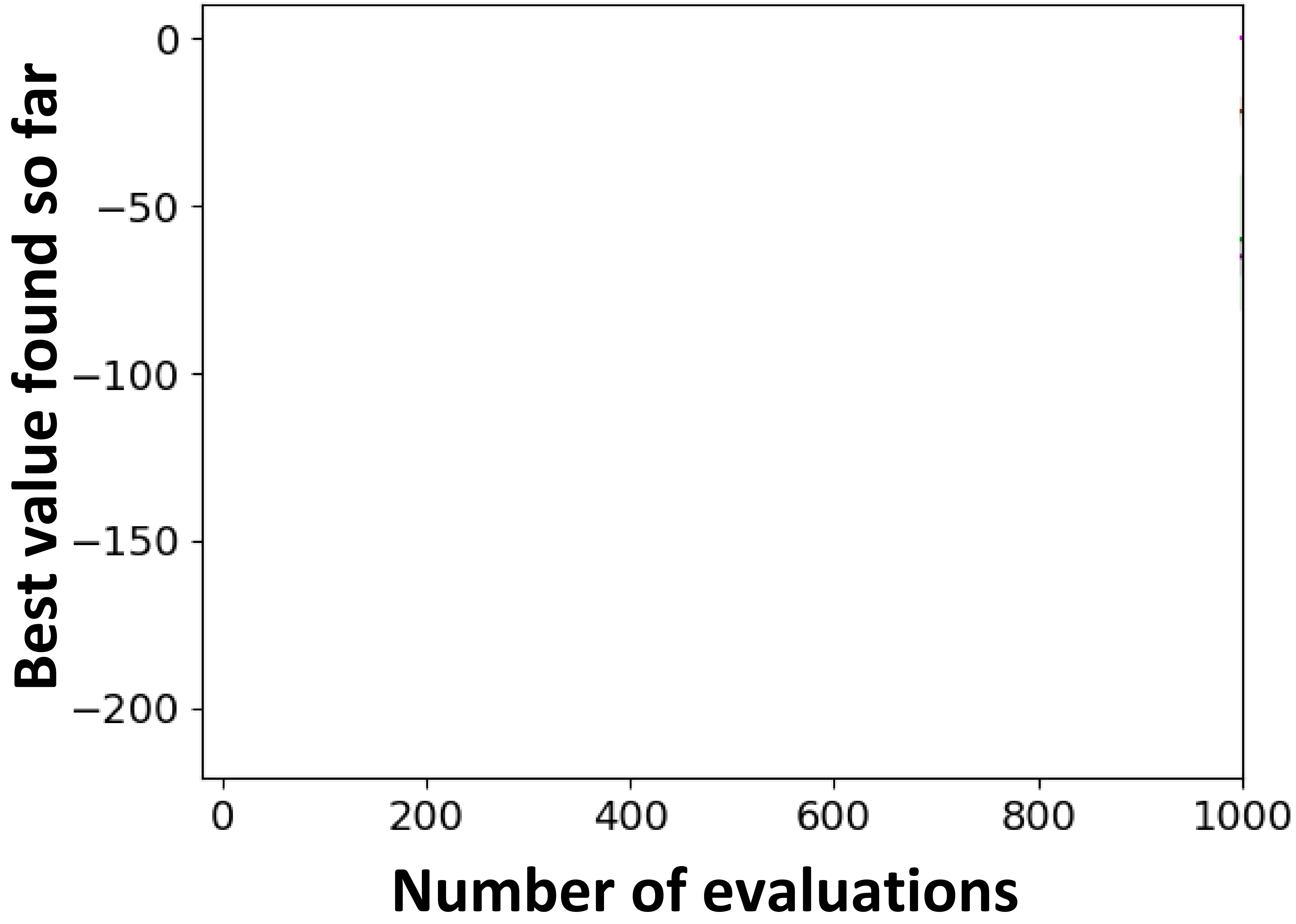
Evaluate $f(x_{t+1})$

Exploitation

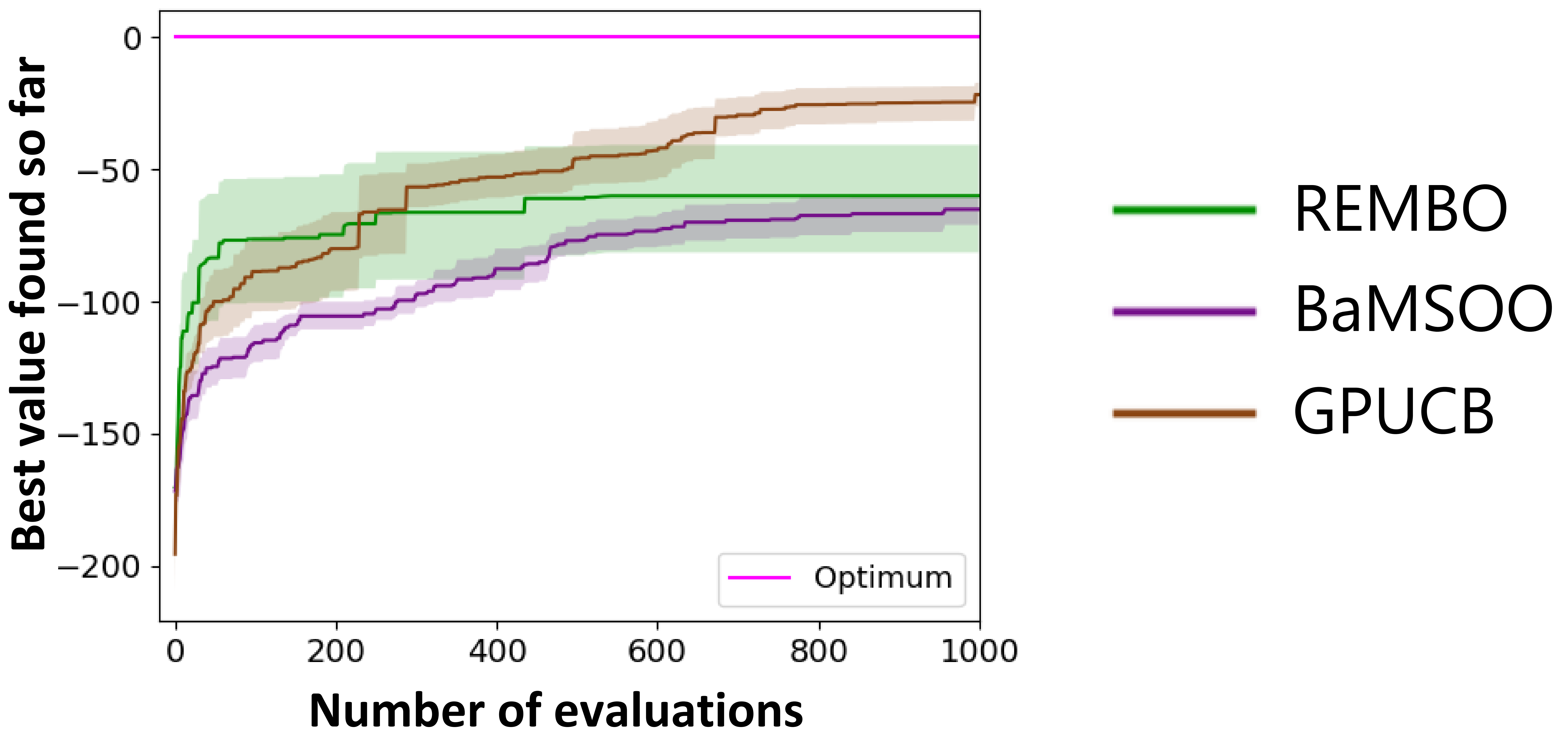
Optimizing Rastrigin function



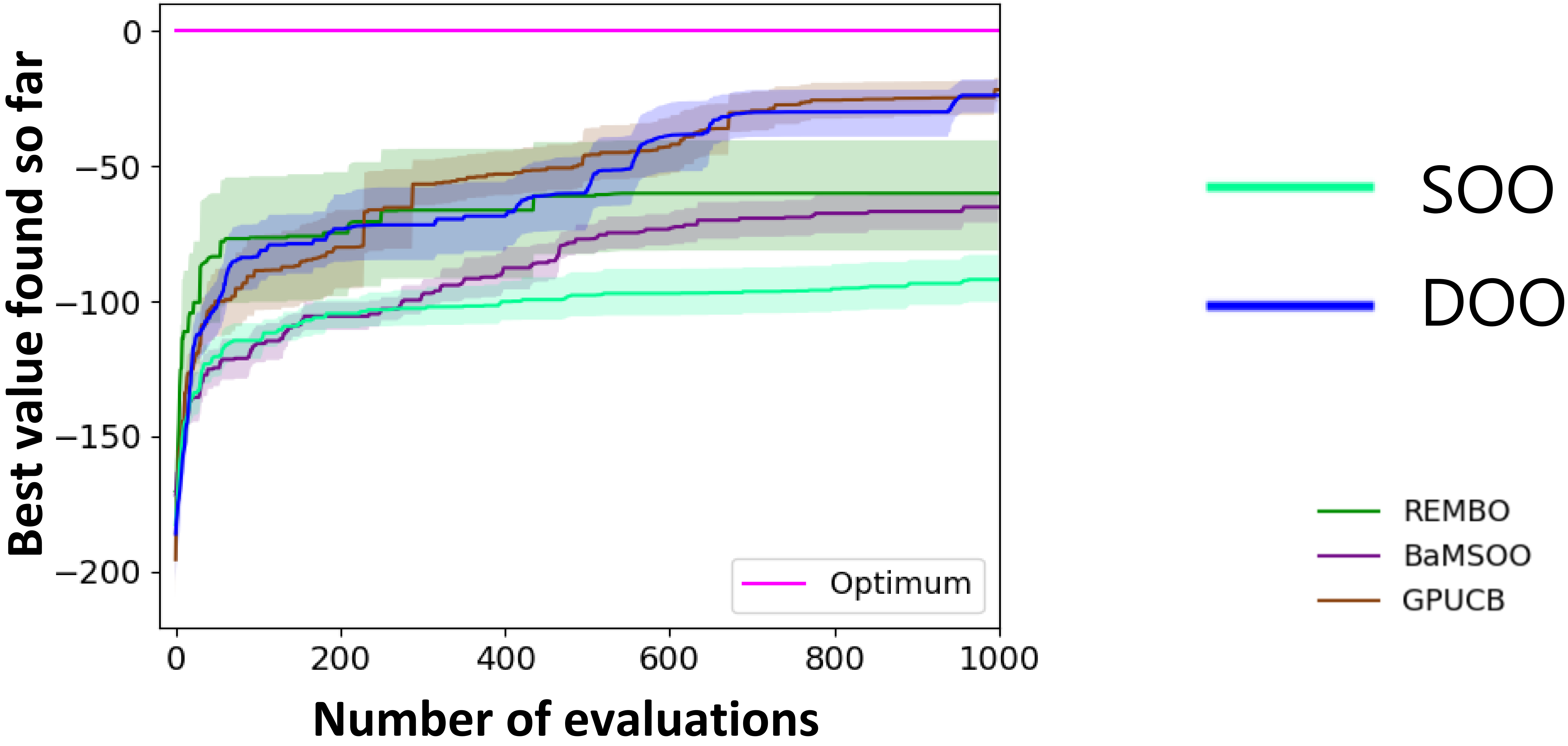
Optimizing **10 dimensional** Rastrigin function



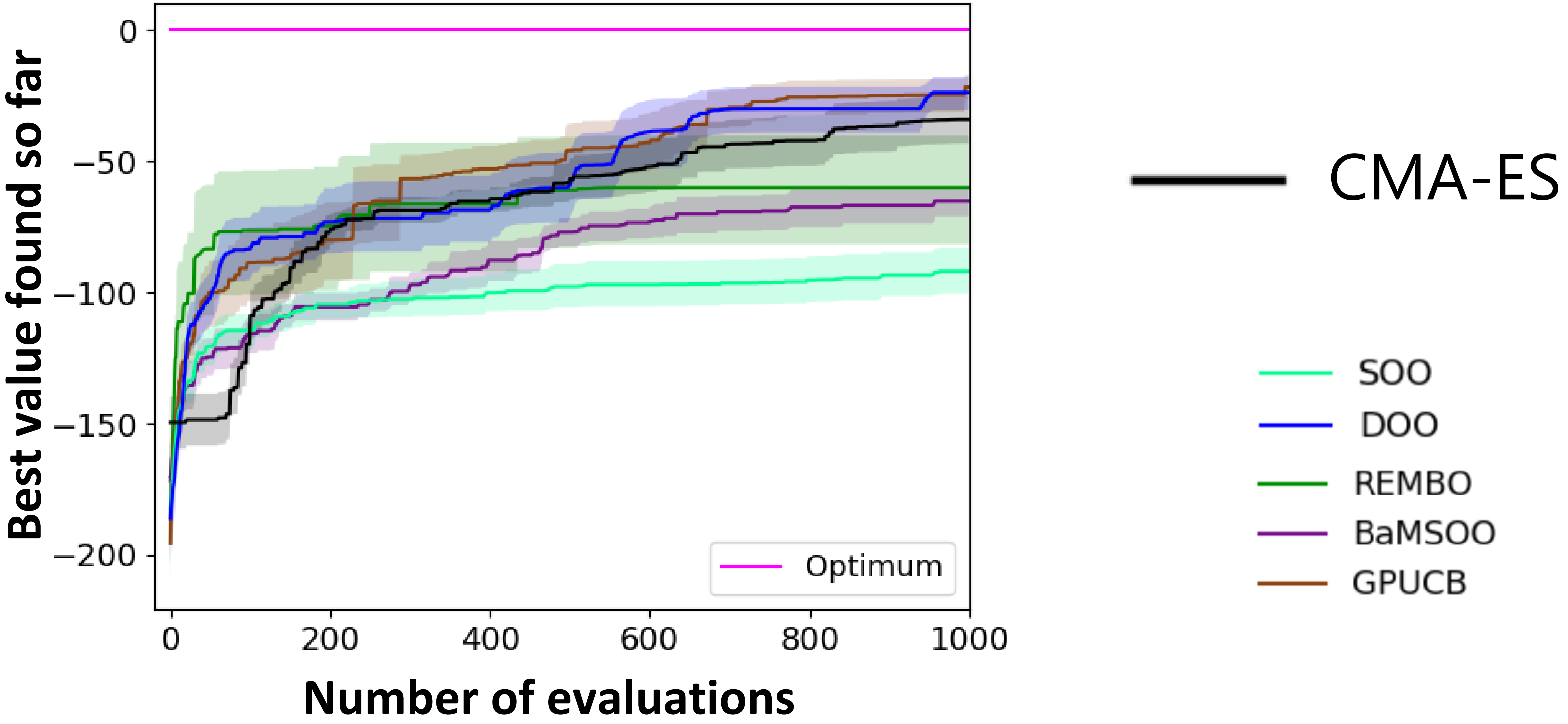
10D – Bayesian optimization methods



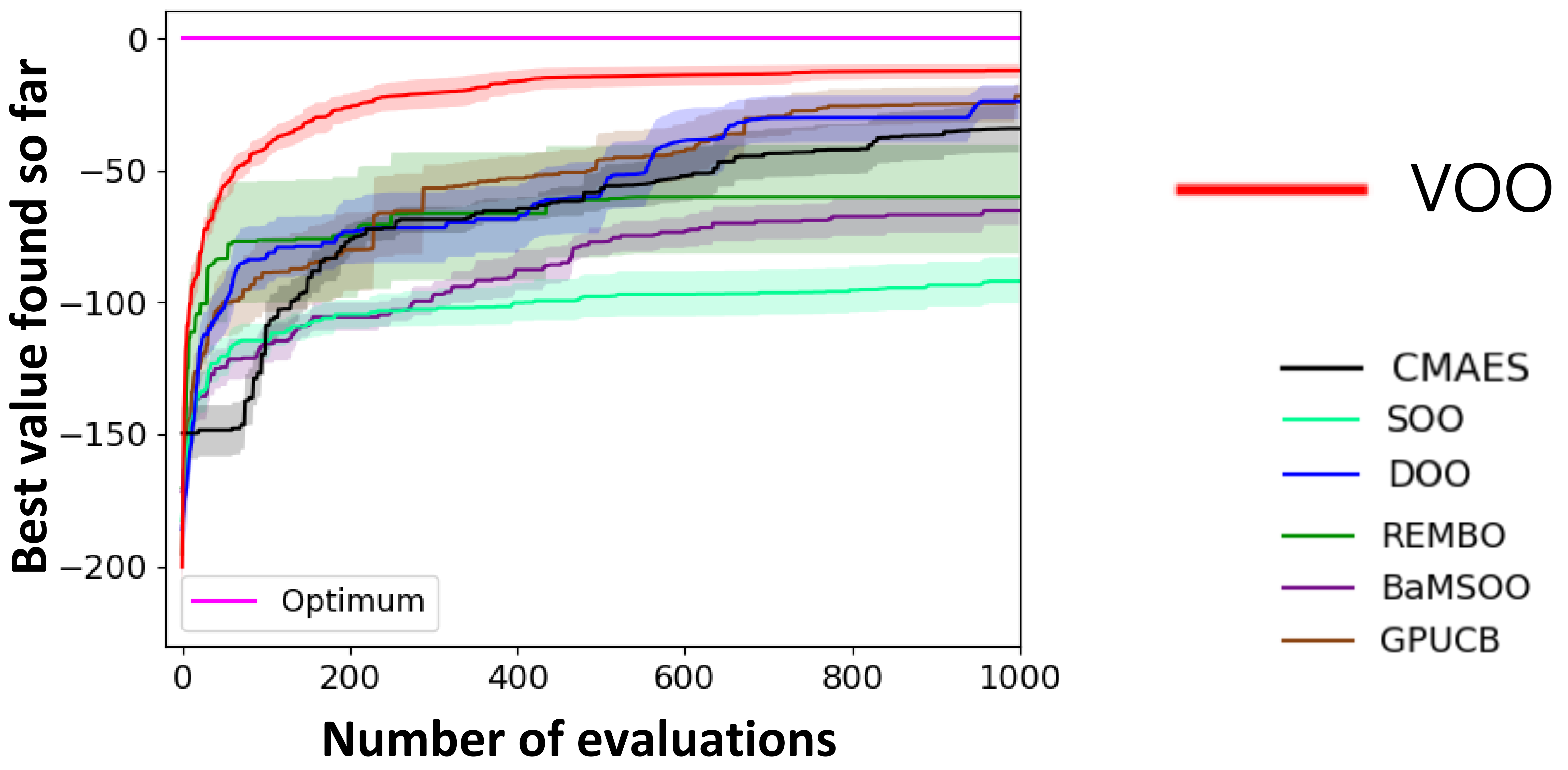
10D – Hierarchical partitioning methods



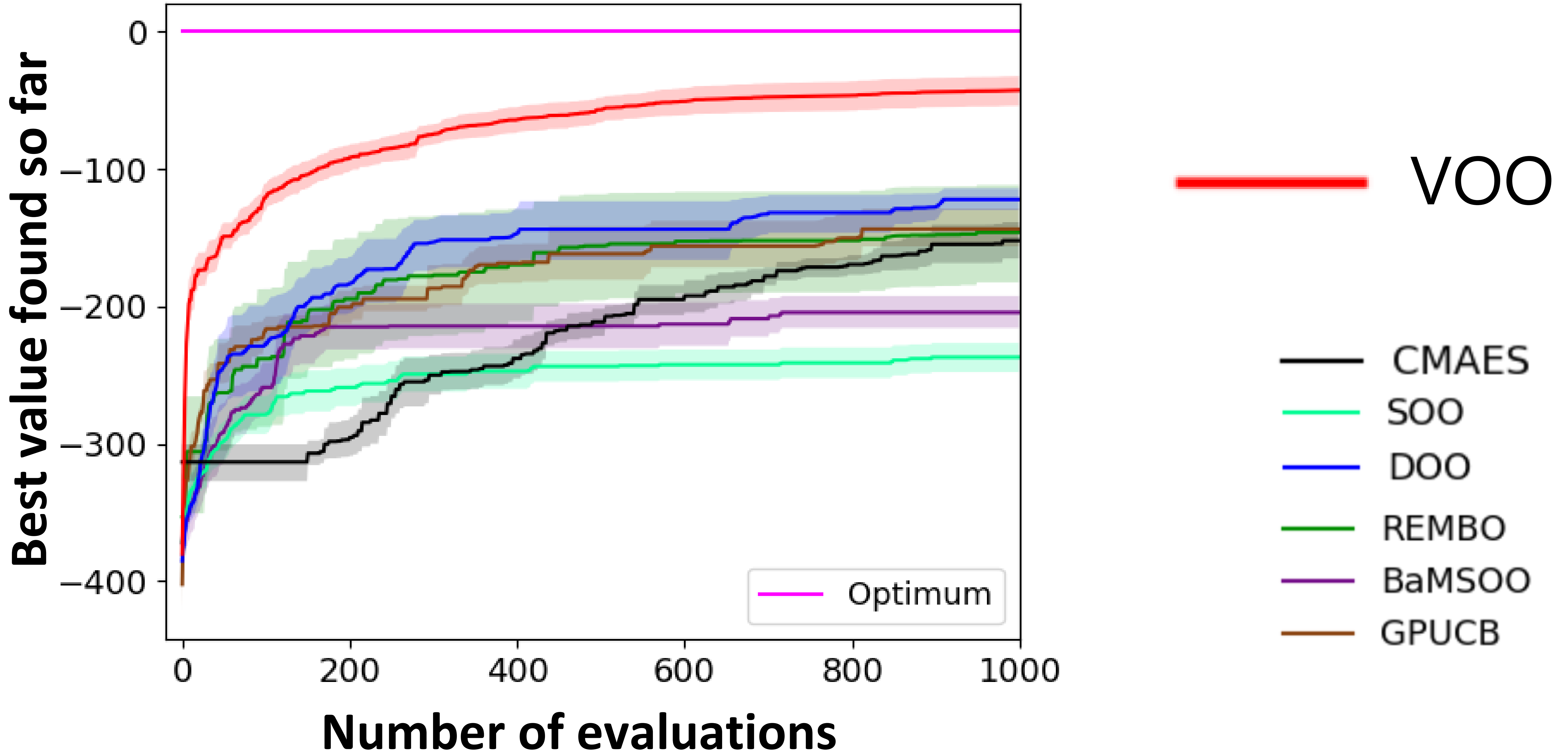
10D – Evolutionary algorithm



10D – Voronoi optimistic optimization



20D – even more drastic difference



From BBFO to MCTS

- So that was when **planning horizon is 1**
- What about **planning horizon >= 1**, for **deterministic environments?**

VOO applied to Trees (VOOT): high-level idea

Assign a VOO agent at each node

VOO applied to Trees (VOOT): high-level idea

Assign a VOO agent at each node

Solve the action optimization problem using the **estimated Q-function**

$$\max_{a \in \mathcal{A}} \hat{Q}(s, a)$$

Our main theoretical result

How many simulations do we need to guarantee

$$V_\star(s_0) - \hat{V}_N(s_0) \leq \eta, \eta > 0$$

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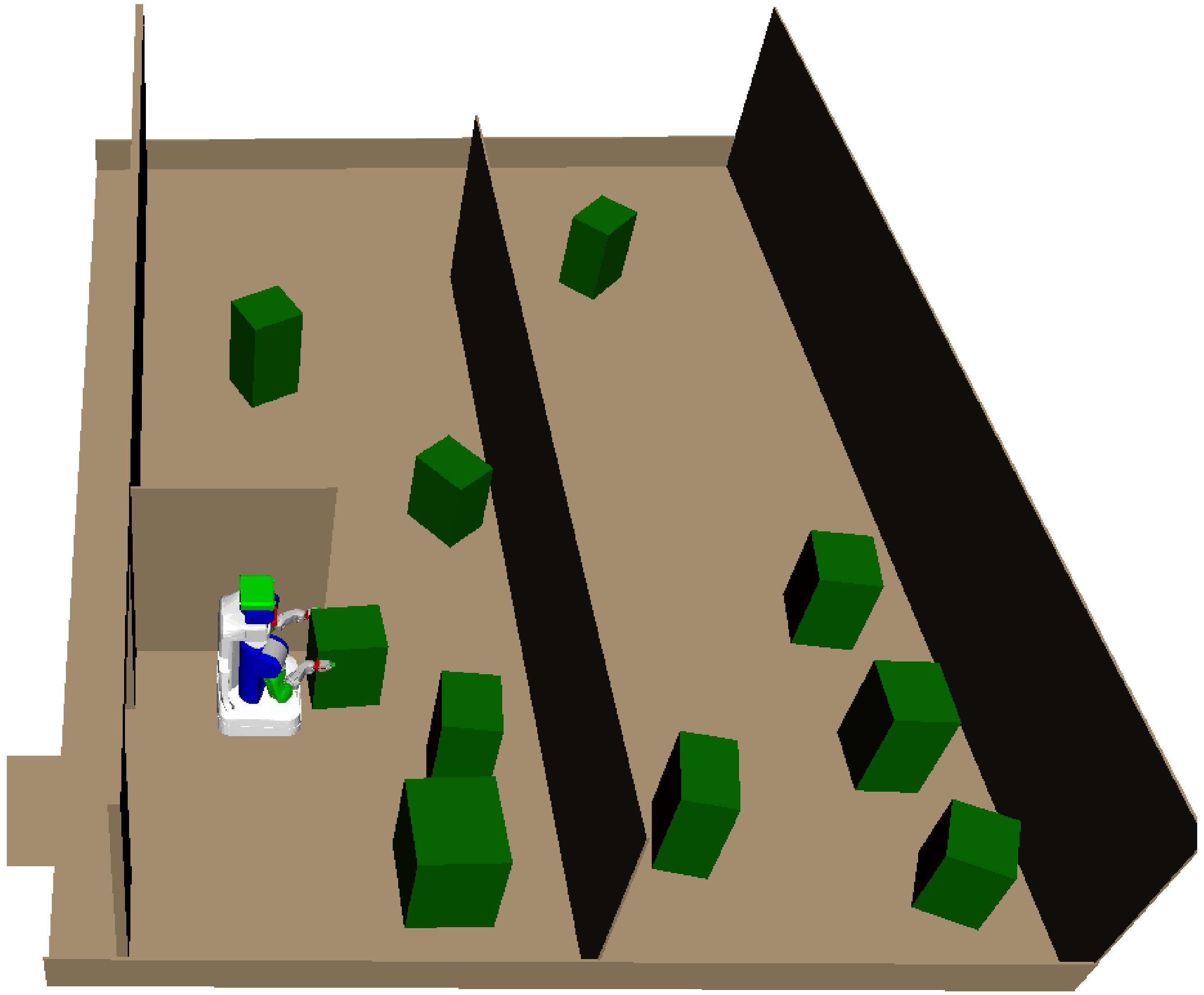
$$V_\star(s_0) - \hat{V}_N(s_0) \leq \eta, \eta > 0$$

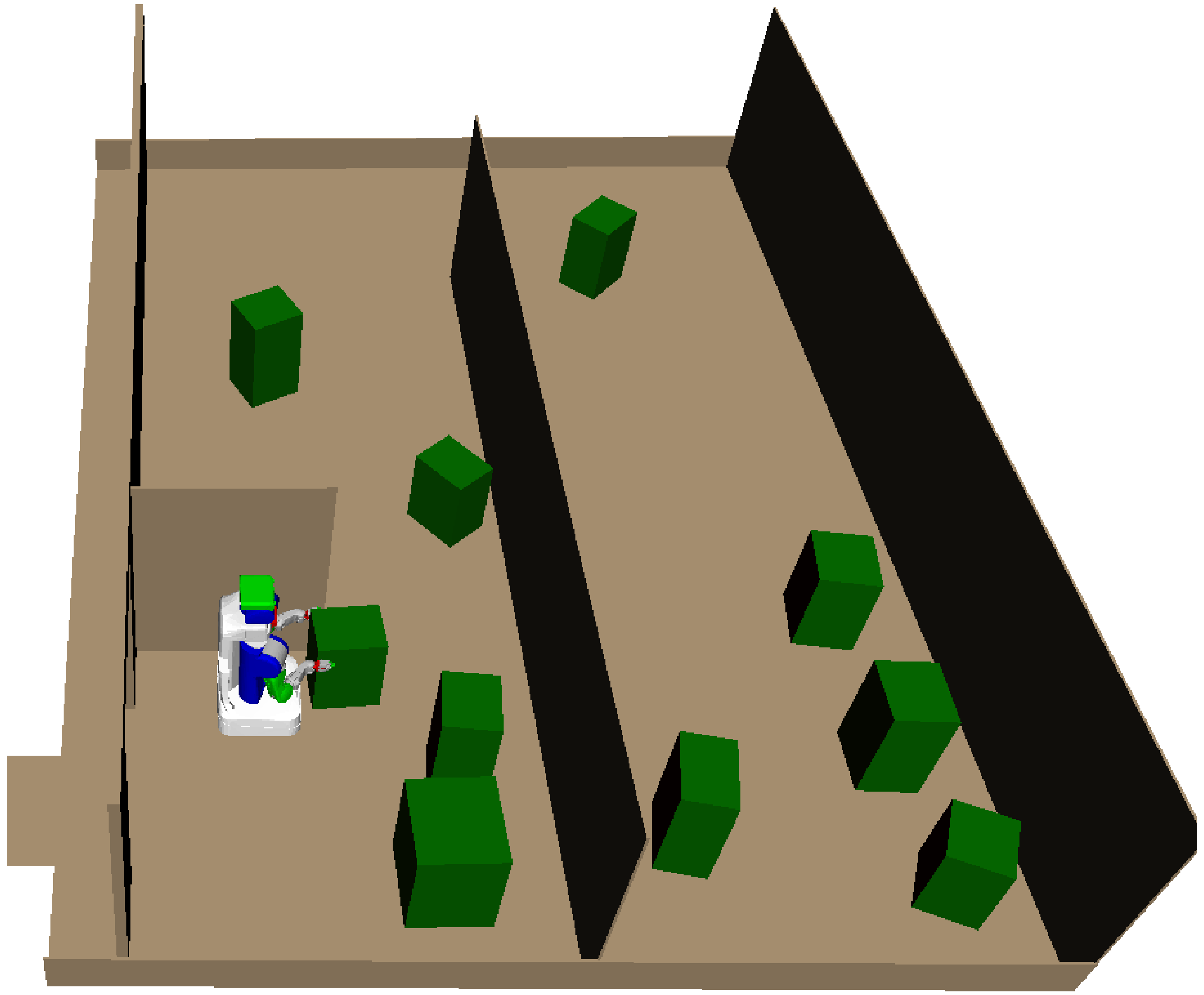
Under mild assumptions, $\mathbb{E}[N] = m^h$

$$m = \log\left(\frac{\eta(1-\gamma)}{2L\delta_{max}C_{max}}\right) \cdot \min(G_{\lambda,\omega}, K_{\nu,\omega,\lambda})$$

Packing problem

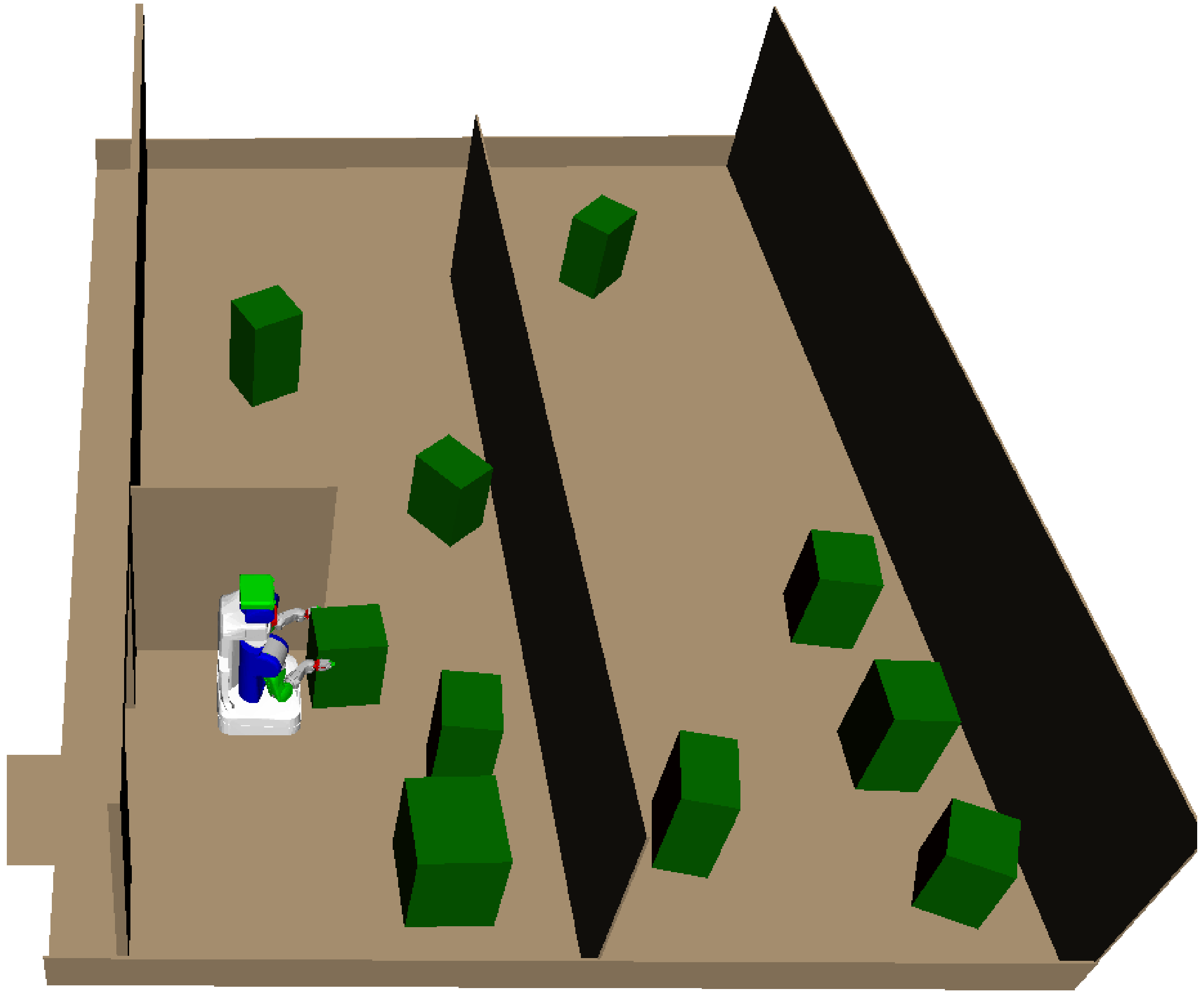


Packing problem



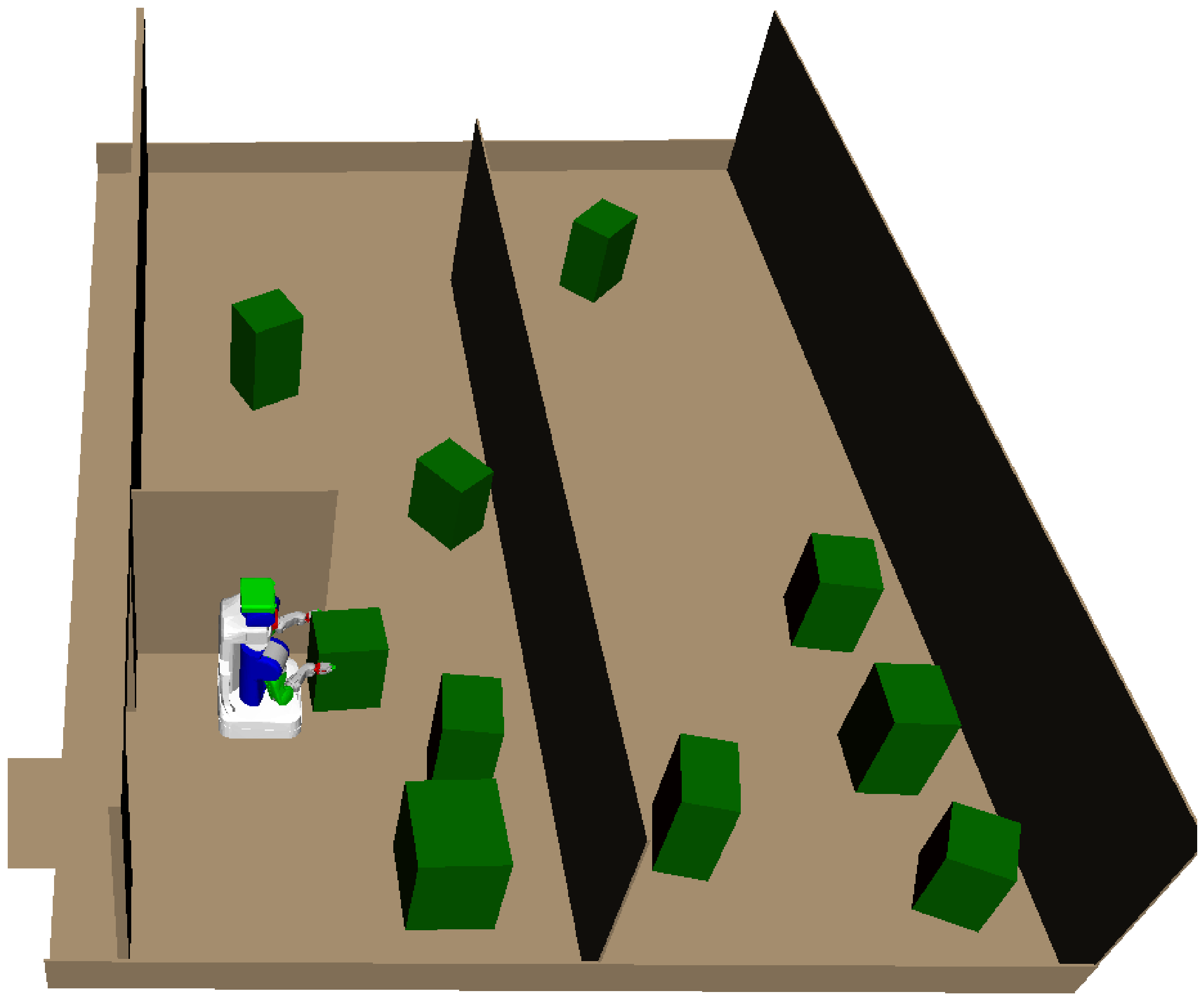
- **Actions**: placements for three boxes (9 dim)

Packing problem



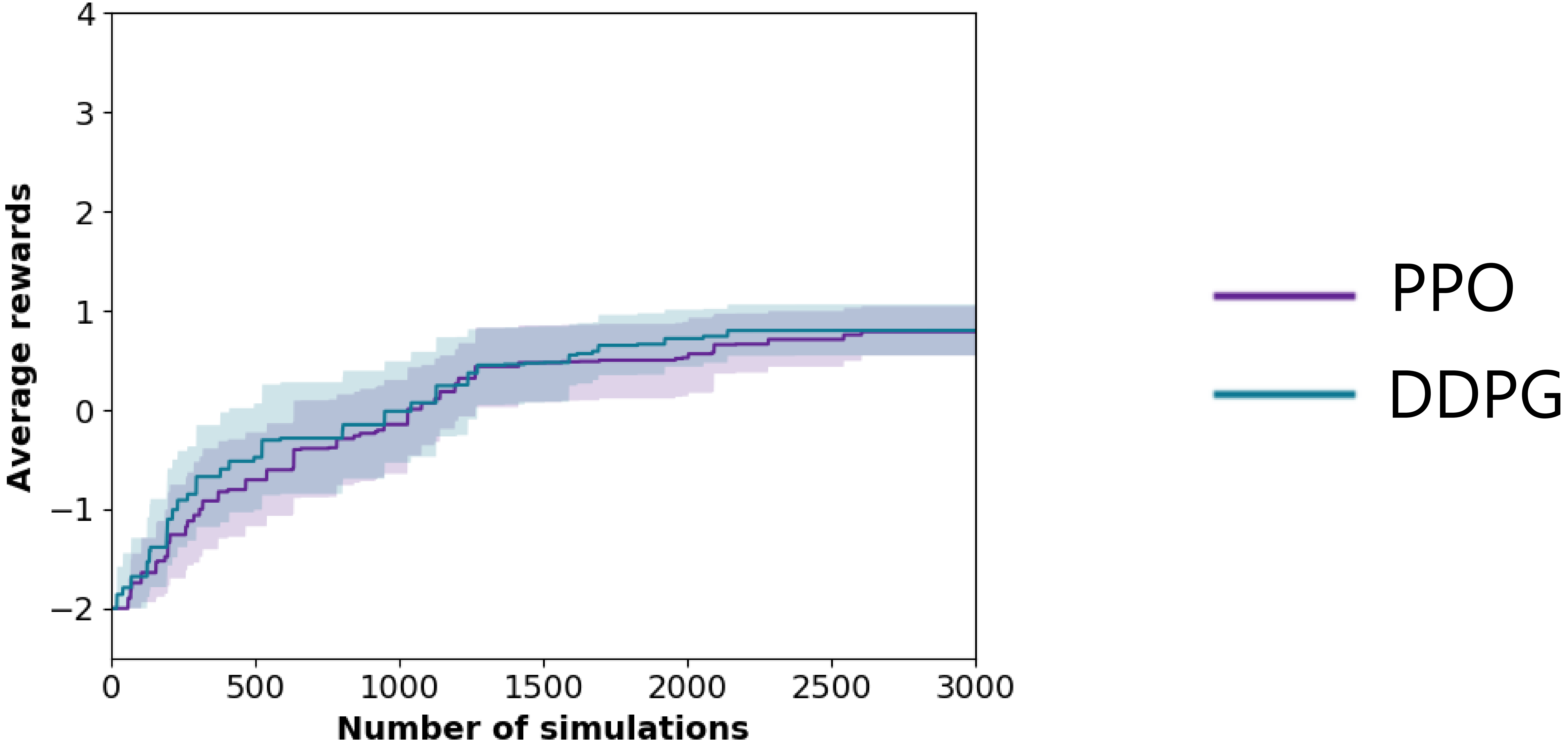
- **Actions**: placements for three boxes (9 dim)
- **Reward function**:
  - 1/d if feasible,
  - r_min otherwise

Packing problem

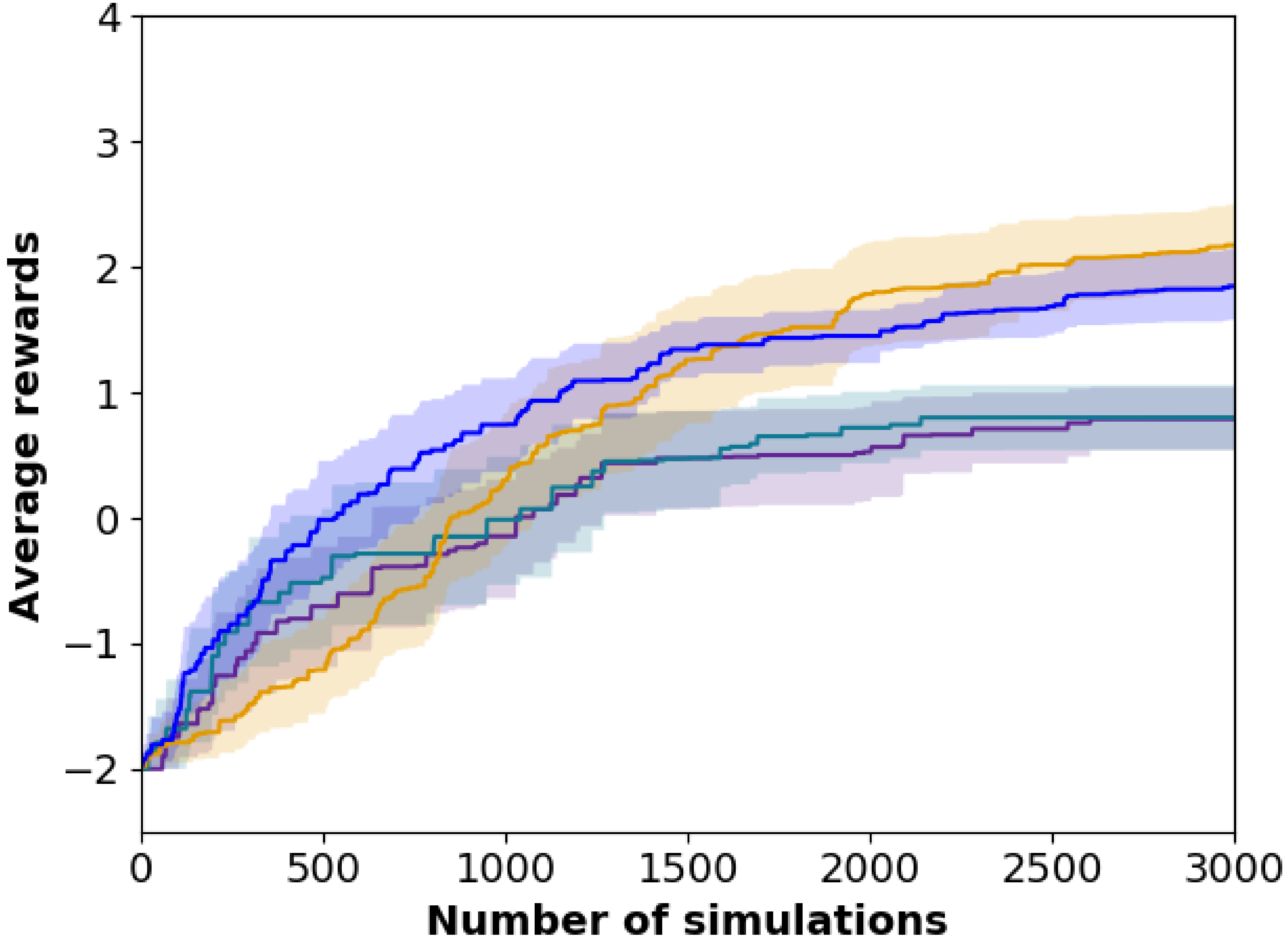


- **Actions**: placements for three boxes (9 dim)
- **Reward function**:
  - 1/d if feasible,
  - r_min otherwise
- **Total boxes to pack**: 20

State-of-the-art **RL algorithms**

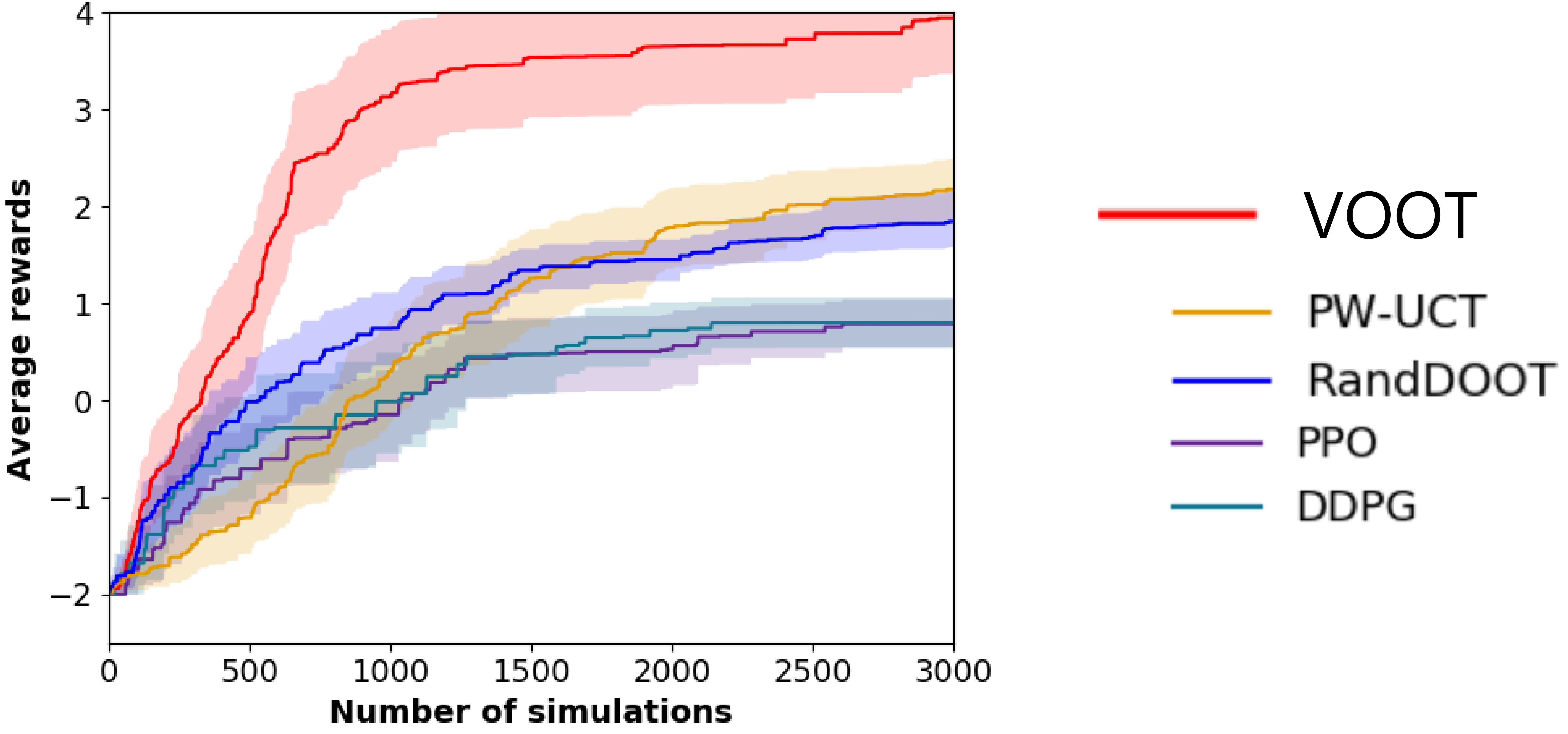


State-of-the-art **continuous-action MCTS**



PW-UCT
DOOT
PPO
DDPG

VOO applied to Trees



Takeaways

Voronoi Optimistic Optimization applied to Trees (VOOT) for **deterministic environment**

- Empirical contribution: improvement over the state-of-the-art, especially in **high-dimensional action-spaces**
- Theoretical contribution: **regret-bound for VOOT**