Tutorial 1

Bayesian Optimization and Reinforcement Learning

Shadan Golestan
golestan@ualberta.ca

Machine Learning Paradigms

Machine Learning Paradigms

Supervised Learning

📊 **Data:** (x, y)

x: features, y: label

🎯 **Goal:** learn a function to map $y \rightarrow x$

💡 **Example:**

Cats: 😸😺😼

Dogs: 🐶🐶🐶

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Unsupervised Learning

📊 **Data:** (x)

x: features, no label

🎯 **Goal:** learn underlying structure

💡 **Example:**

These are similar things 😸😺😼

These are similar things 🐶🐶🐶

Machine Learning Paradigms

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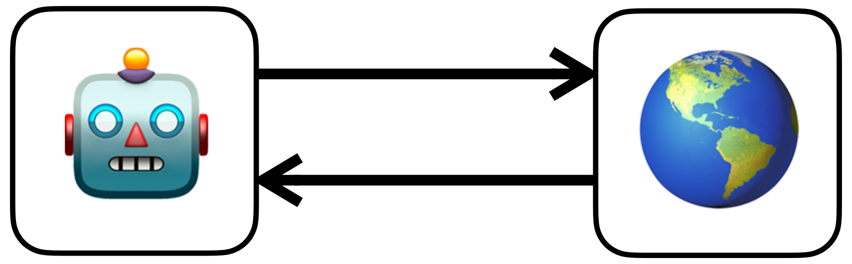
Sequential Decision Making

📊 **Data:**



🎯 **Goal:** maximize some reward

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🤖 eats 🍎 because it keeps 🤖 alive

Machine Learning Paradigms

Supervised Learning

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Dogs: 🐶🐶🐶

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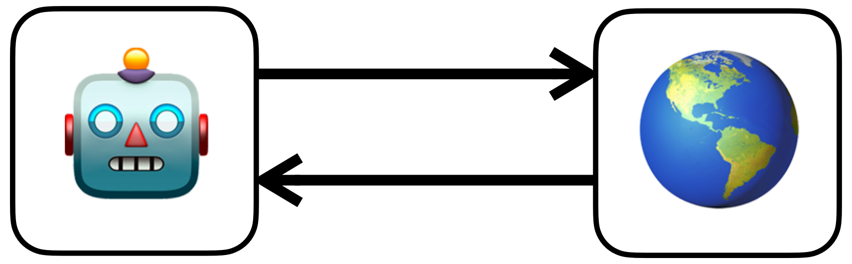

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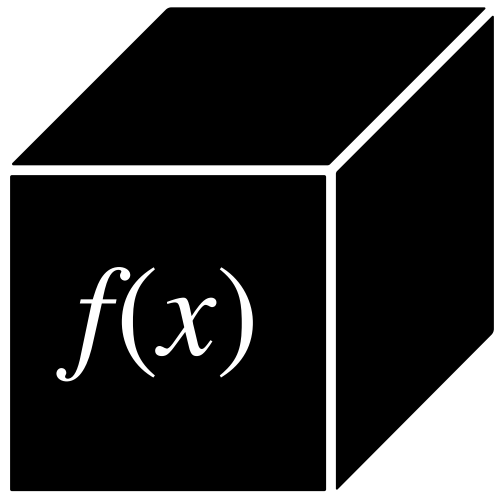
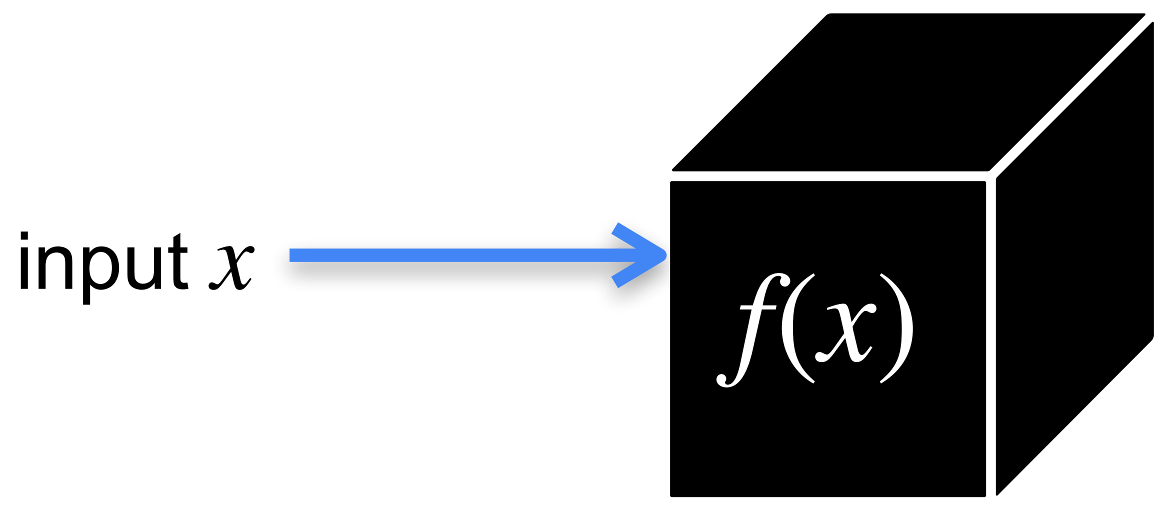
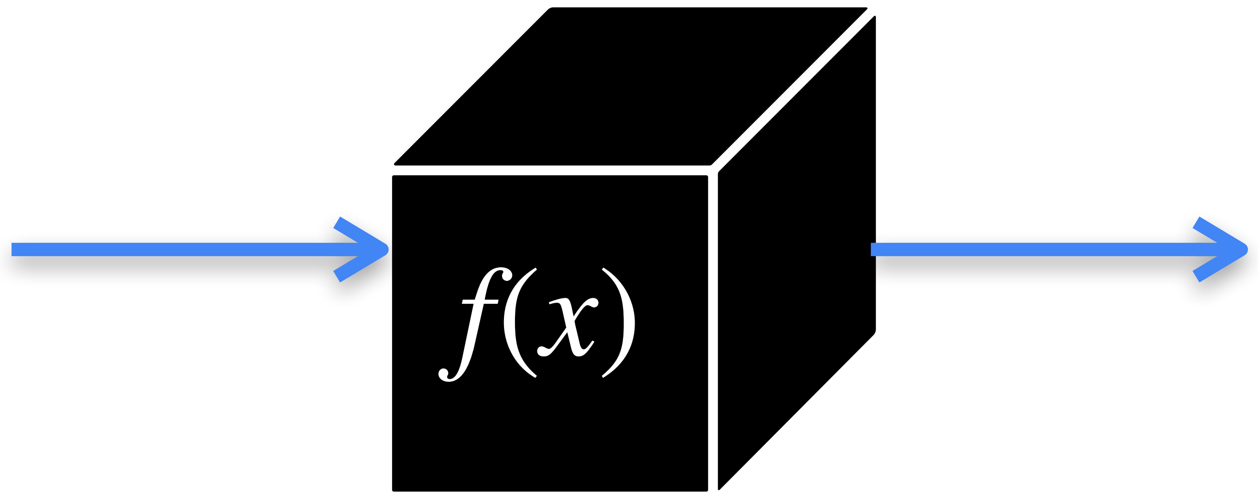


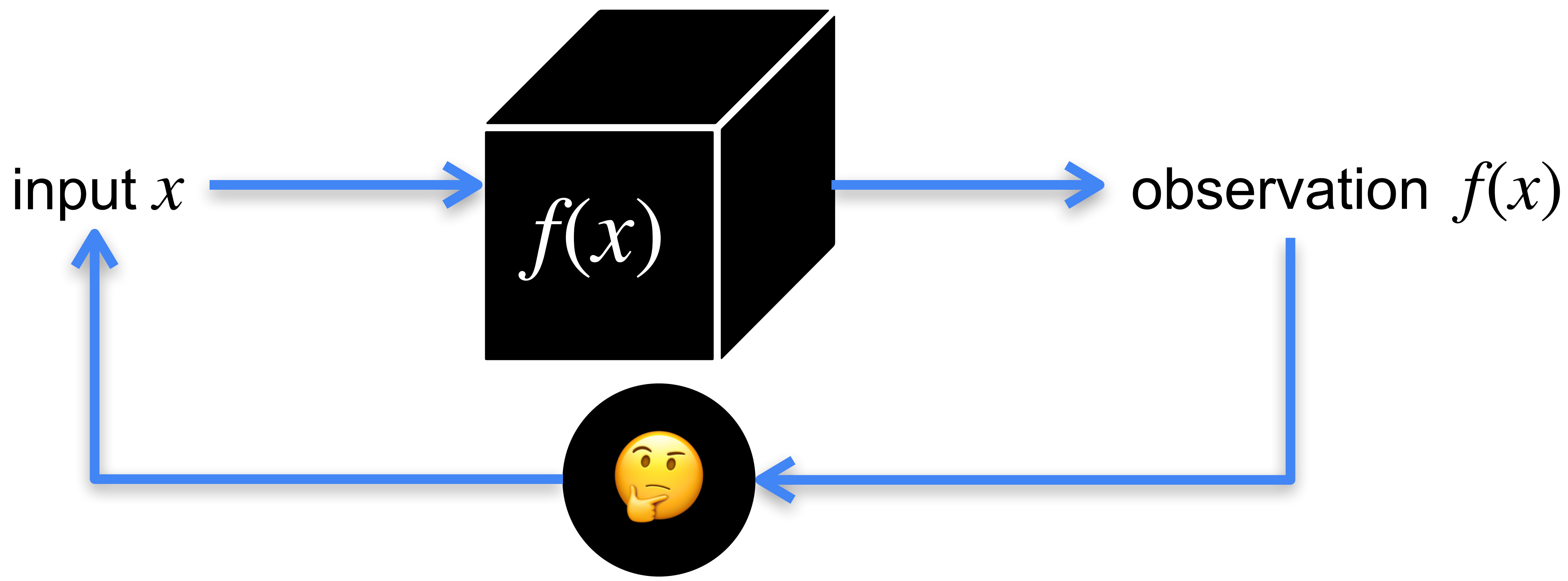
Sequential Decision Making



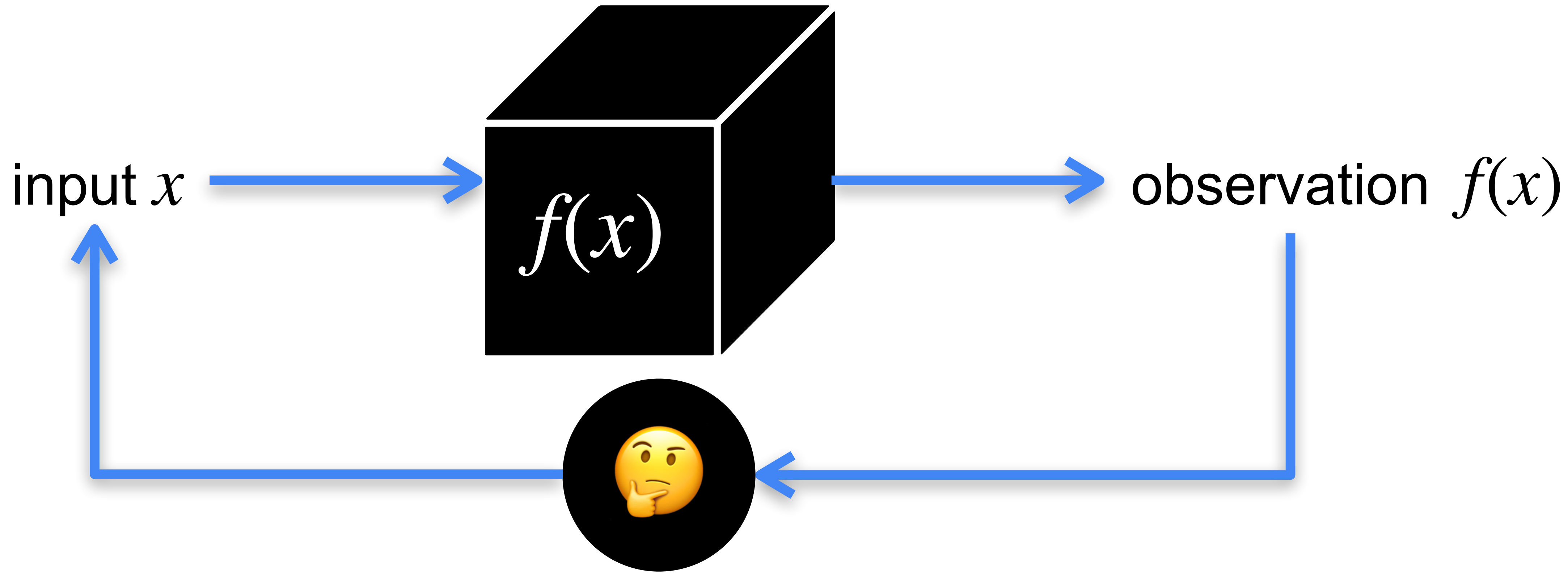
Sequential Decision Making

input x  observation $f(x)$

Sequential Decision Making



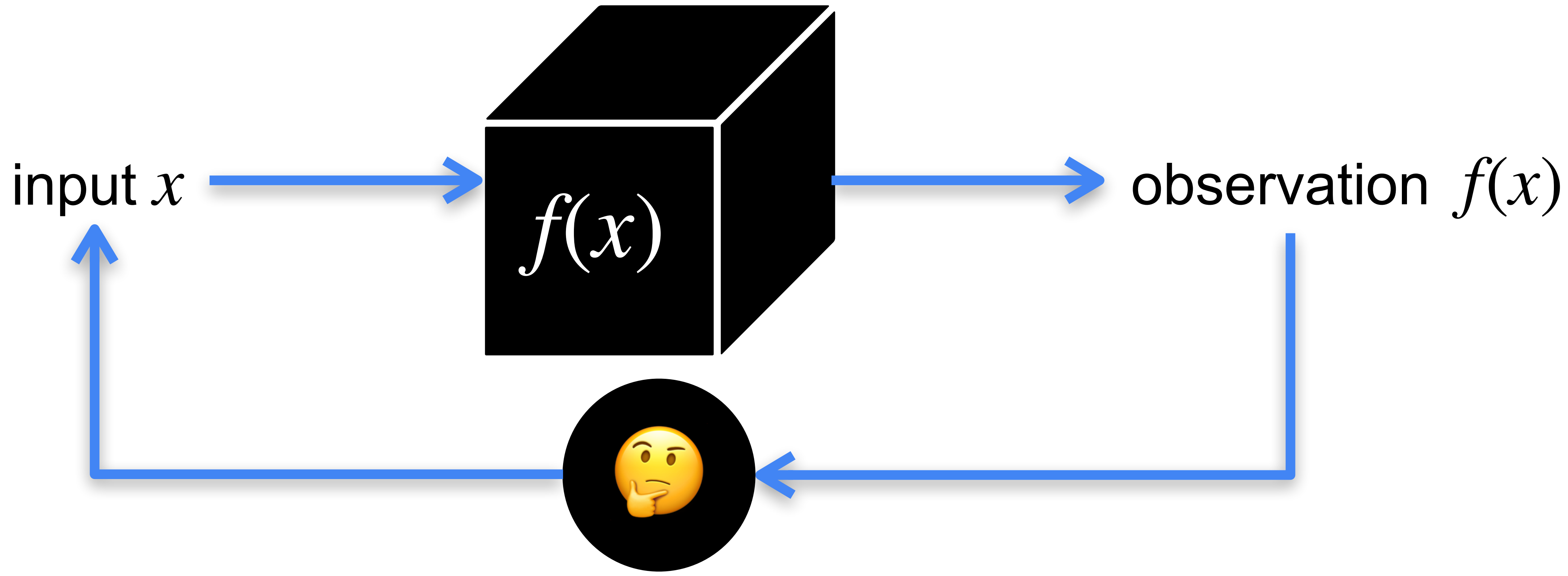
Sequential Decision Making



Estimation of Distribution Algorithms (Bayesian Optimization)

Reinforcement Learning

Sequential Decision Making



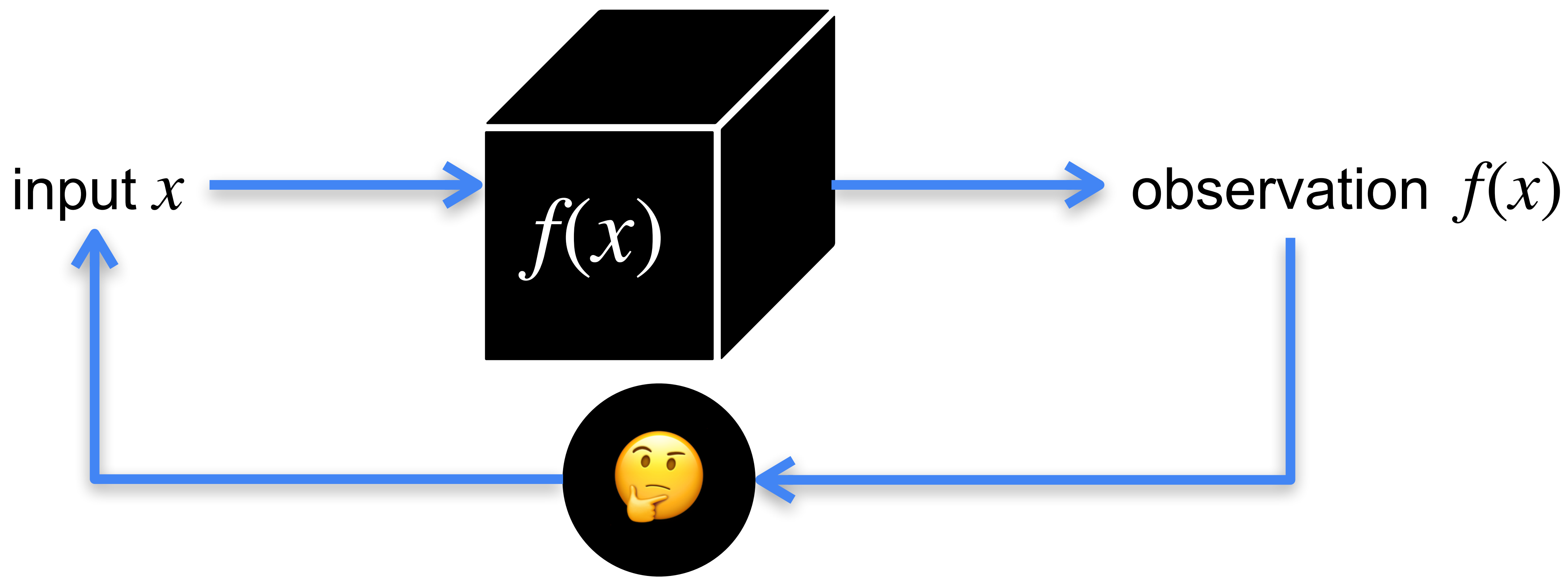
Estimation of Distribution Algorithms (Bayesian Optimization)

📦 **Function** $f(x)$

does not change with x (static)

Reinforcement Learning

Sequential Decision Making



Estimation of Distribution Algorithms (Bayesian Optimization)	Reinforcement Learning
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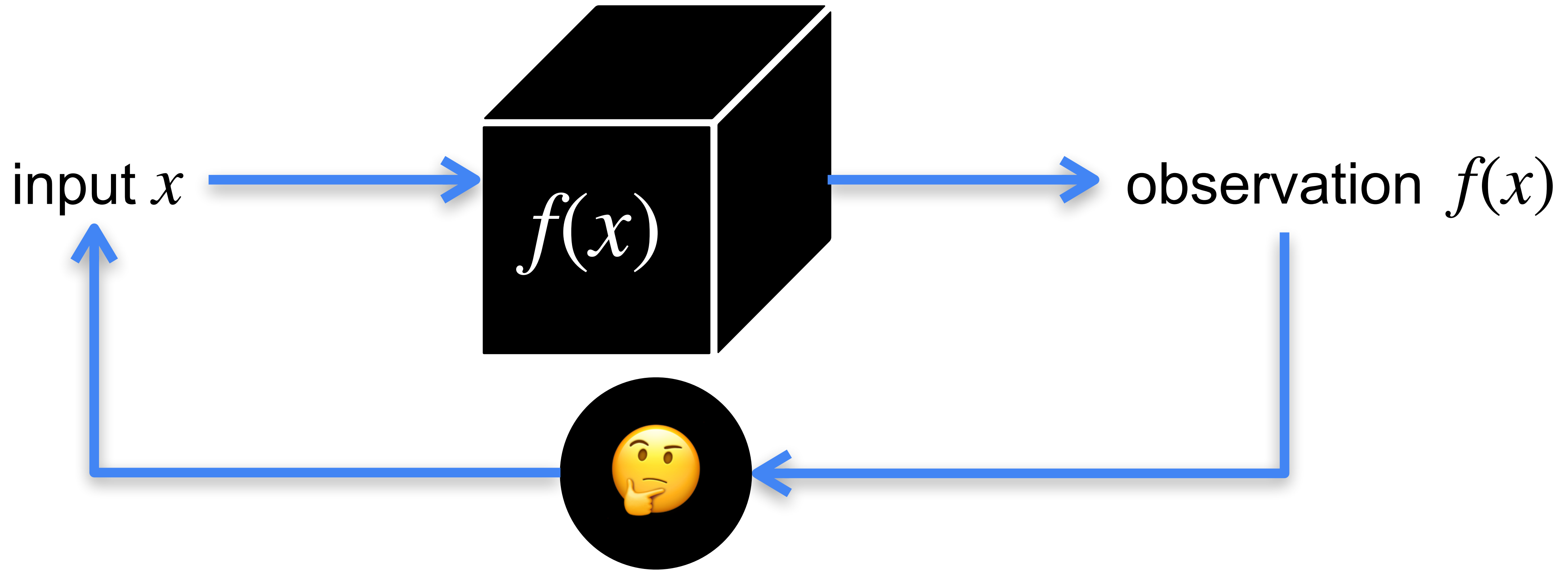

Estimation of Distribution Algorithms (Bayesian Optimization)	Reinforcement Learning
📦 **Function** $f(x)$ does not change with x (static)	📦 **Function** $f(x)$ changes with x (dynamic)
🎯 **Goal:** finding the best x	

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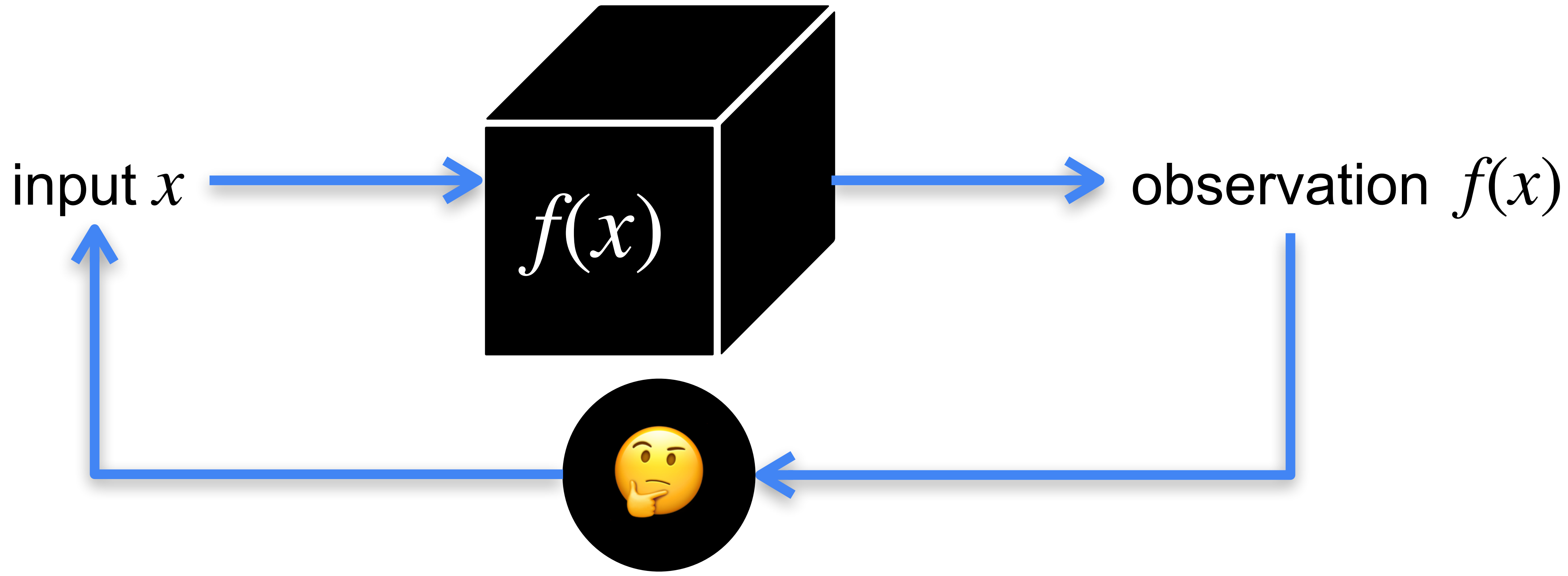

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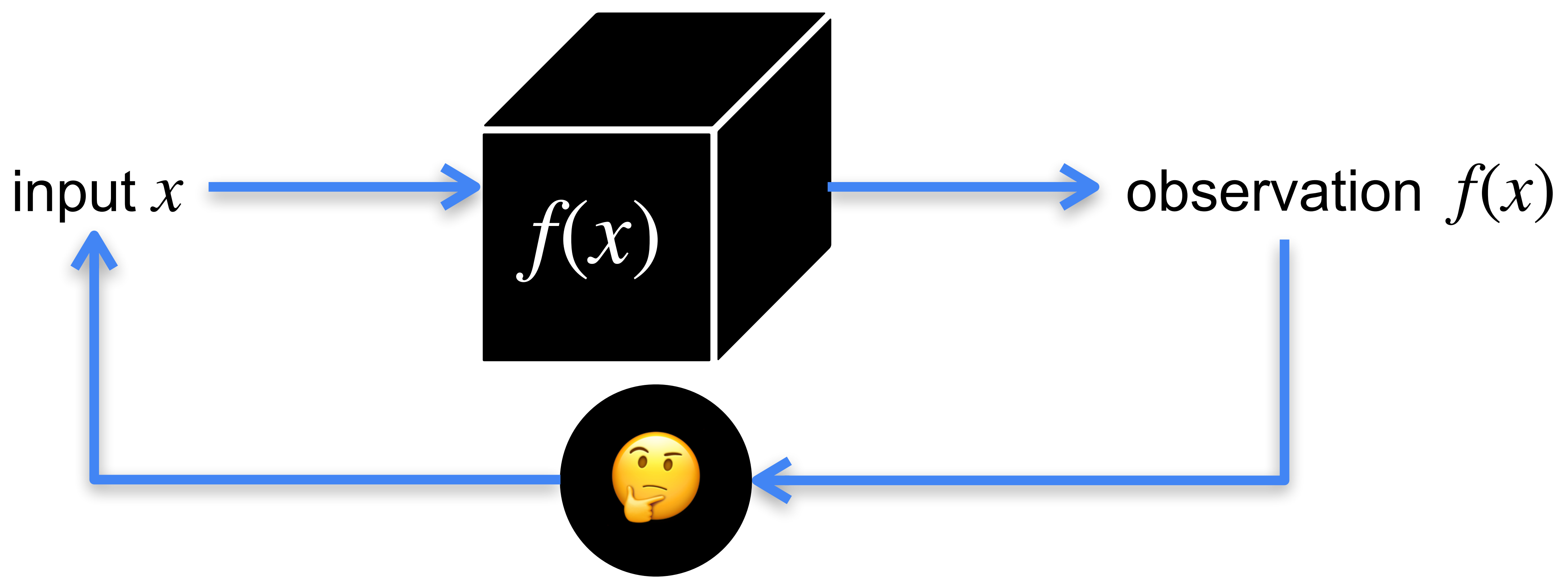
Reinforcement Learning

📦 **Function** $f(x)$ changes with x (dynamic)

🎯 **Goal:** finding a policy that gives the best x at each state of $f(x)$

Sequential Decision Making



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⚙️ **Process:** learn and improve decisions iteratively

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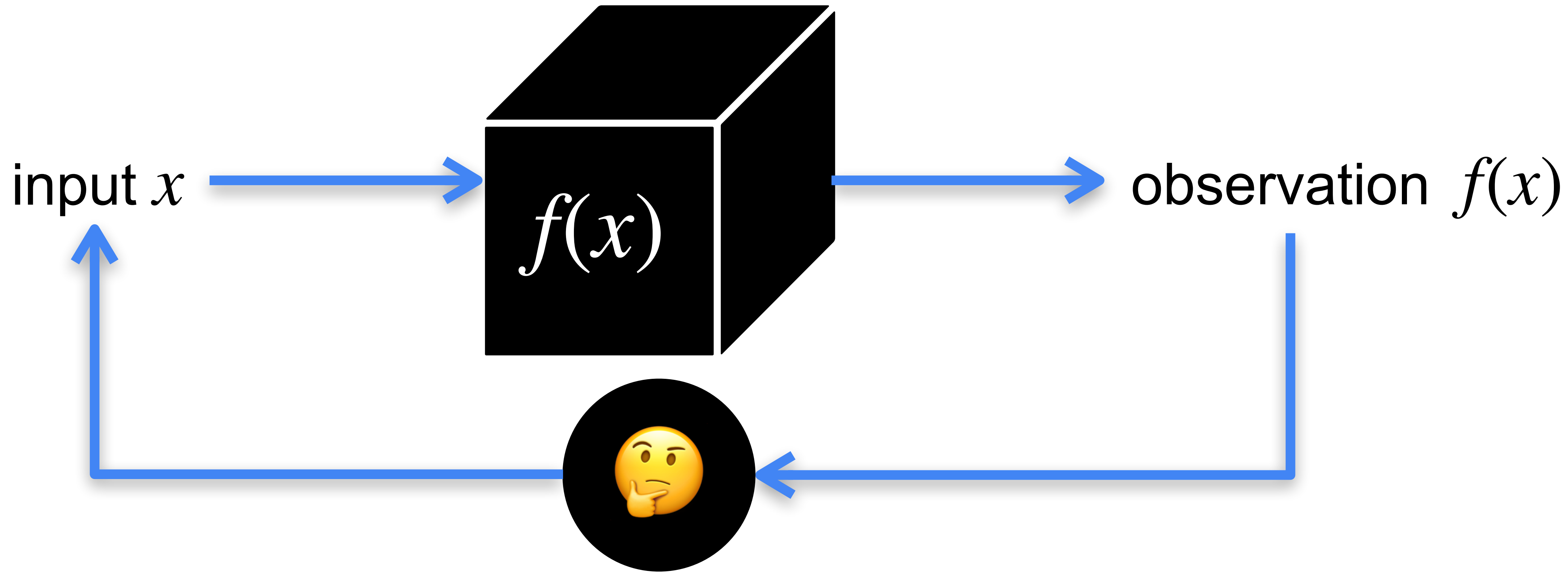

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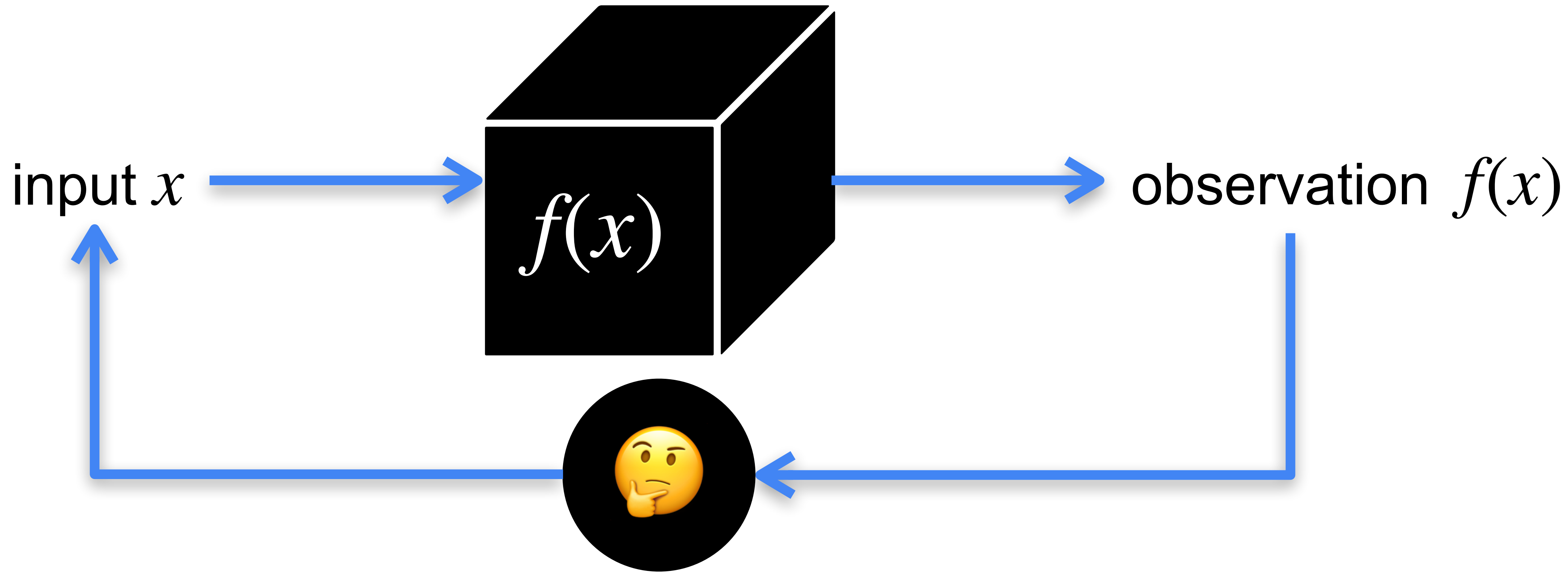

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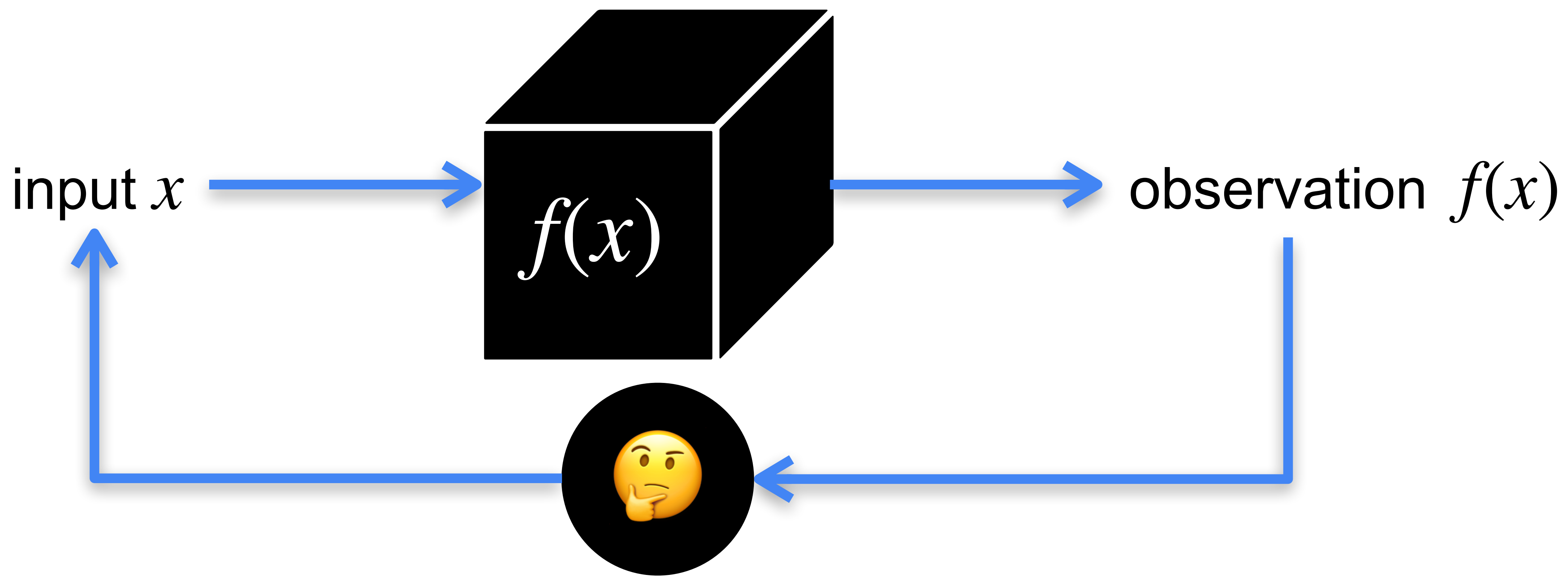

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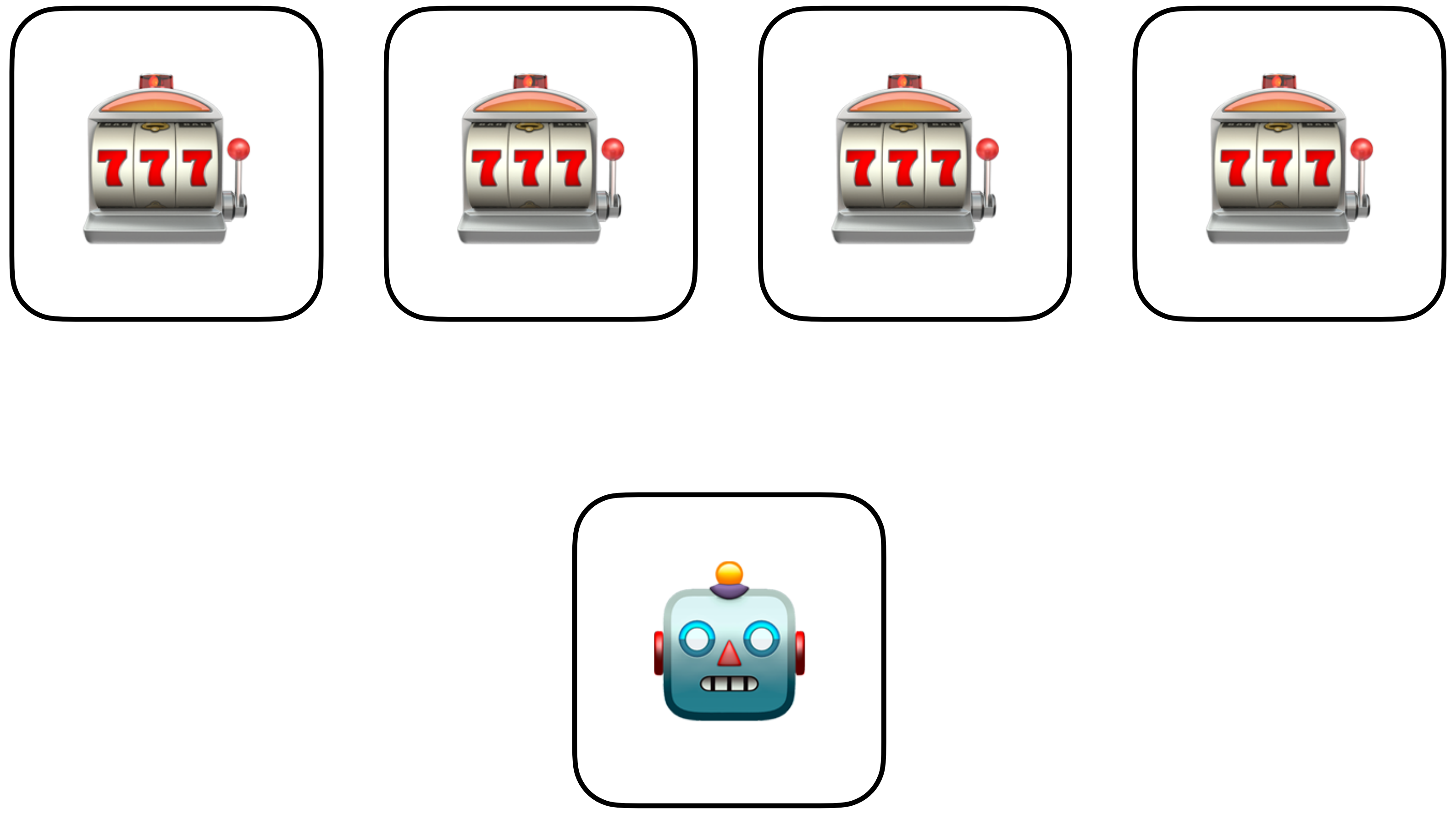

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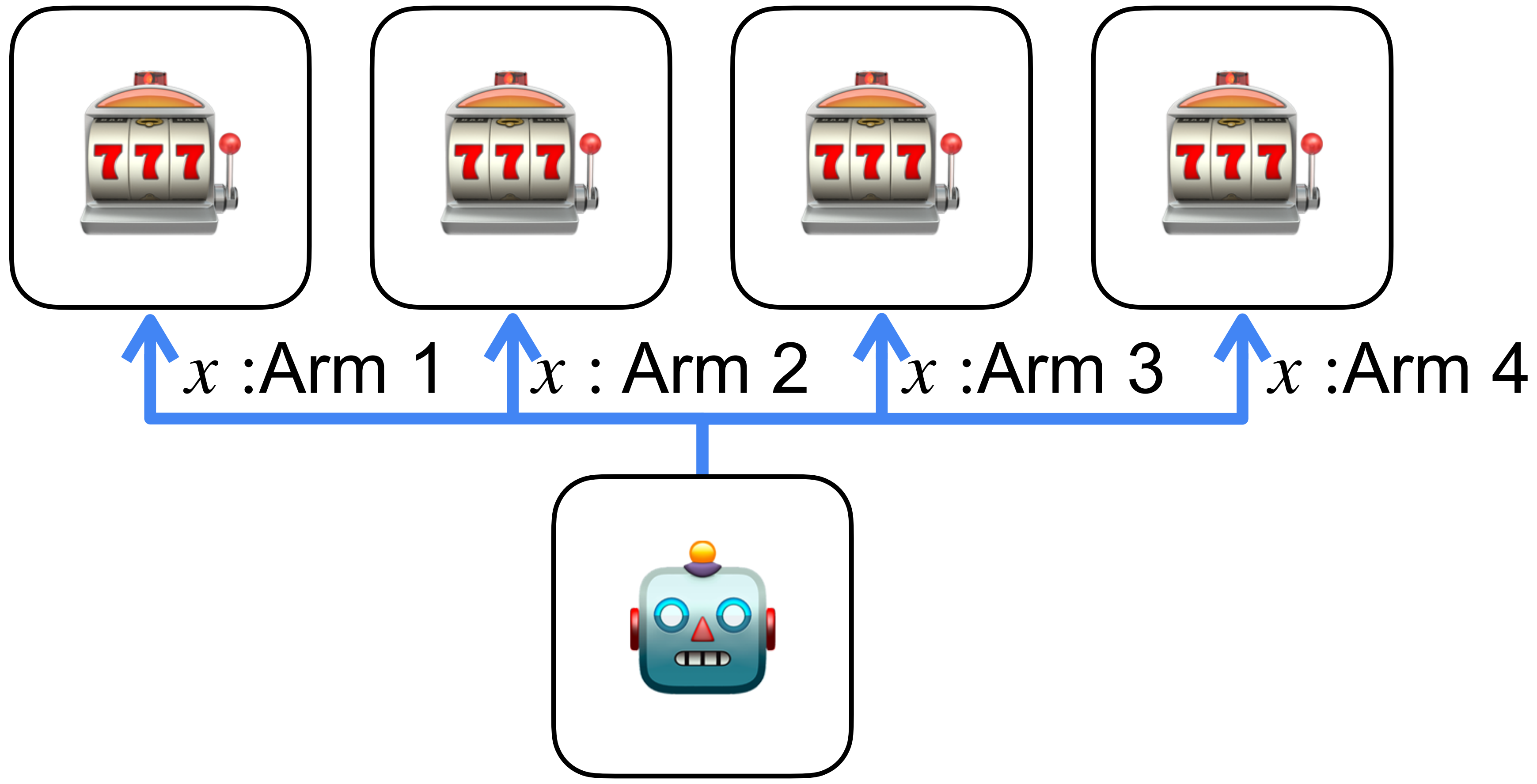

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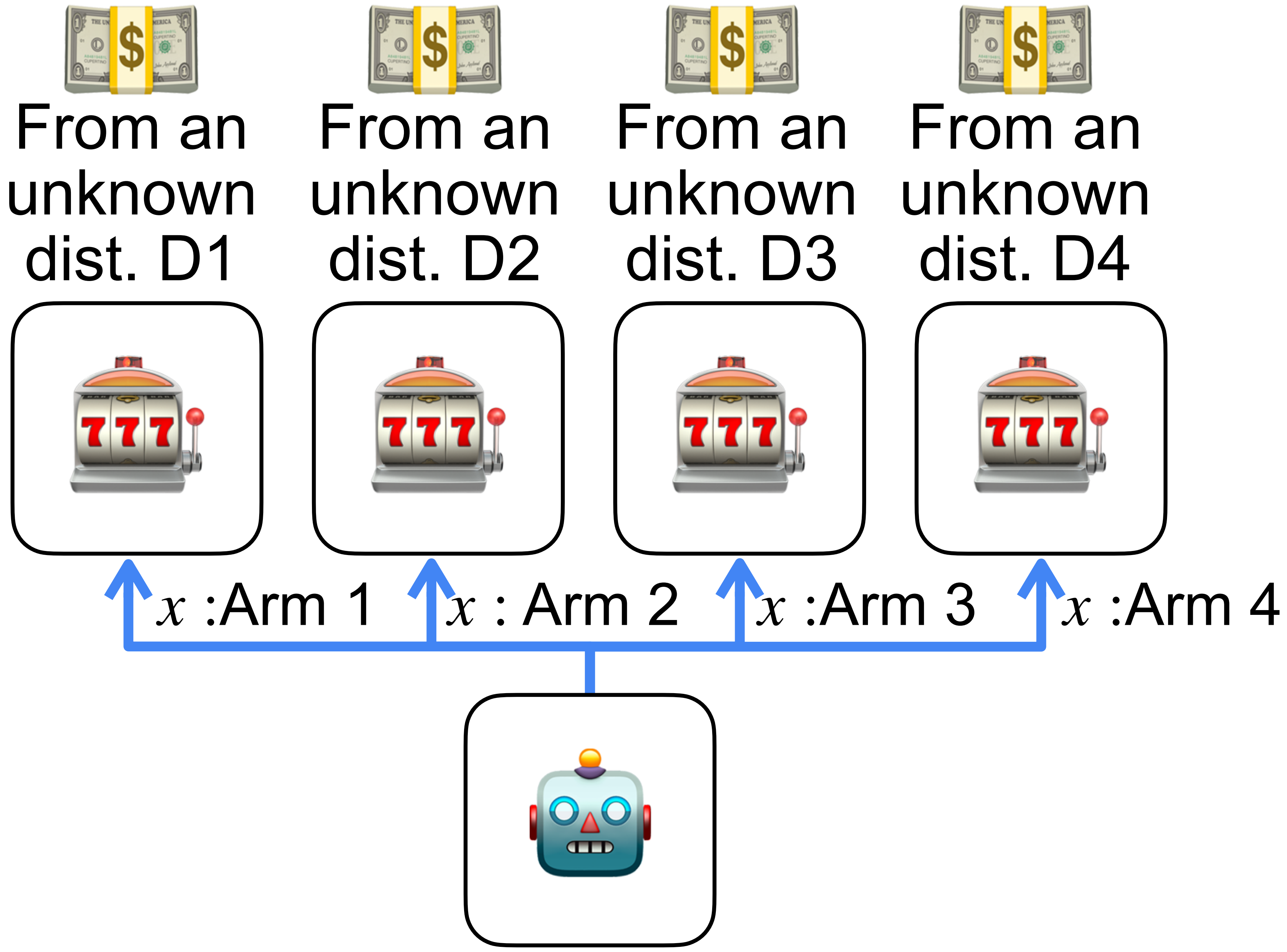

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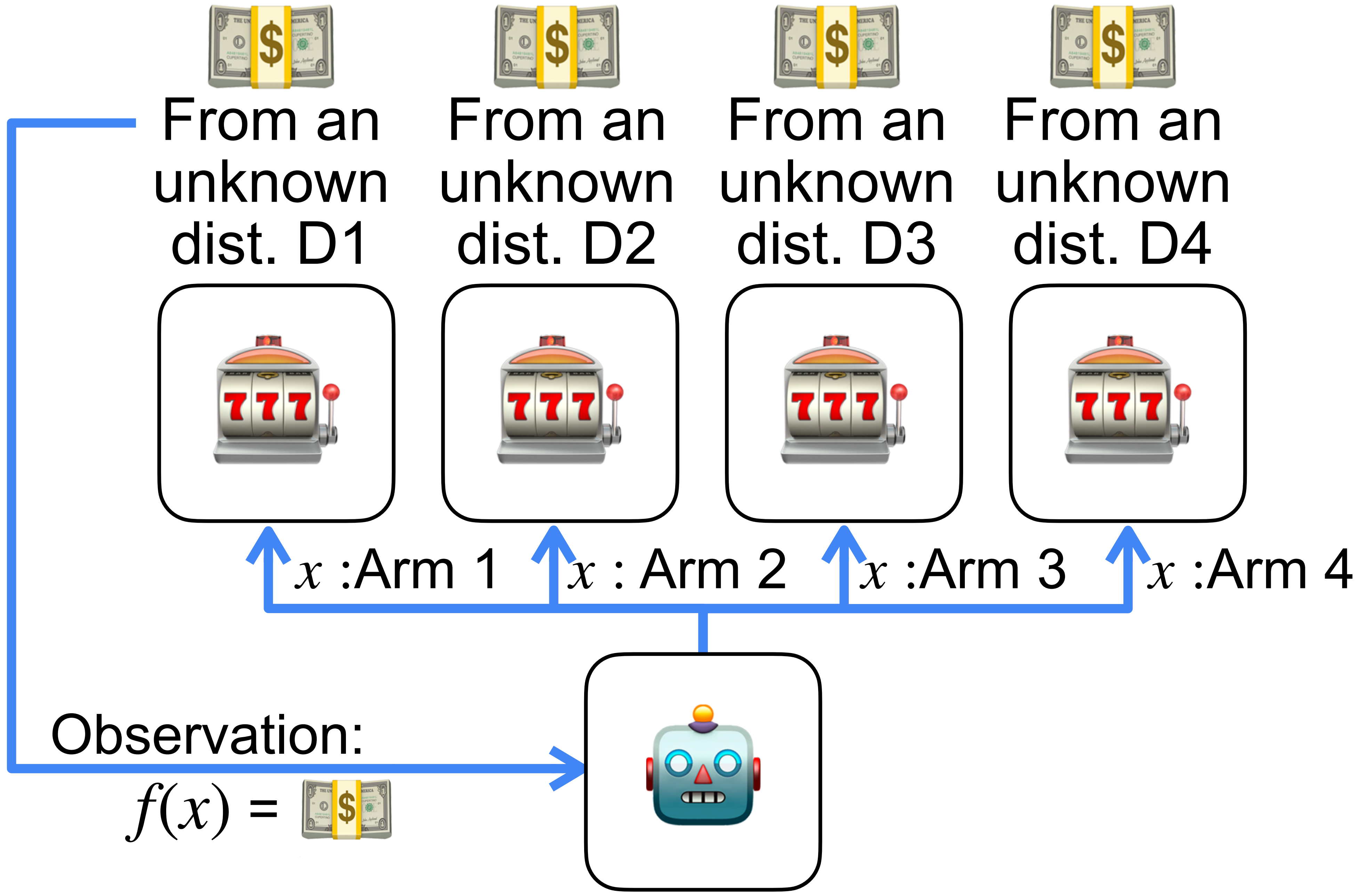

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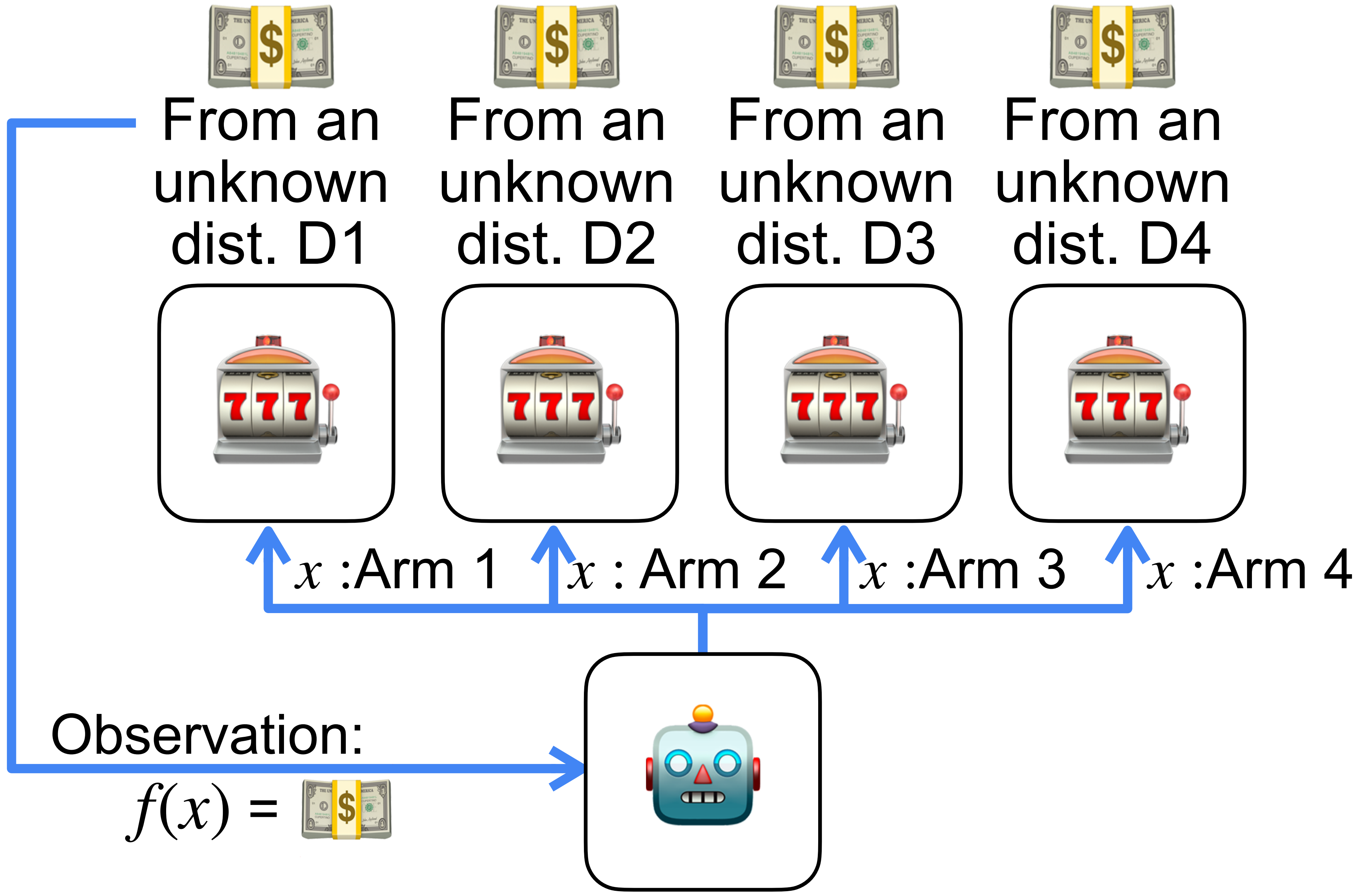

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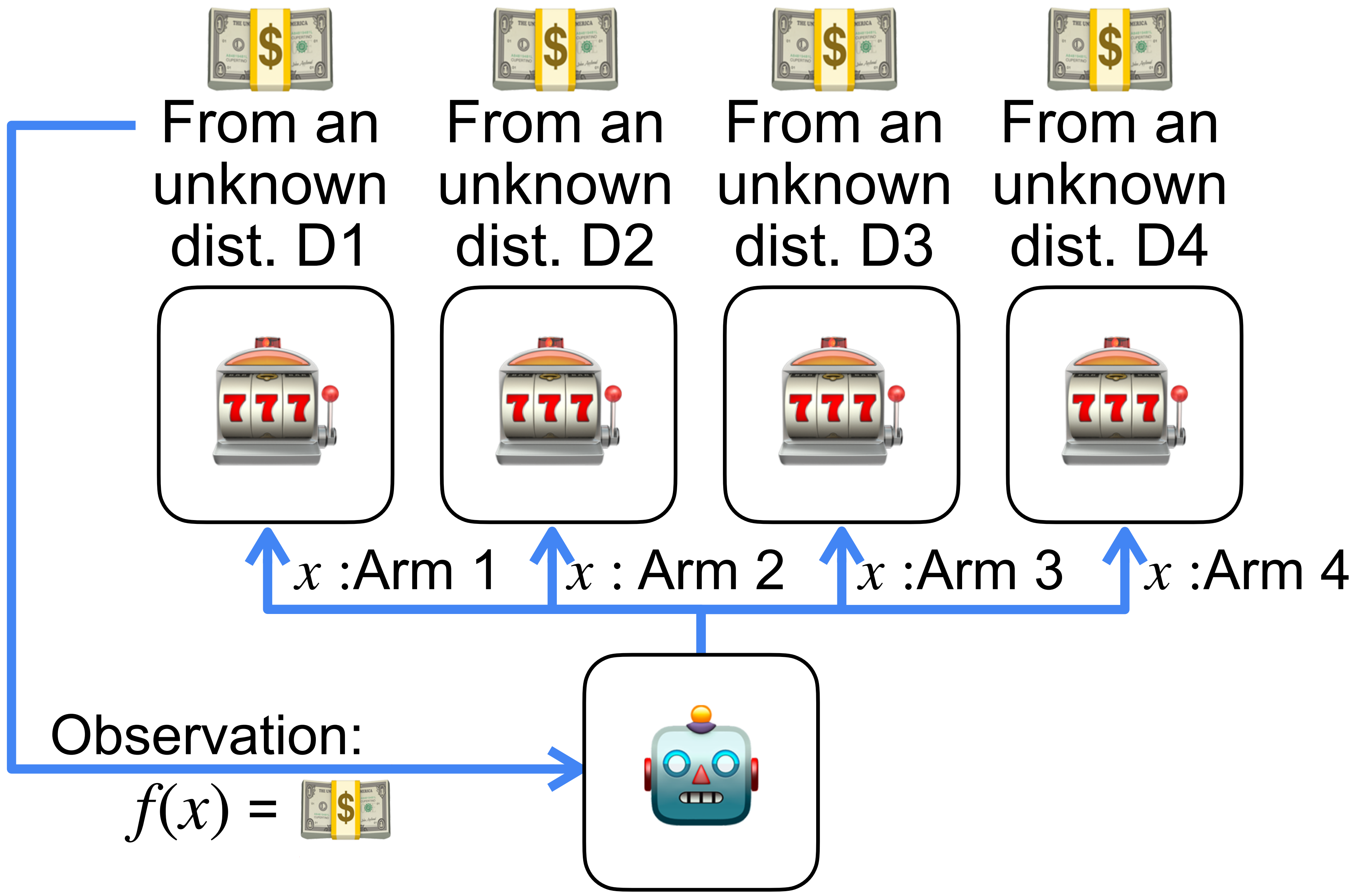

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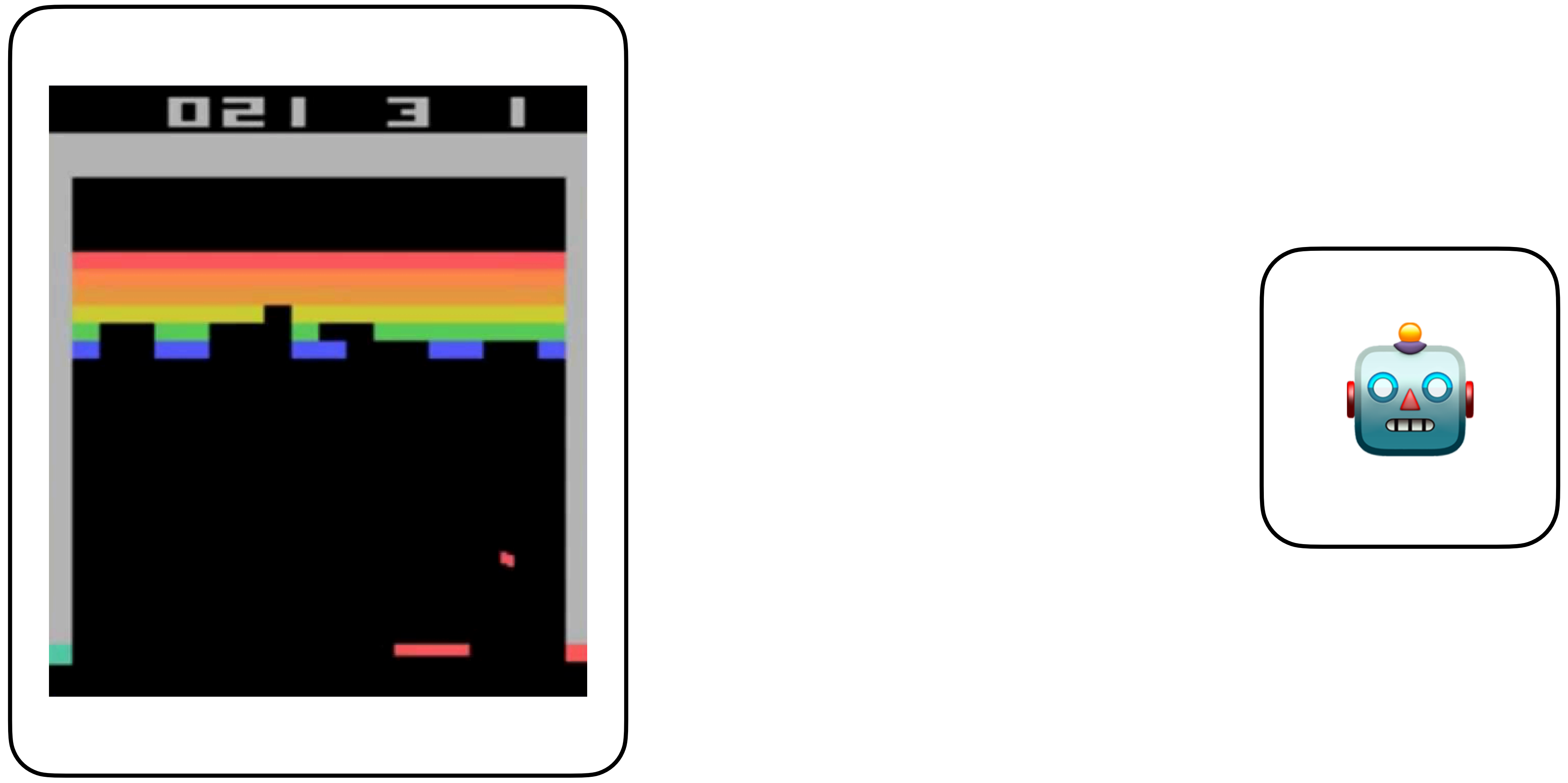

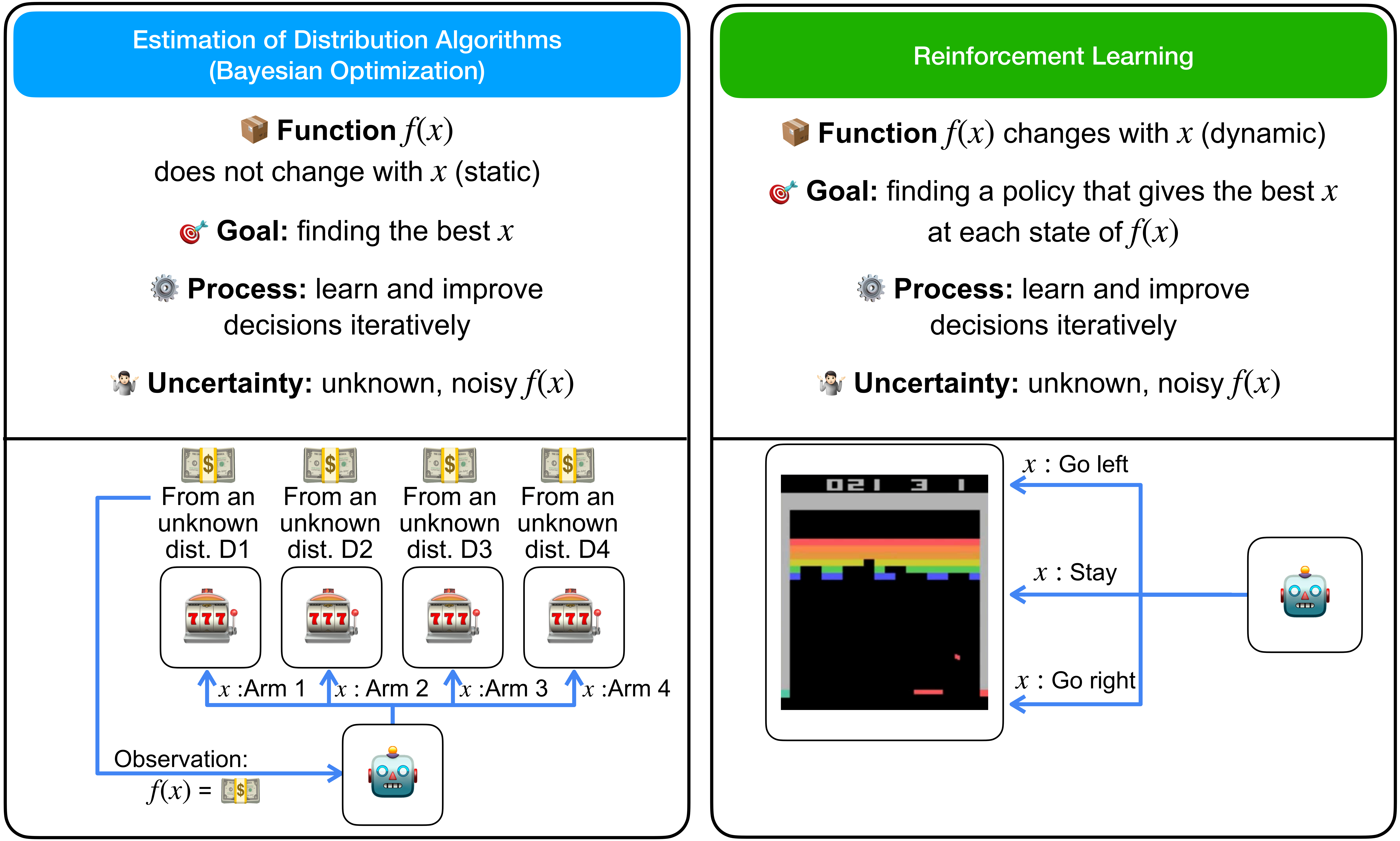
Estimation of Distribution Algorithms
(Bayesian Optimization)
Function $f(x)$
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Goal: finding the best x
Process: learn and improve
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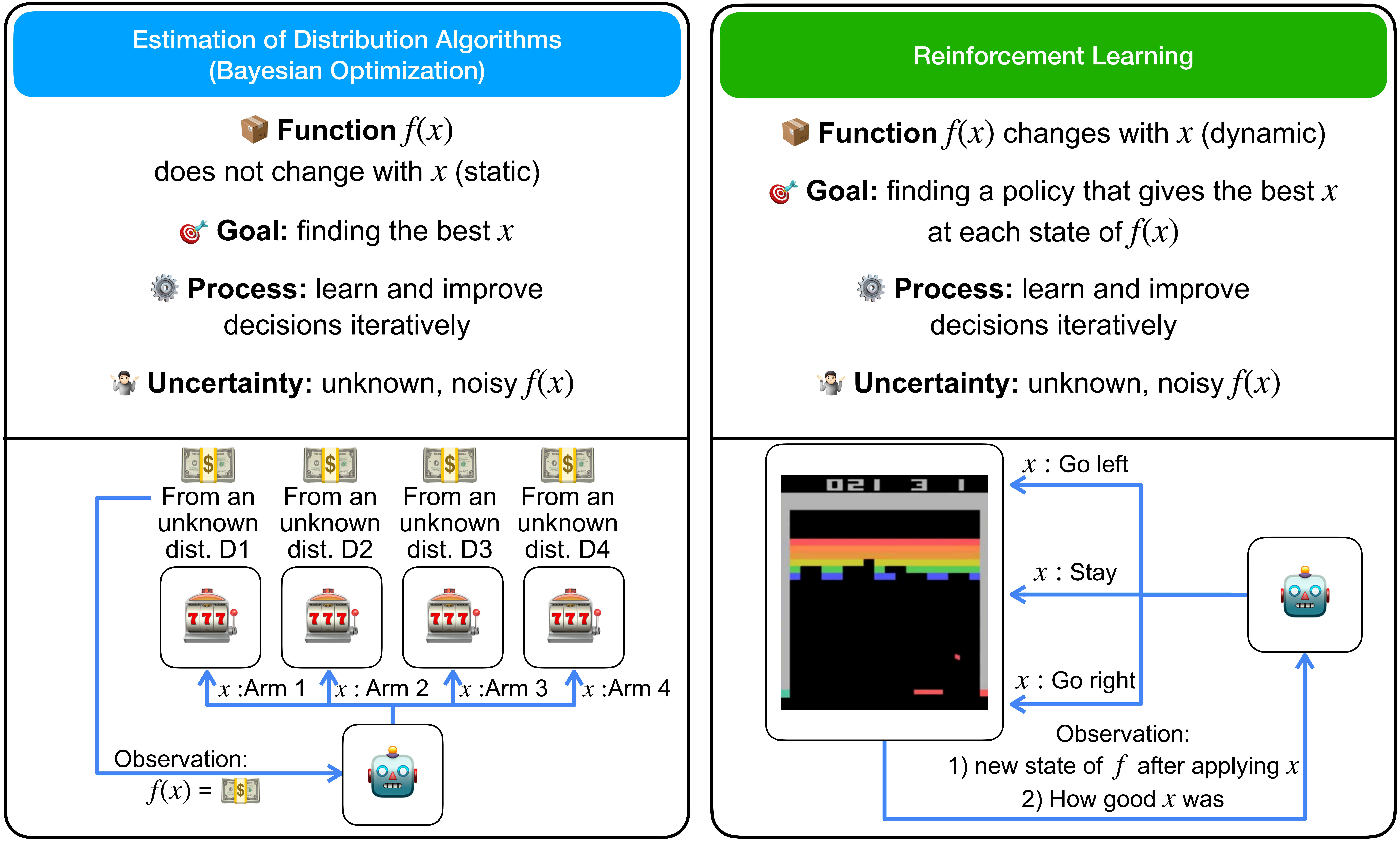
Uncertainty: unknown, noisy $f(x)$
From an unknown dist. D1
From an unknown dist. D2
From an unknown dist. D3
From an unknown dist. D4
x :Arm 1
x : Arm 2
x :Arm 3
x :Arm 4
Observation:
$f(x)$ =
Reinforcement Learning
Function $f(x)$ changes with x (dynamic)
Goal: finding a policy that gives the best x
at each state of $f(x)$
Process: learn and improve
decisions iteratively
Uncertainty: unknown, noisy $f(x)$
x : Go left
x : Stay
x : Go right



Estimation of Distribution Algorithms
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Process: learn and improve decisions iteratively
Uncertainty: unknown, noisy $f(x)$
x : Go left
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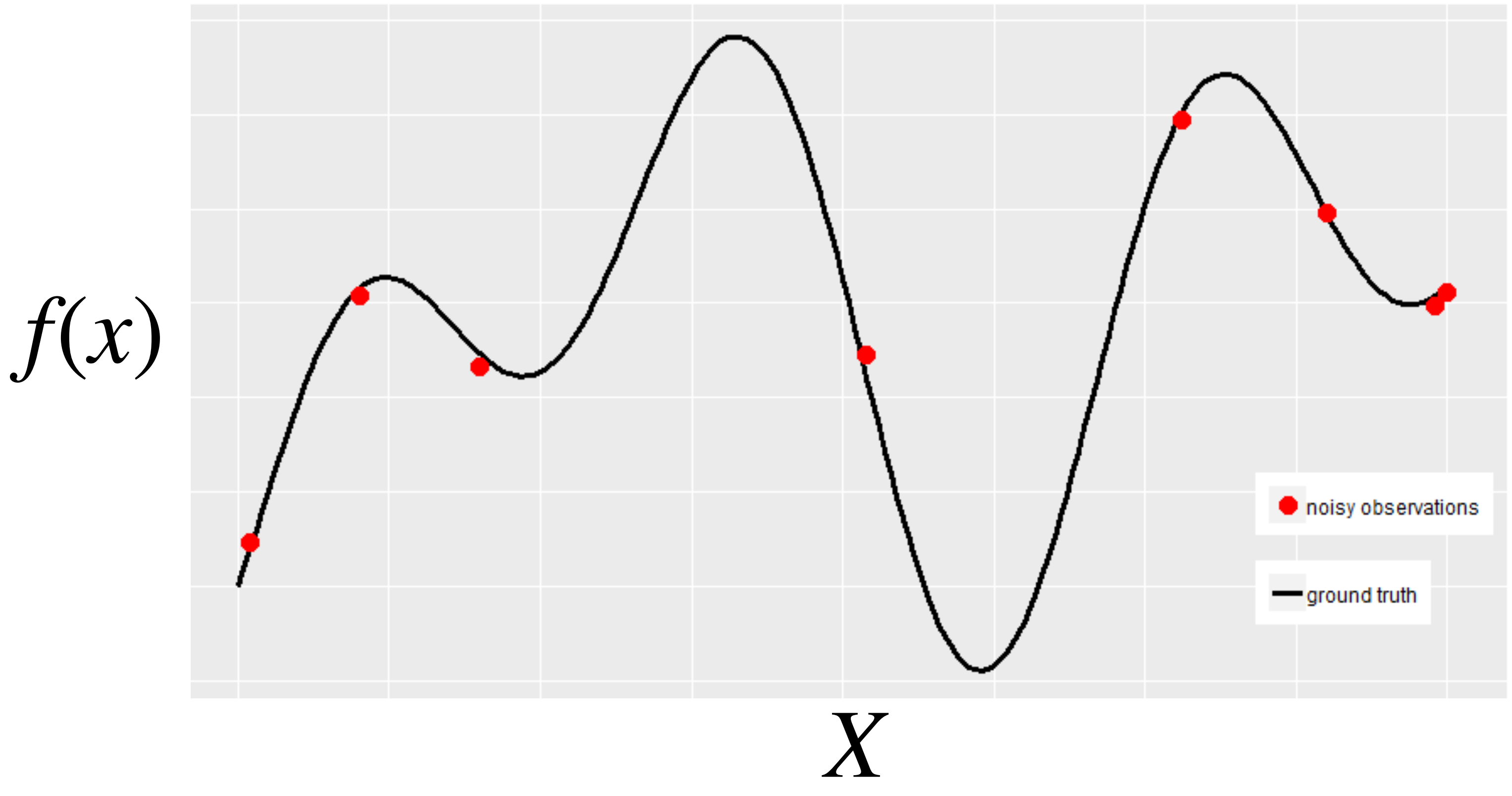
x : Go right
Observation:
1) new state of f after applying x
2) How good x was

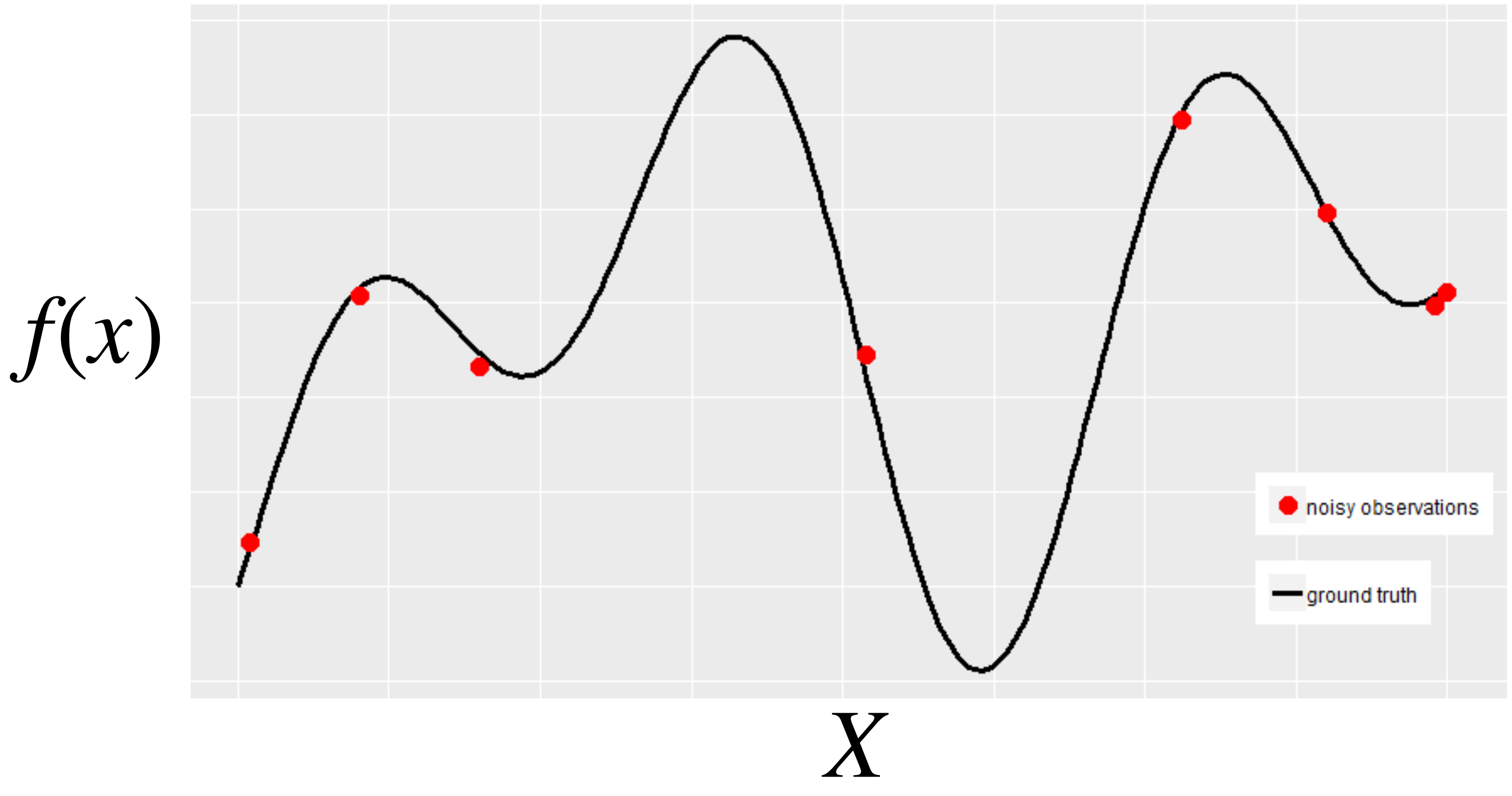
Bayesian Optimization

Bayesian Optimization

Bayesian Optimization

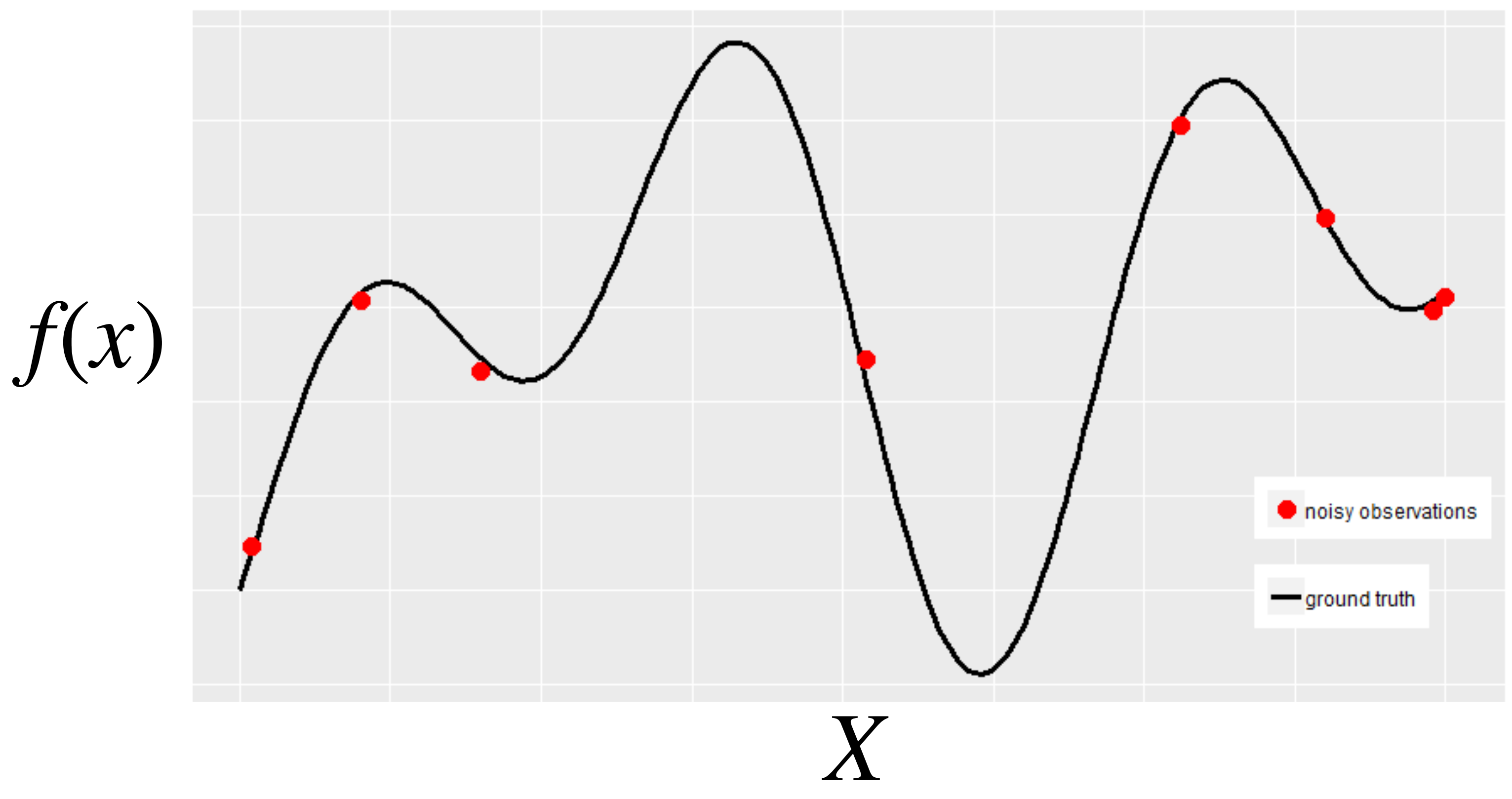


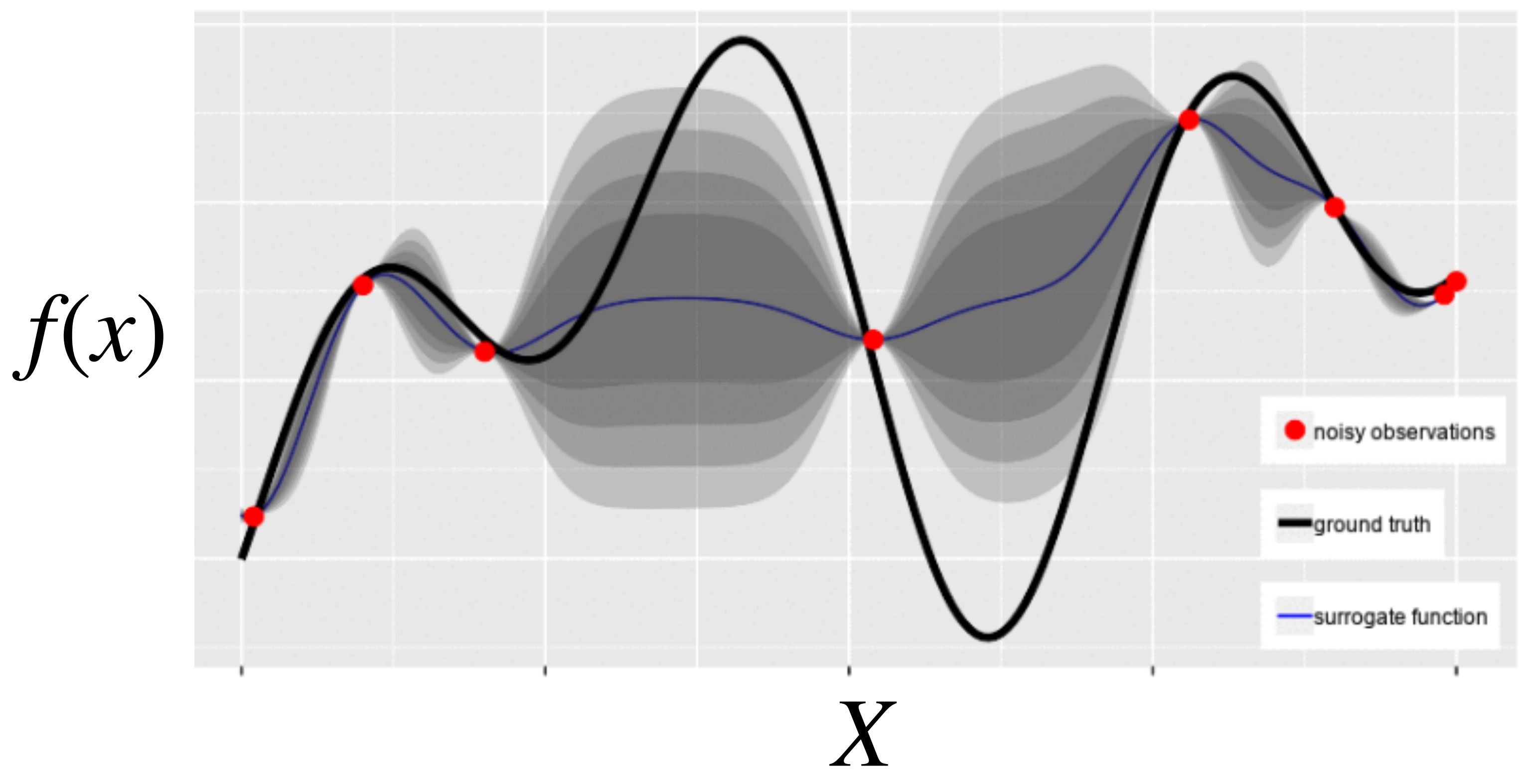
Bayesian Optimization



1) initial sample

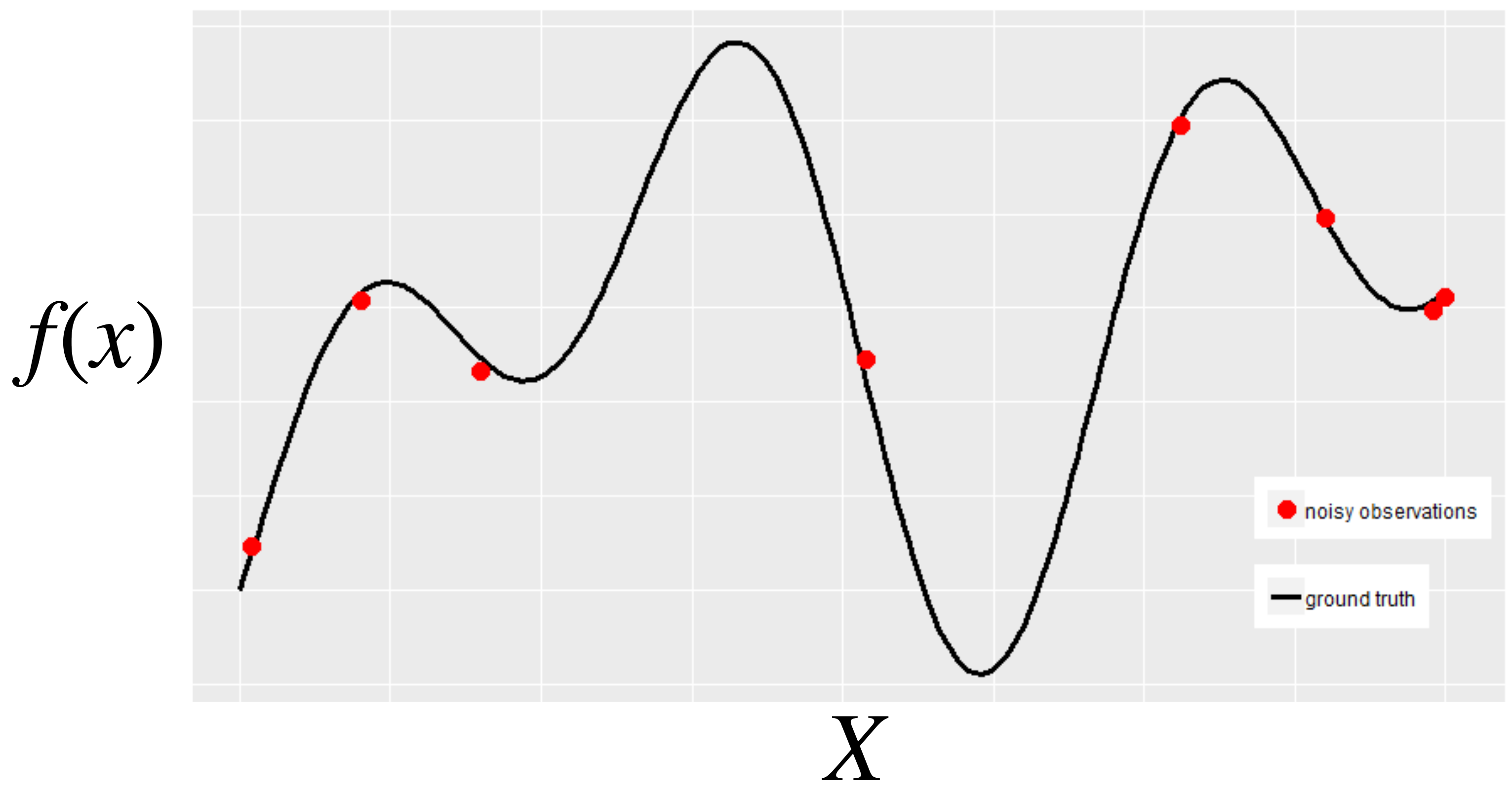
Bayesian Optimization

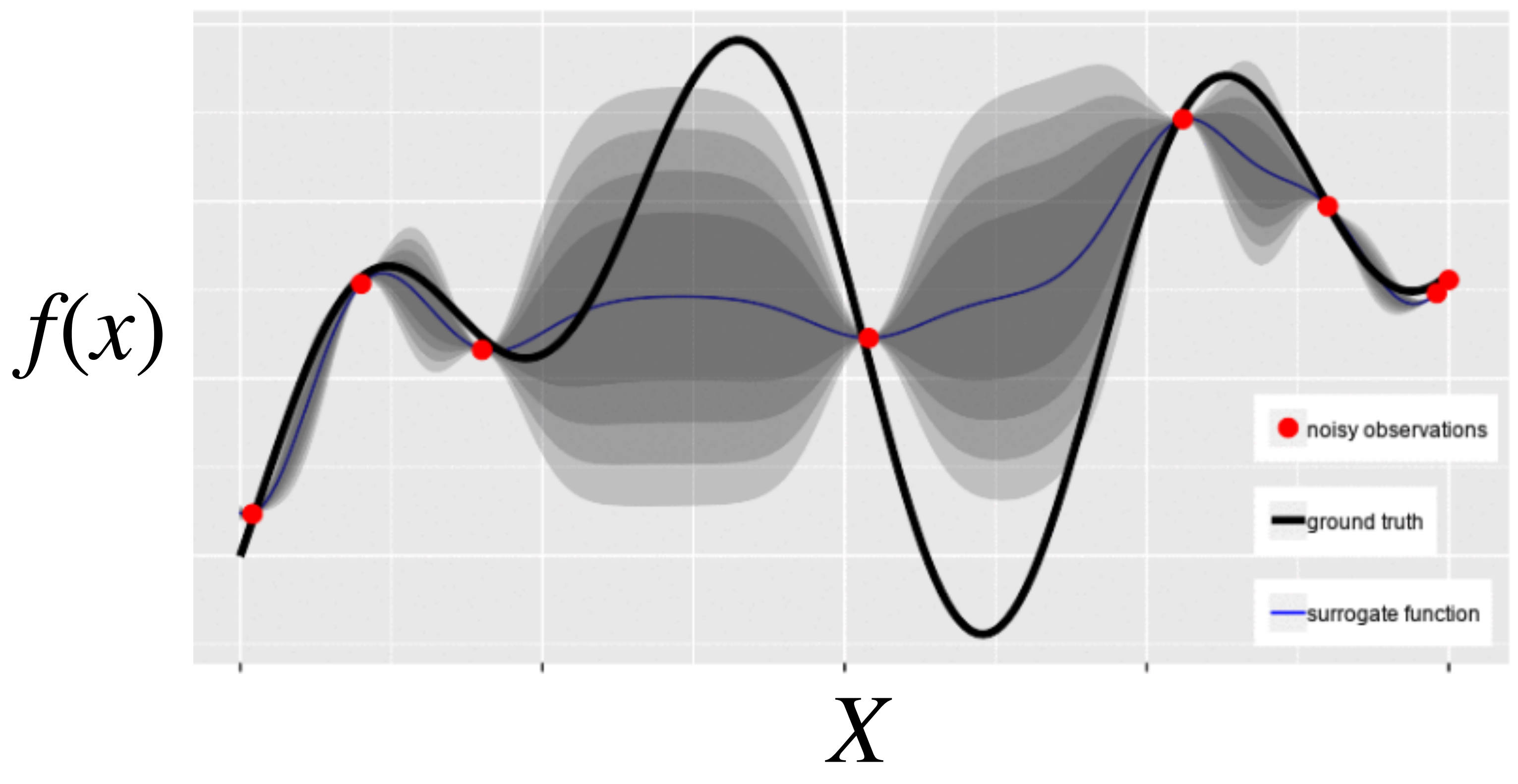


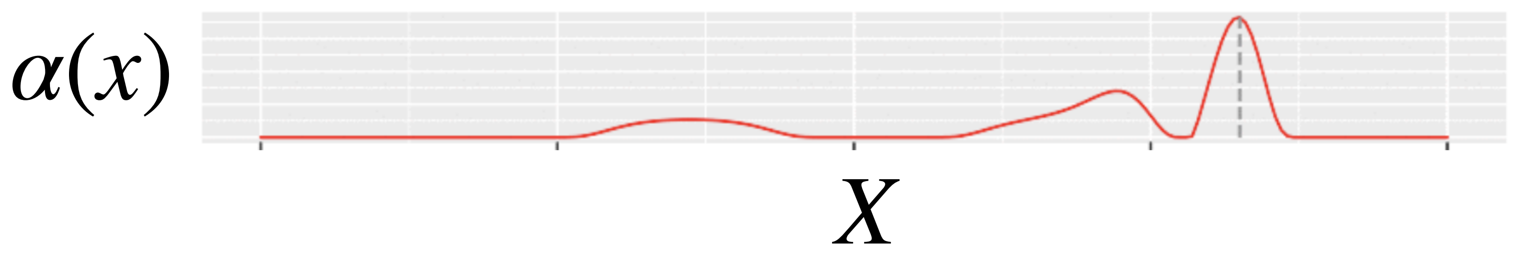


1) initial sample
2) fit a surrogate model given samples

Bayesian Optimization







1) initial sample
2) fit a surrogate model given samples
3) obtain an acquisition function $\alpha(x)$

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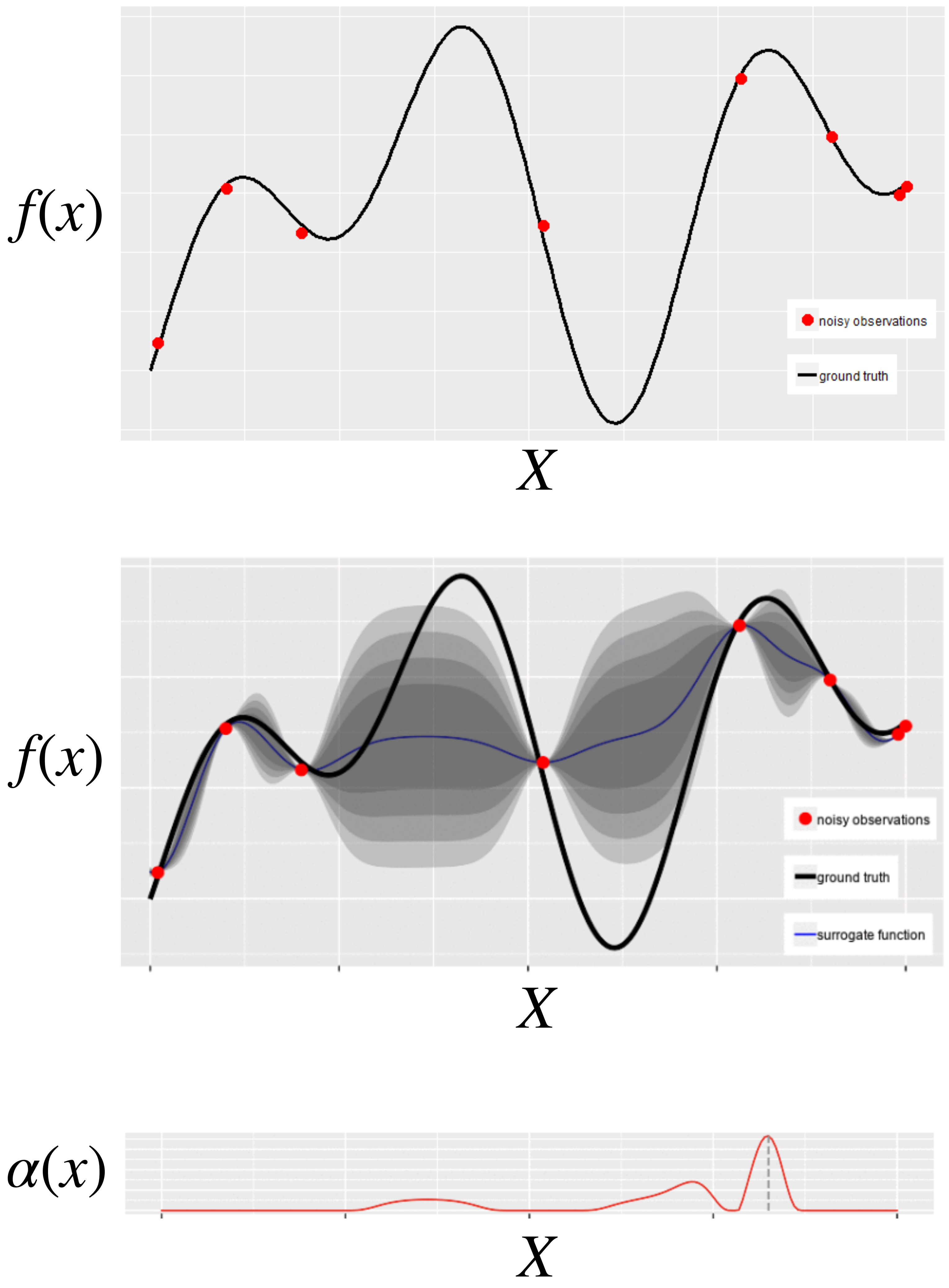
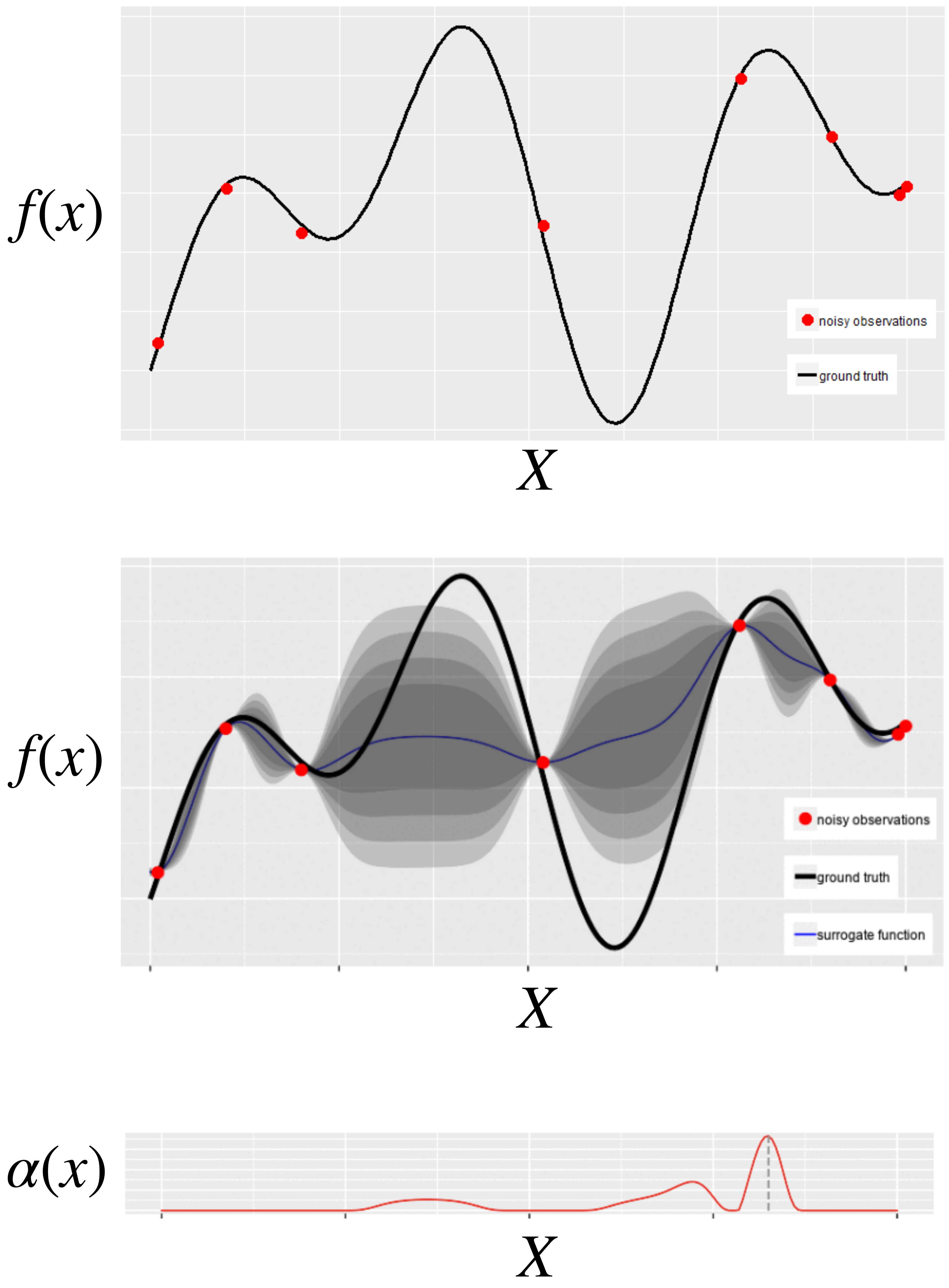
Bayesian Optimization



1) initial sample
2) fit a surrogate model given samples
3) obtain an acquisition function $\alpha(x)$
4) optimize $\alpha(x)$

$$x_{next} = \arg \underset{x \in X}{max} \ \alpha(x)$$

Bayesian Optimization



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$$x_{next} = \underset{x \in X}{\arg\,max}\ \alpha(x)$$

5) sample x_{next}

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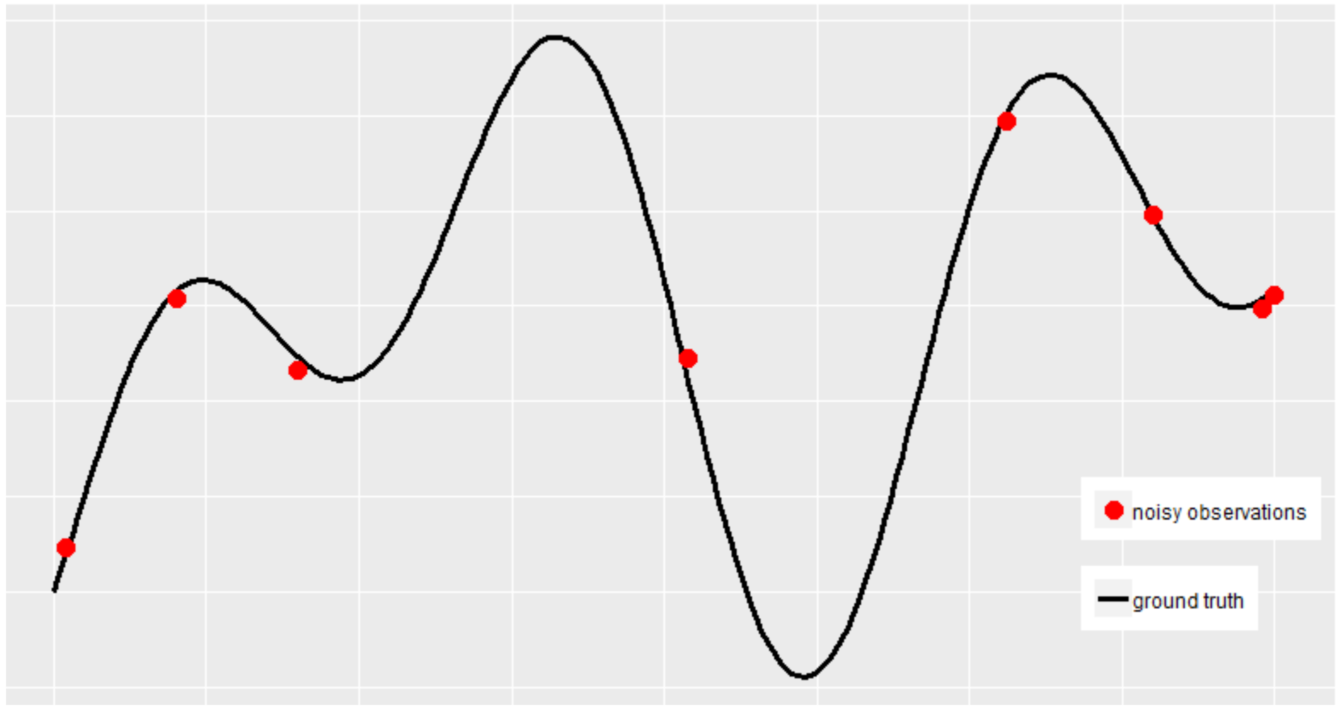
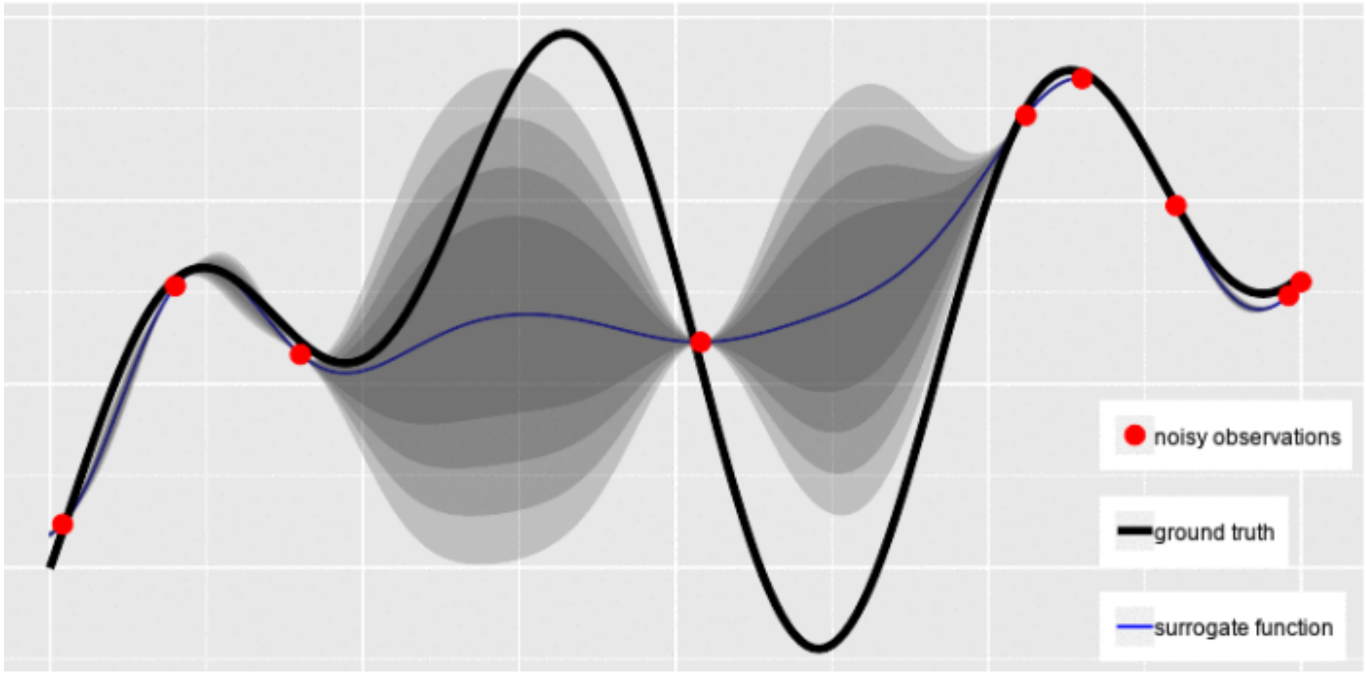
Bayesian Optimization

$f(x)$



X

$f(x)$



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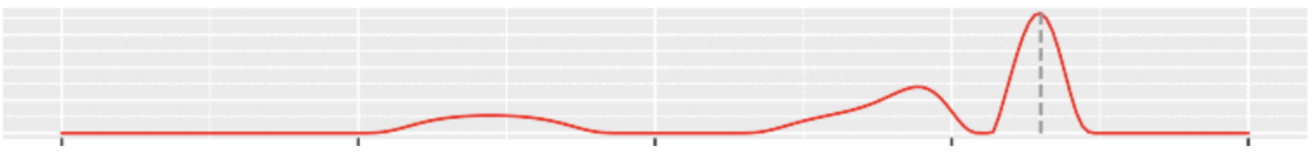
$\alpha(x)$



X

1) initial sample
2) fit a surrogate model given samples
3) obtain an acquisition function $\alpha(x)$
4) optimize $\alpha(x)$

$$x_{next} = \arg \max_{x \in X} \alpha(x)$$

5) sample x_{next}
6) update surrogate model

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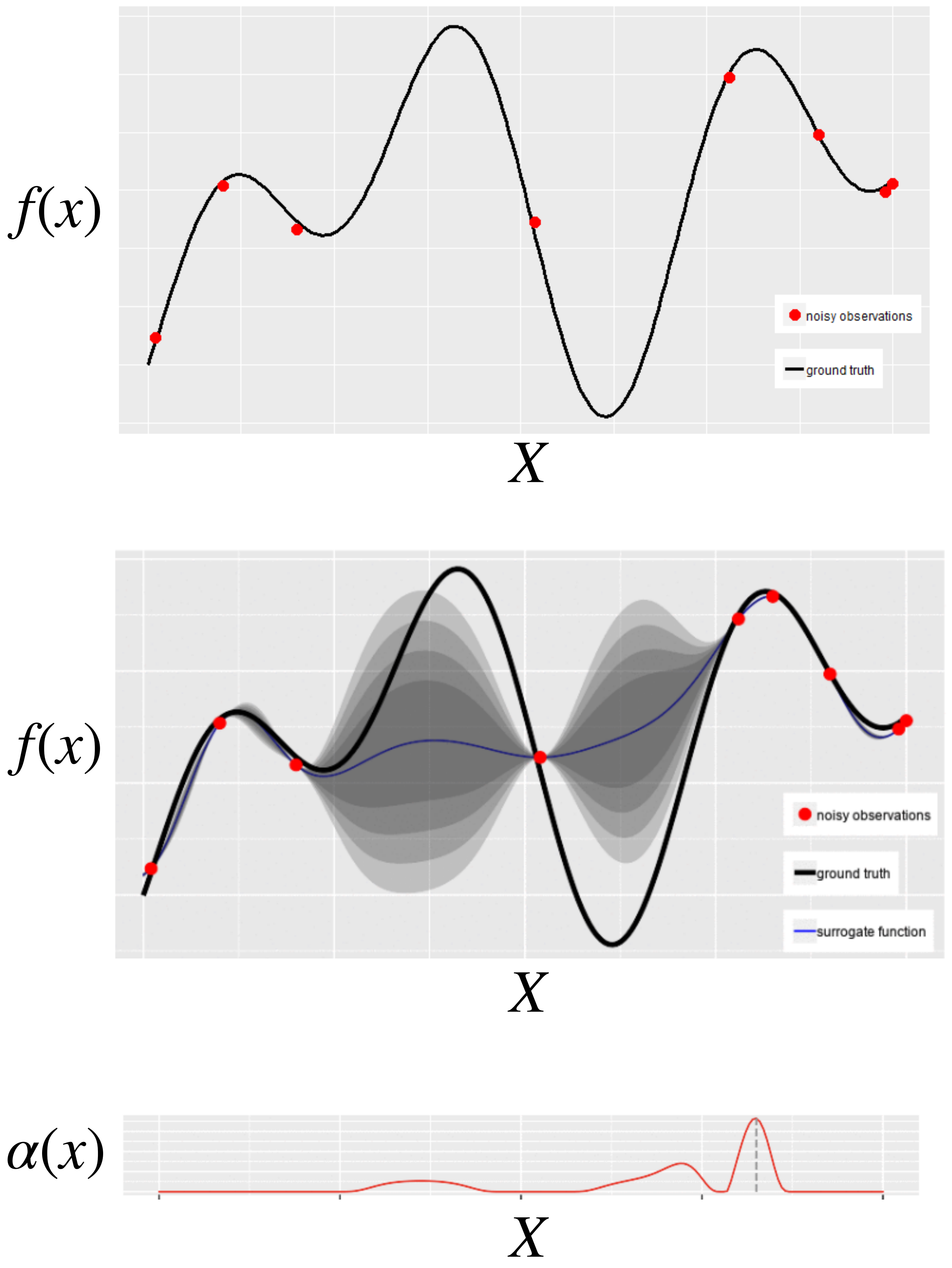
Bayesian Optimization



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5) sample x_{next}
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7) iterate from 3

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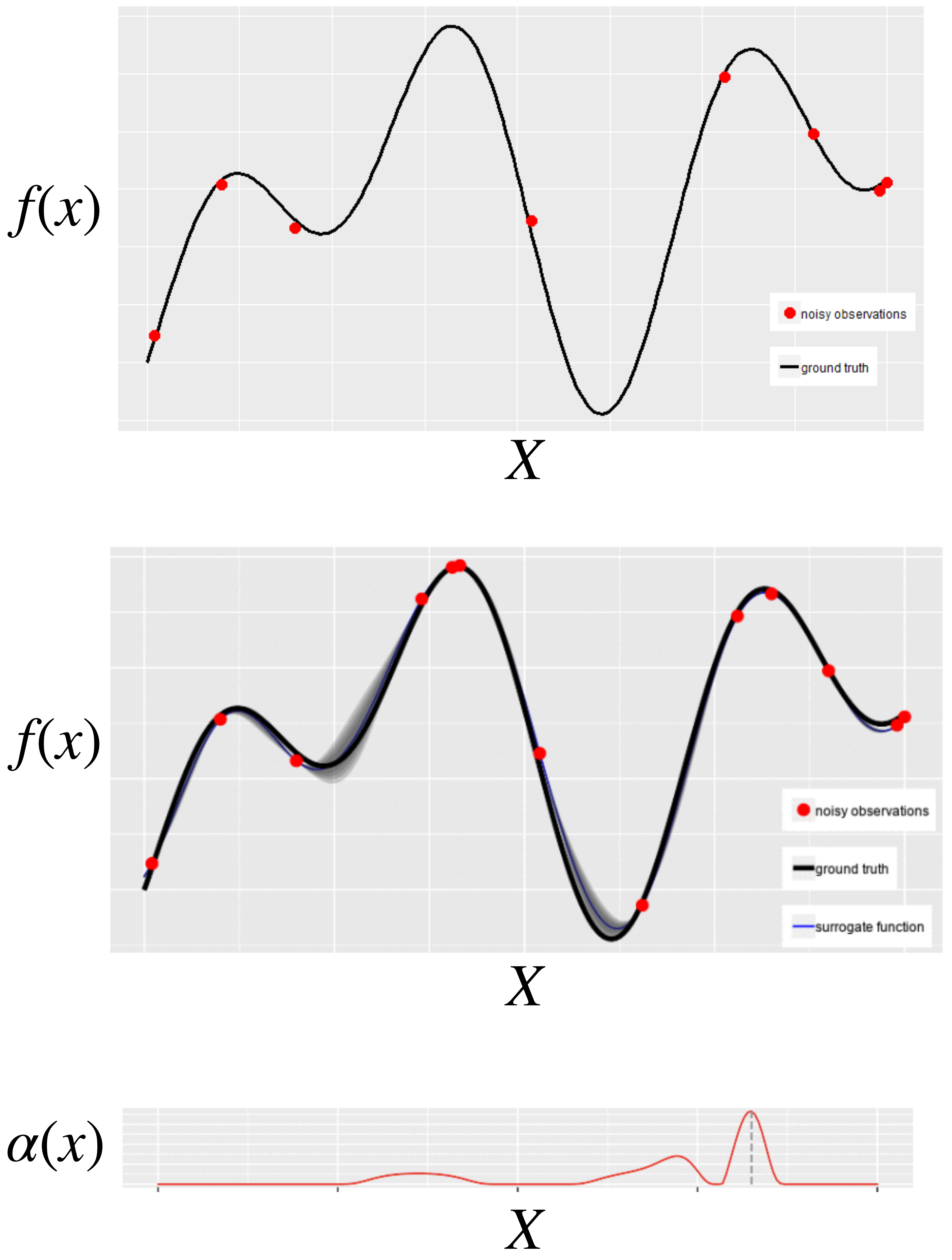

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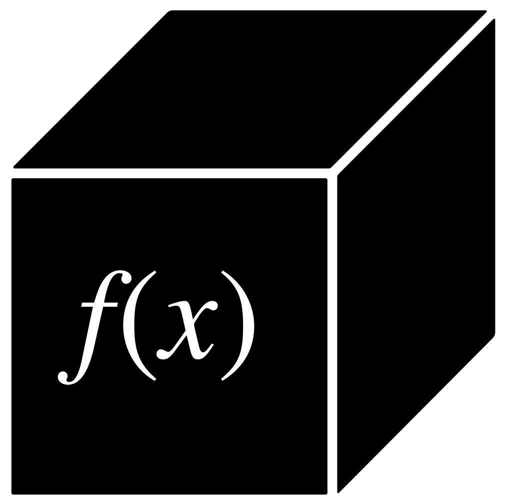
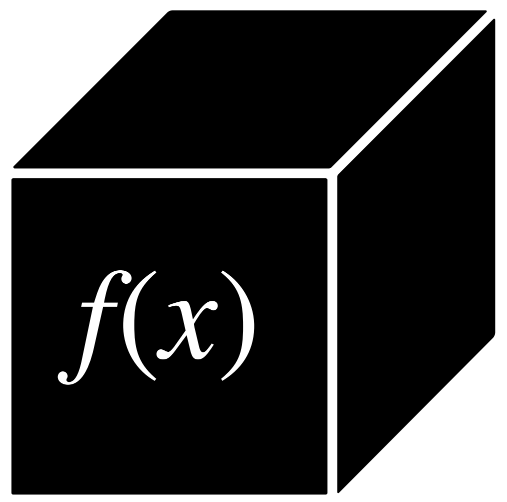
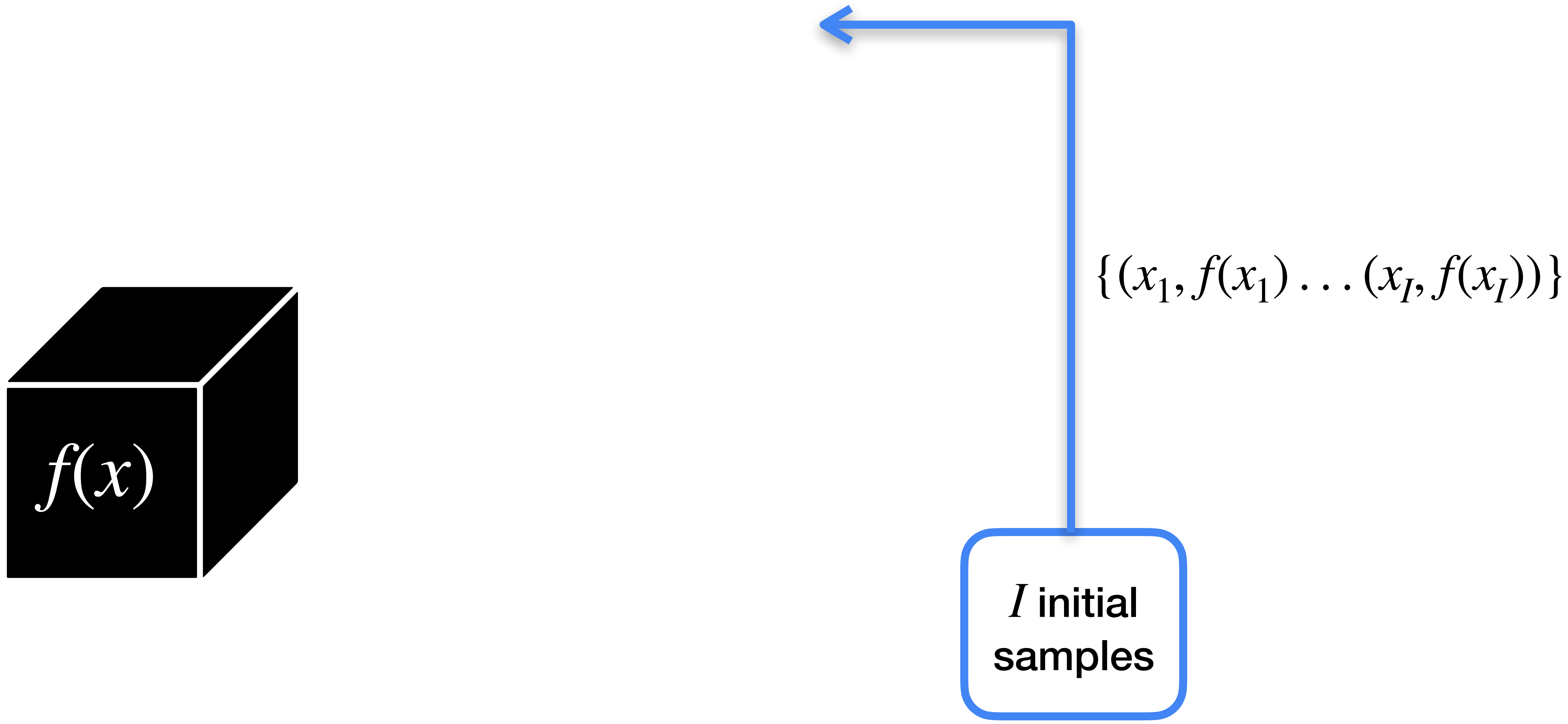


Bayesian Optimization



I initial samples

Bayesian Optimization



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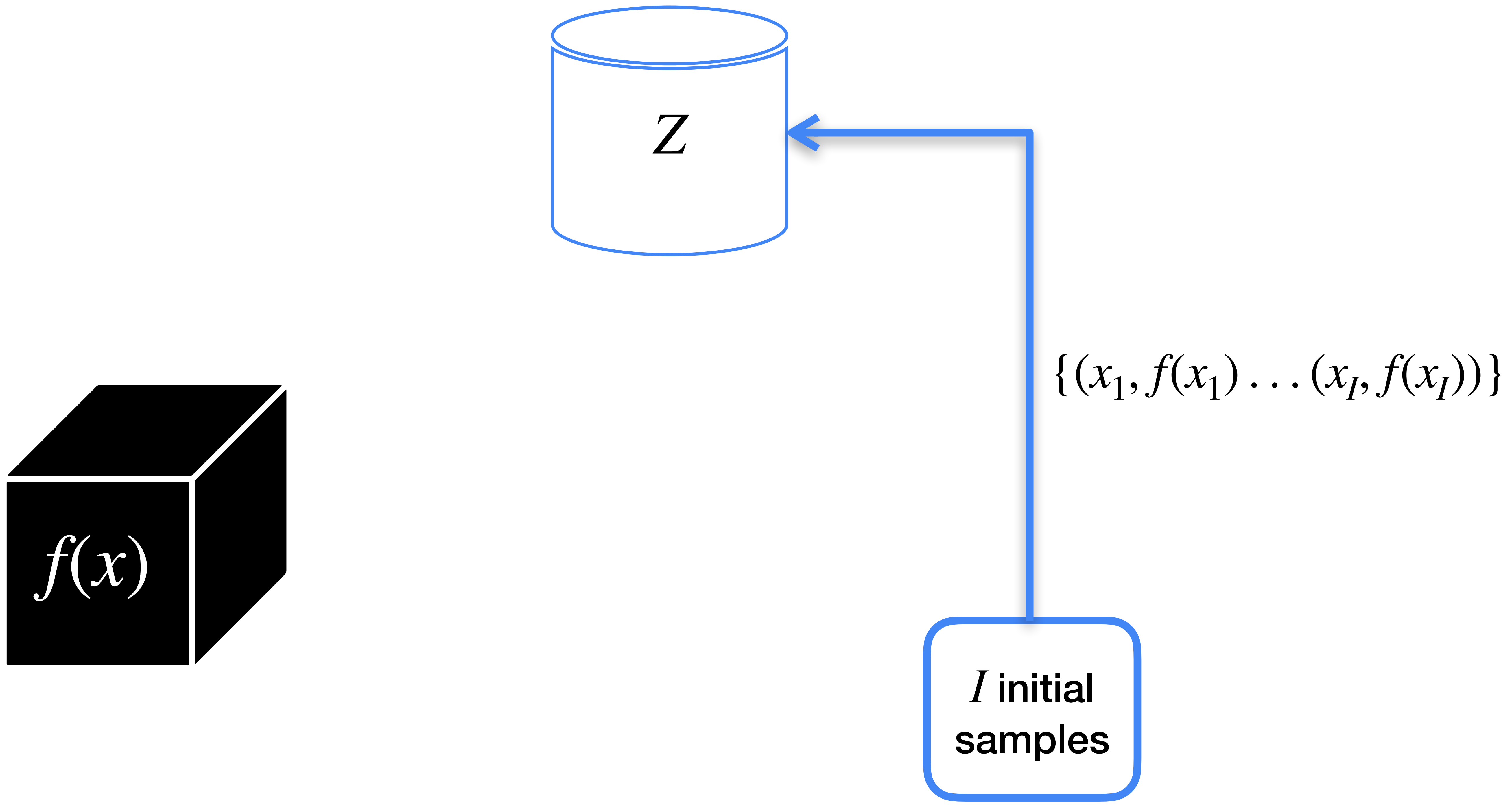

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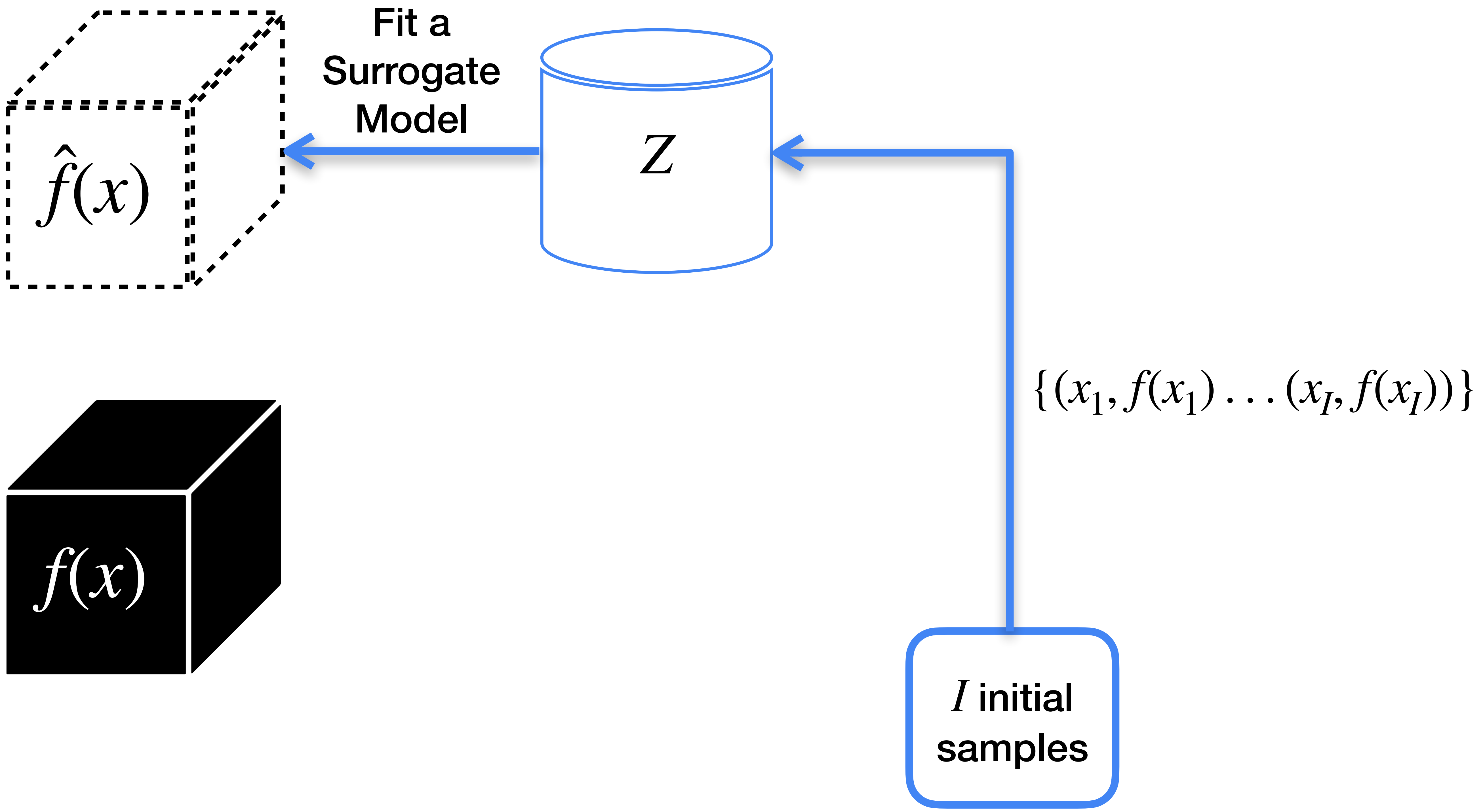

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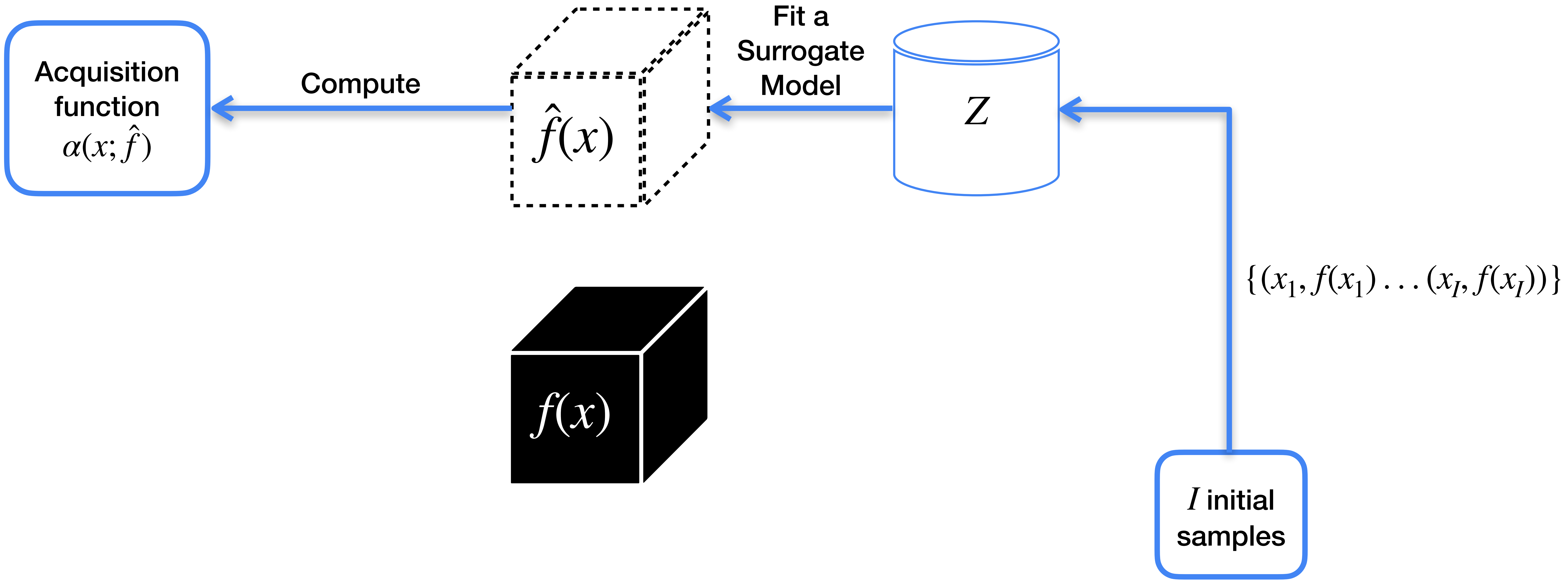

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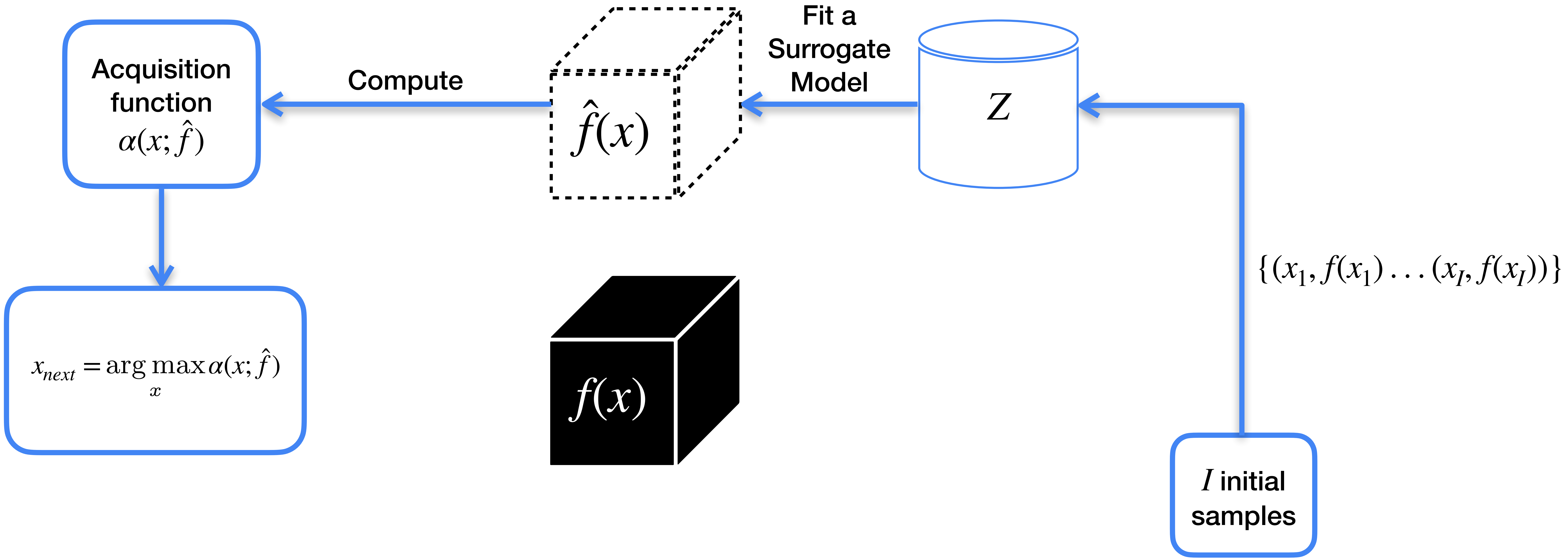

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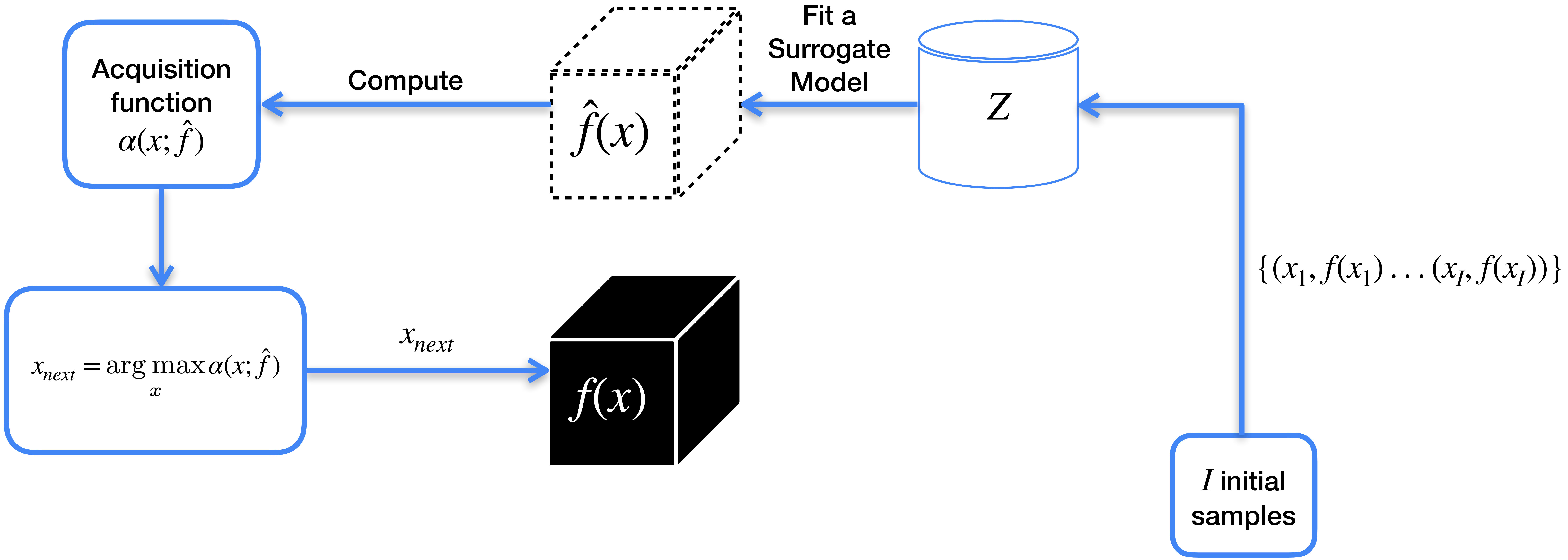

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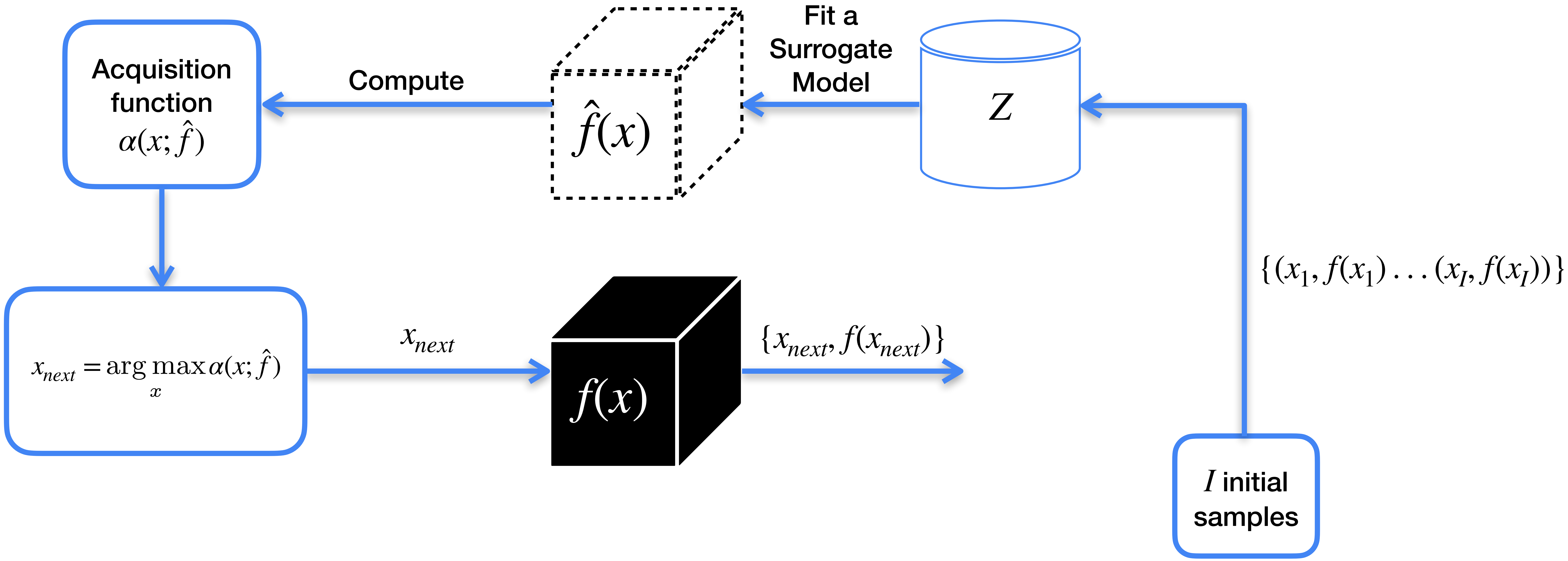

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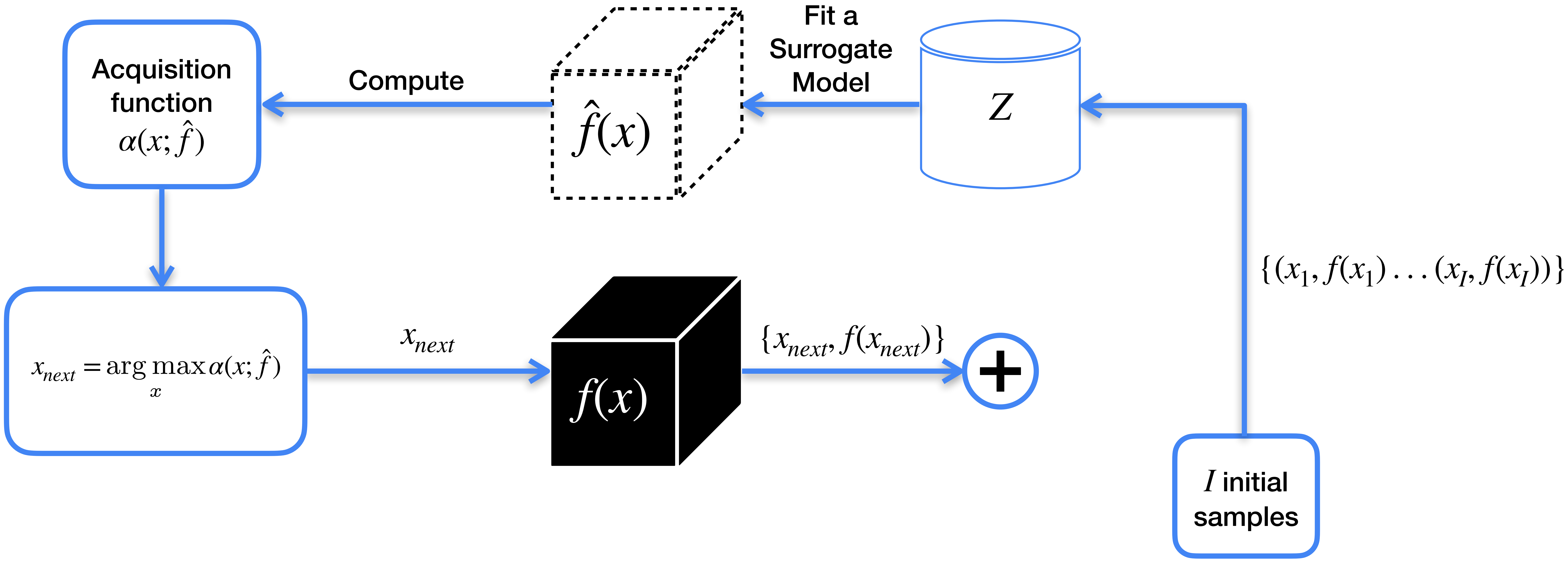

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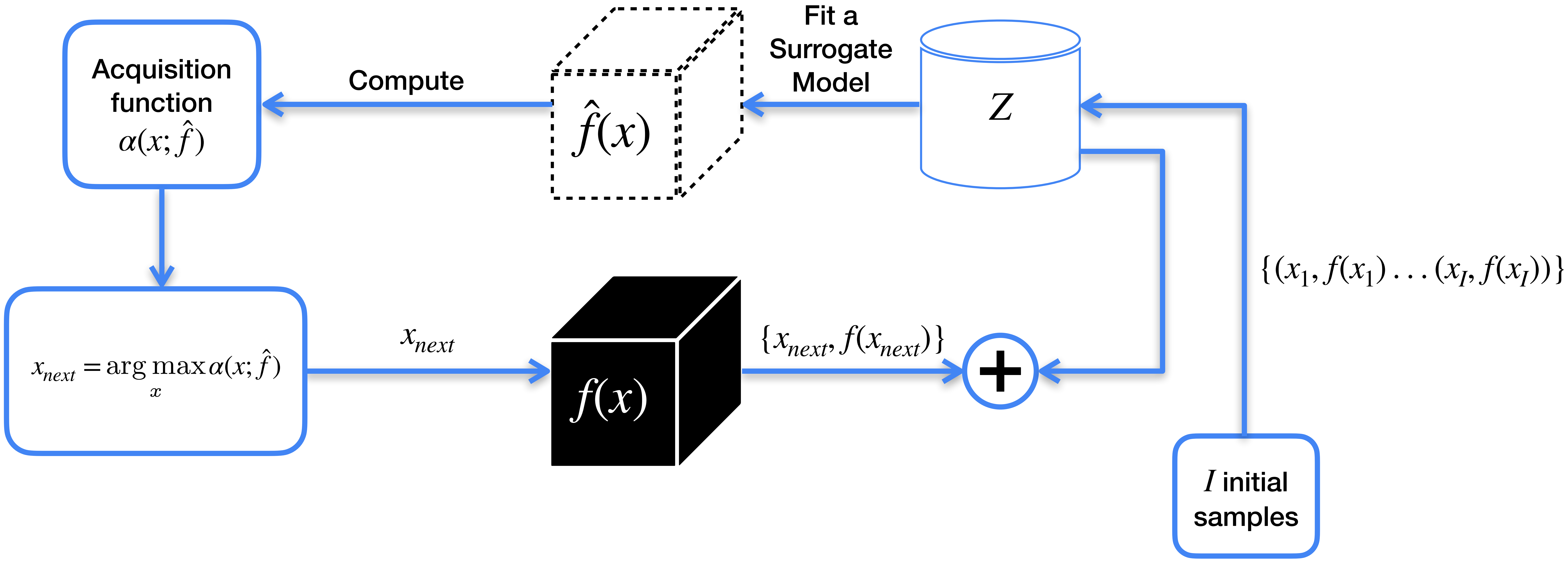

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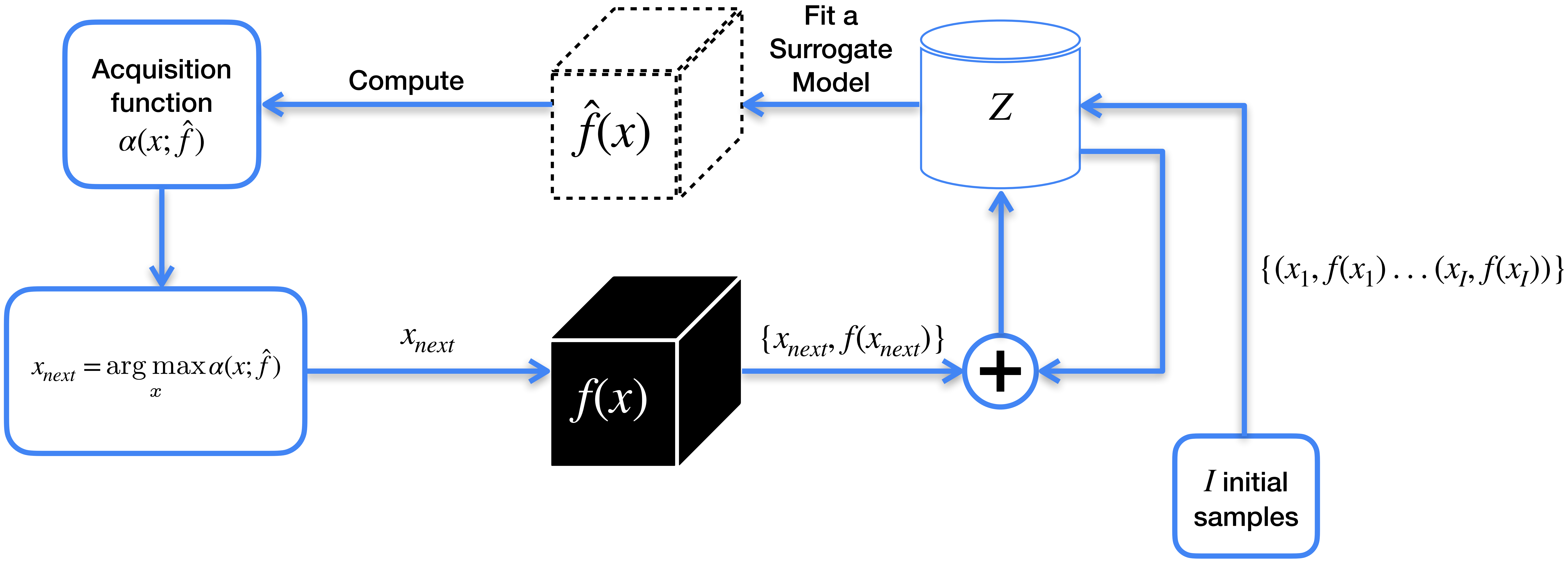

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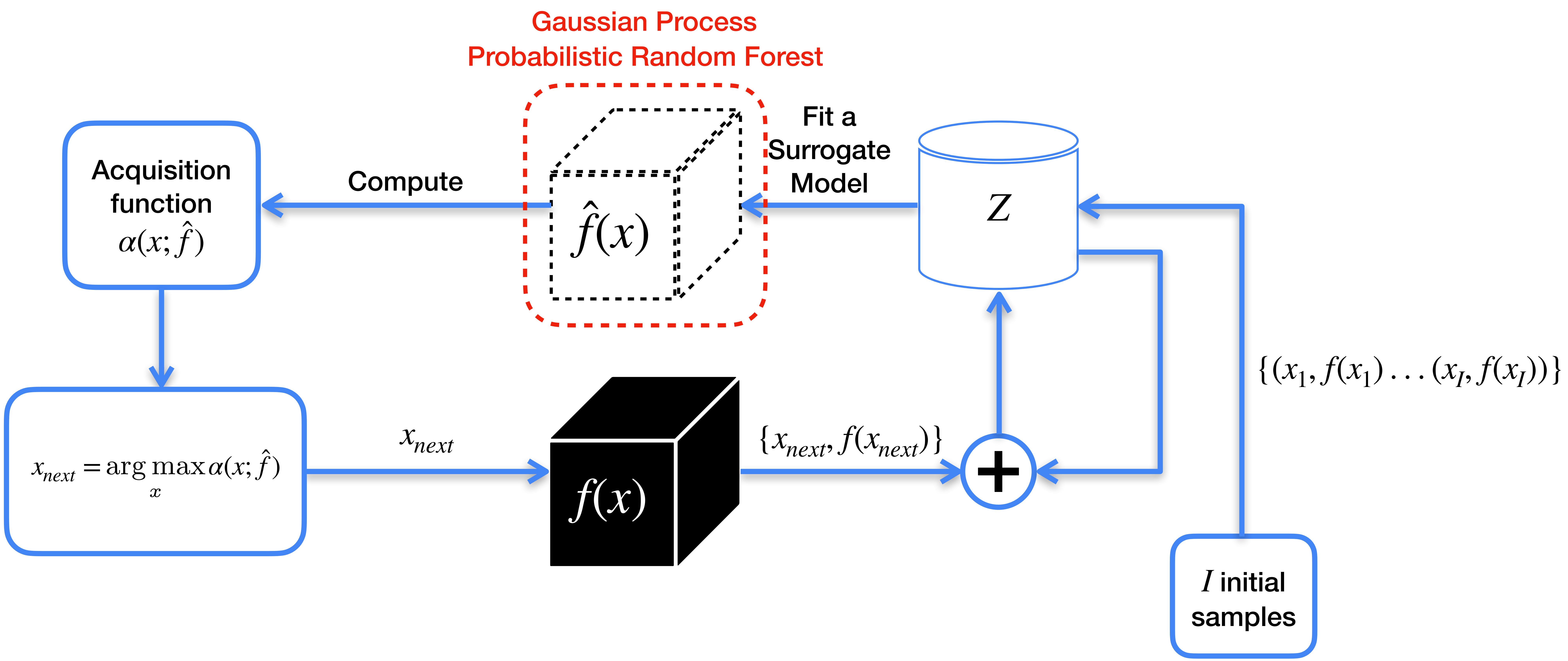

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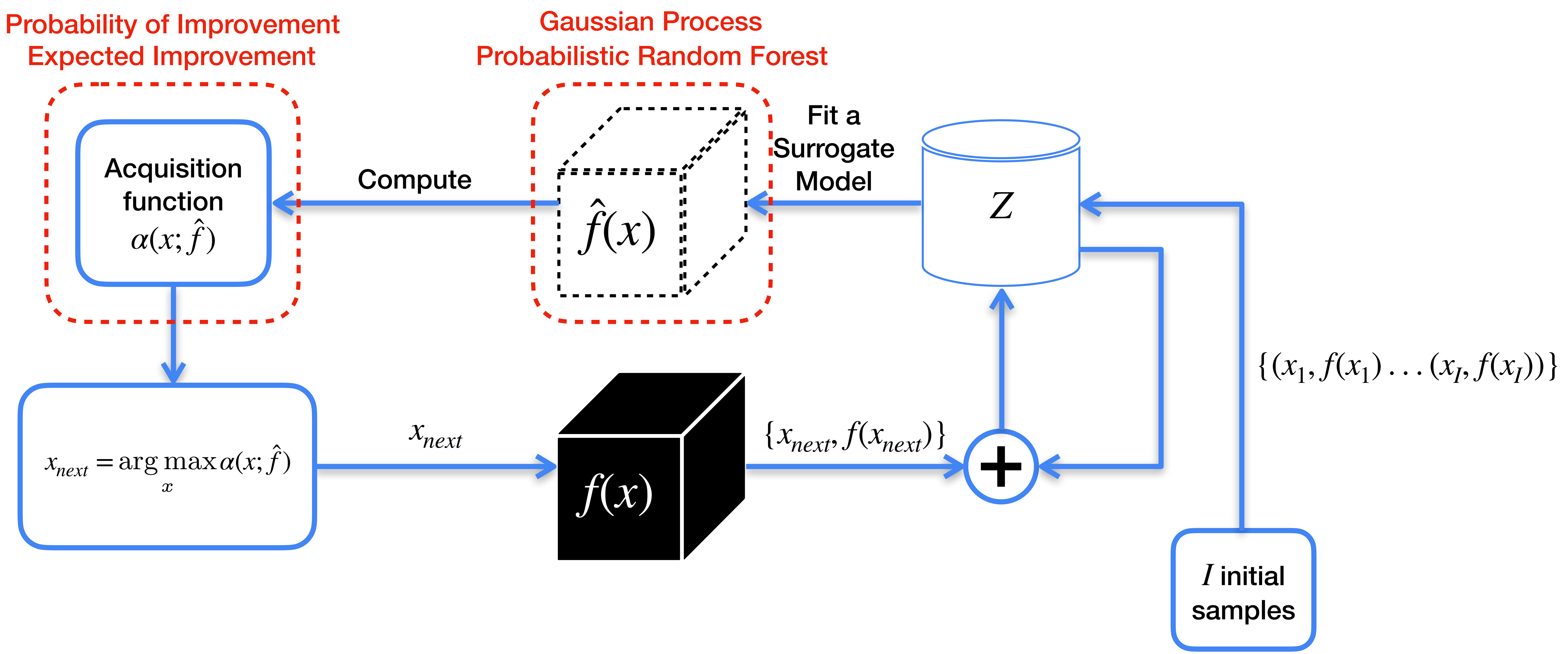

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Bayesian Optimization

Real-World Applications

Bayesian Optimization

Real-World Applications

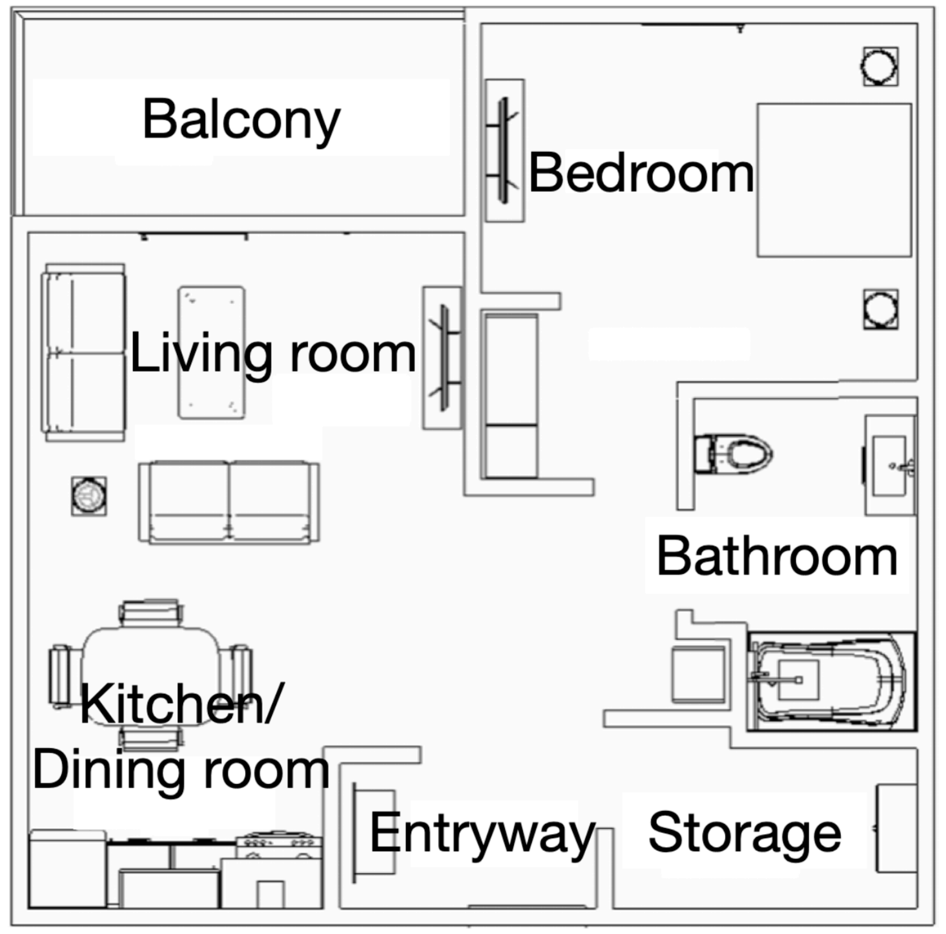
System Design Optimization

Bayesian Optimization

Real-World Applications

System Design Optimization

Sensor Placement Optimization



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Bayesian Optimization

Real-World Applications

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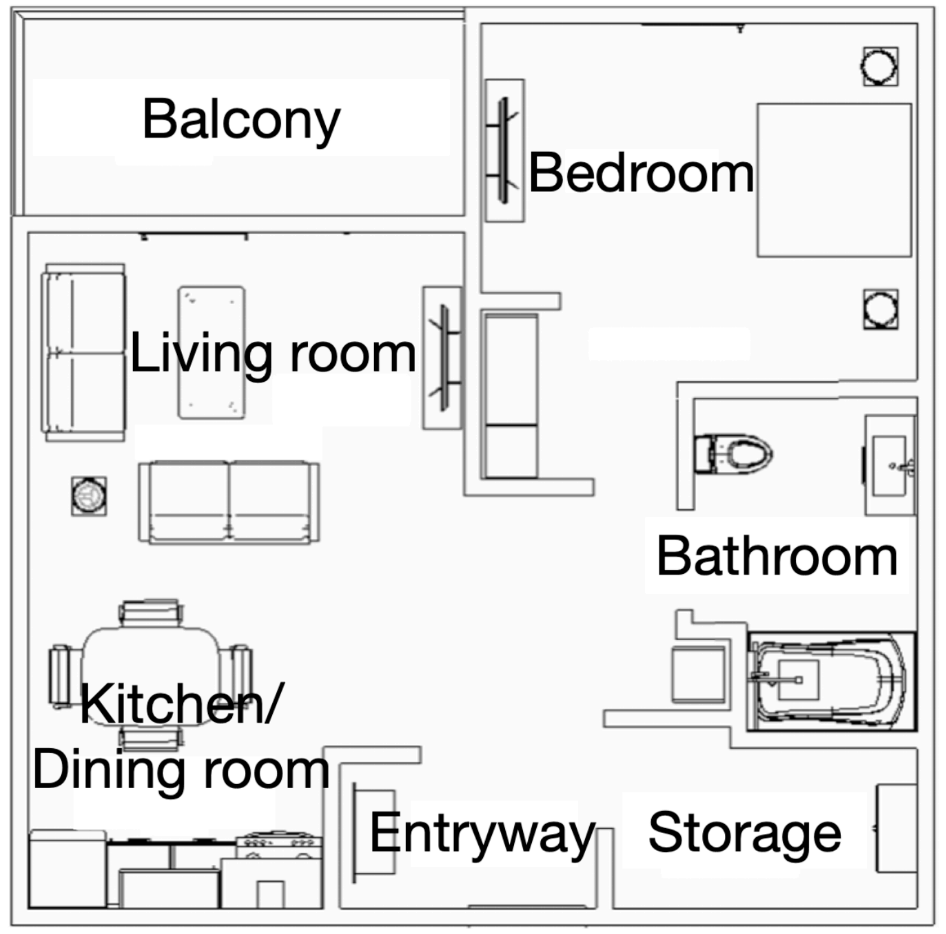

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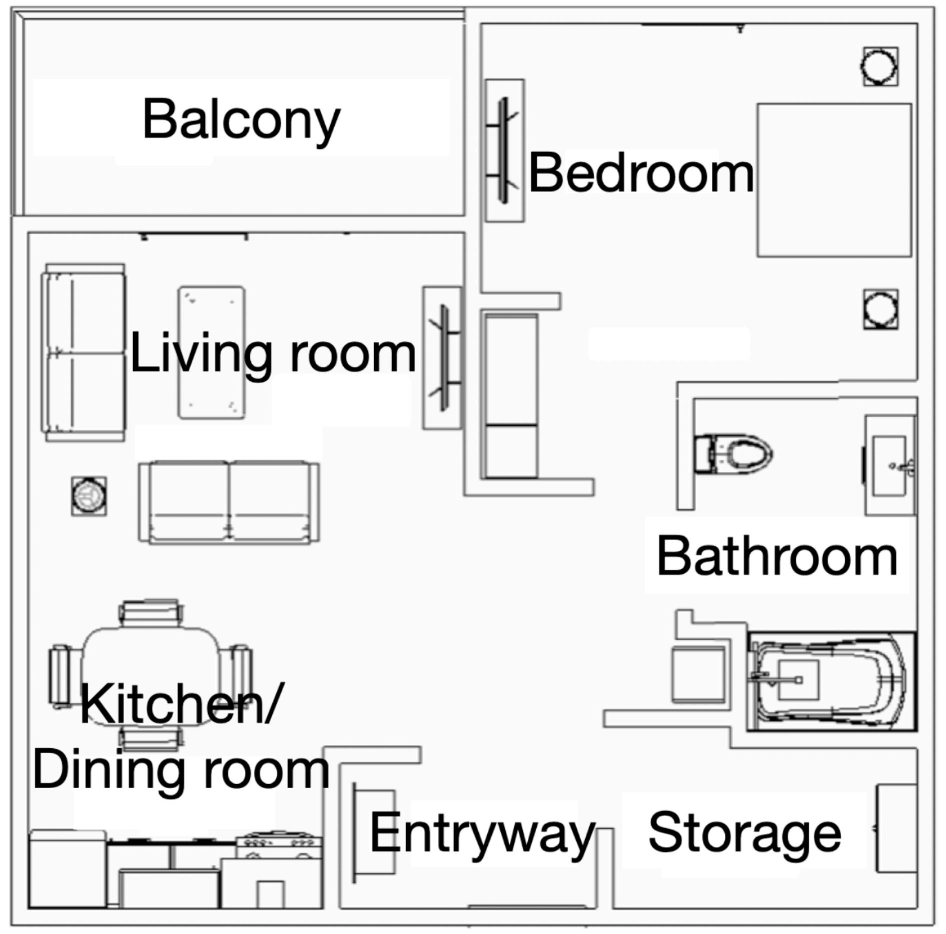

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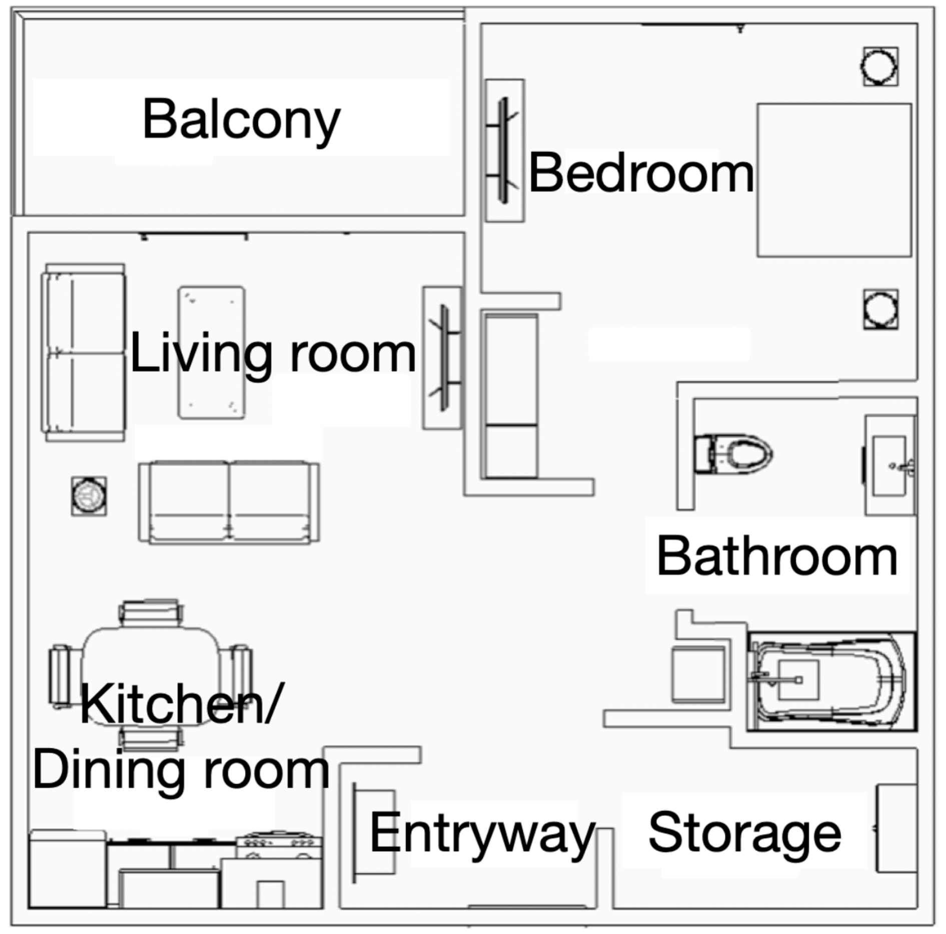
Bayesian Optimization

Real-World Applications

System Design Optimization

AutoML (Hyperparameter Optimization)

Sensor Placement Optimization



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Bayesian Optimization

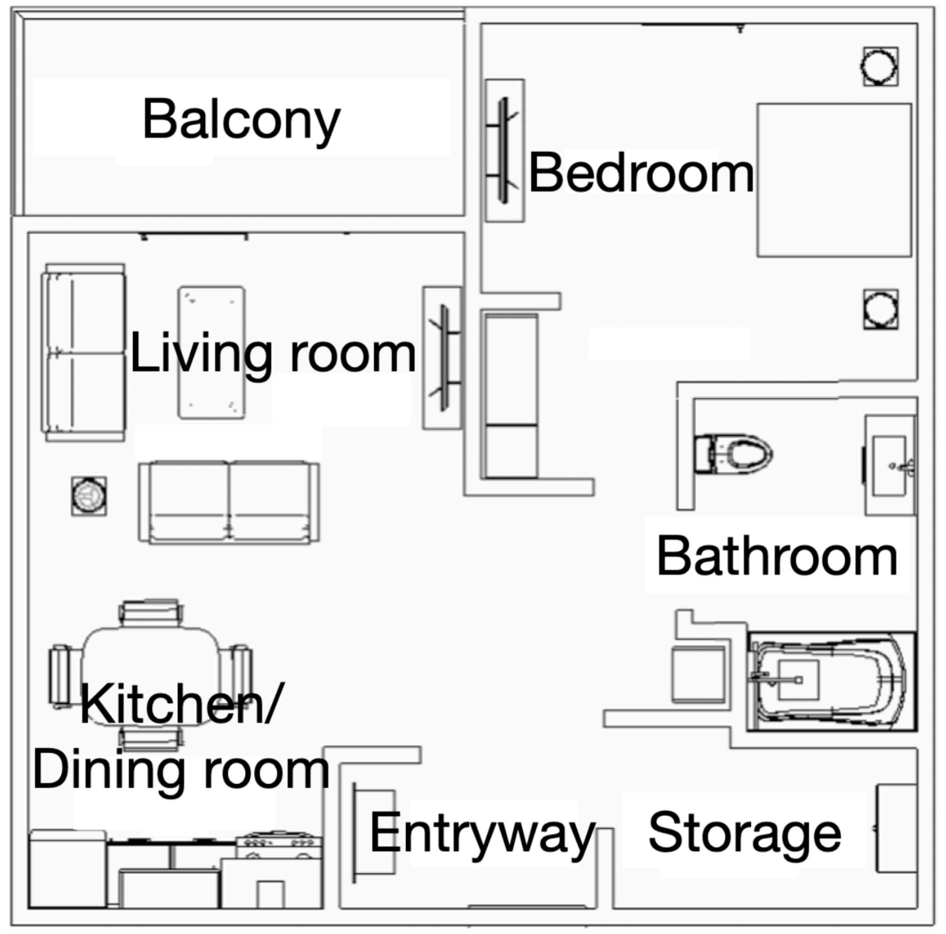
Real-World Applications

System Design Optimization

AutoML (Hyperparameter Optimization)

Automatic LQR Tuning Based on Gaussian Process Global Optimization

Sensor Placement Optimization



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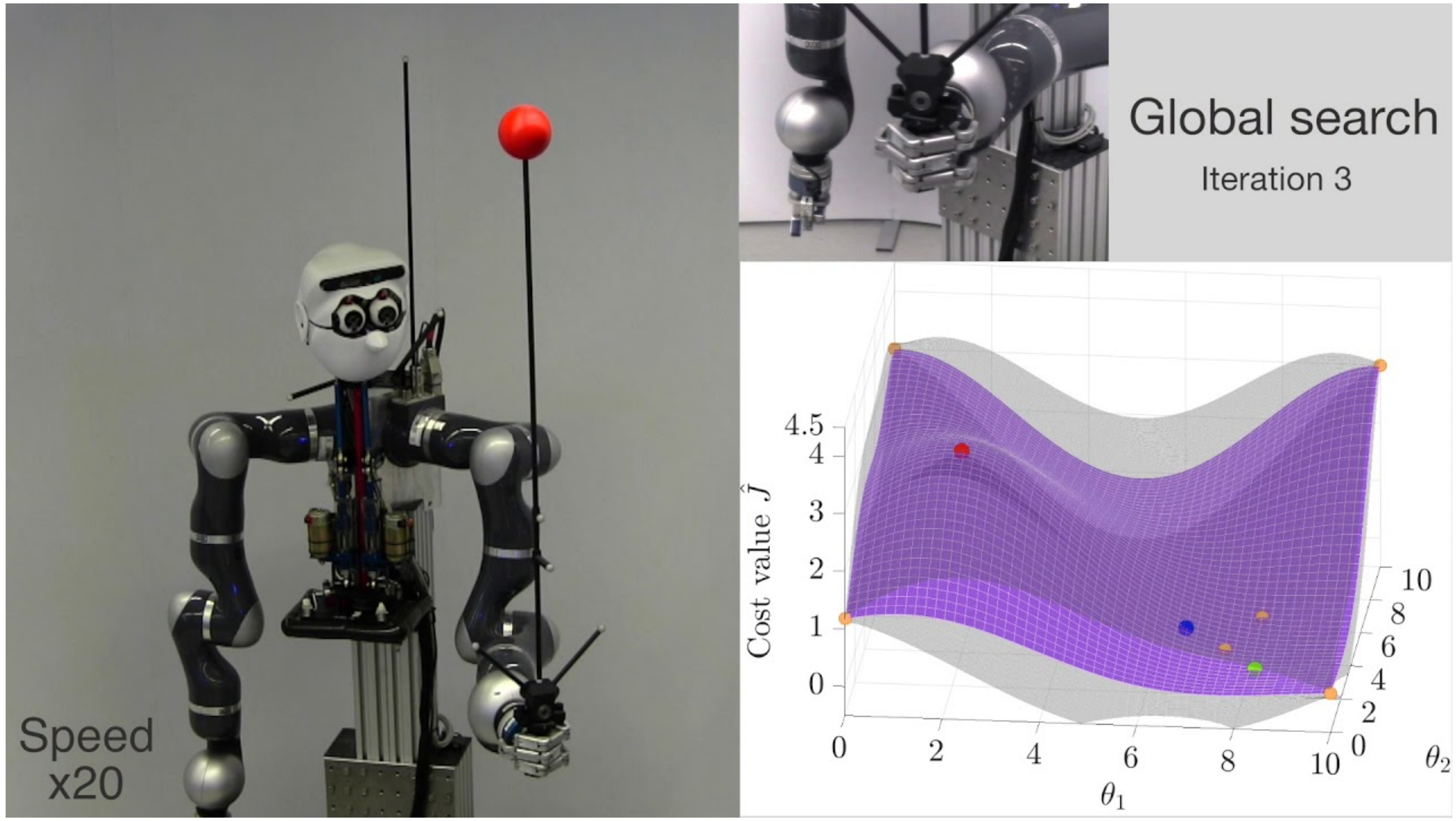

https://am.is.mpg.de/research_projects/cont-learn-bayes-opt

Reinforcement Learning

Reinforcement Learning

Introduction

- **Learning by interaction**
  - **Nature-inspired:** Learn how to achieve a particular task by trial and error

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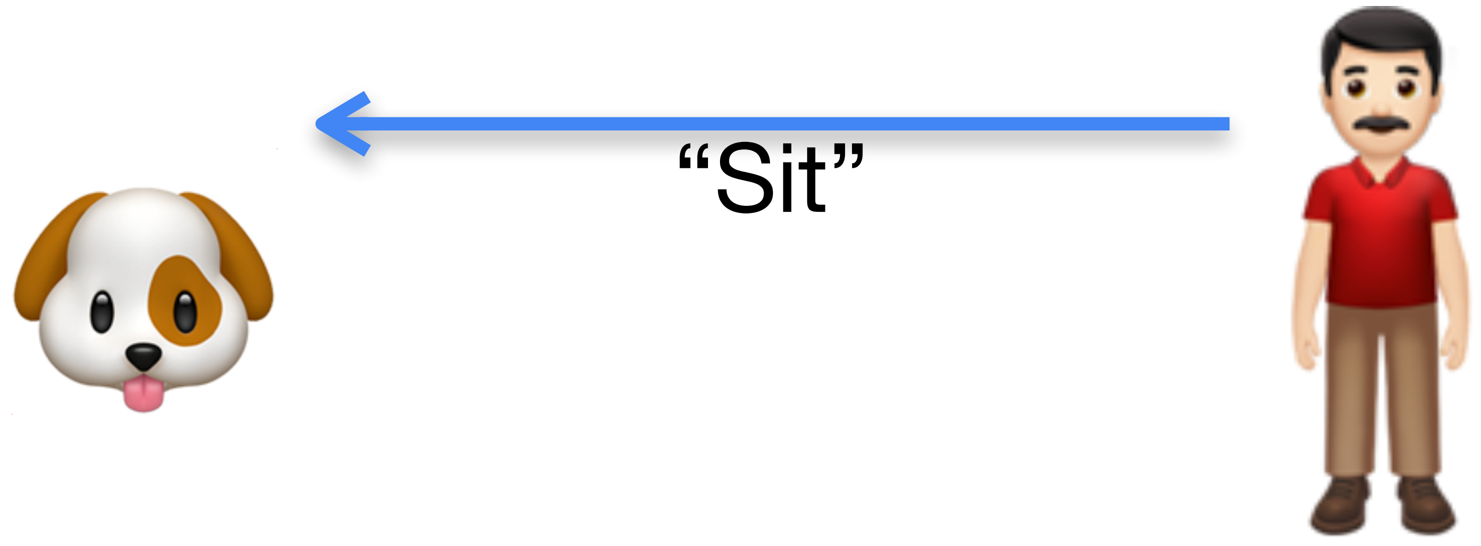

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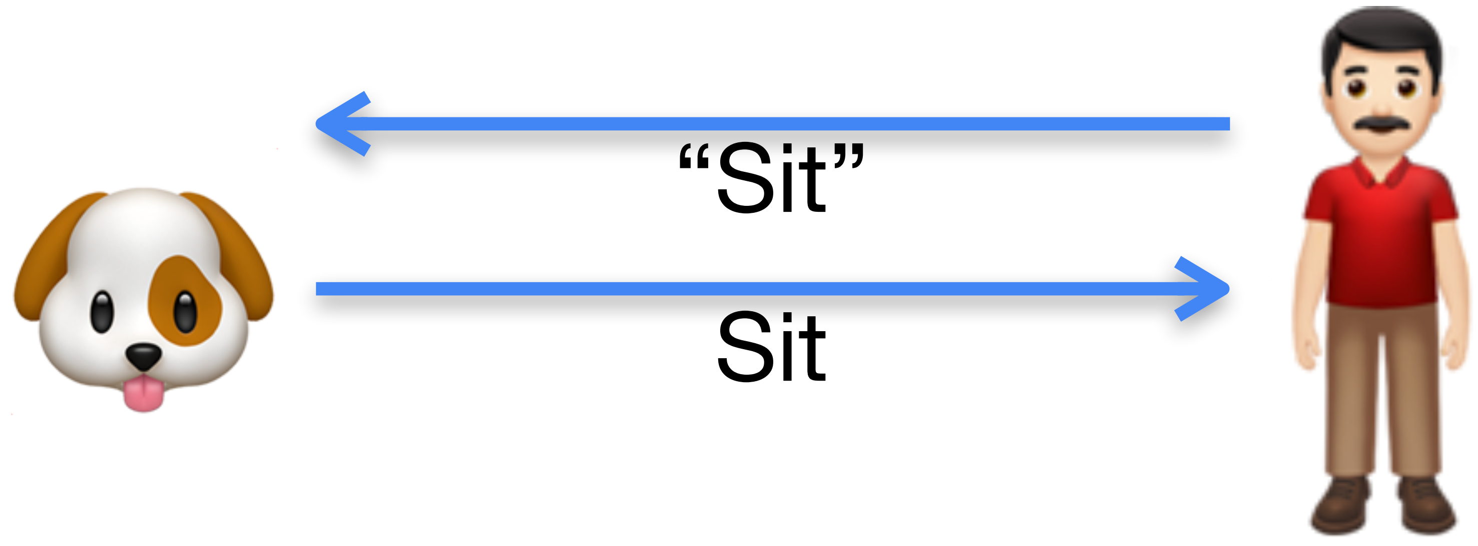

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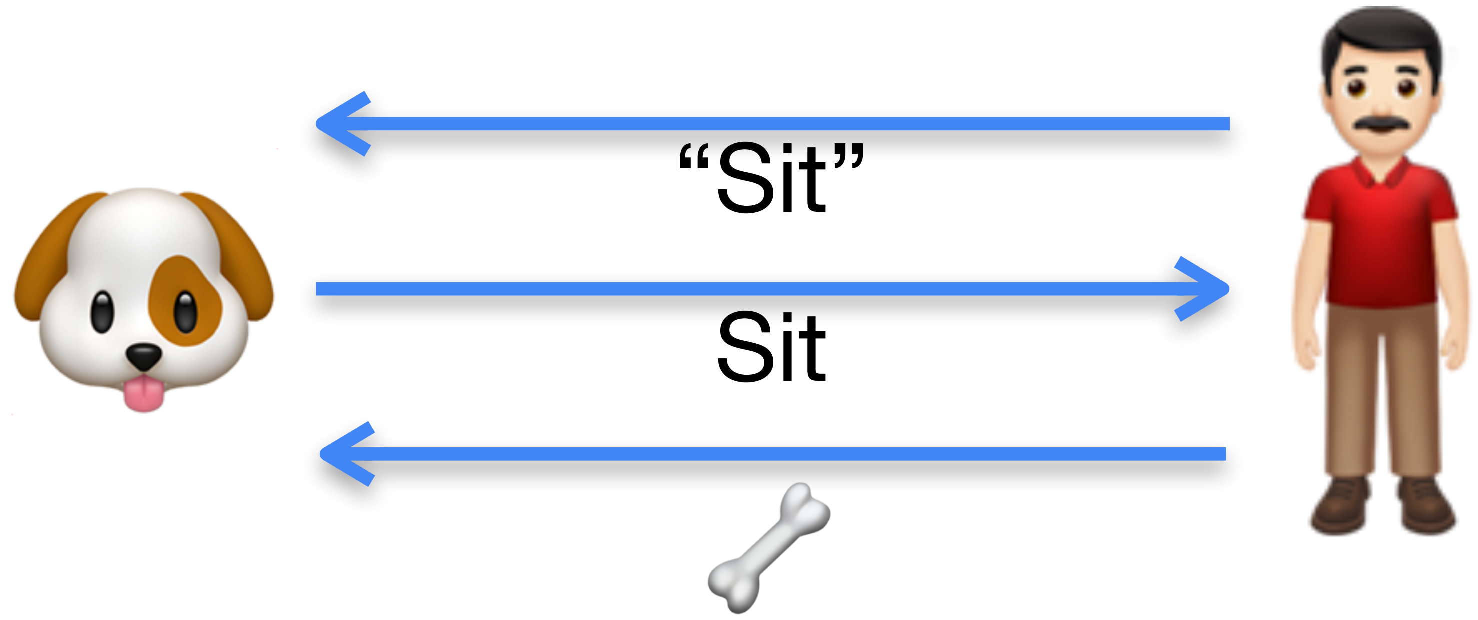

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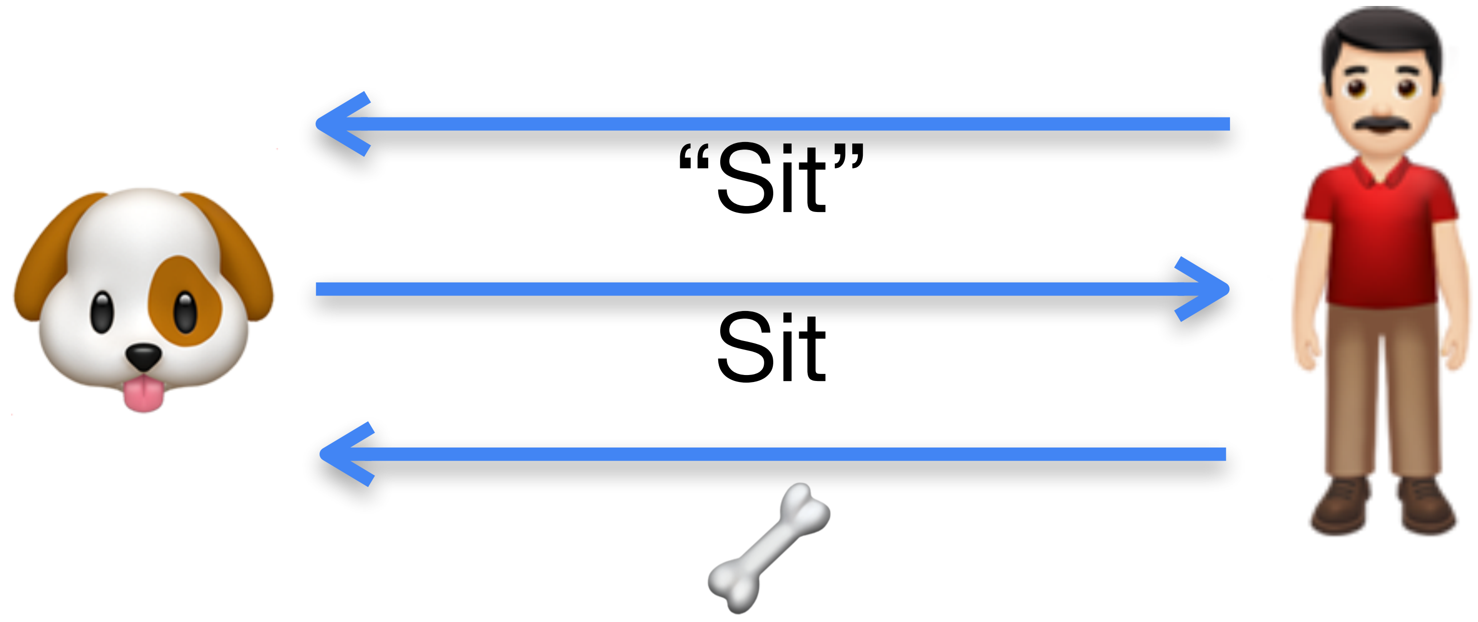
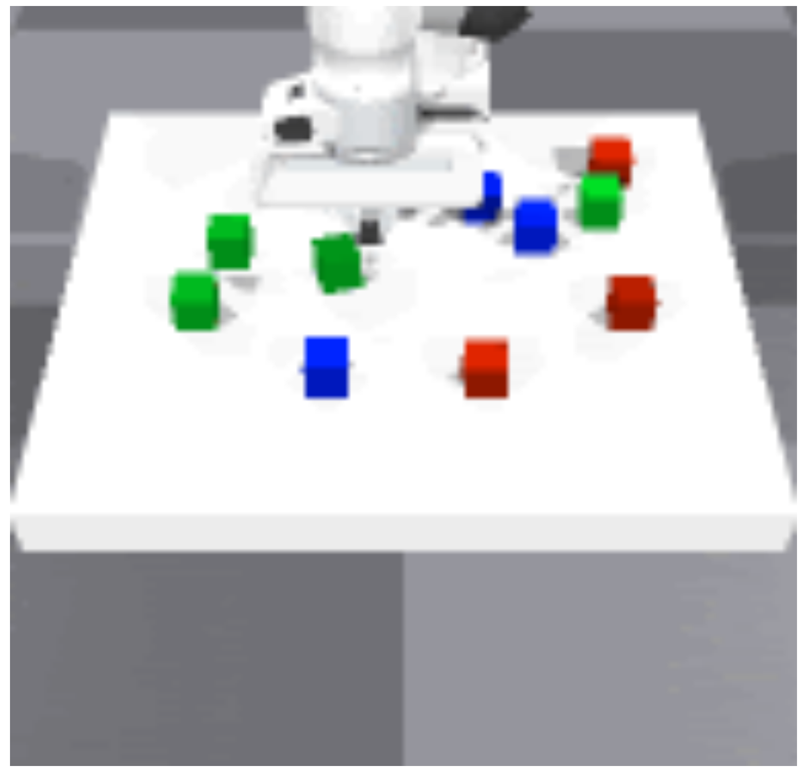


Object manipulation



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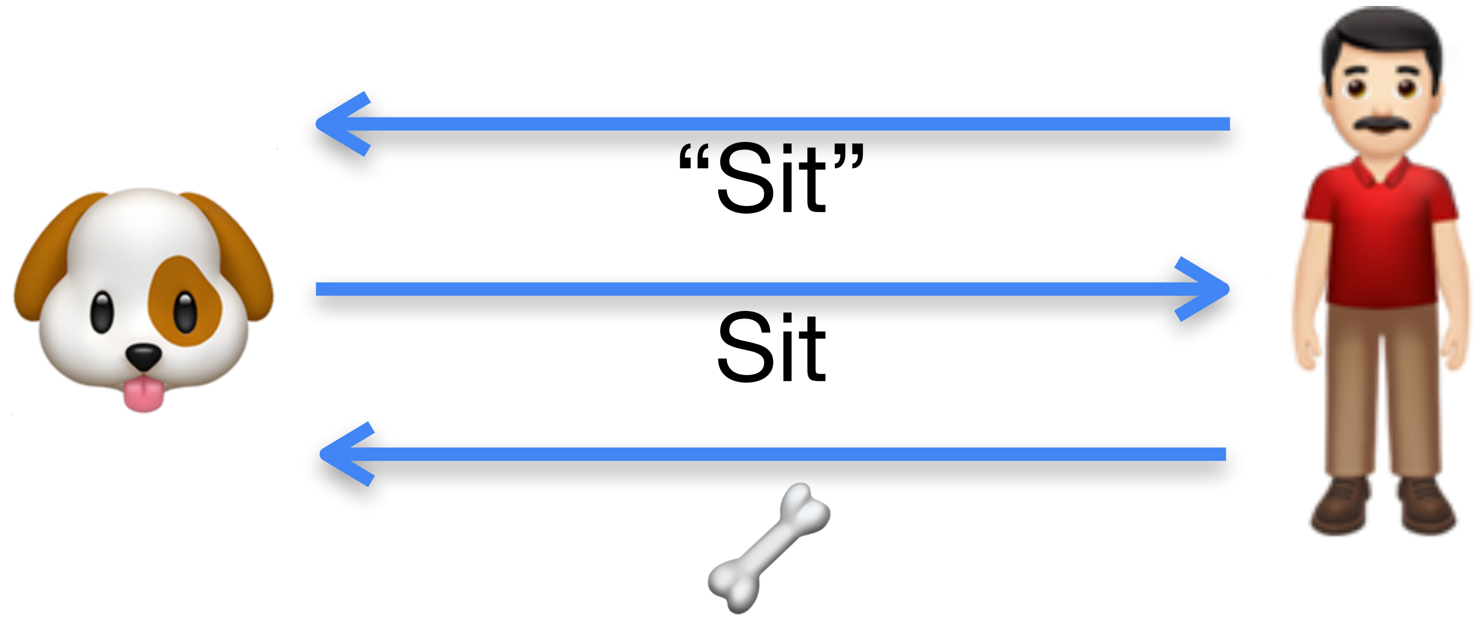

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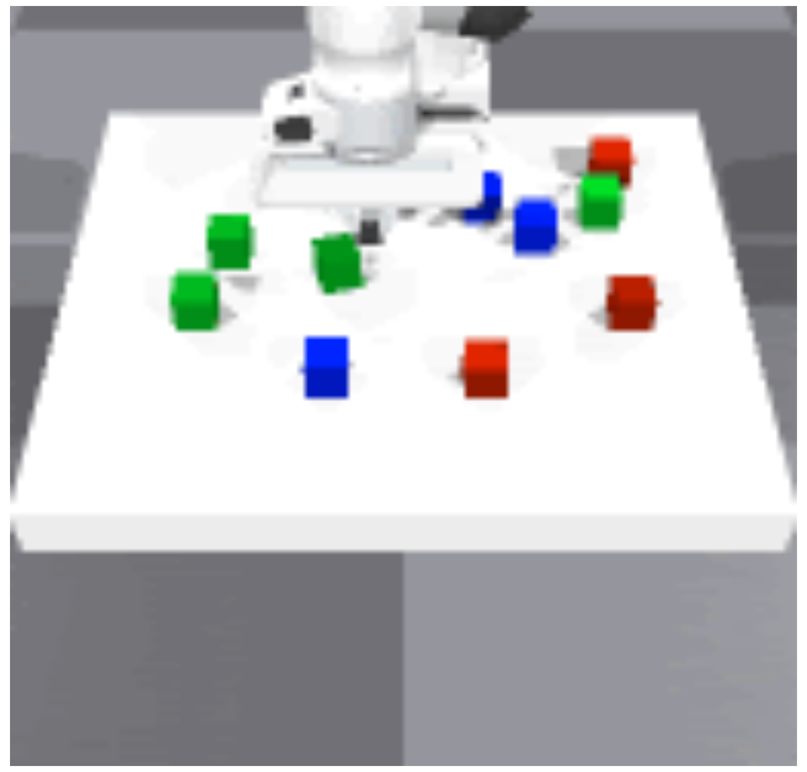

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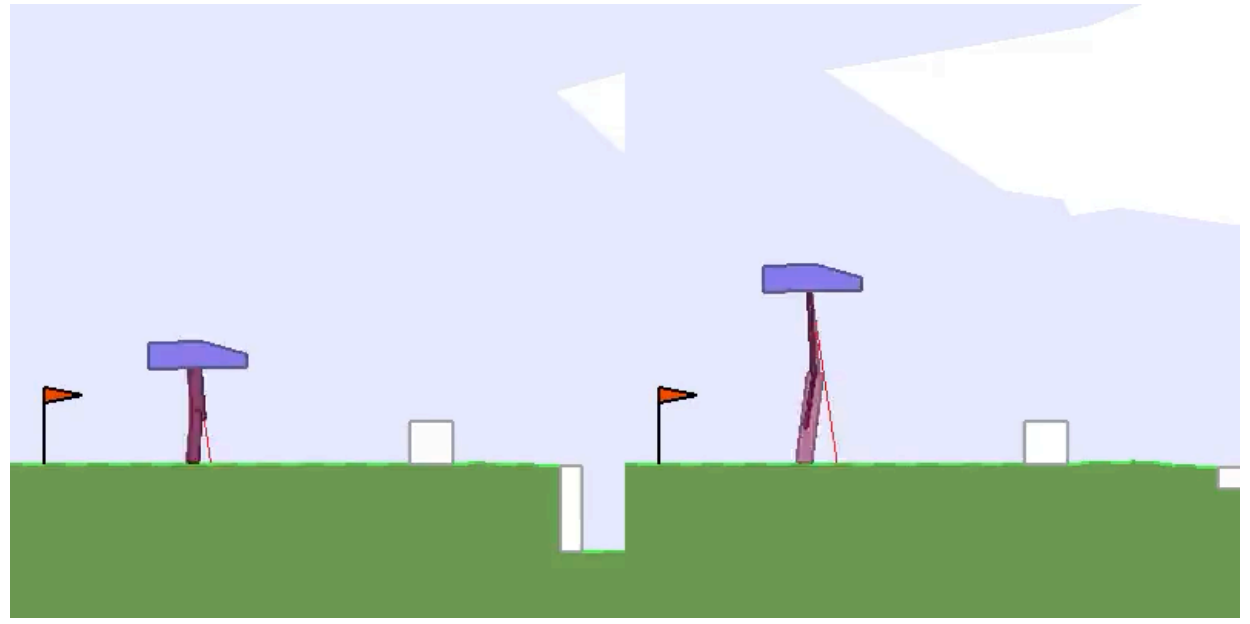

Learning to navigate

Learns a body design jointly with the navigation task

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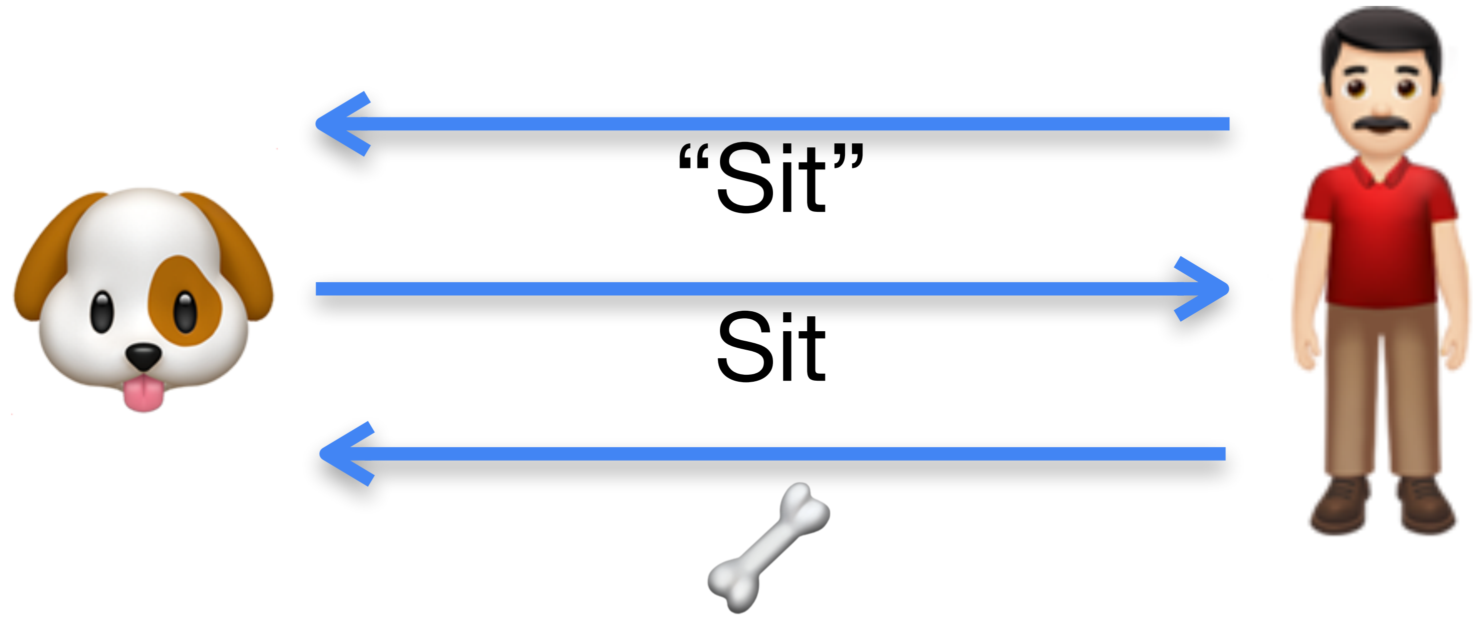

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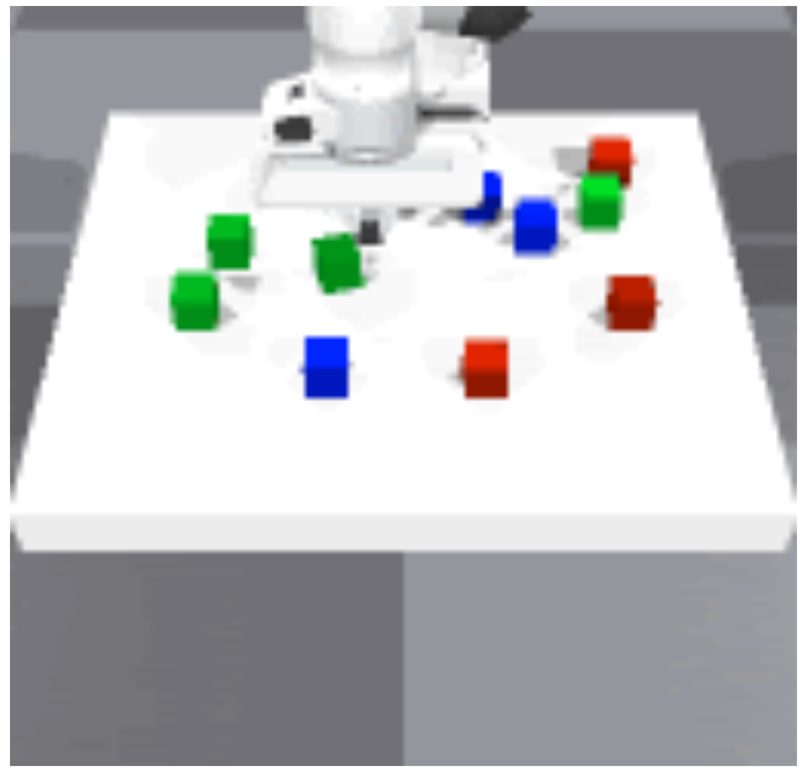

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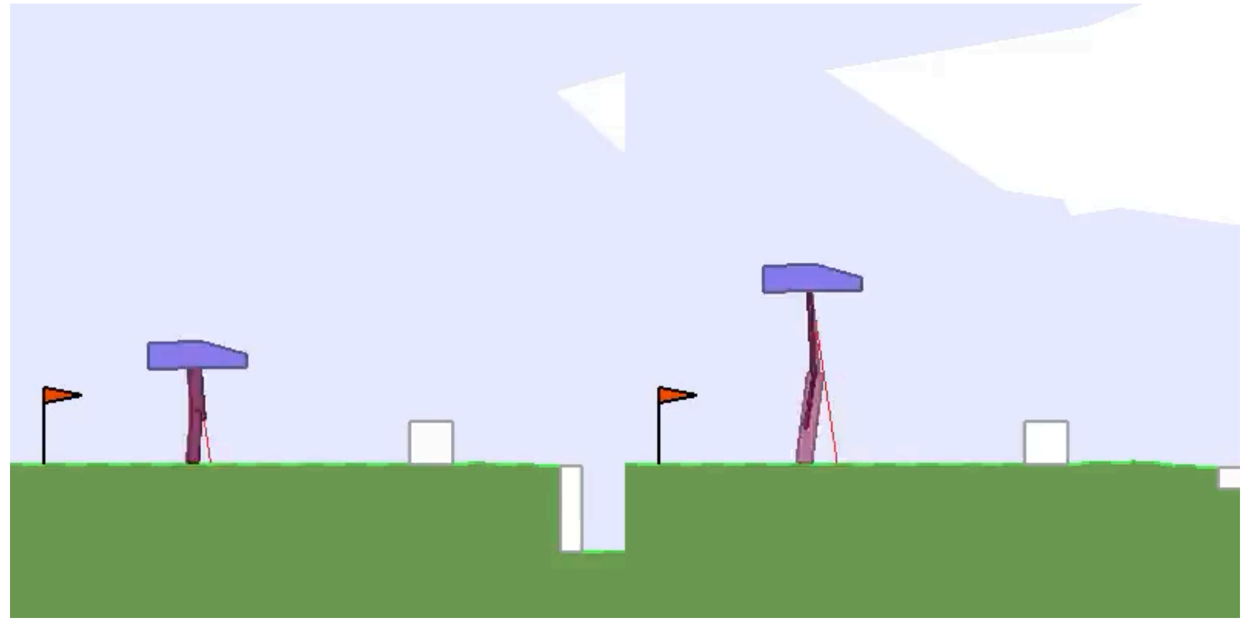

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Adaptation

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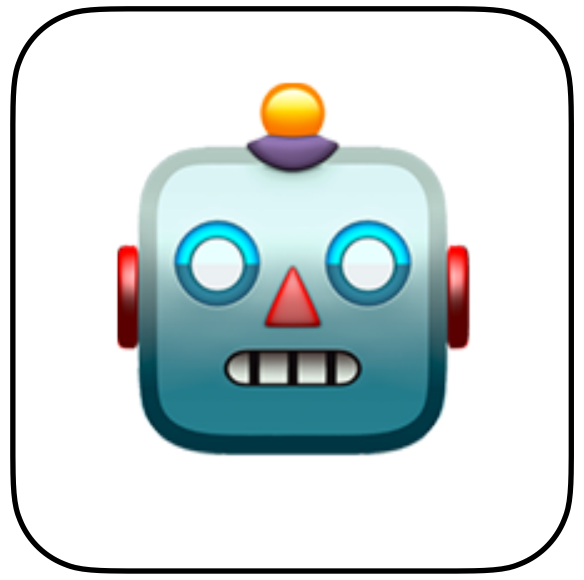
Reinforcement Learning

Core Concepts and Terminology

Reinforcement Learning

Core Concepts and Terminology

Agent:
the entity that
takes actions
e.g., robots



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Reinforcement Learning

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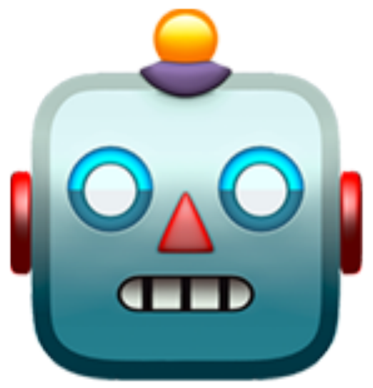

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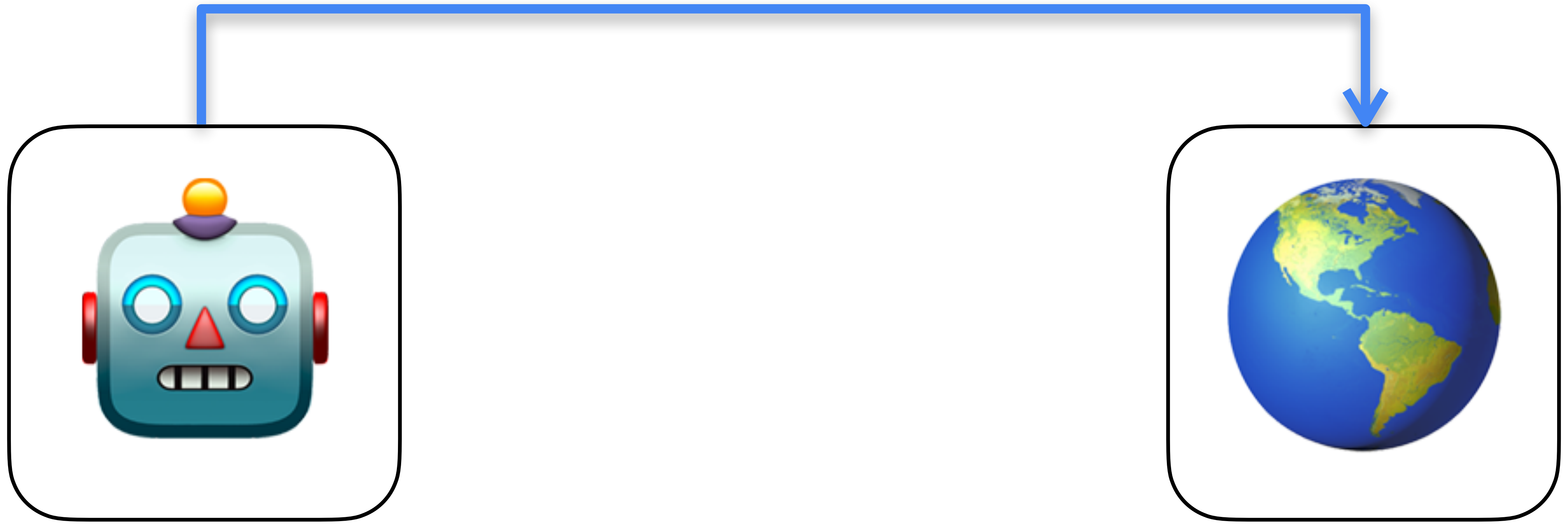
Reinforcement Learning

Core Concepts and Terminology

Actions (a_t):
the allowed moves
e.g. joints movements,
grab/drop objects



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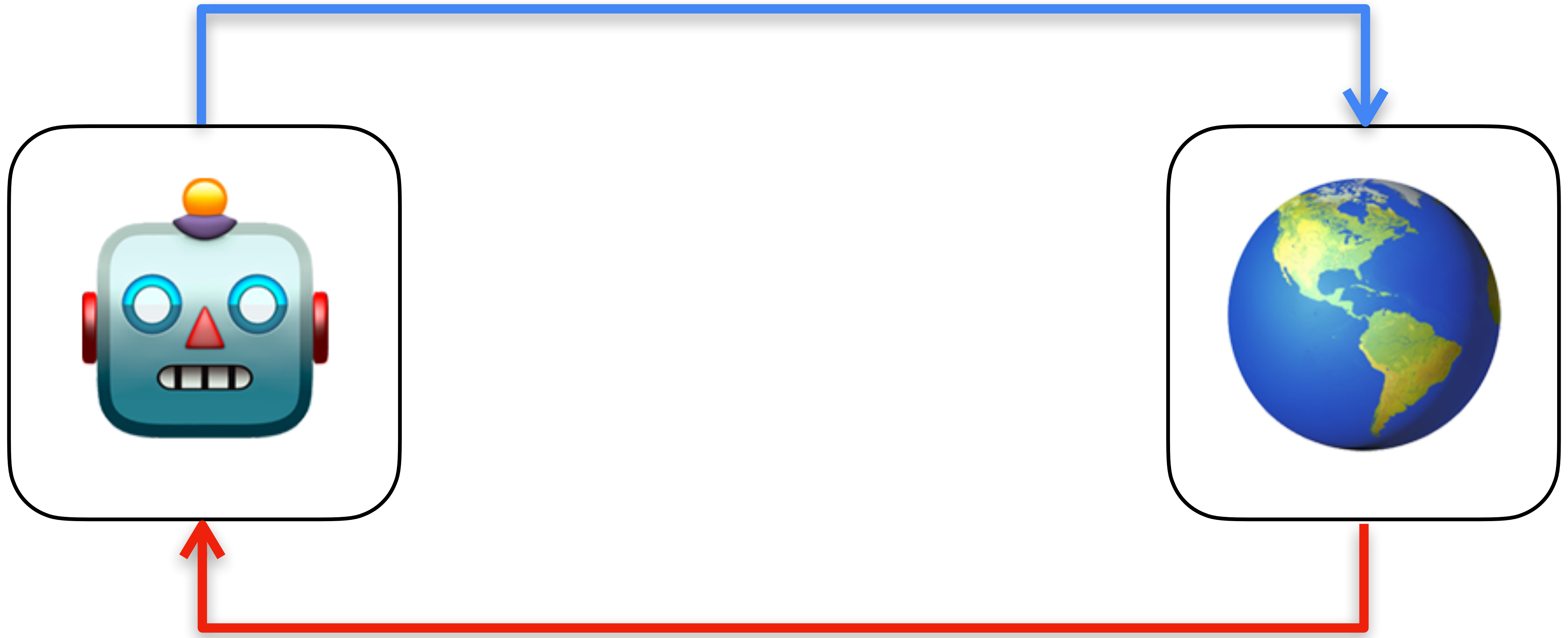

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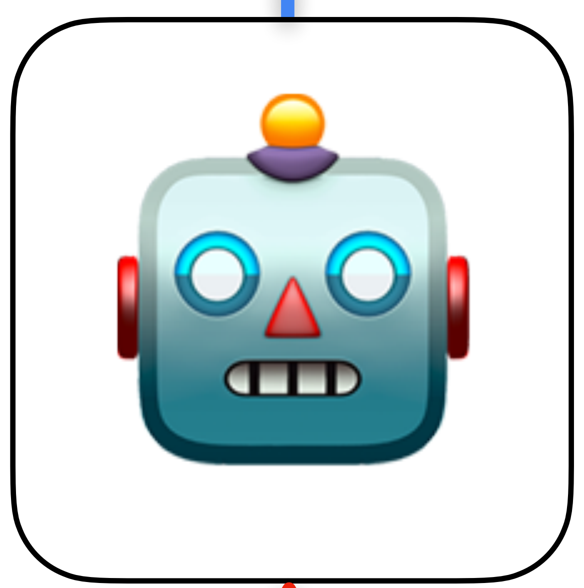

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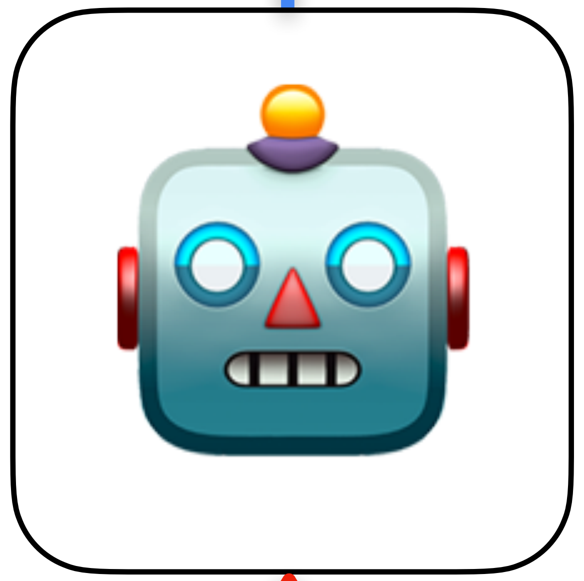

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States (s_{t+1})
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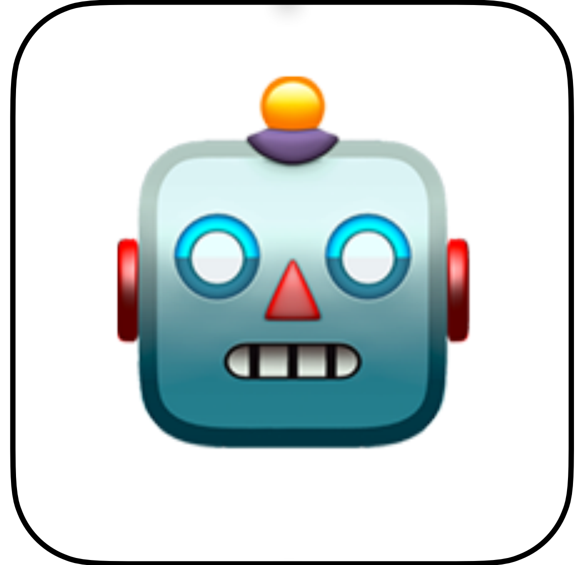

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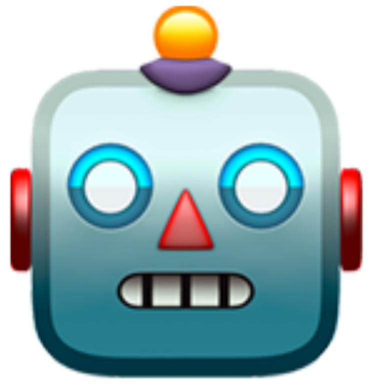

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Sum of Reward (R_t)

$$R_t = \sum_{i=t}^{H} r_t$$

H is a horizon (can be ∞)

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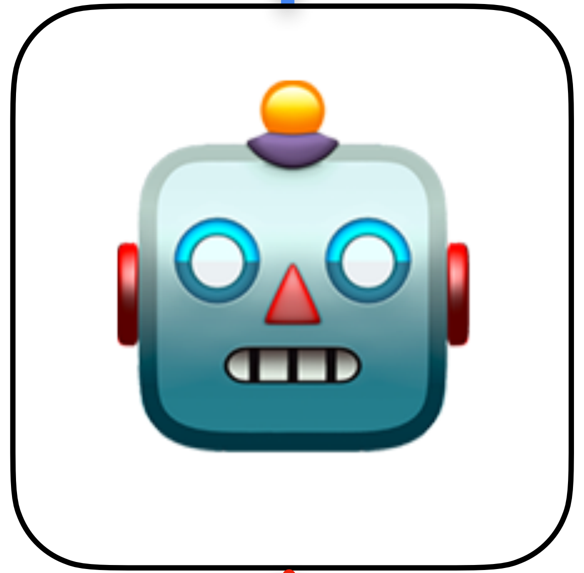

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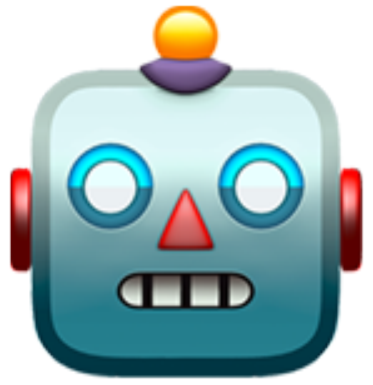

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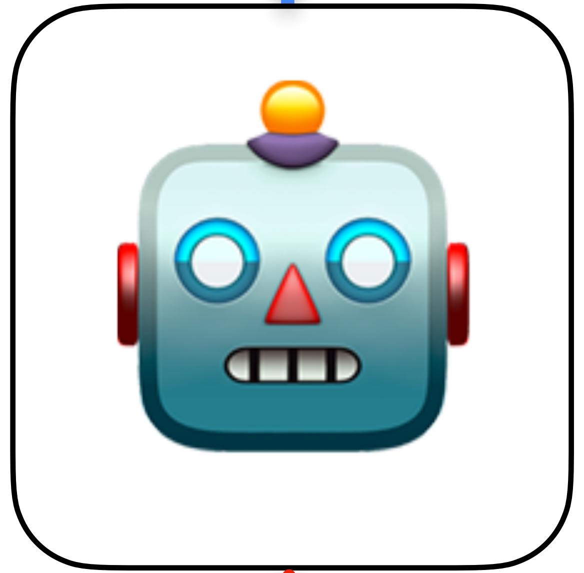

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💵 now OR 💵 1 year later

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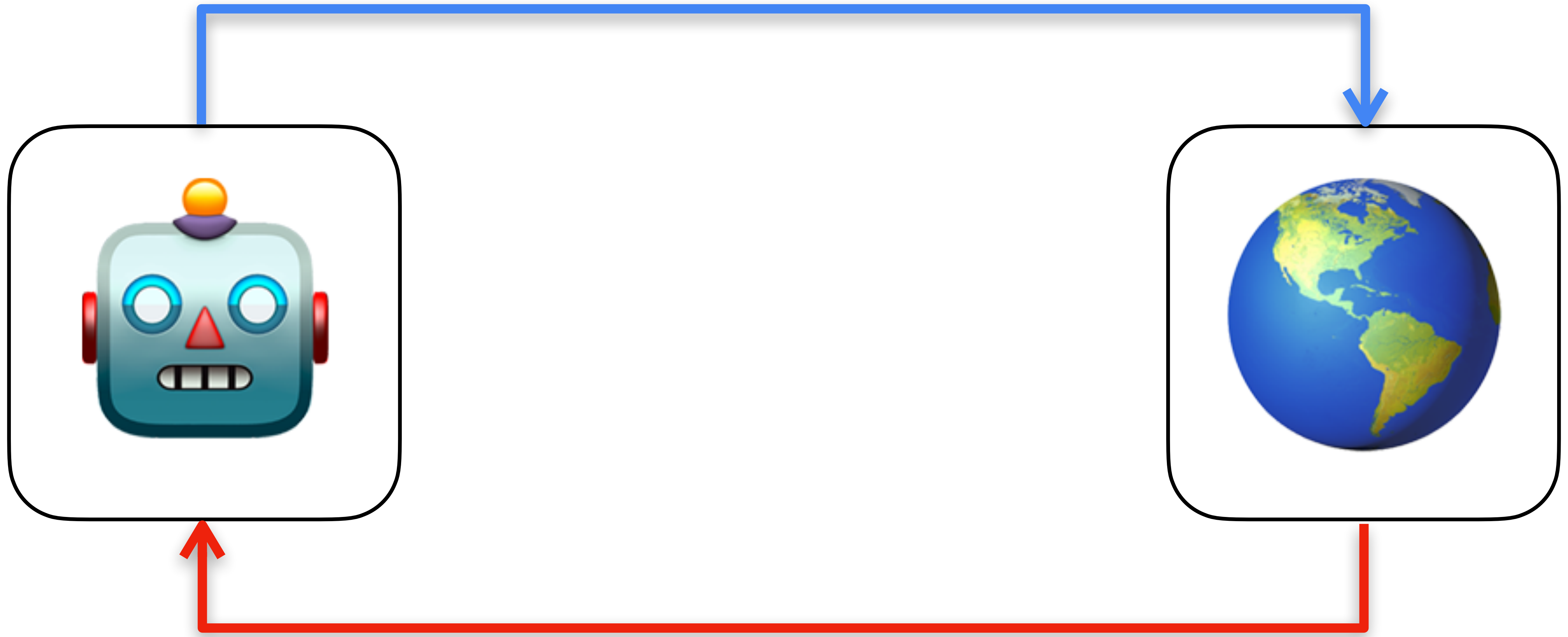

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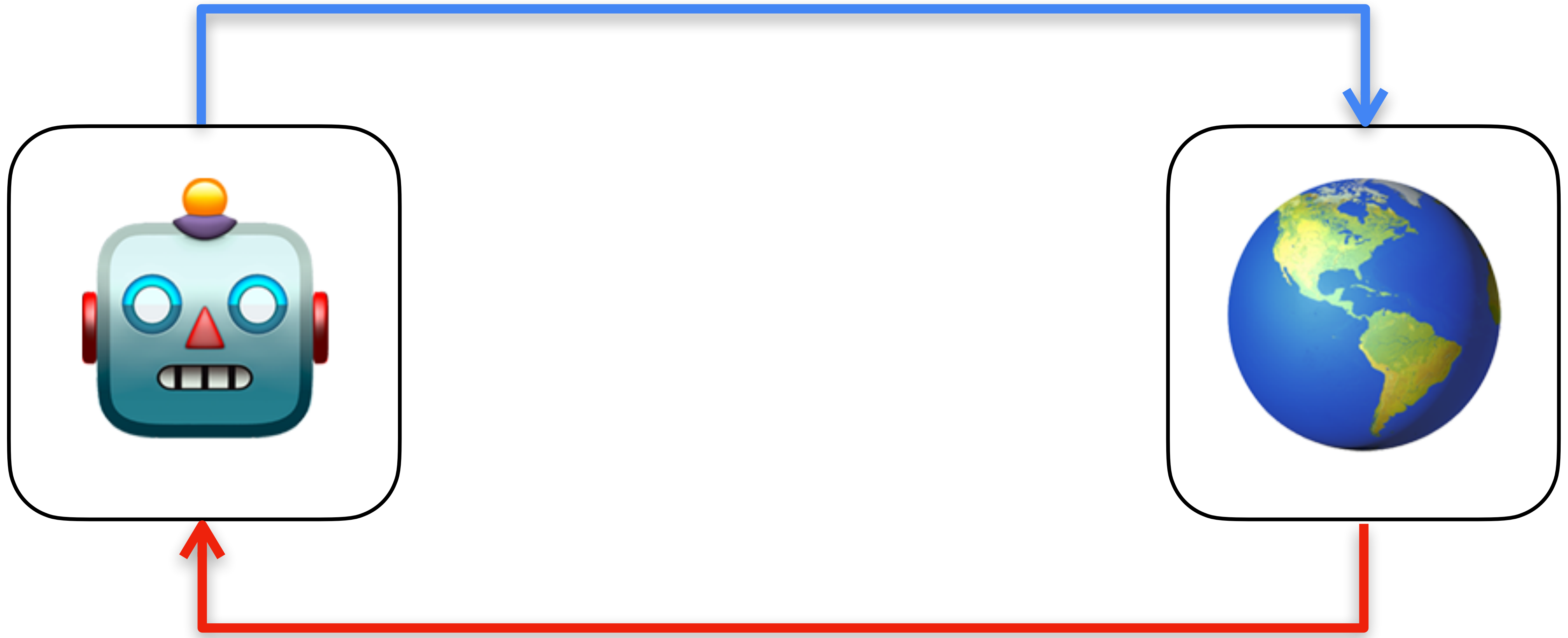

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Reinforcement Learning

Core Concepts and Terminology

Q-function

$$Q(s_t, a_t)$$

expected total future reward that the agent can receive in state s_t by taking action a_t

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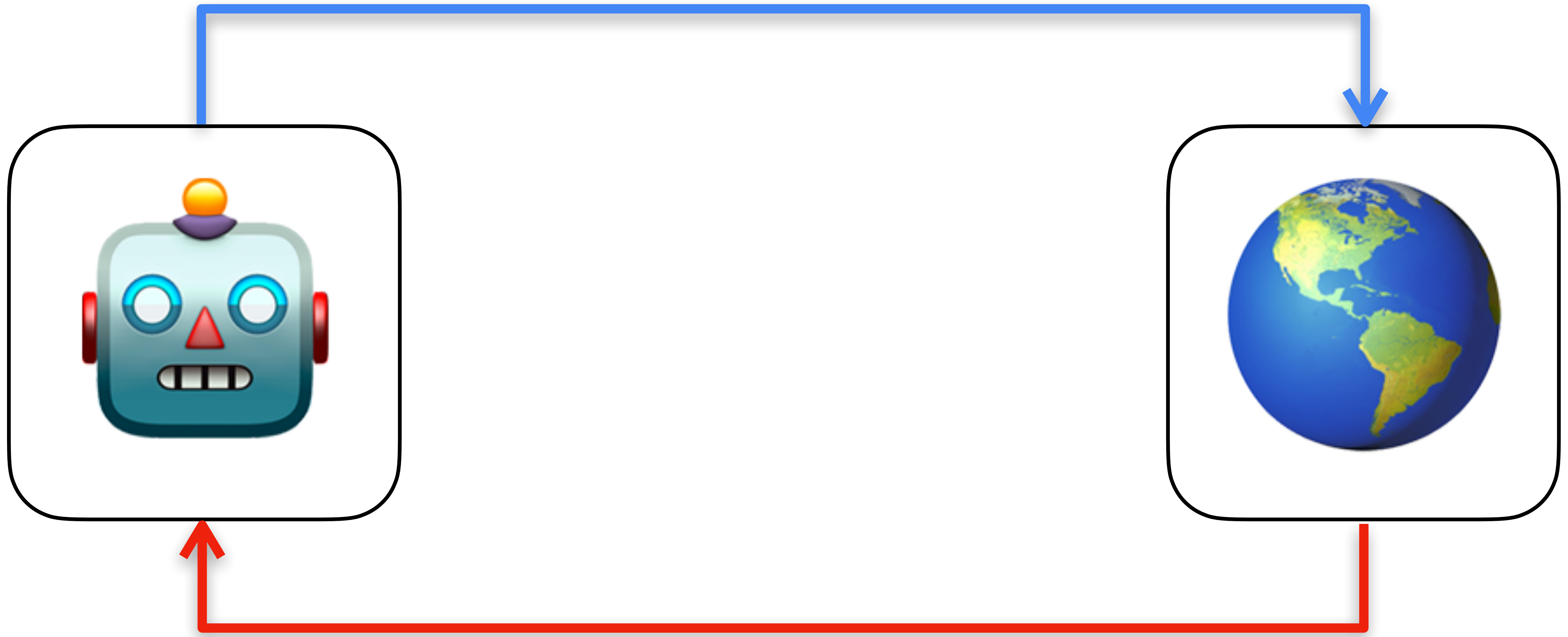

Observations:
changes of the environment observable by the agent
e.g. objects locations

Reward (r_t) **States (s_{t+1})**

Discounted Sum of Reward (R_t)

Reinforcement Learning

Core Concepts and Terminology

Q-function

$Q(s_t, a_t)$

expected total future reward that the agent can receive in state s_t by taking action a_t

$$Q(s_t, a_t) = E[R_t \,|\, s_t, a_t]$$

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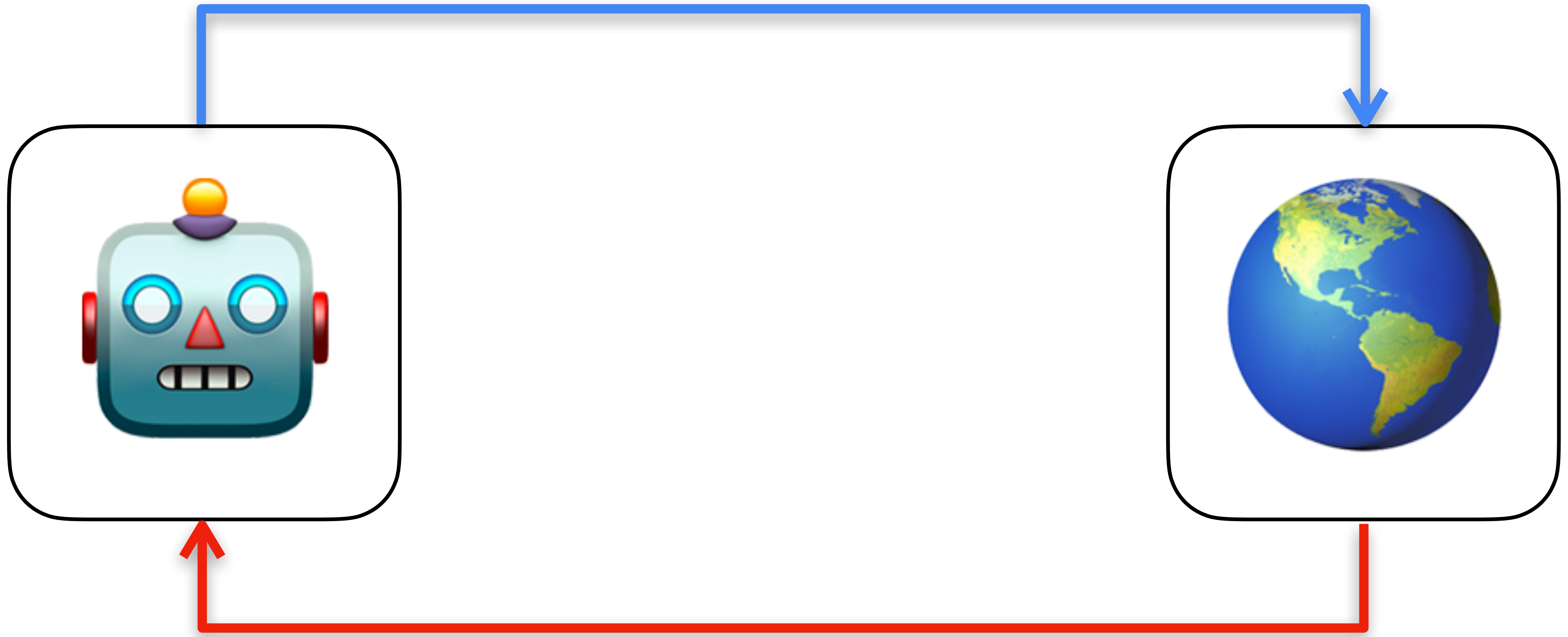

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Reinforcement Learning

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If the agent "magically" knows $Q(s_t, a_t)$, how it should take action a_t at any given state?

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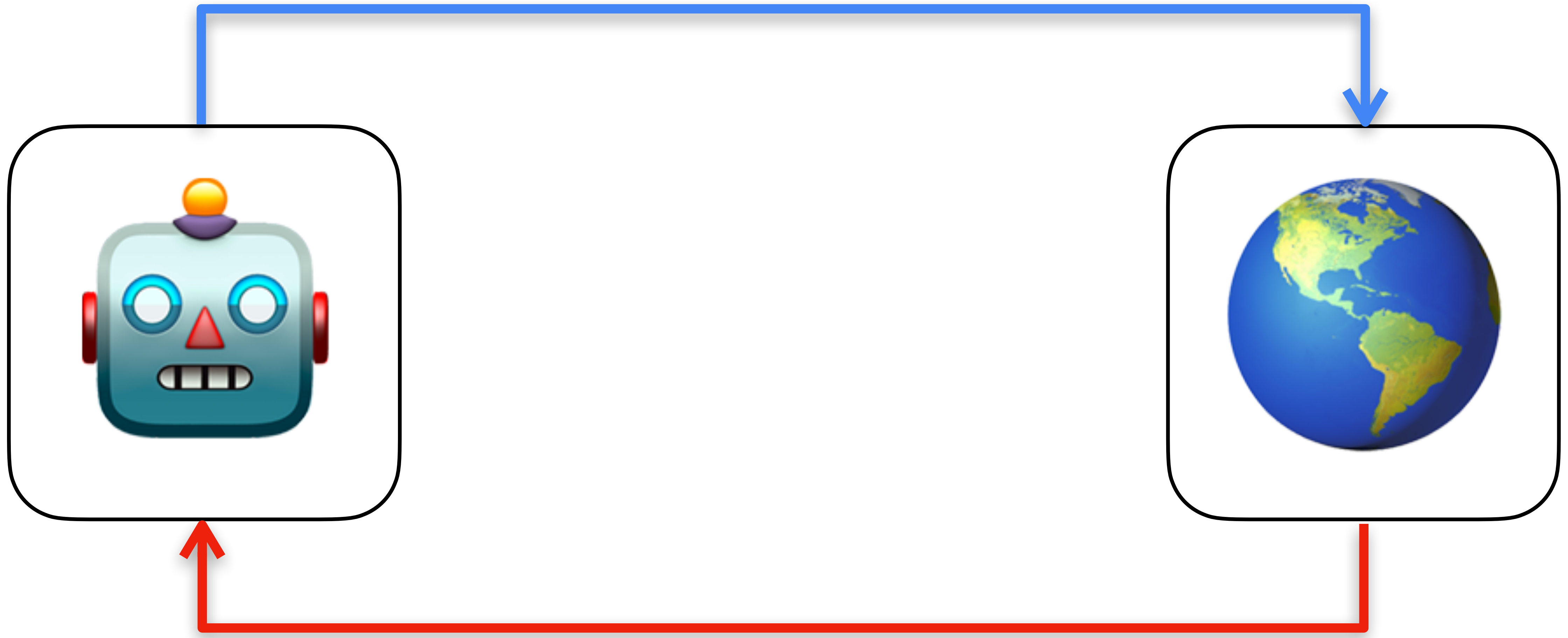

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best action to take at any given state s

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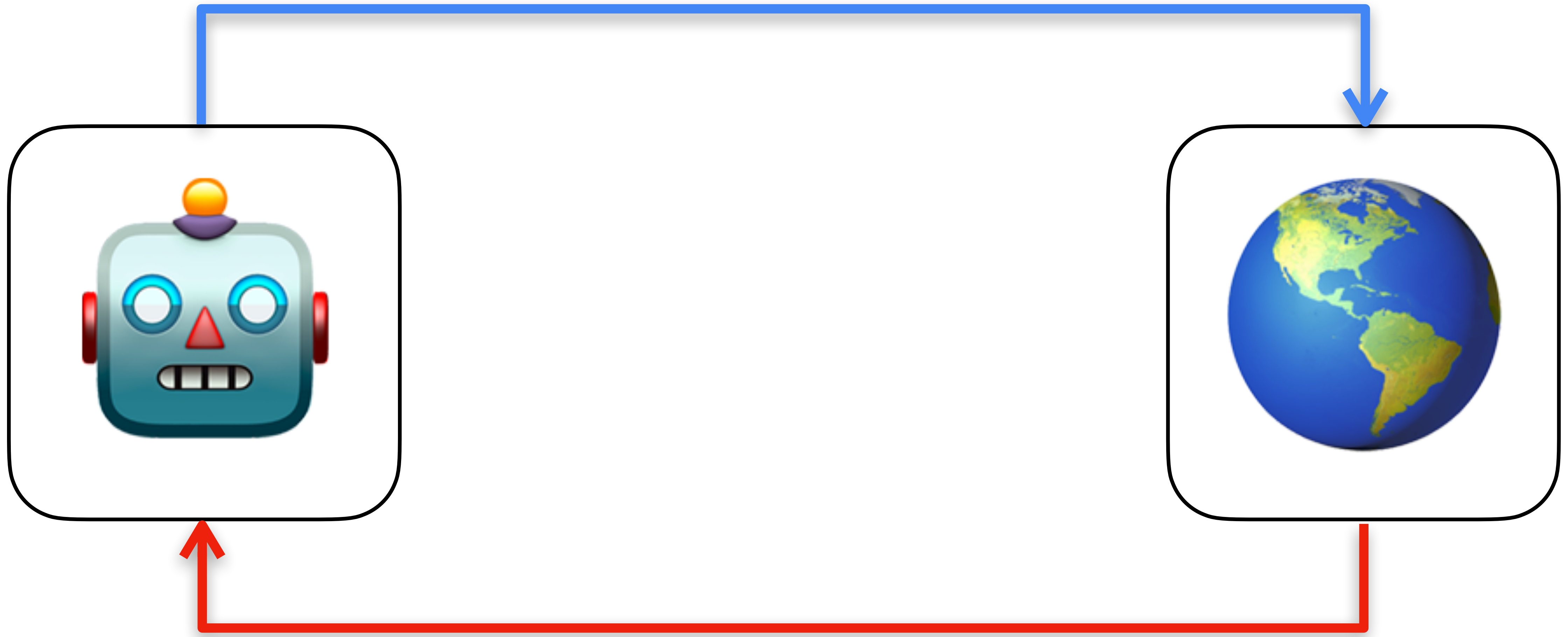

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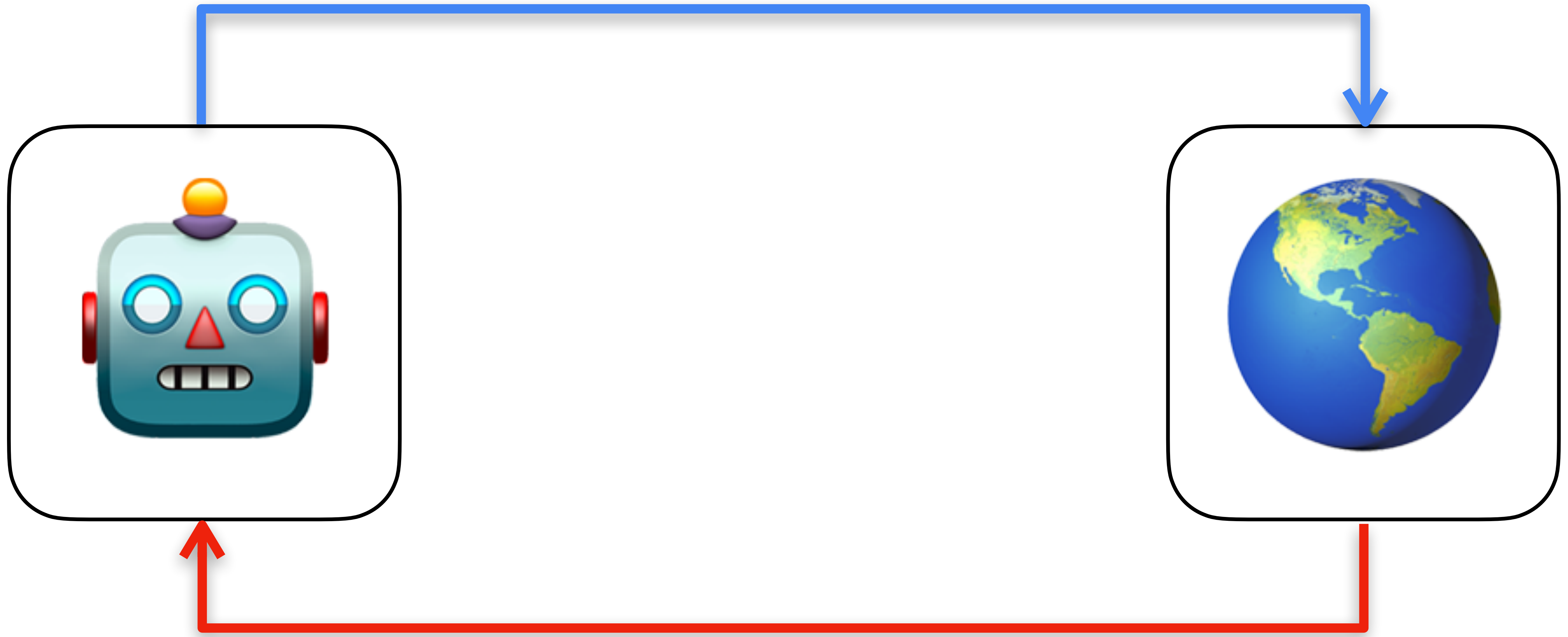

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Reinforcement Learning

Core Concepts and Terminology

Action

states

	a_0	a_1	a_2	...
s_0	$Q(s_0, a_0)$	$Q(s_0, a_1)$	$Q(s_0, a_2)$	...
s_1	$Q(s_1, a_0)$	$Q(s_1, a_1)$	$Q(s_1, a_2)$	...
s_2	$Q(s_2, a_0)$	$Q(s_2, a_1)$	$Q(s_2, a_2)$	...
...	...	...	...	...

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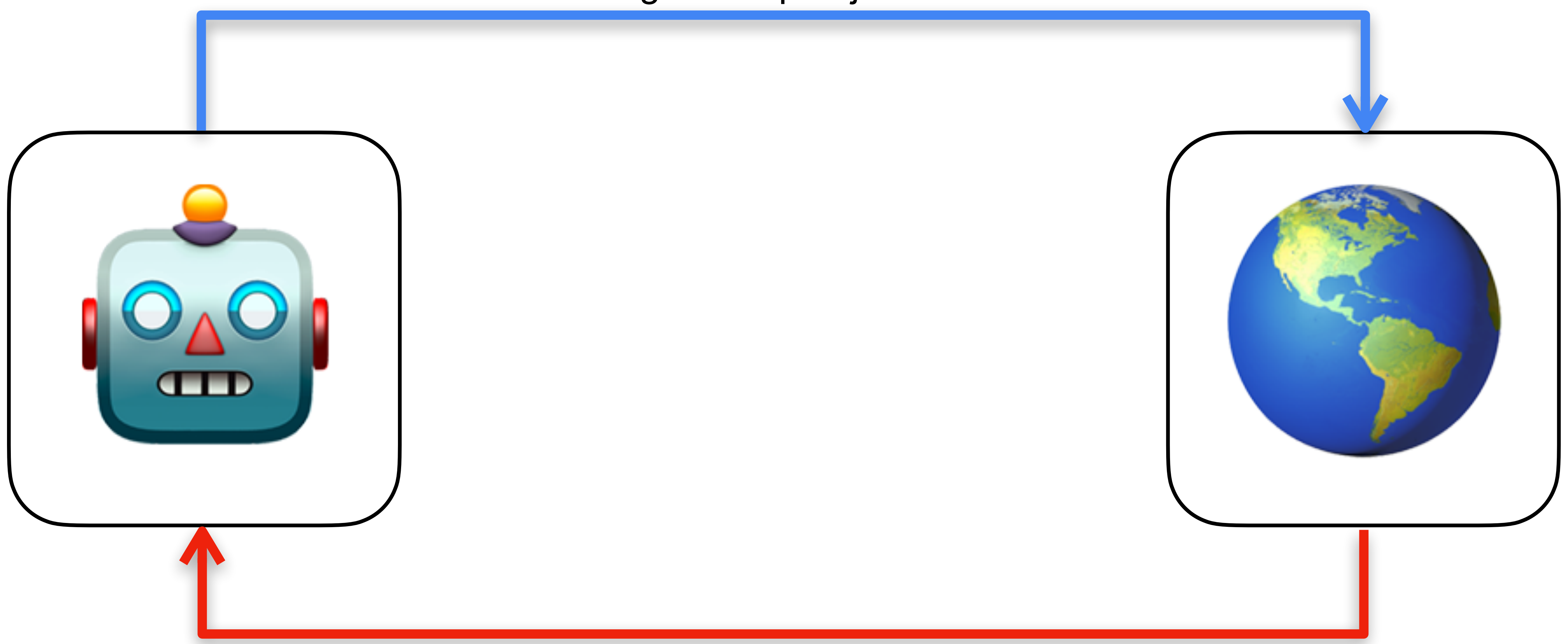

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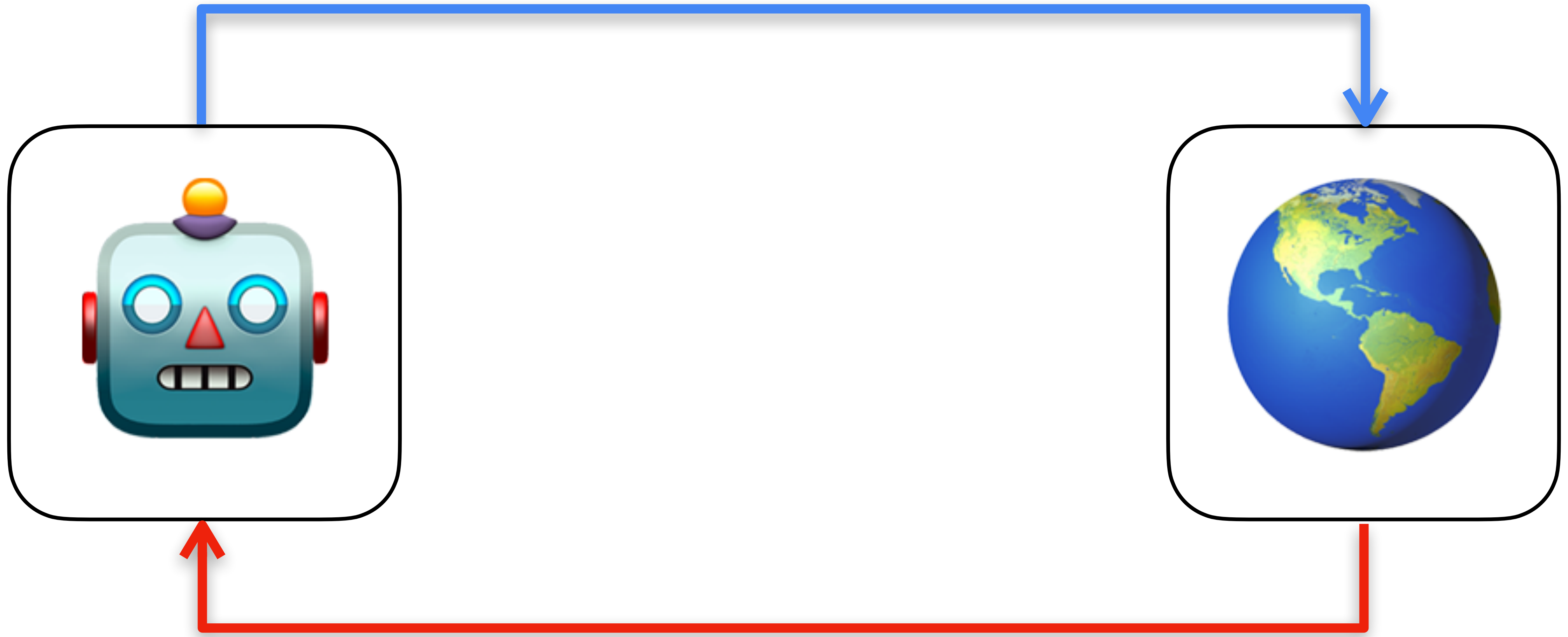

Environment:
the world where the agent exists in
e.g., an assembly line

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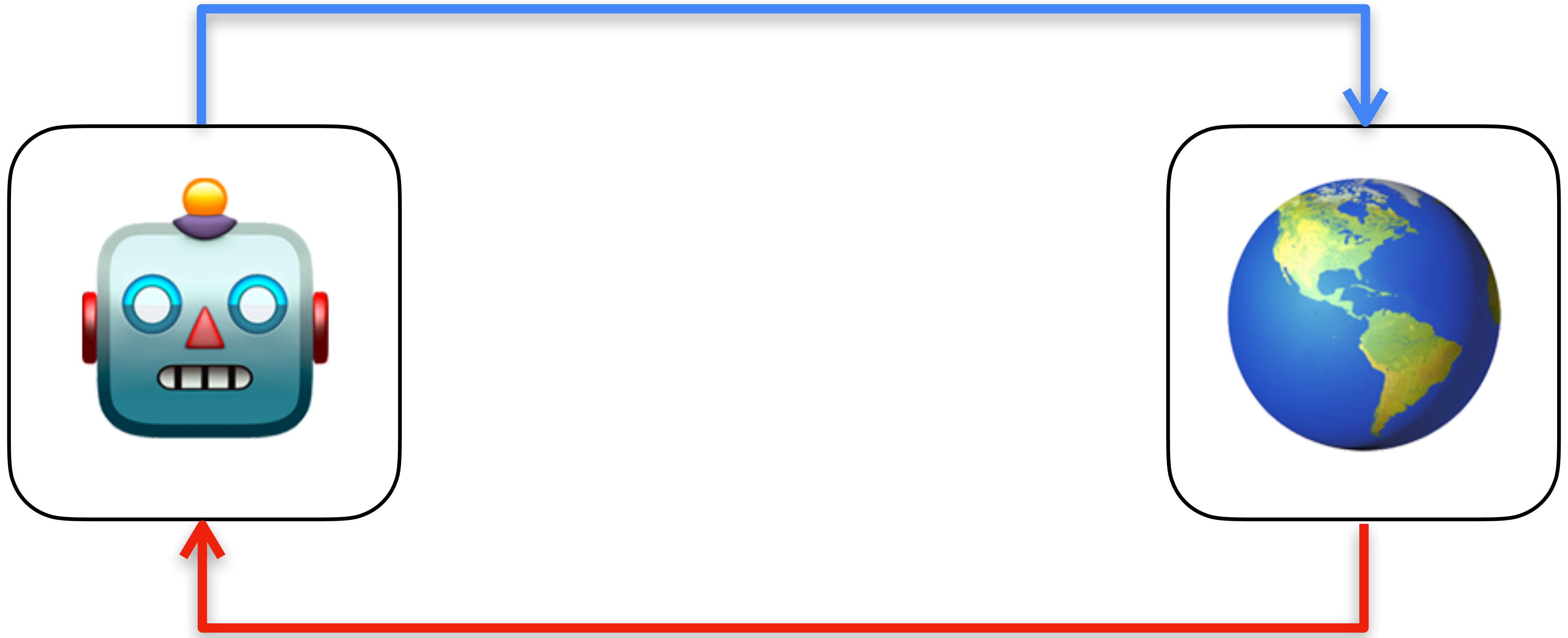

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Reinforcement Learning

Q-Learning

Reinforcement Learning

Q-Learning

1. Initialize π

Reinforcement Learning

Q-Learning

1. Initialize π
2. $t = 0$

Reinforcement Learning

Q-Learning

1. Initialize π
2. $t = 0$
3. Initialize $s_t = s_0$

Reinforcement Learning

Q-Learning

1. Initialize π
2. $t = 0$
3. Initialize $s_t = s_0$
4. Loop:

Reinforcement Learning

Q-Learning

1. Initialize π
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4. Loop:
    4.1. Take $a_t = \pi(s_t)$

Reinforcement Learning

Q-Learning

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3. Initialize $s_t = s_0$
4. Loop:
   4.1. Take $a_t = \pi(s_t)$
   4.2. Observe (r_t, s_{t+1})

Reinforcement Learning

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4. Loop:
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    4.3. $Q(s_t, a_t) =$

Reinforcement Learning

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Reinforcement Learning

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Reinforcement Learning

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Reinforcement Learning

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Reinforcement Learning

Q-Learning

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4. Loop:
    - 4.1. Take $a_t = \pi(s_t)$
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    - 4.5. $t = t + 1$

Reinforcement Learning

Deep Q Network (DQN)

Main Idea: use neural networks to model Q-Function

Reinforcement Learning

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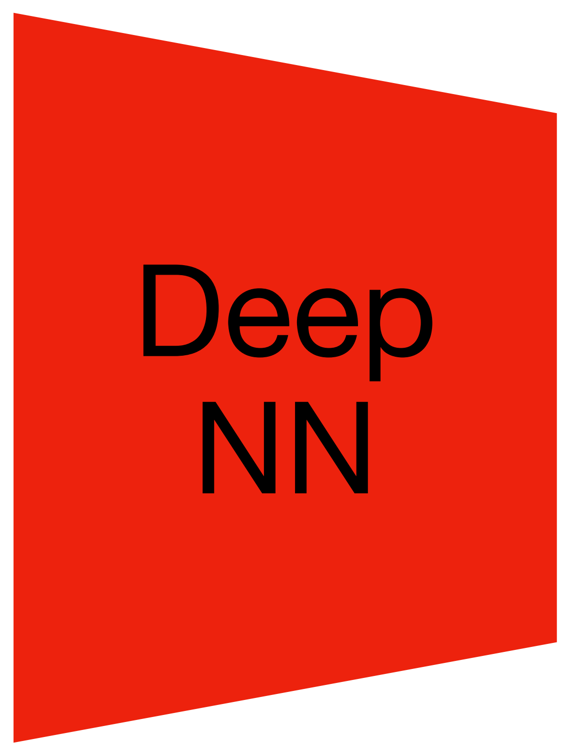

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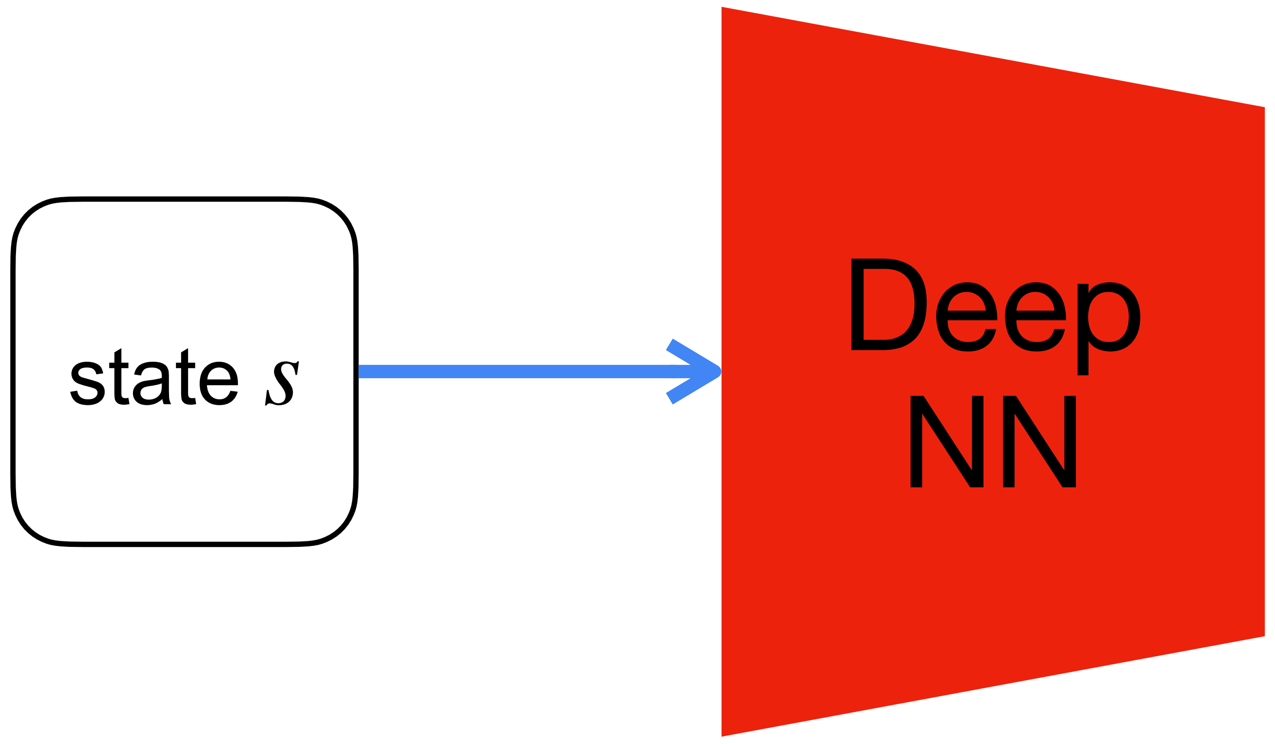

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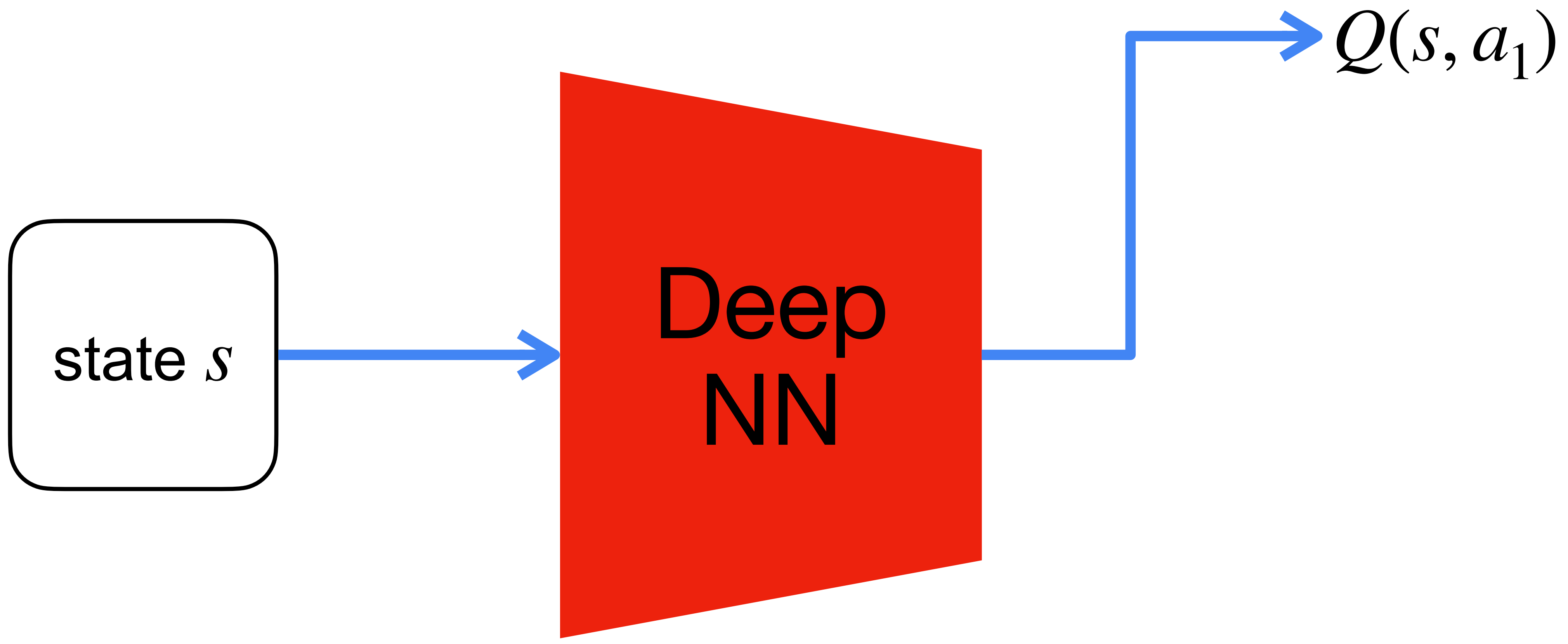

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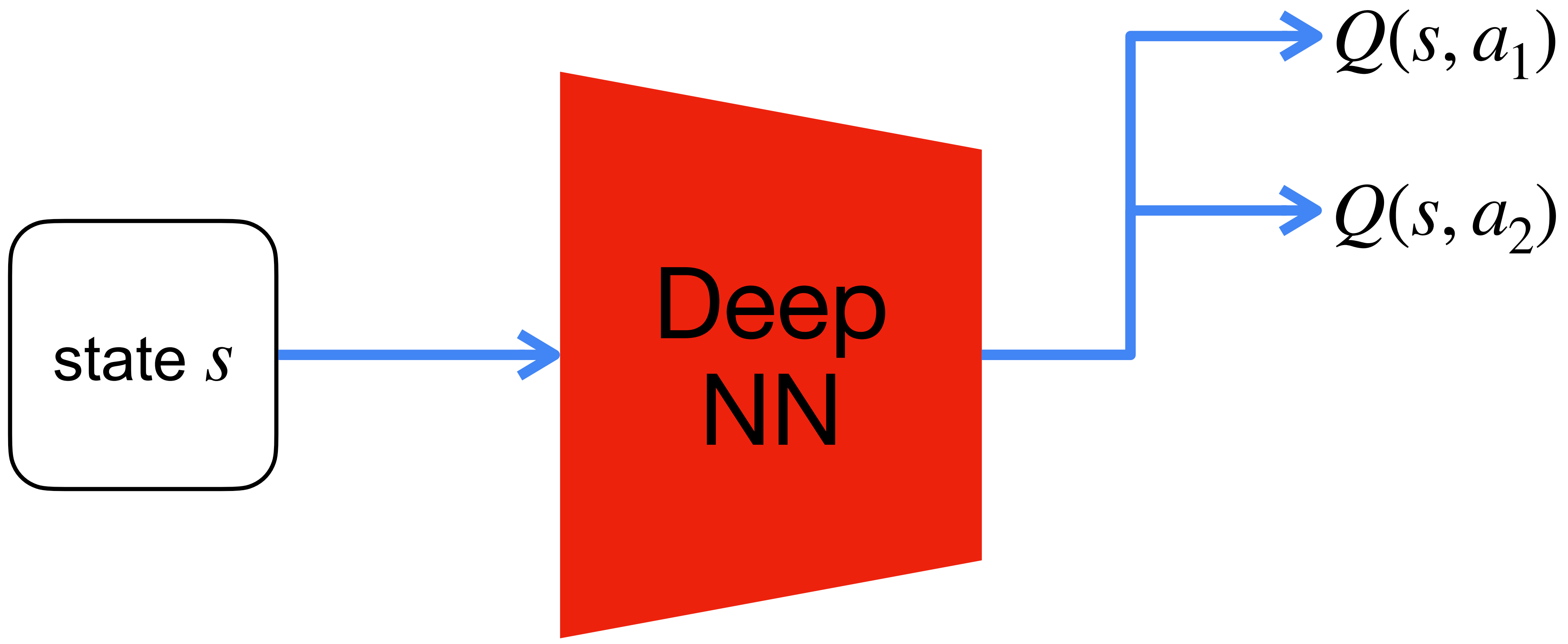

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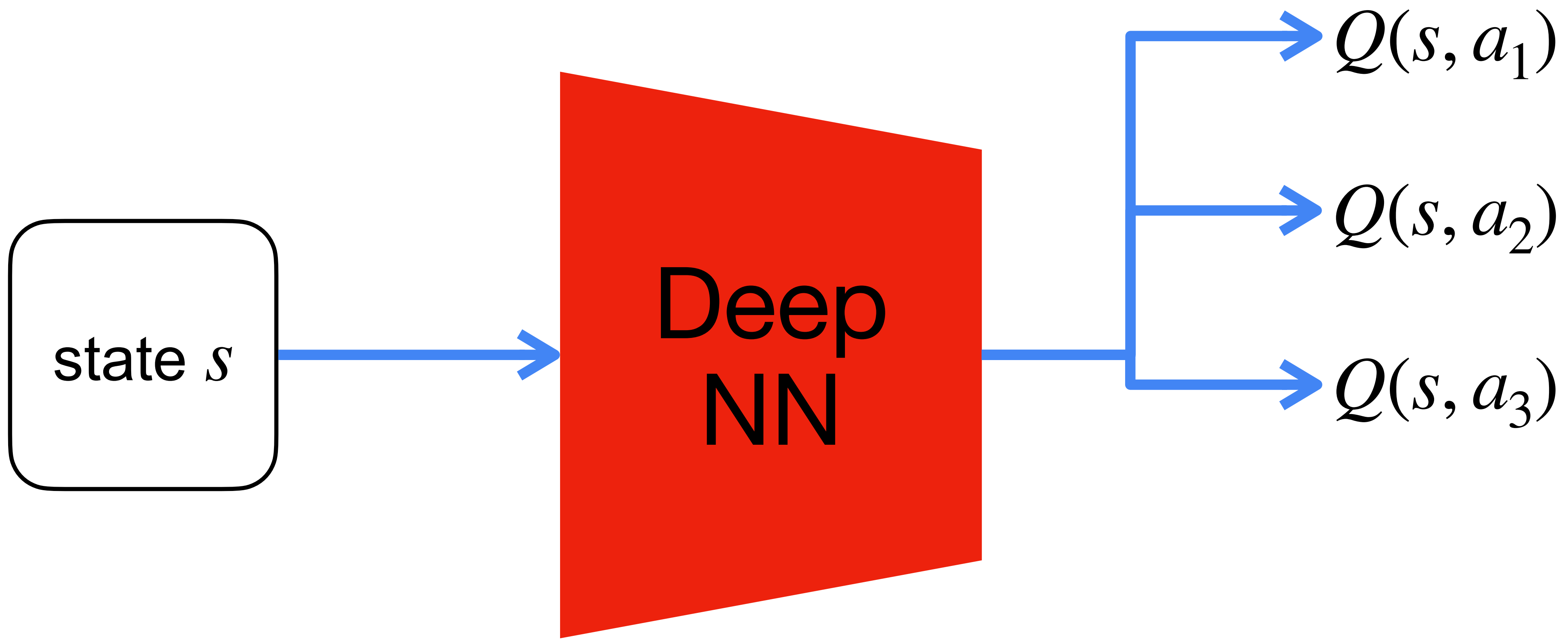

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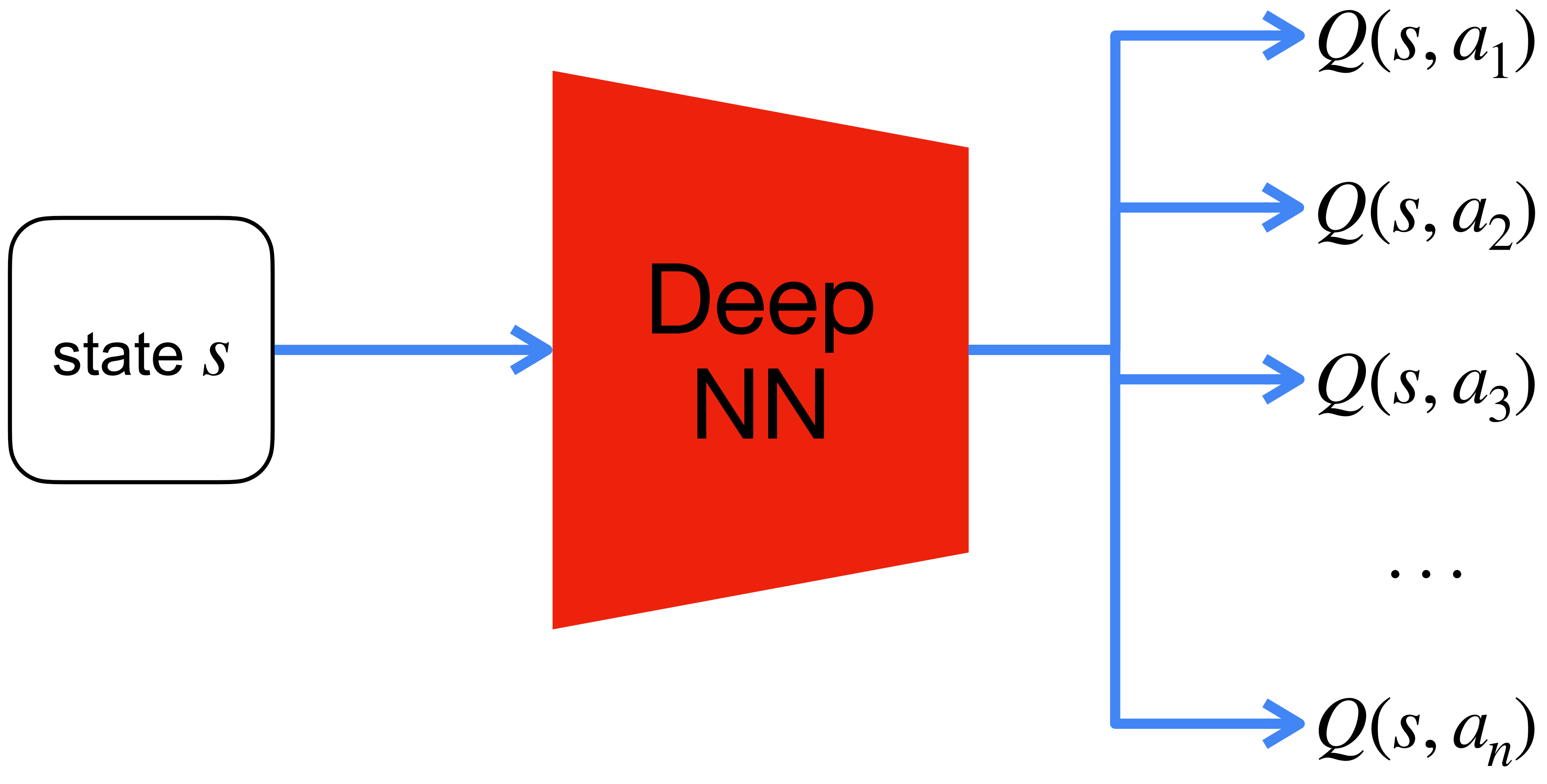

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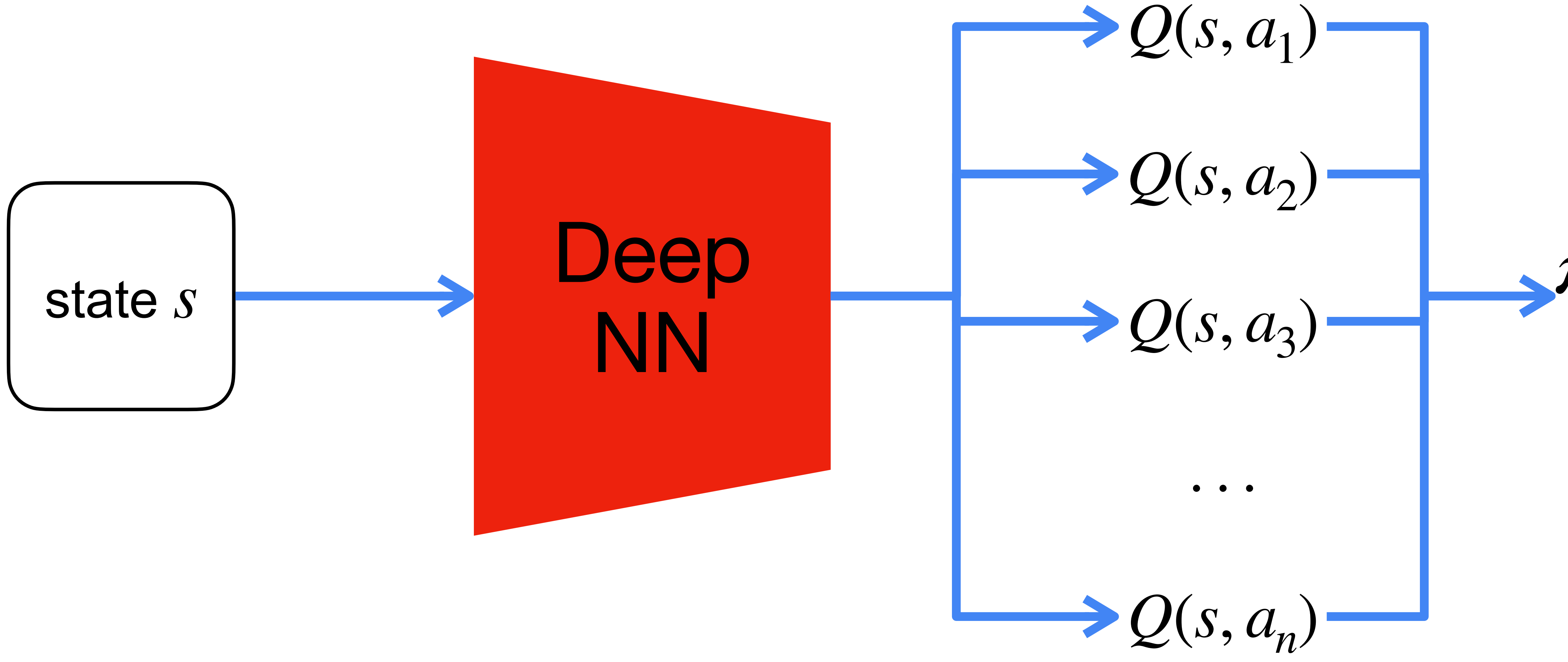

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Reinforcement Learning

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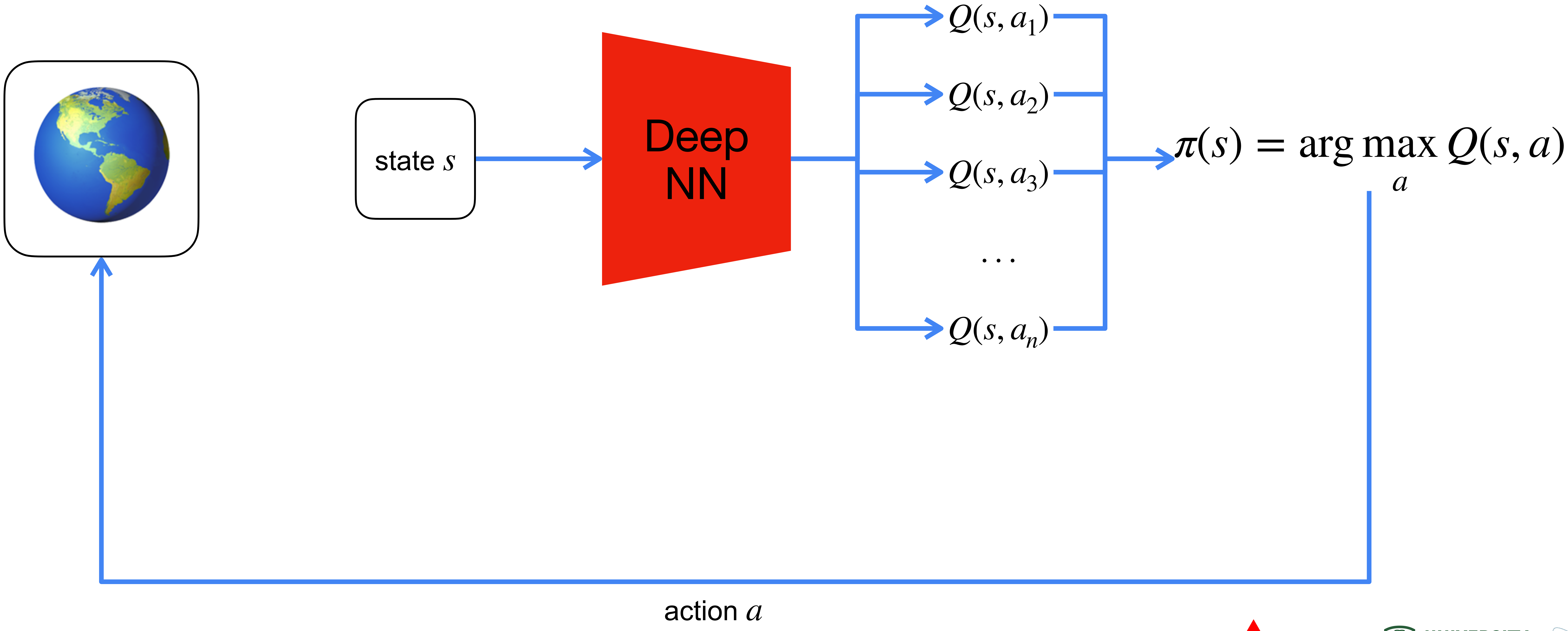

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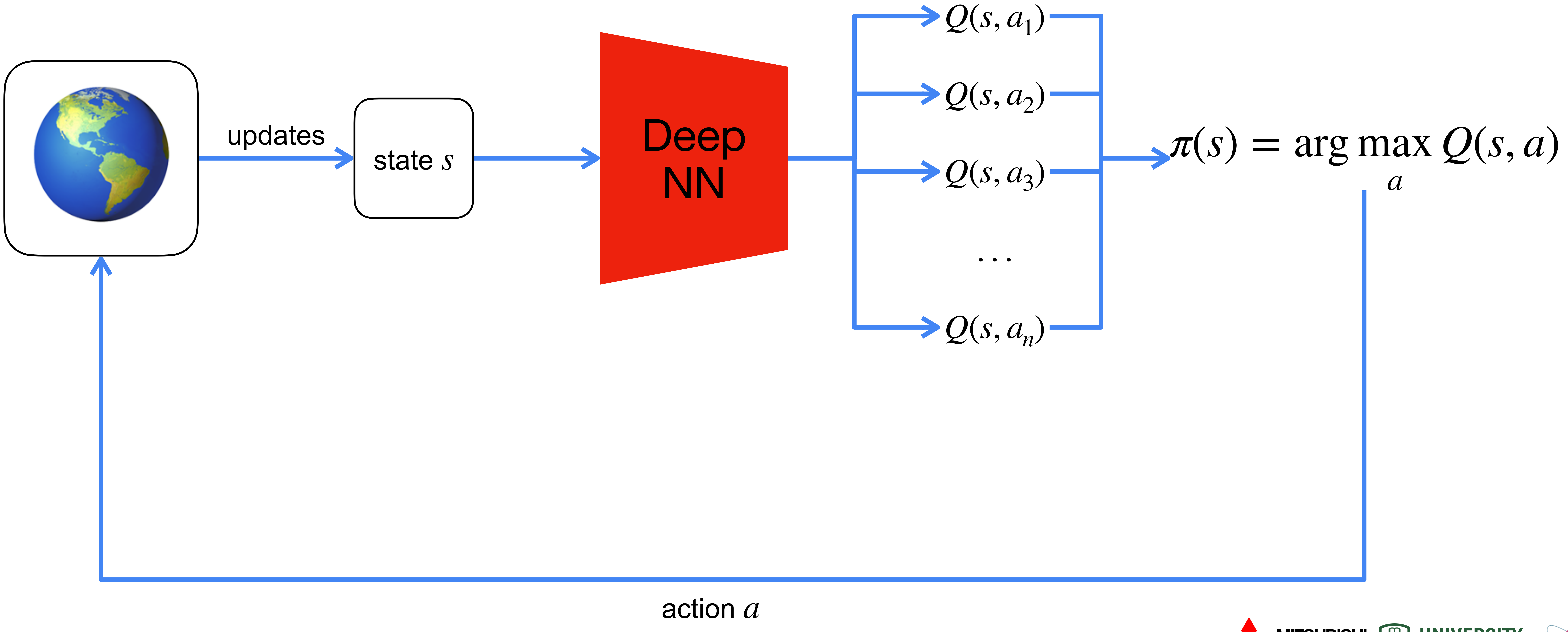

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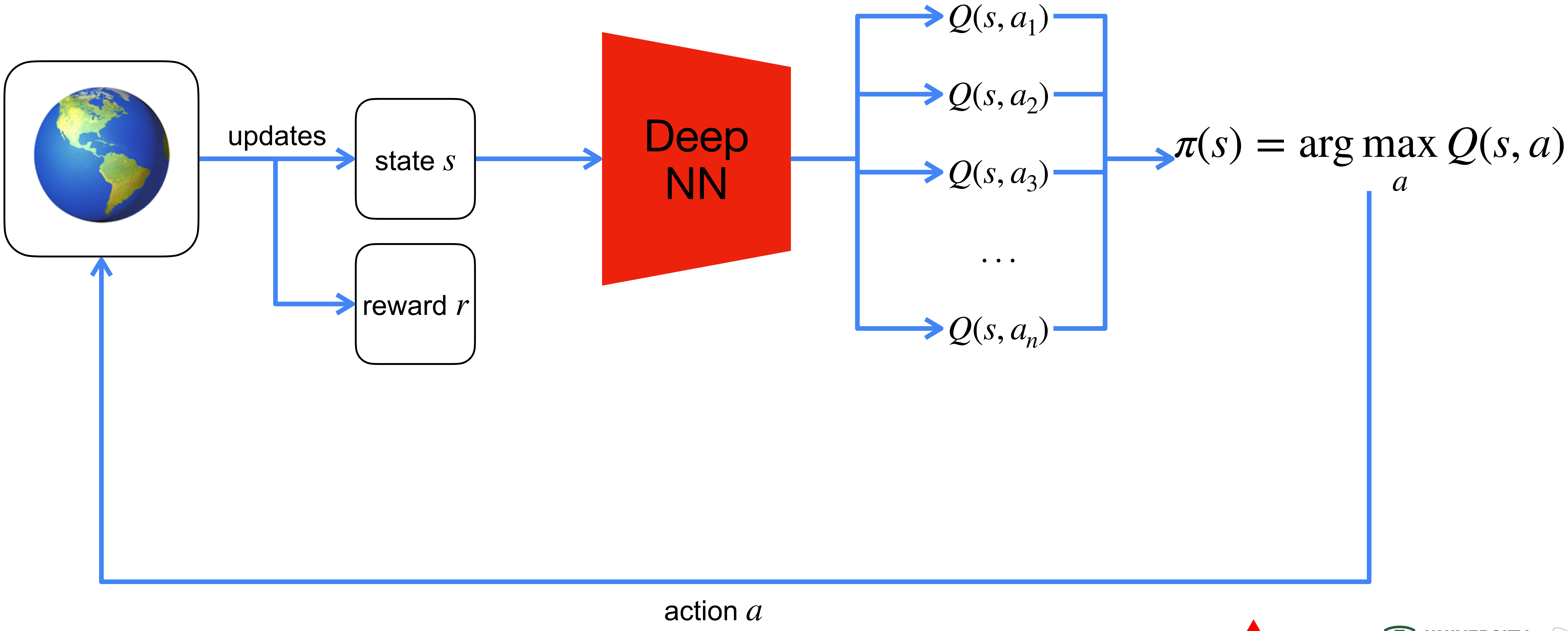

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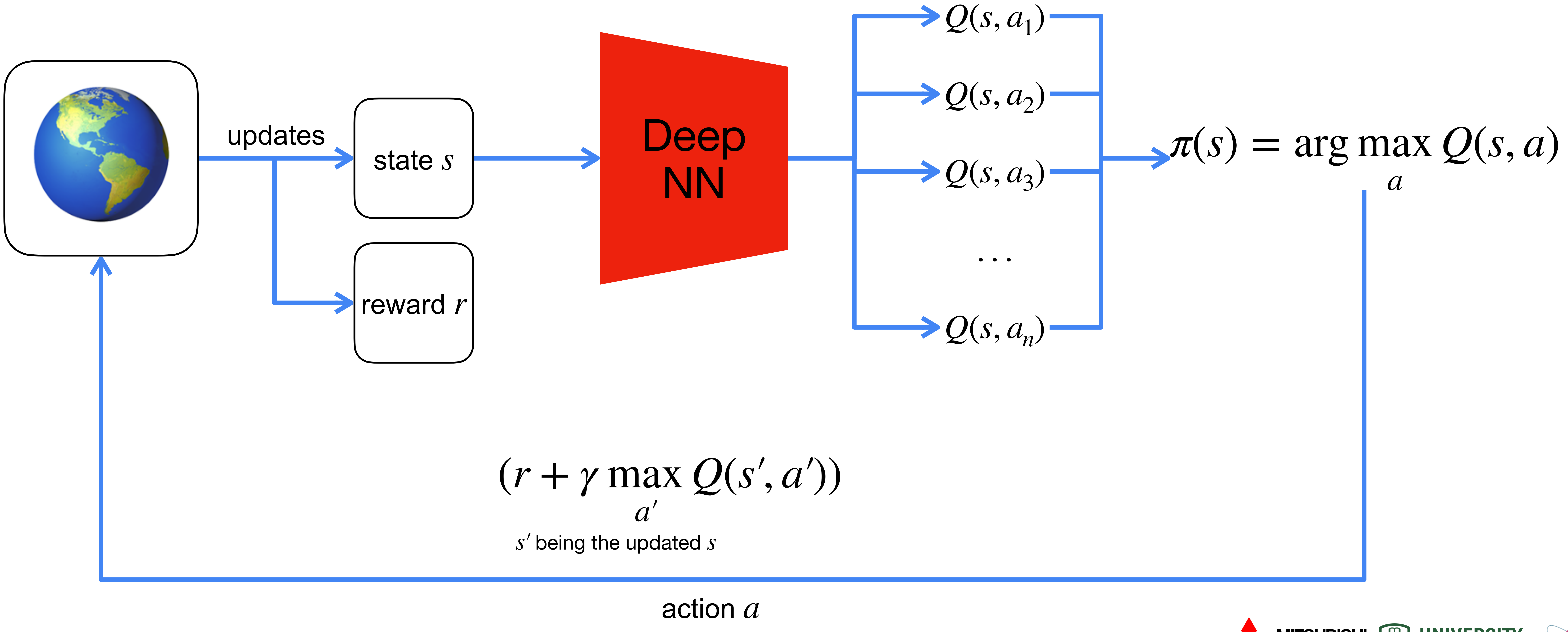

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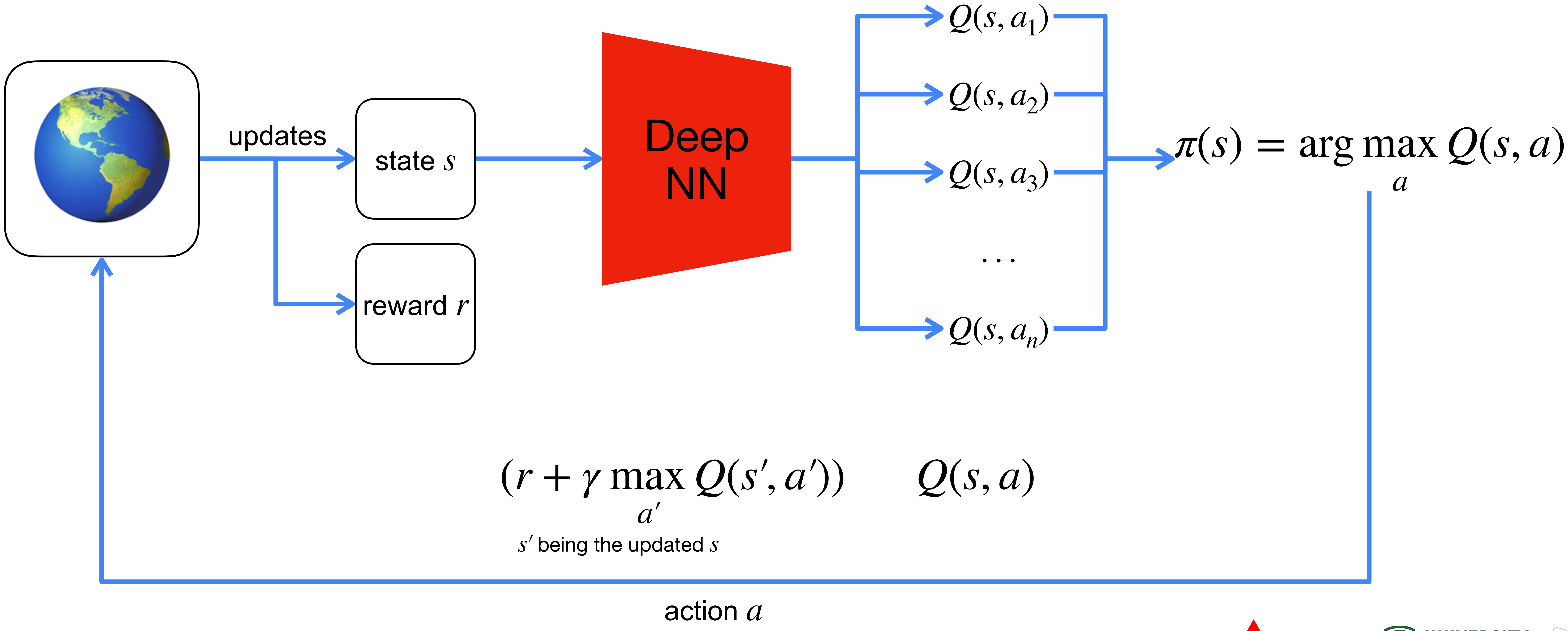

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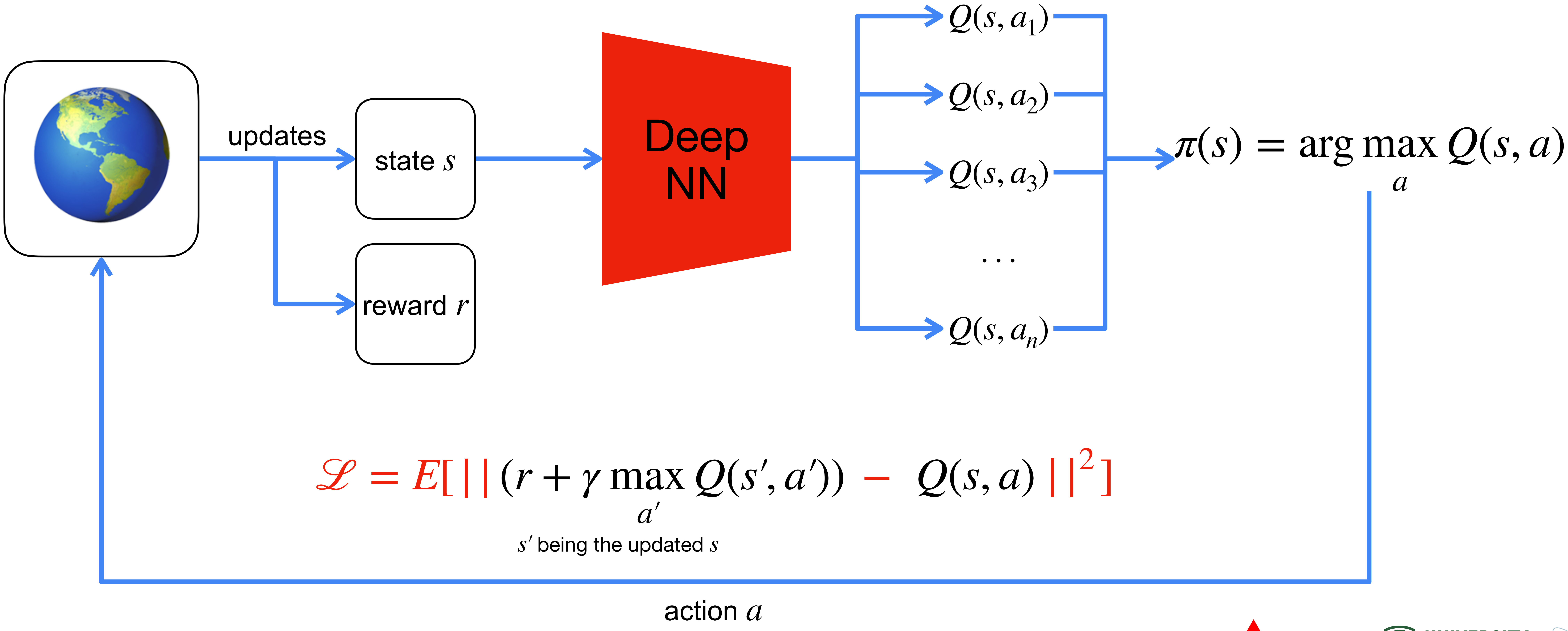
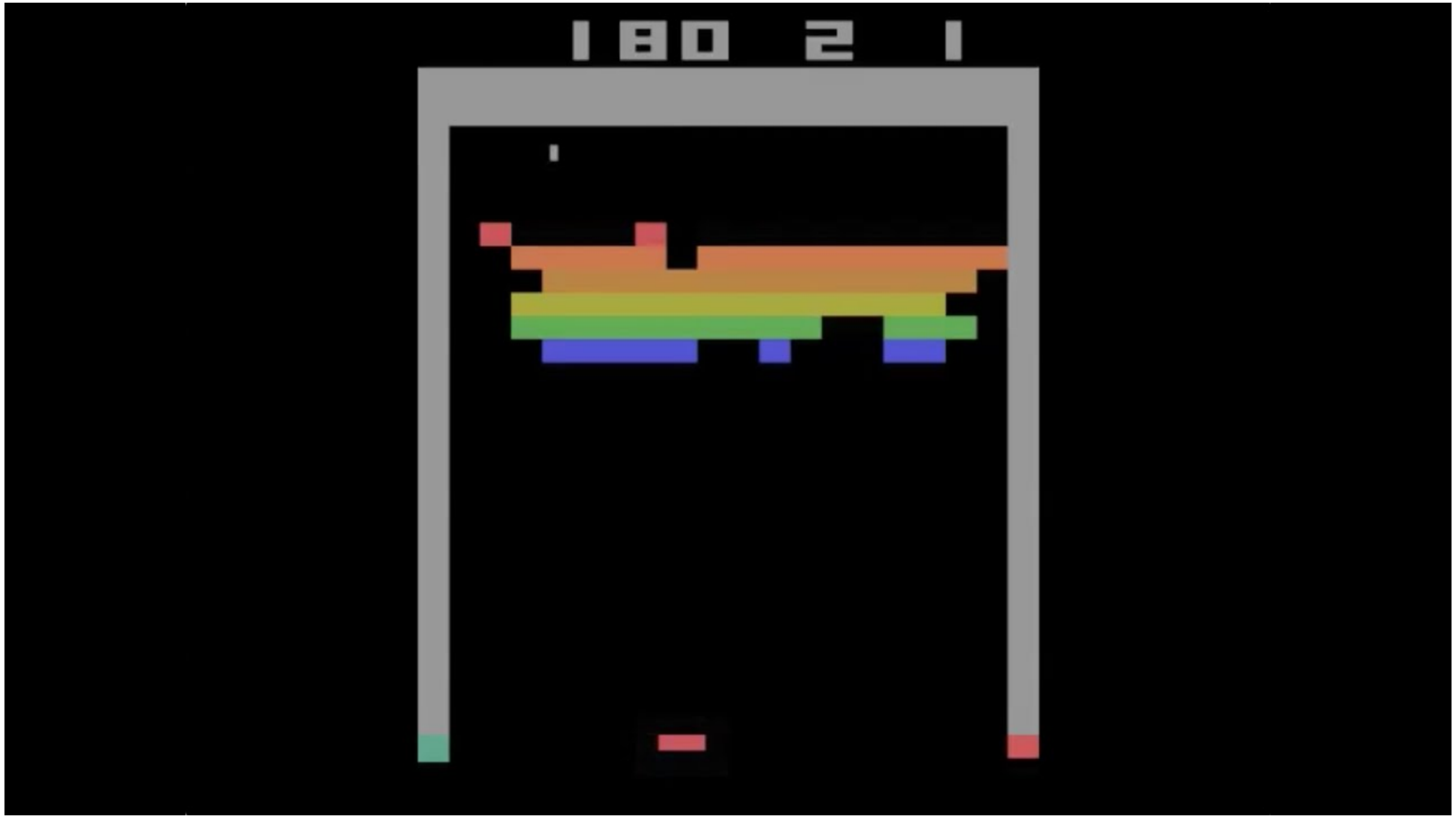


Reinforcement Learning

Real-World Applications



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Reinforcement Learning

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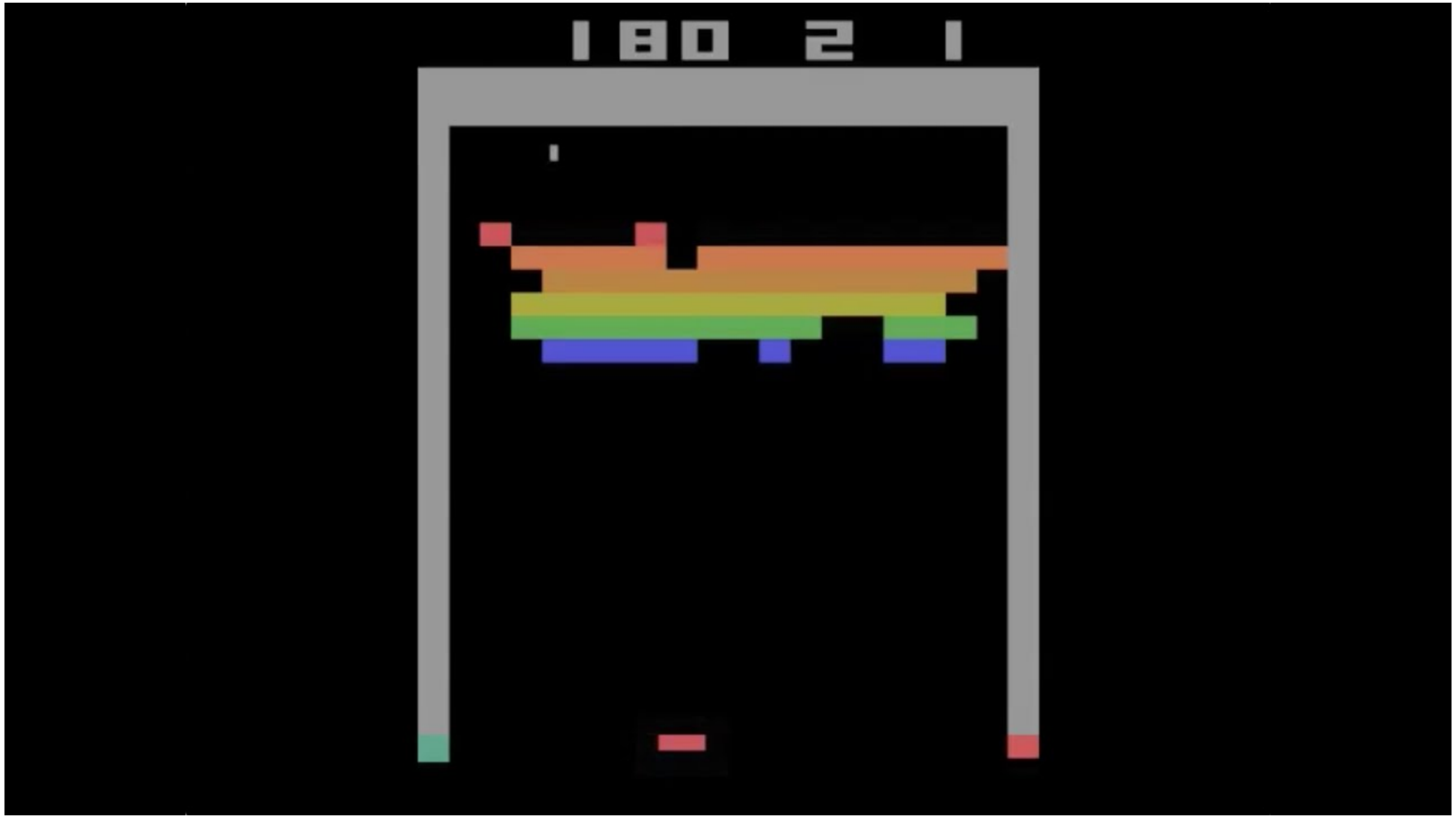

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BO or RL?

Bayesian Optimization	Reinforcement Learning

BO or RL?

Bayesian Optimization

Reinforcement Learning

Environment

Static

Dynamic

BO or RL?

Bayesian Optimization		Reinforcement Learning
Static	**Environment**	Dynamic
Deterministic	**Action**	Stochastic

BO or RL?

	Bayesian Optimization	Reinforcement Learning
Environment	Static	Dynamic
Action	Deterministic	Stochastic
Reward	Direct and immediate	Delayed and/or Sparse

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