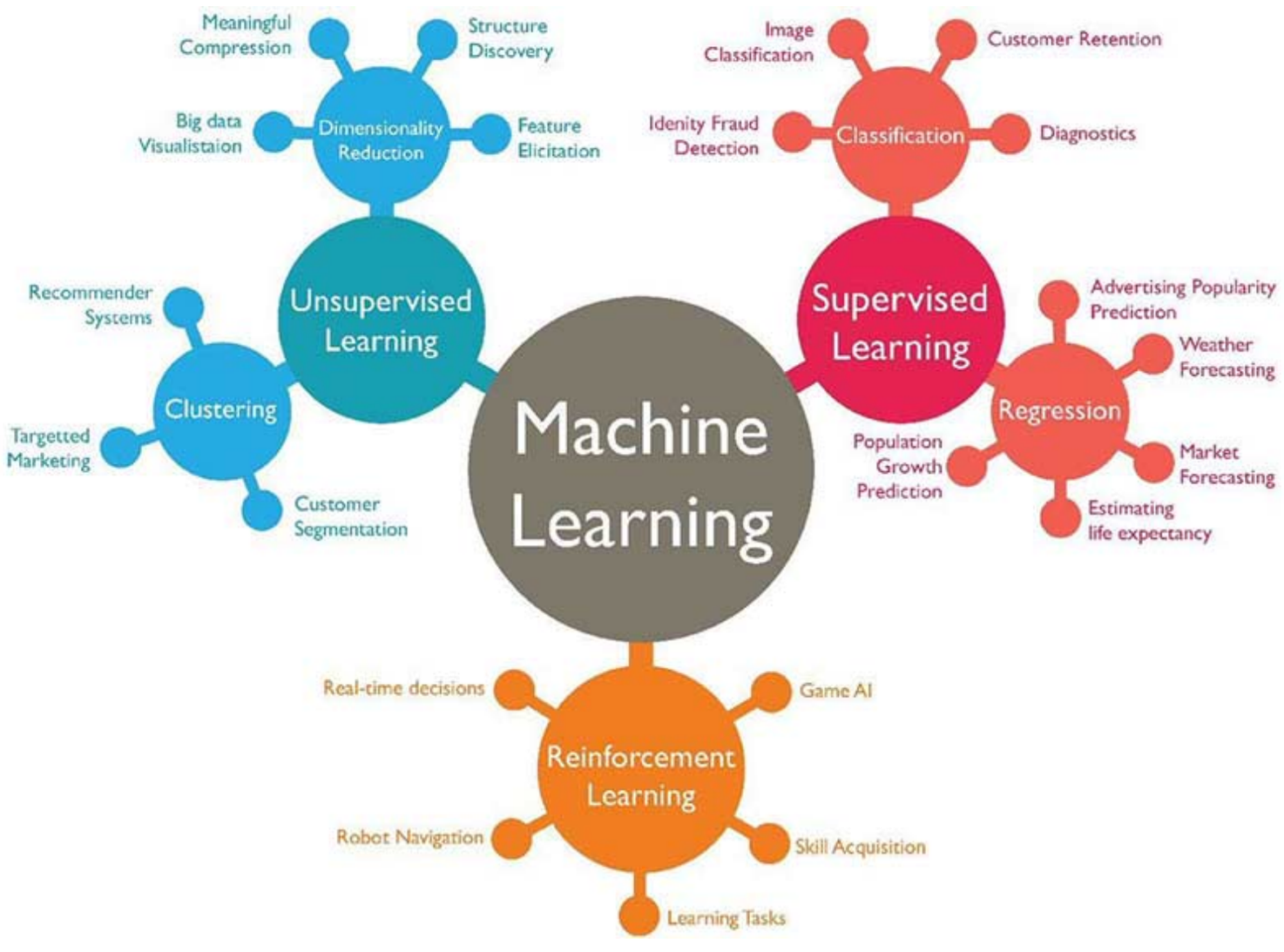
MPI-PKS

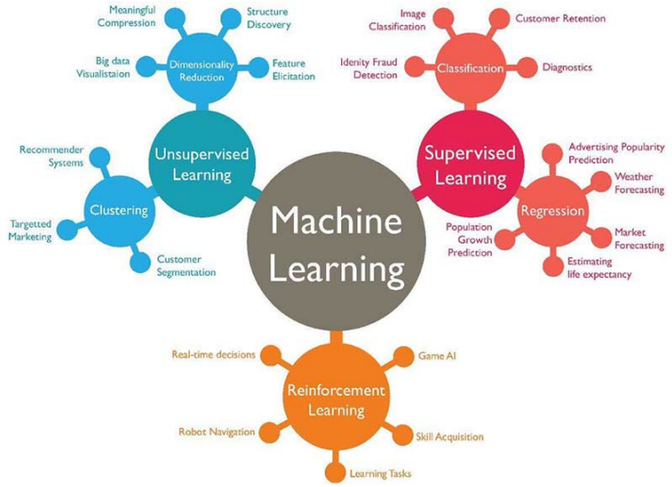
From Quantum Matter to Quantum Computers

Max Planck Institute
for the Physics of Complex Systems

INTRODUCTION TO REINFORCEMENT LEARNING

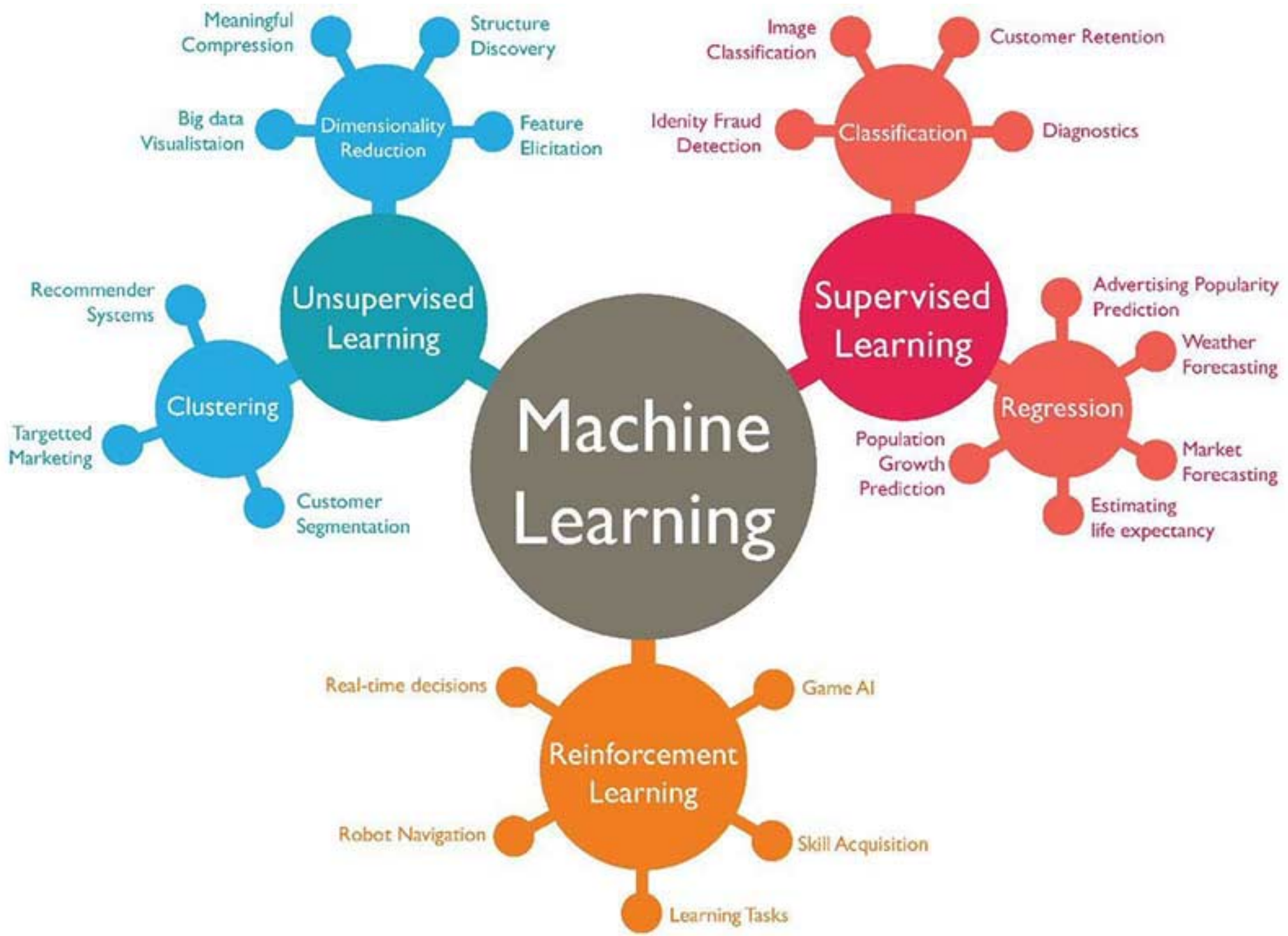


Overview

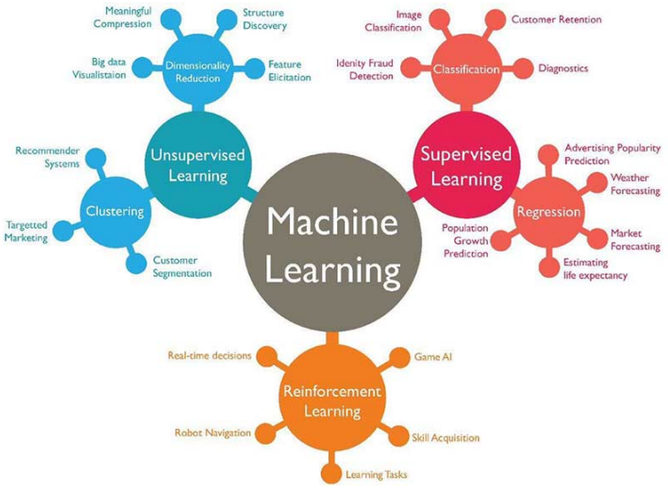


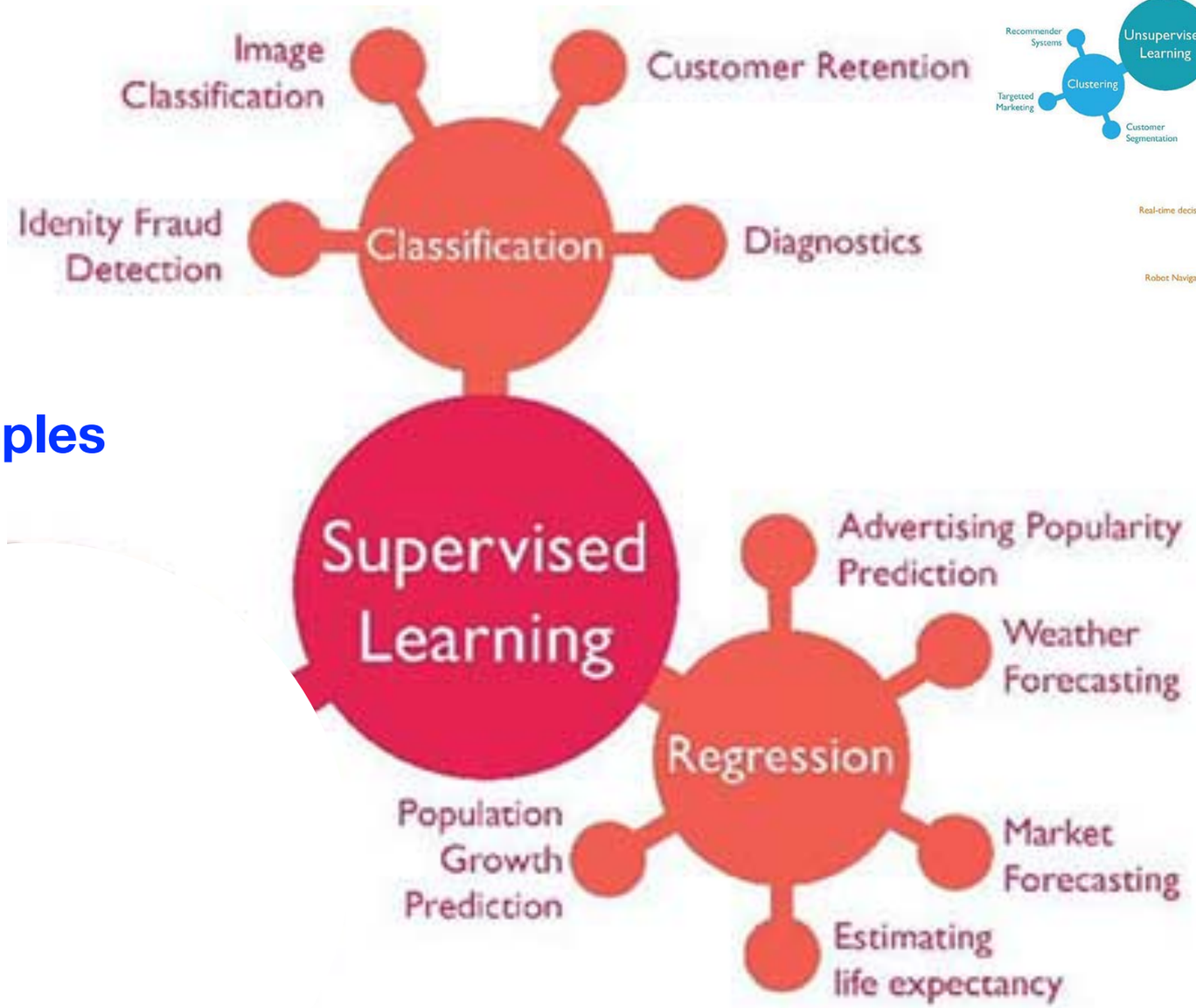
- What is Reinforcement Learning (RL)?
- RL framework in a nutshell
- RL algorithms
- Applications of RL in quantum physics

Machine Learning



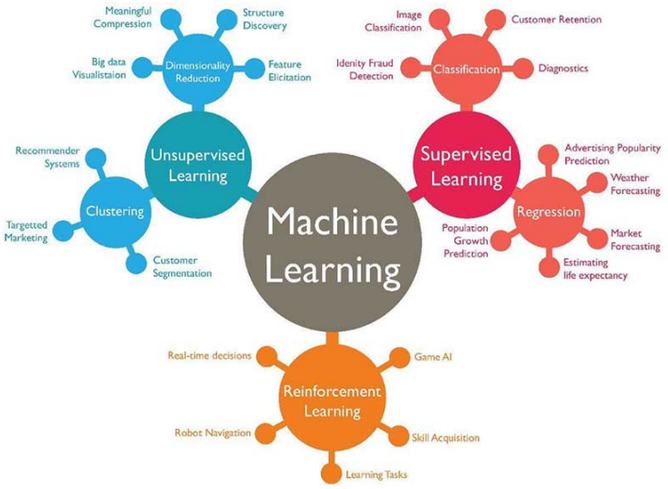
Supervised Learning

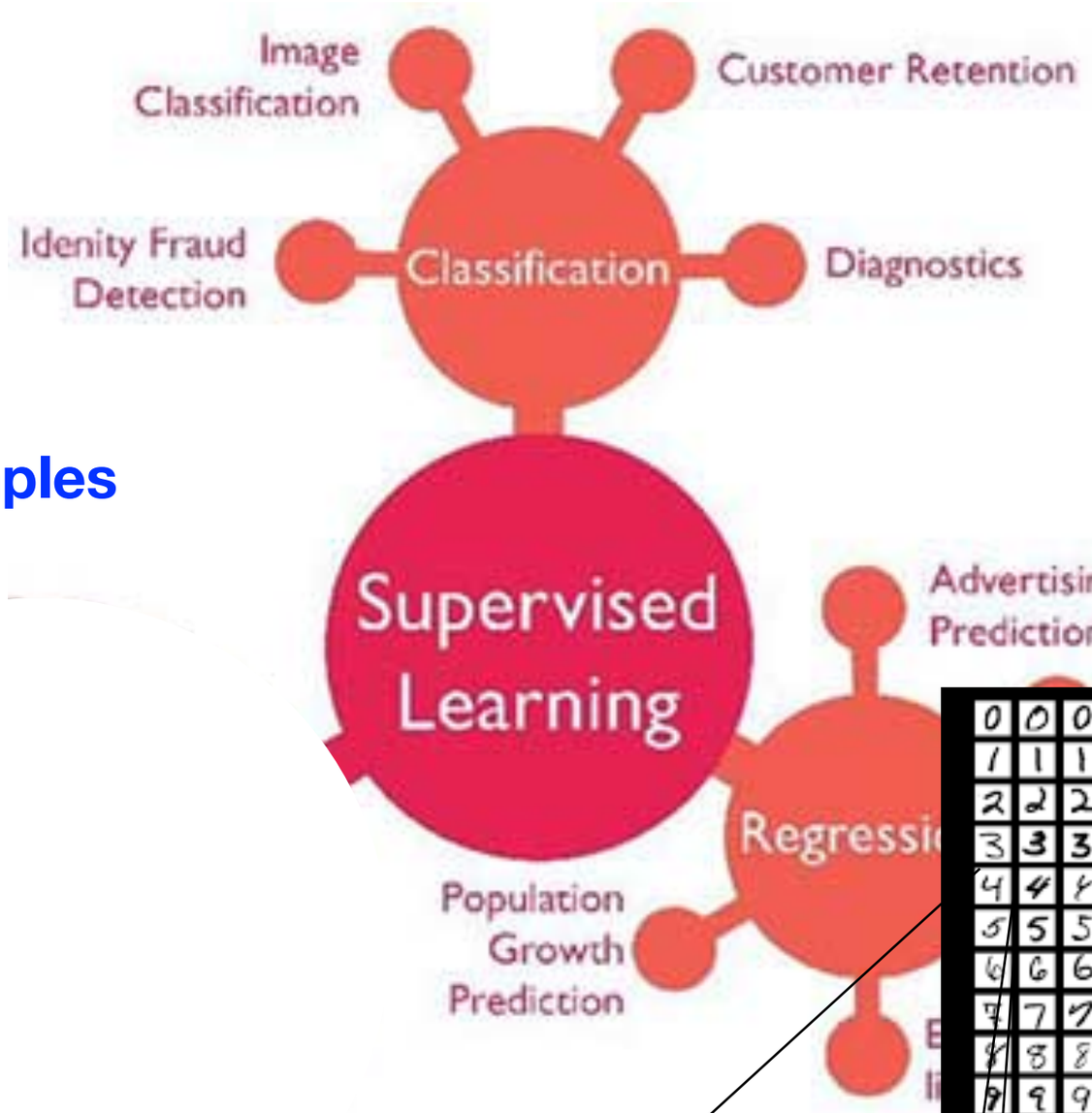




learning from examples
(labeled data)

Supervised Learning





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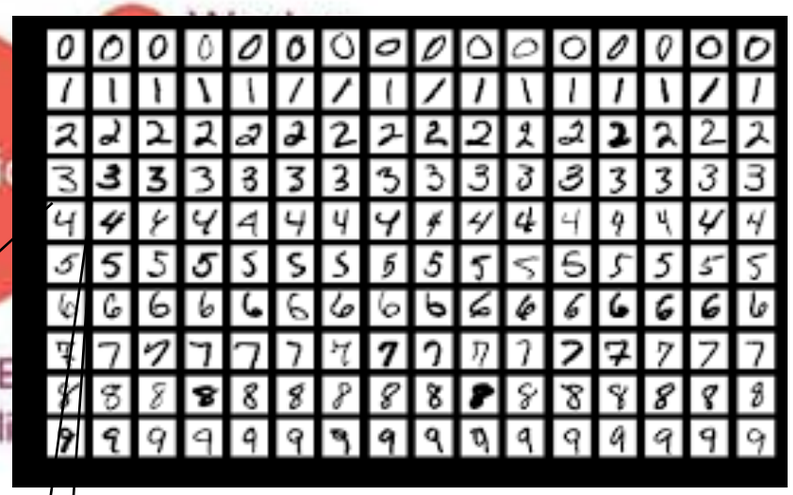
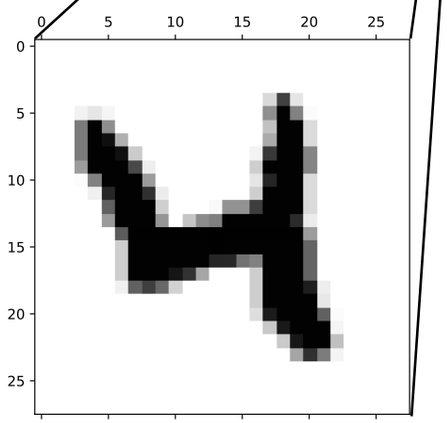
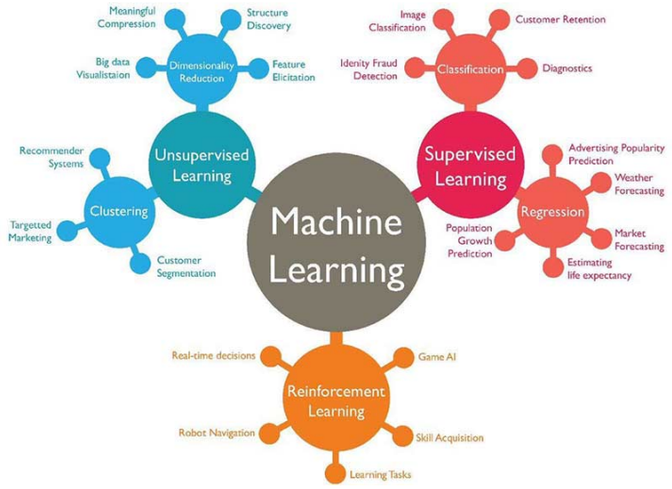




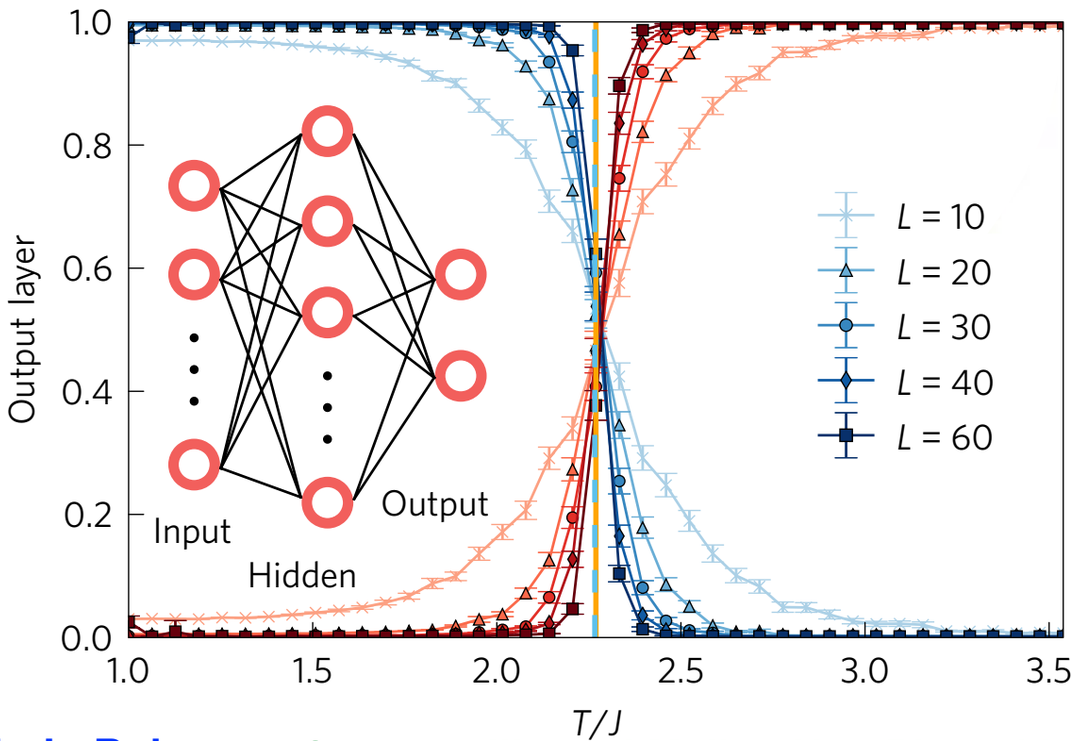
recognize hand-written digits

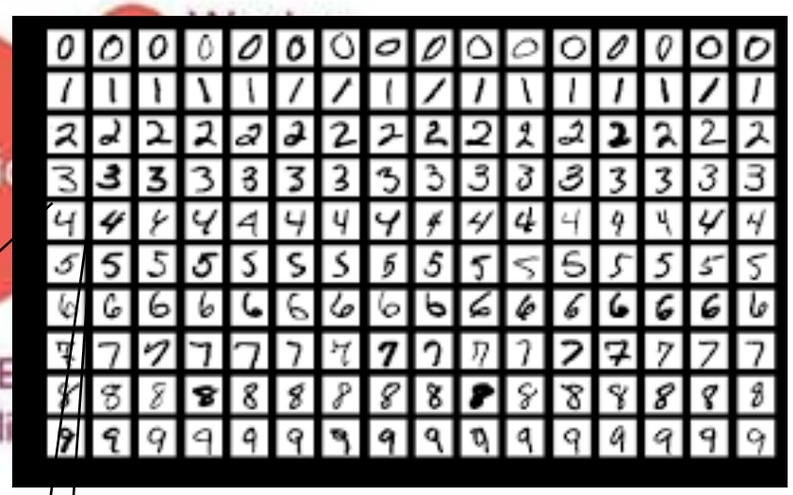
Supervised Learning

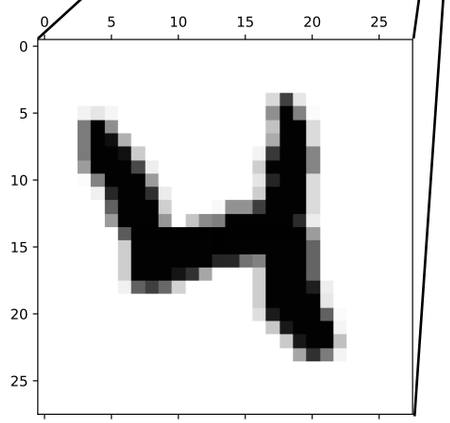


learning from examples (labeled data)

classify phases of matter, determine critical point from data







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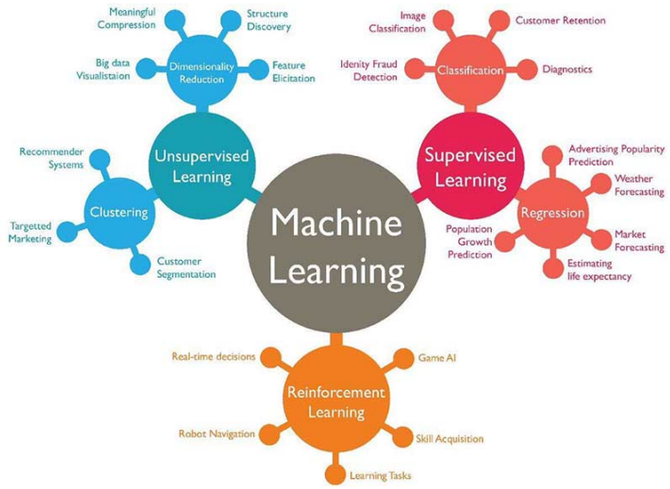
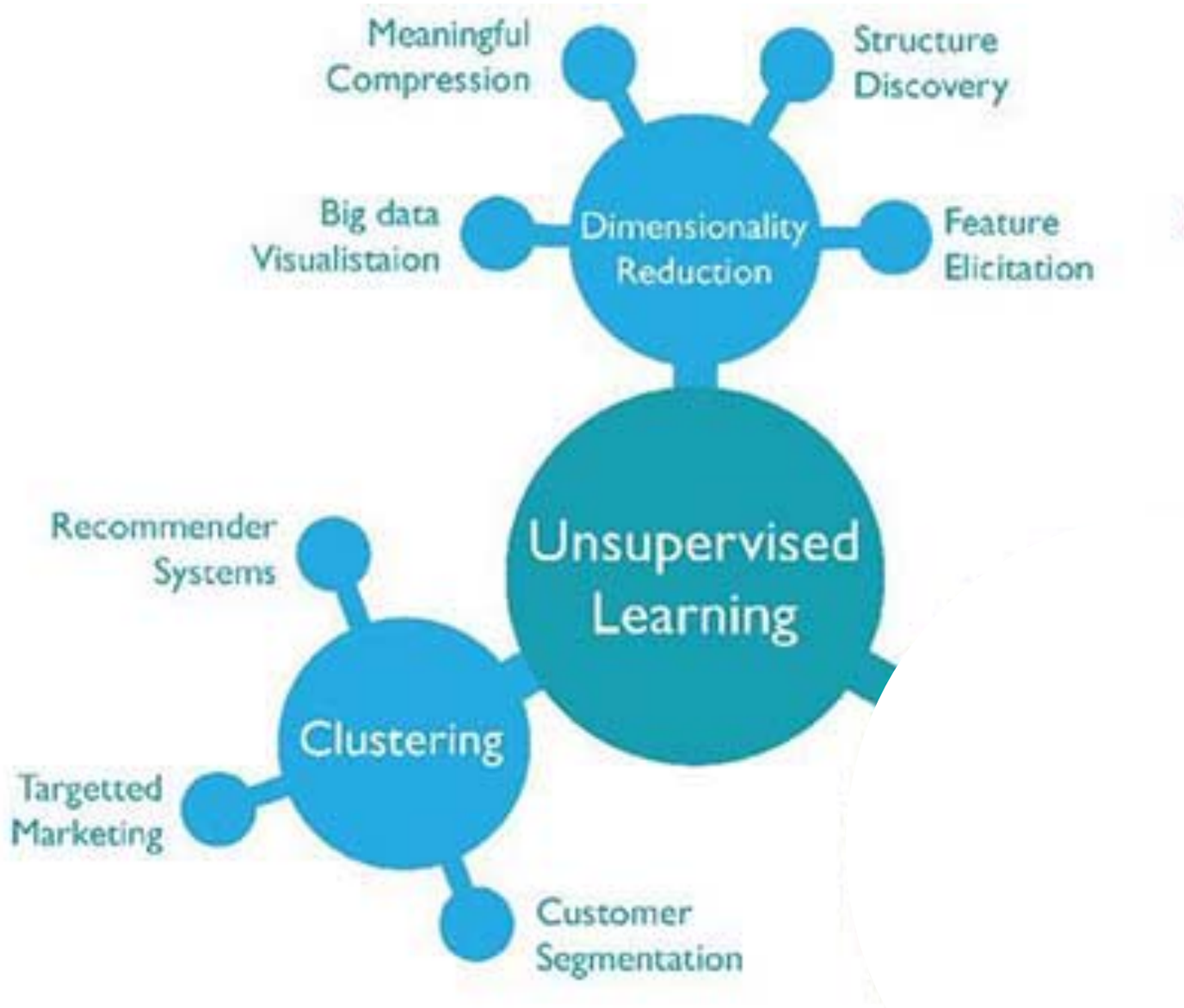
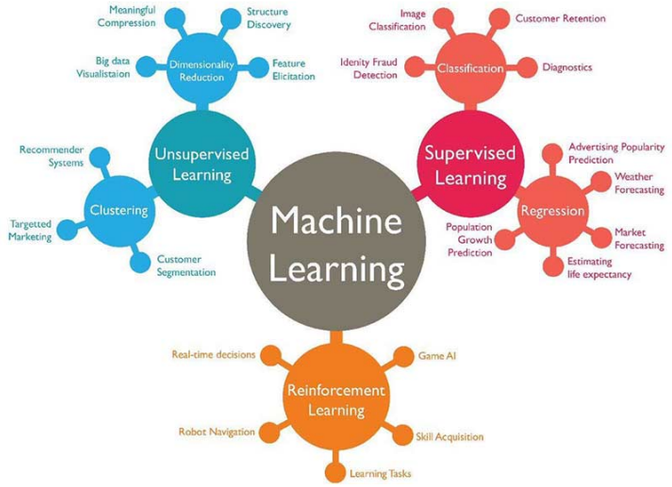
Unsupervised Learning





learning the structure of unlabeled data

Unsupervised Learning



learning the structure of unlabeled data

Neural Quantum States

recall: variational wave functions

$$|\psi(\theta)\rangle$$

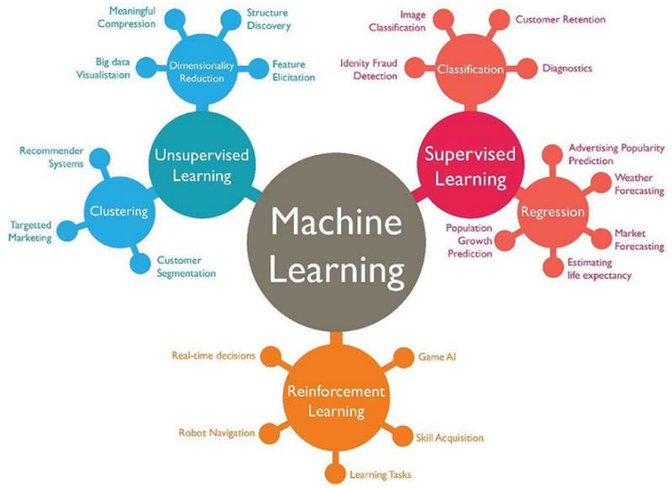
$$\psi(x;\theta) \propto \exp\left(-\frac{(x-\theta_1)^2}{2\theta_2^2}\right)$$

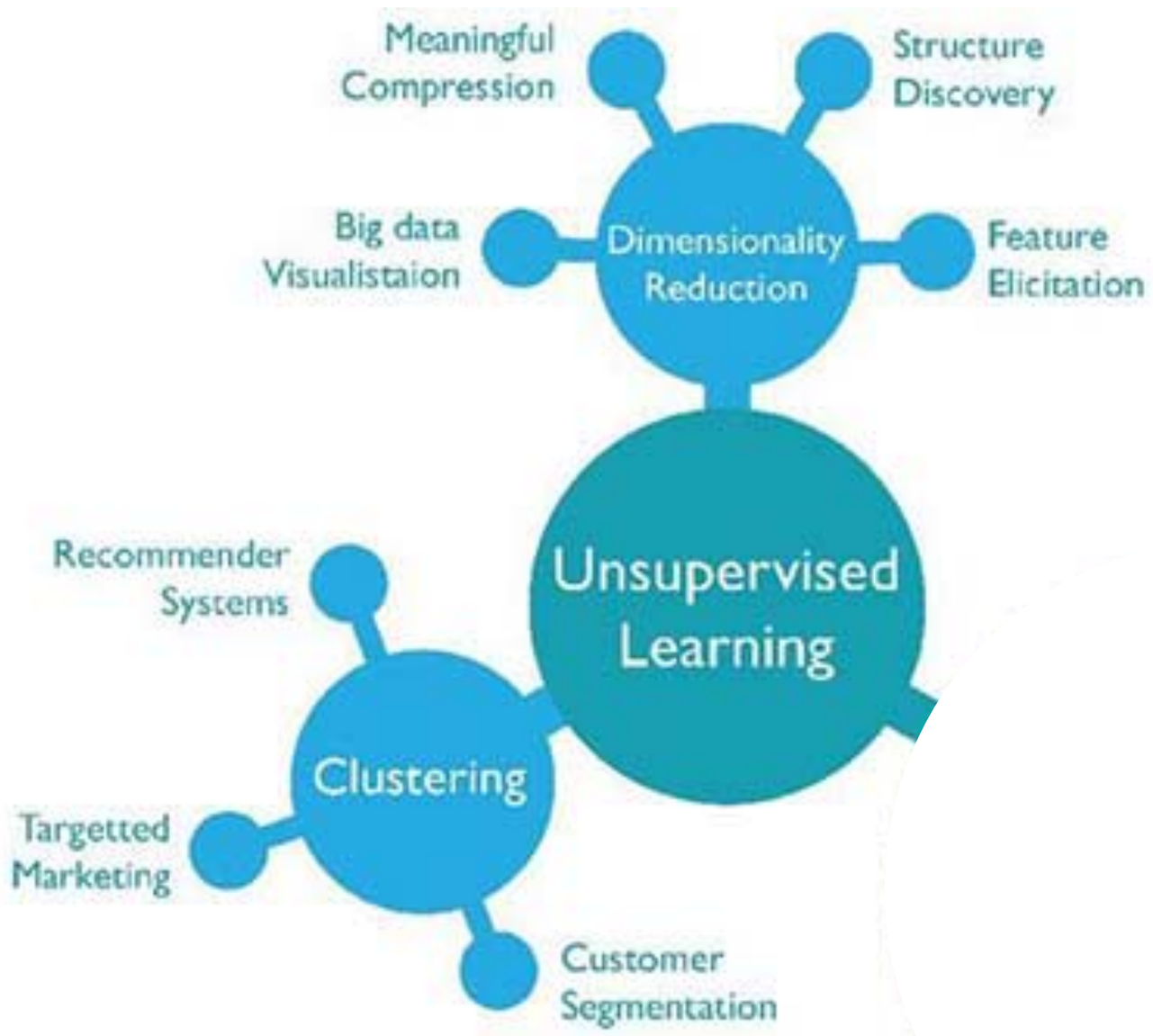
$$E(\theta) = \langle\psi(\theta)|H|\psi(\theta)\rangle$$

$$\partial_\theta E(\theta) \stackrel{!}{=} 0$$

Carleo and Troyer, Science 2017
Schmitt and Heyl, PRL 2020
+ many more

Unsupervised Learning





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Neural Quantum States $|\psi(\theta)\rangle$

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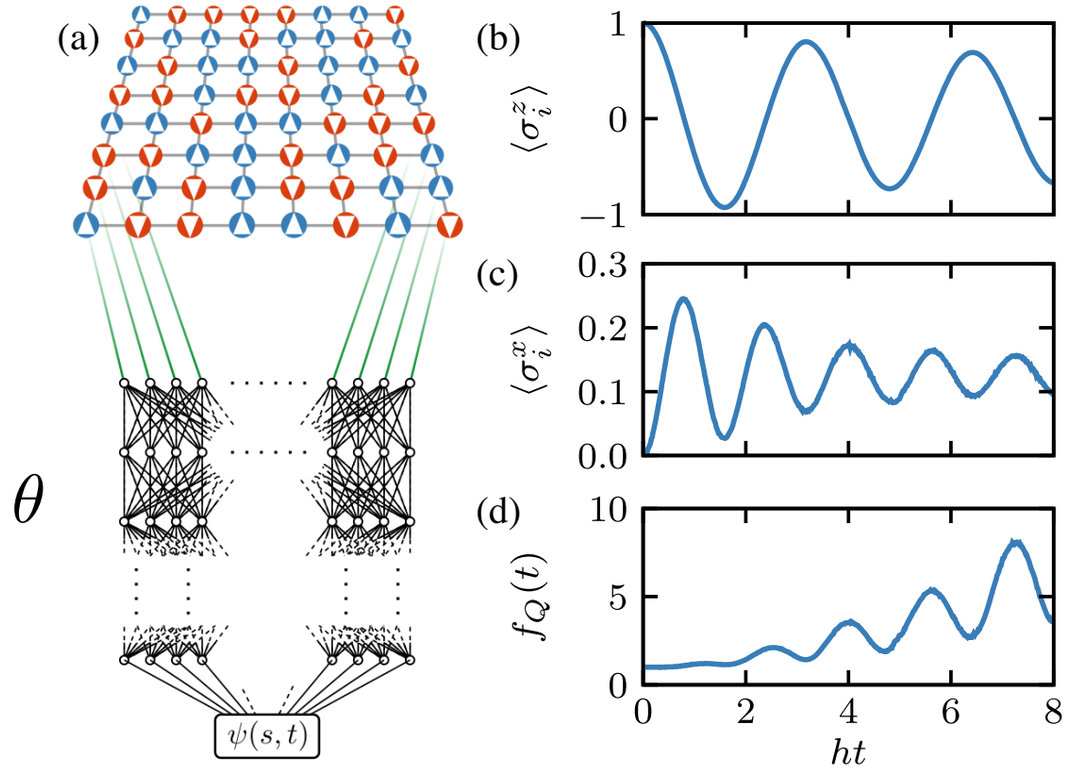

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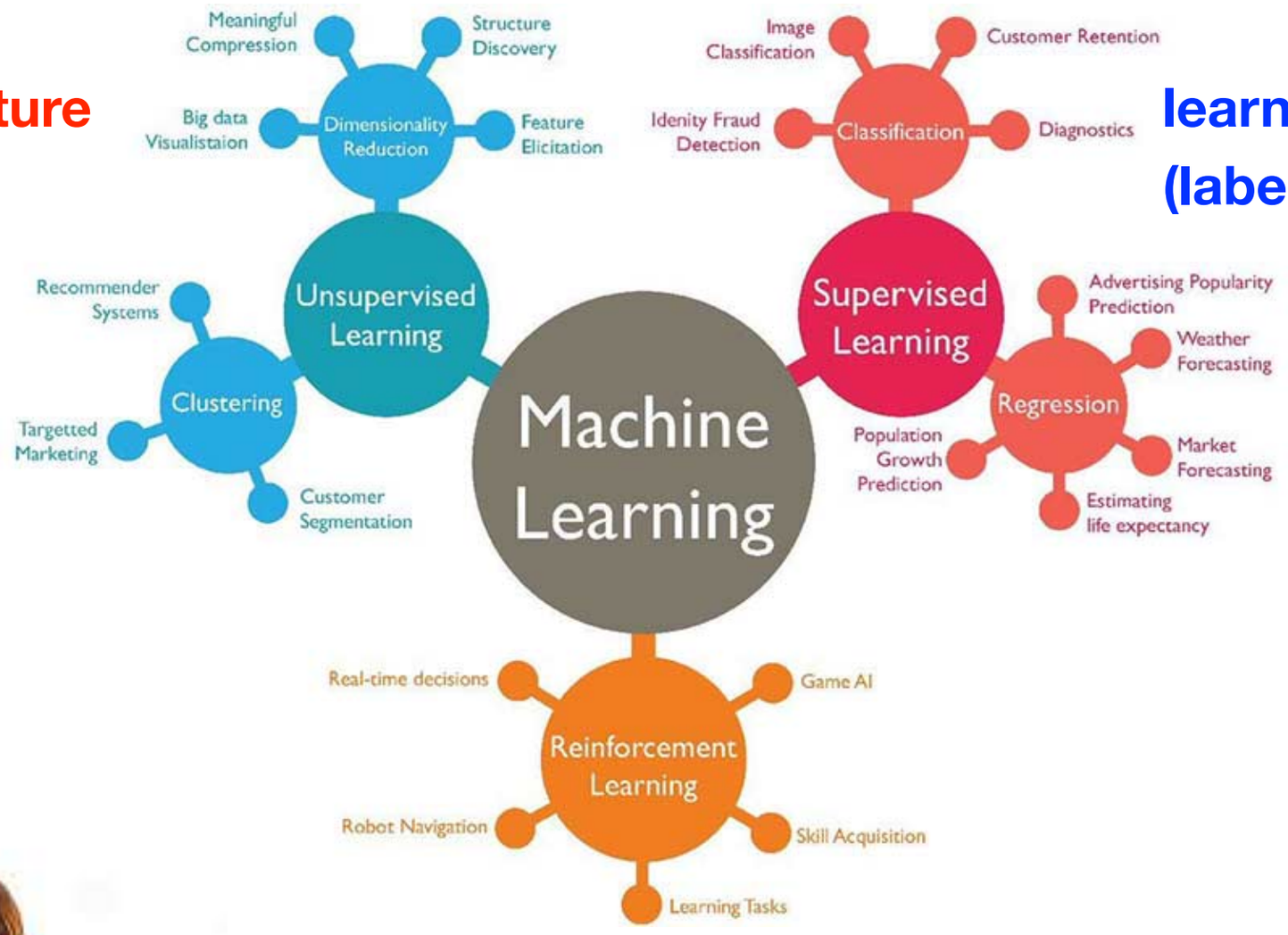
Reinforcement Learning

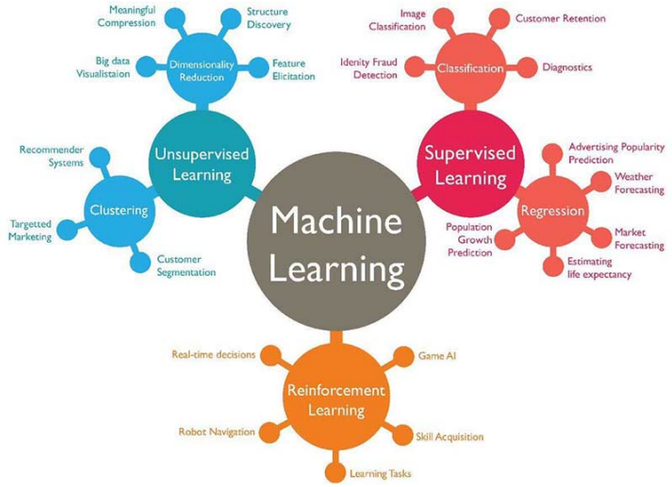
learning the structure of unlabeled data



learning from examples (labeled data)

learning from experience

Overview



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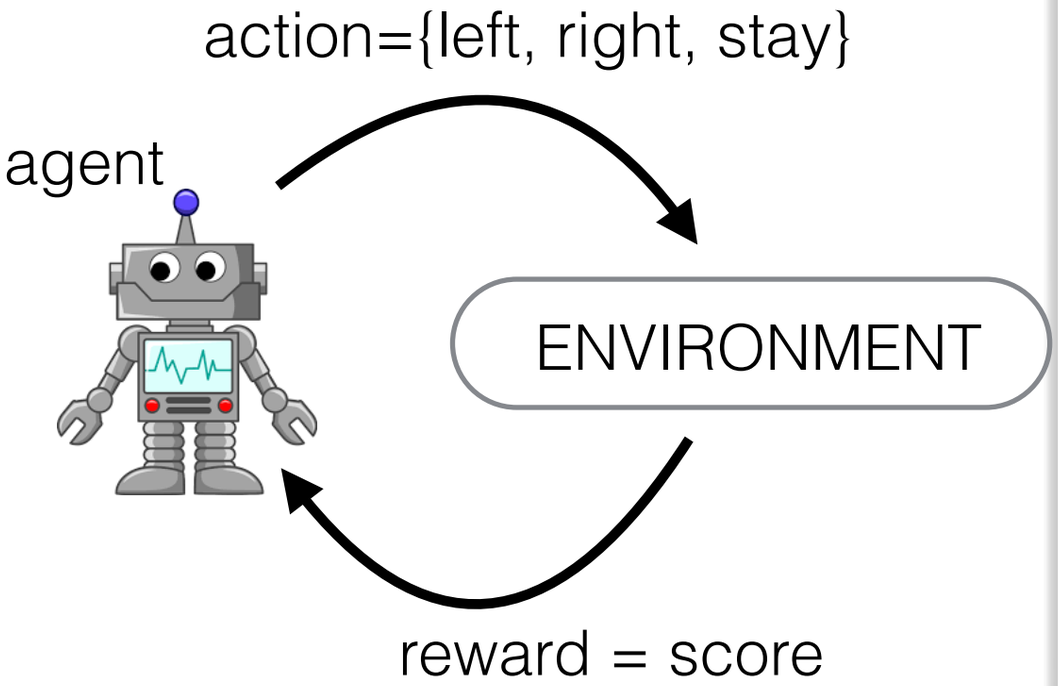
What is Reinforcement Learning?



What is Reinforcement Learning Useful for?

Mastering the game of Go with deep neural networks and tree search

Silver, et. al, Nature *529* 484–489 (2016)

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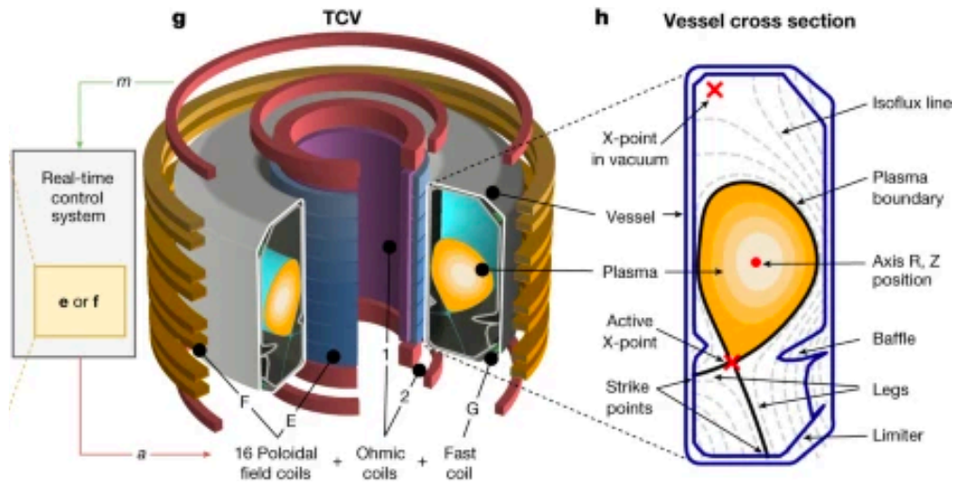
Magnetic control of tokamak plasmas through deep RL



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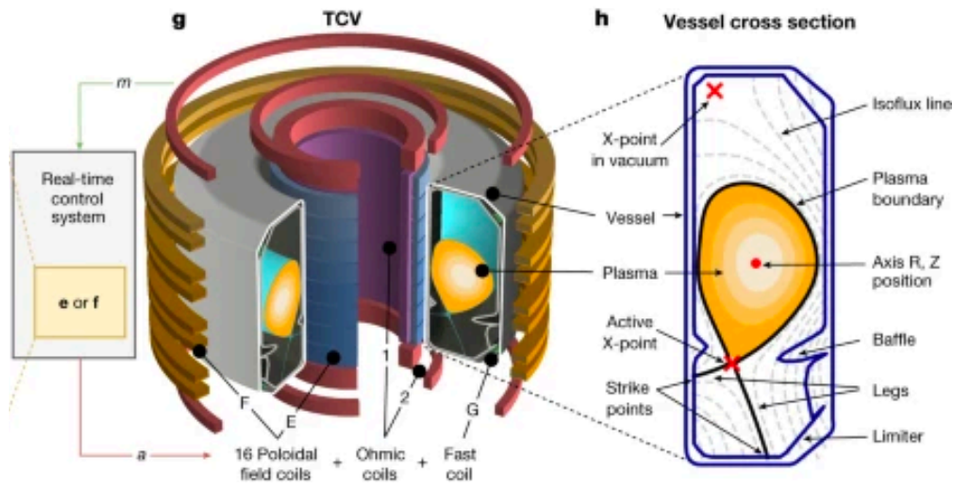

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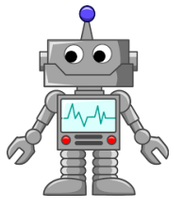
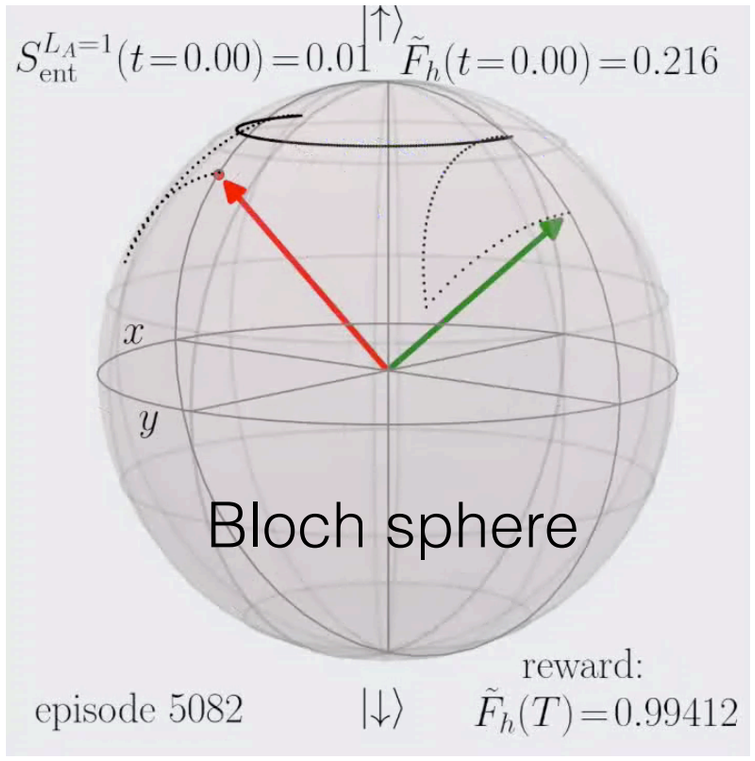
RL-aided quantum technologies





quantum control

quantum error correction

quantum gate design

quantum circuit design

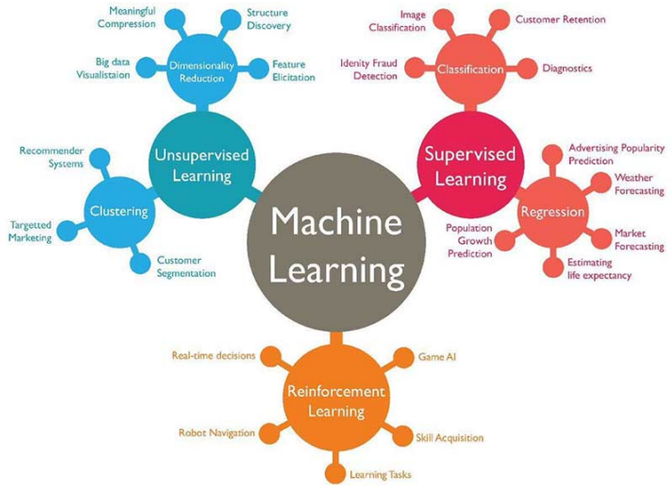
When should you consider using RL?

- *model-free:* requires no pre-knowledge of the controlled physical system

- *adaptive:* transfers acquired knowledge that might allow us to identify connections between unrelated phenomena

- *autonomous:* provides novel insights into automating complex manipulation protocols

Overview



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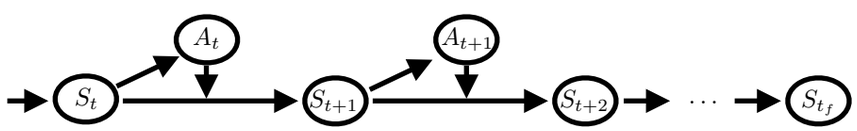
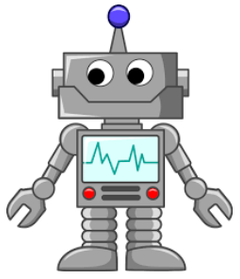
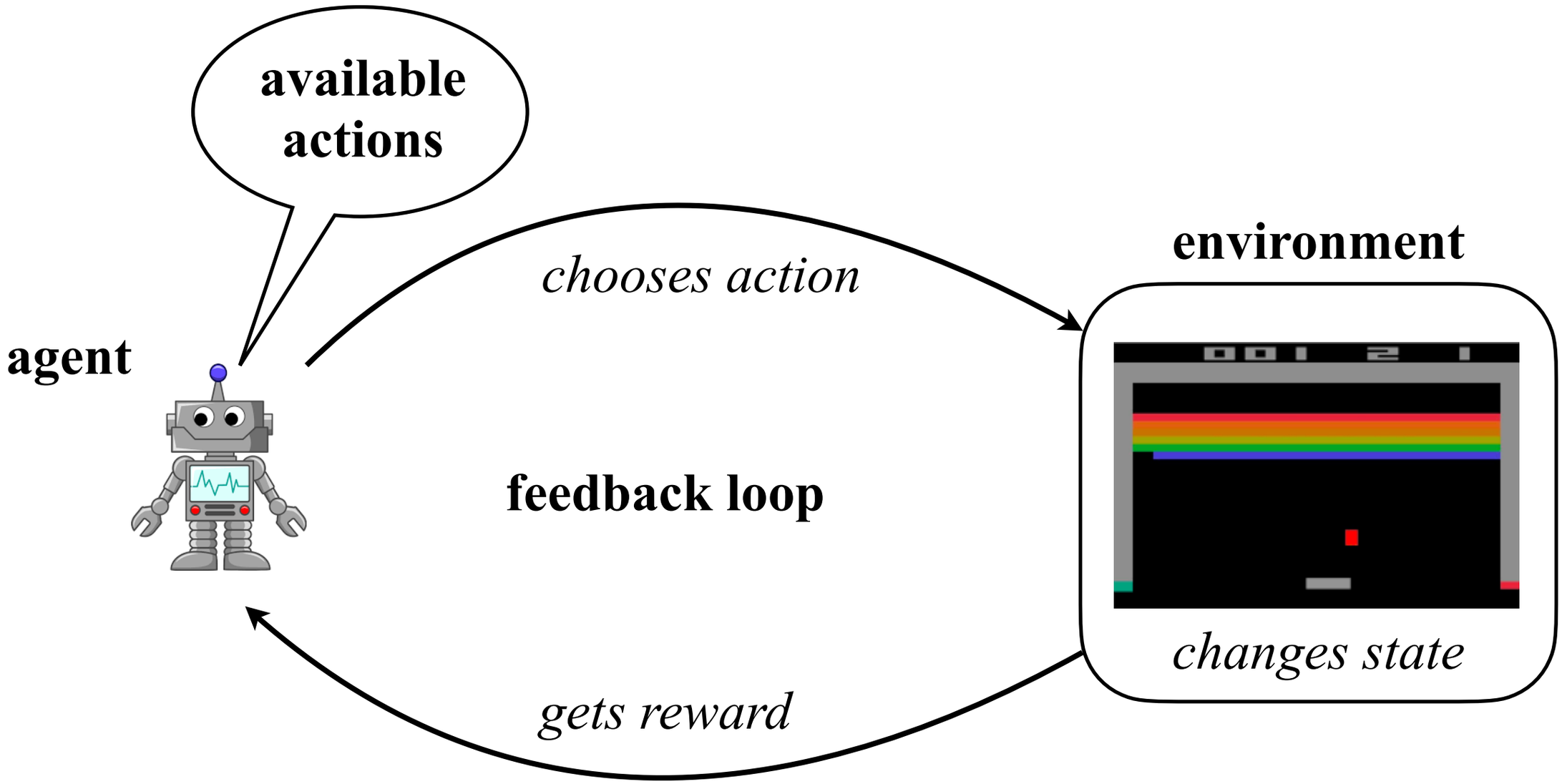




Reinforcement Learning (RL) in a Nutshell

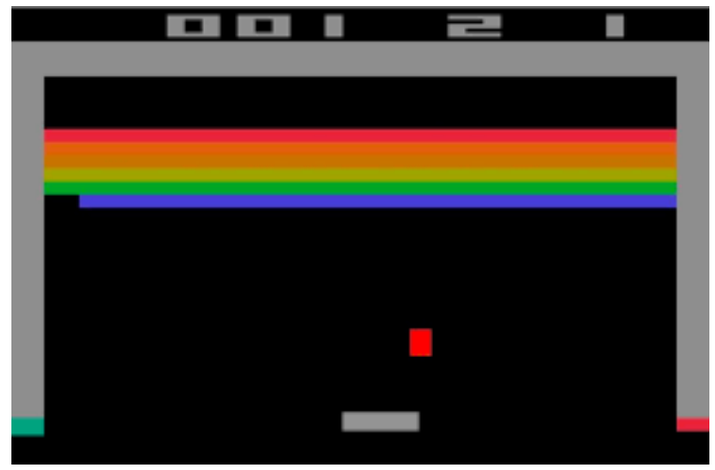
→ RL formalism



RL in a Nutshell

→ RL formalism

- action space $\mathcal{A} = \{\text{left},\ \text{stay},\ \text{right}\}$
- state space $\mathcal{S}$ pixelized image of the screen
- reward space $\mathcal{R} = \text{score}$



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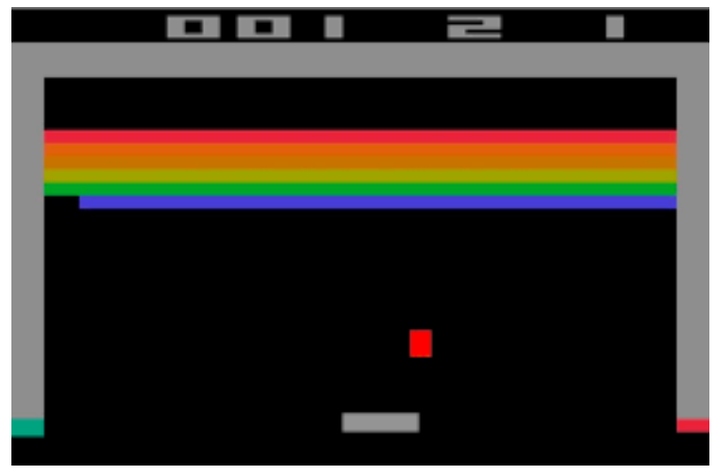
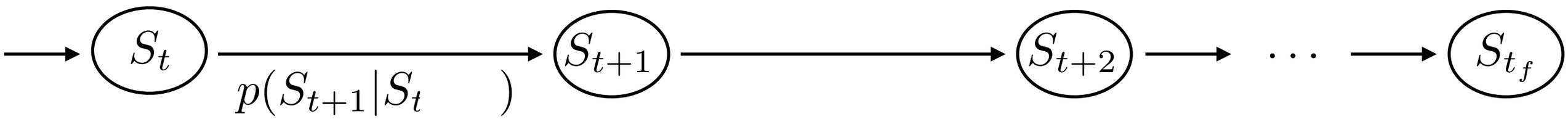


→ RL episode is a Markov decision process



- transition probability: $p(S_{t+1}|S_t\quad)$

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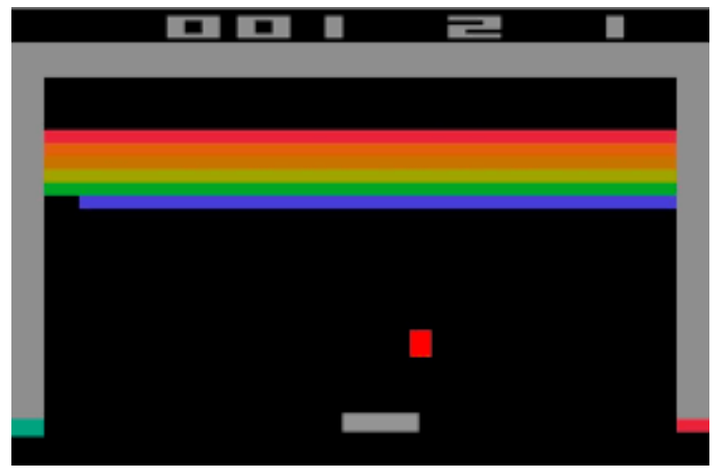

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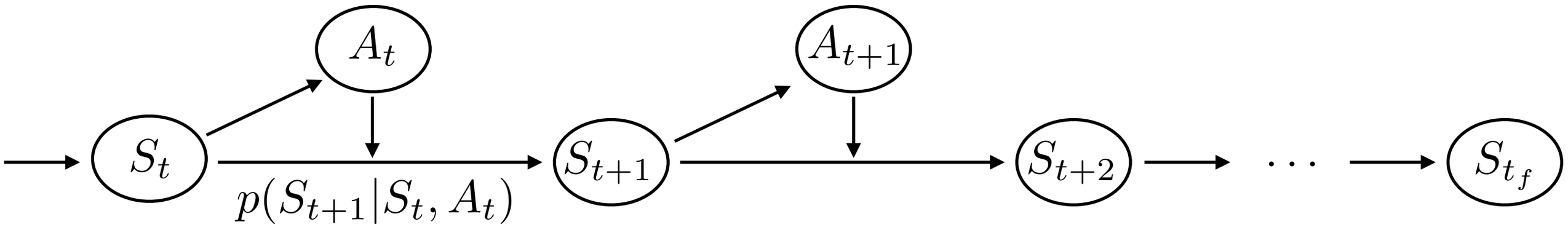
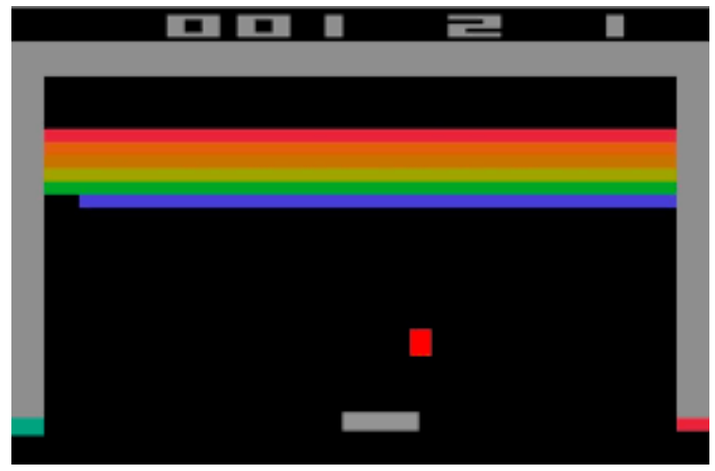


- transition probability: $p(S_{t+1}|S_t, A_t)$

RL in a Nutshell

→ RL formalism



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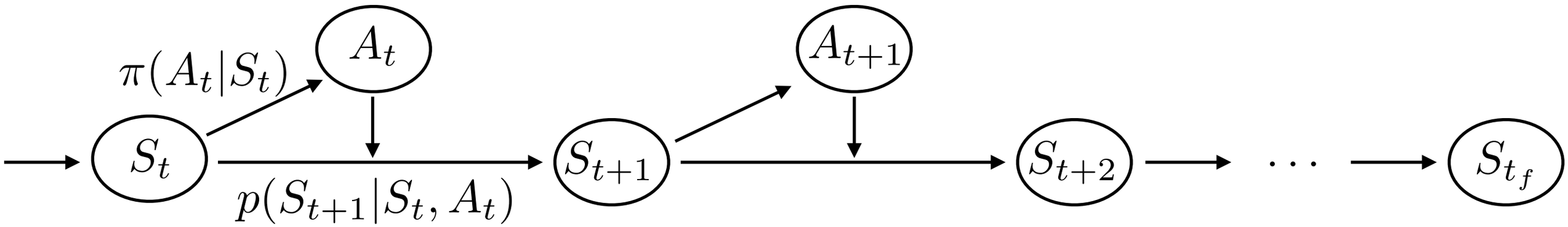

- transition probability: $p(S_{t+1}|S_t, A_t)$
- policy: $\pi(A_t|S_t)$ probability to take action A_t in the state S_t

RL in a Nutshell

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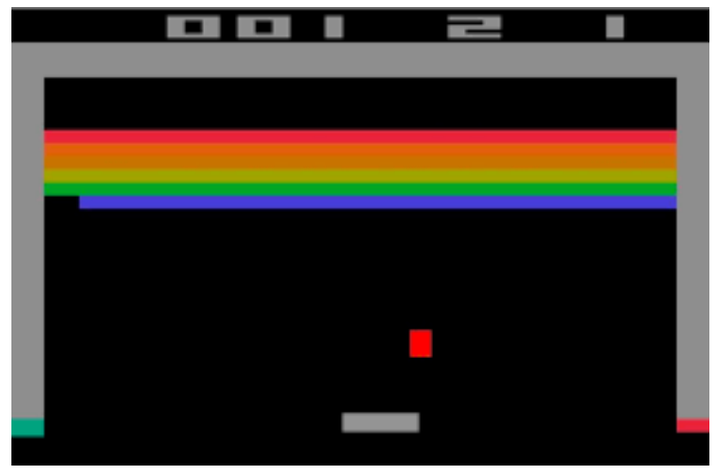

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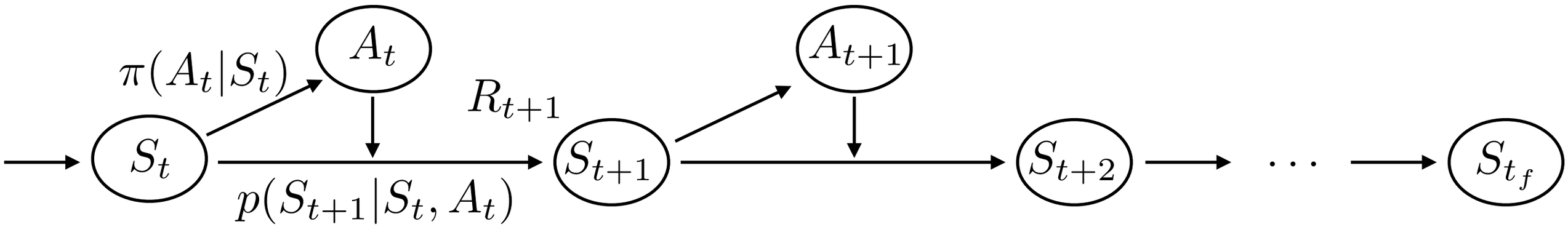

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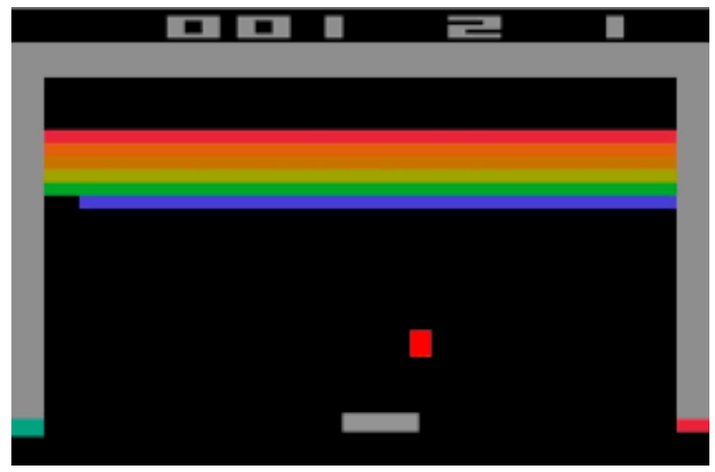

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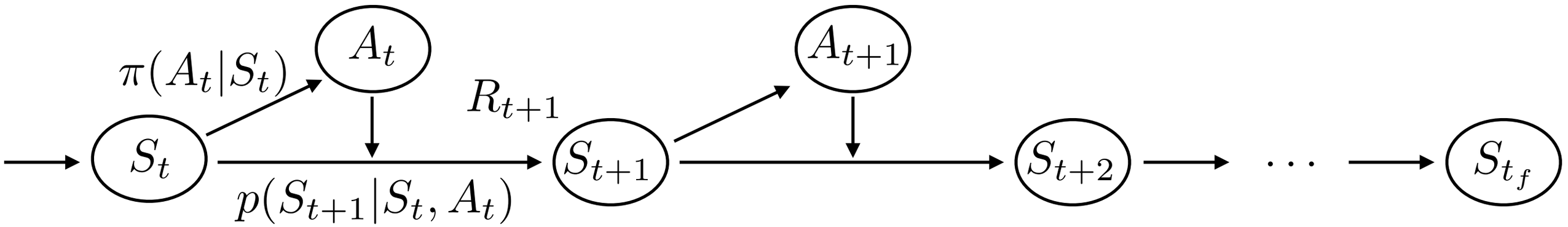
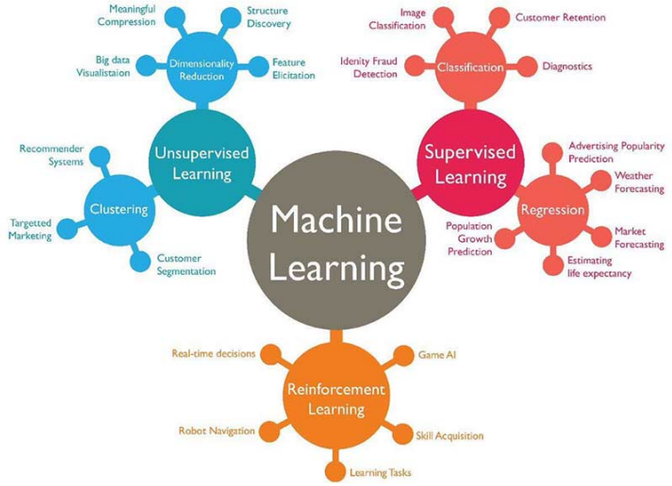


→ RL **objective**: *find policy* which maximizes the total *expected return*

$$J = \mathbb{E}_{a\sim\pi(a|s)}[R_{t+1} + \cdots + R_{t_f}|S_0 = s]$$

Overview



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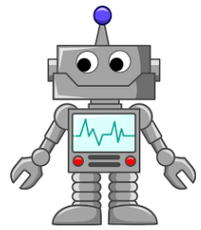
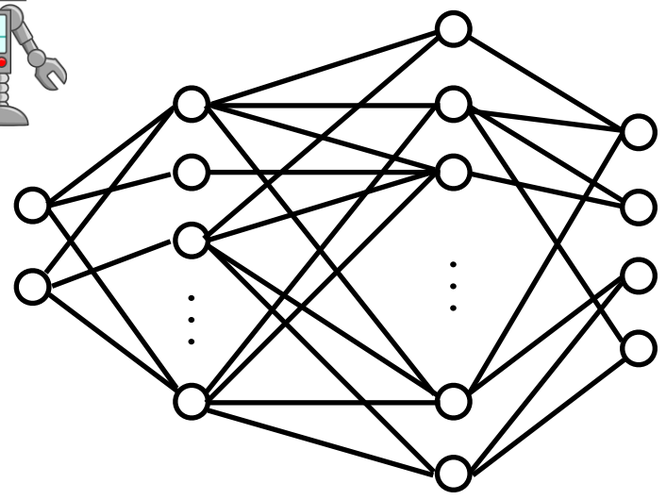
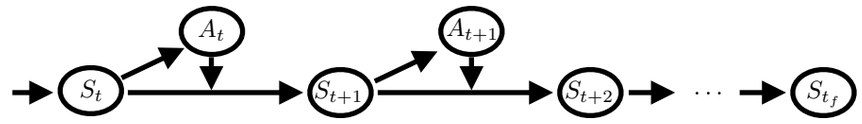




Policy Gradient



→ *in practice:* **evaluate** RL objective by sampling trajectories

$$J = \mathbb{E}_{a\sim\pi(a|s)}\left[\sum_t R_t \middle| S_0 = s\right] \approx \frac{1}{N_{\mathrm{MC}}}\sum_{j=1}^{N_{\mathrm{MC}}}\sum_t R_t(\tau_j)$$

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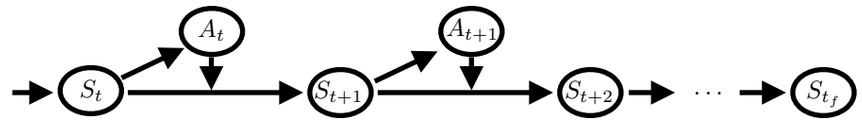

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- parametrize policy: $\pi(a|s) \approx \pi_\theta(a|s)$

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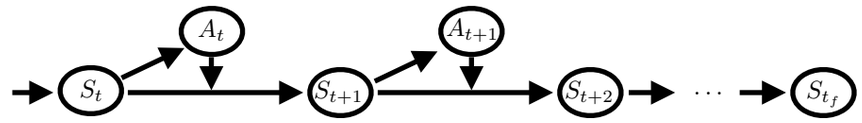

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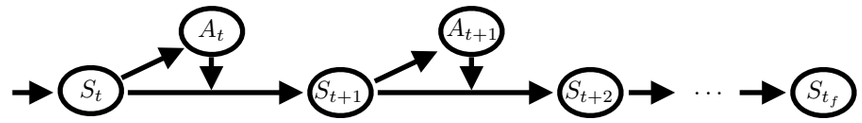

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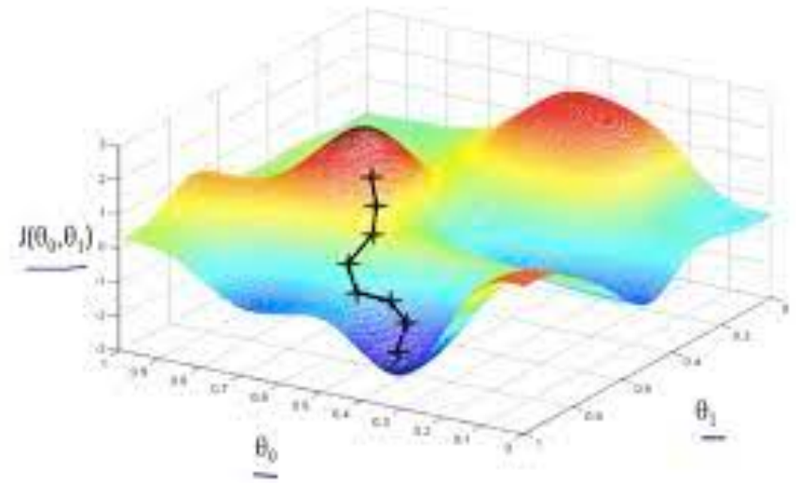
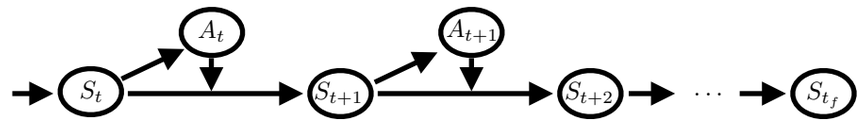
$$\theta_{\mathrm{new}} = \theta_{\mathrm{old}} + \alpha\nabla_\theta J(\theta)$$



Policy Gradient



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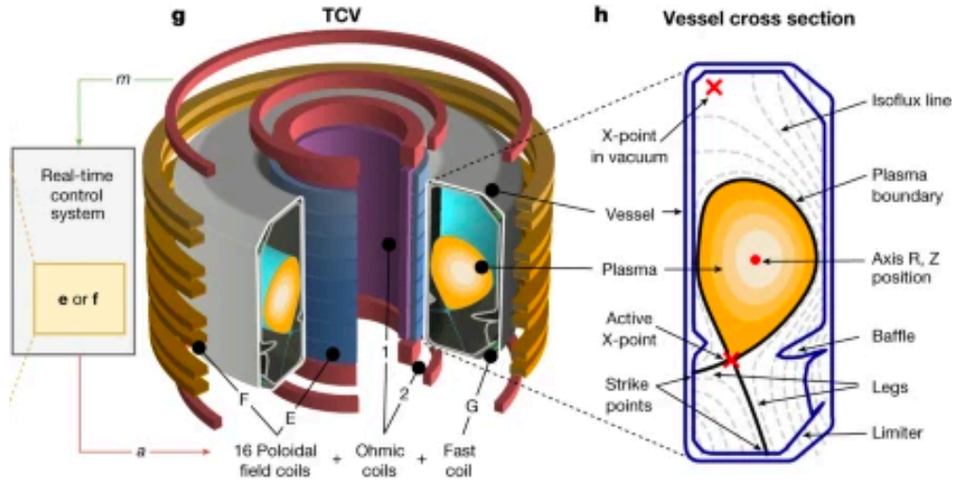

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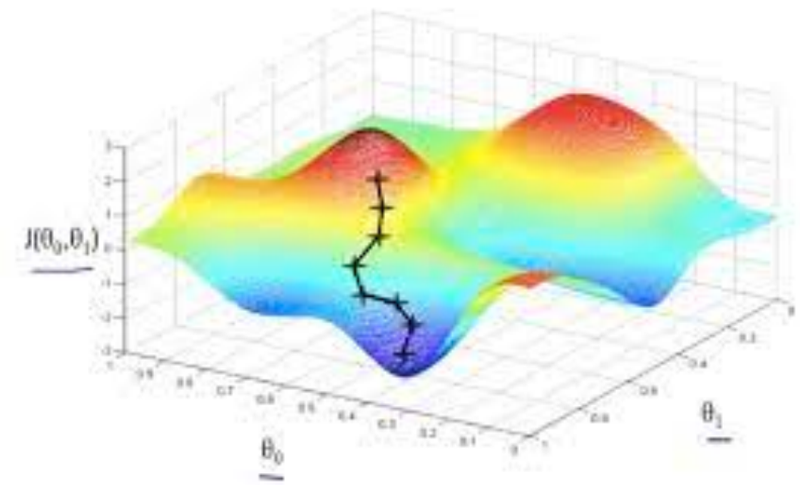
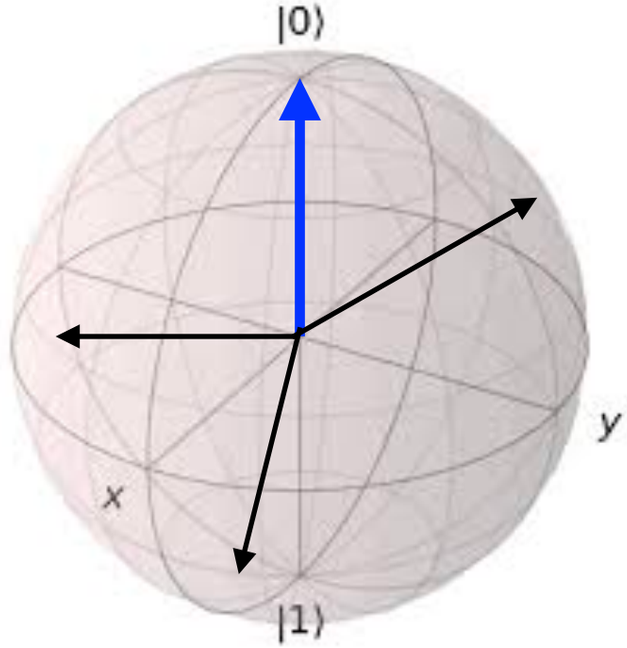


RL for Quantum State Initialization

Bloch sphere



→ **quantum control:** two-level system

- **task:** prepare $|0\rangle$ using infinitesimal rotations

$$U_\alpha = \exp\left(-i\frac{\delta t}{2}\sigma^\alpha\right) \qquad \alpha = x, y, z$$

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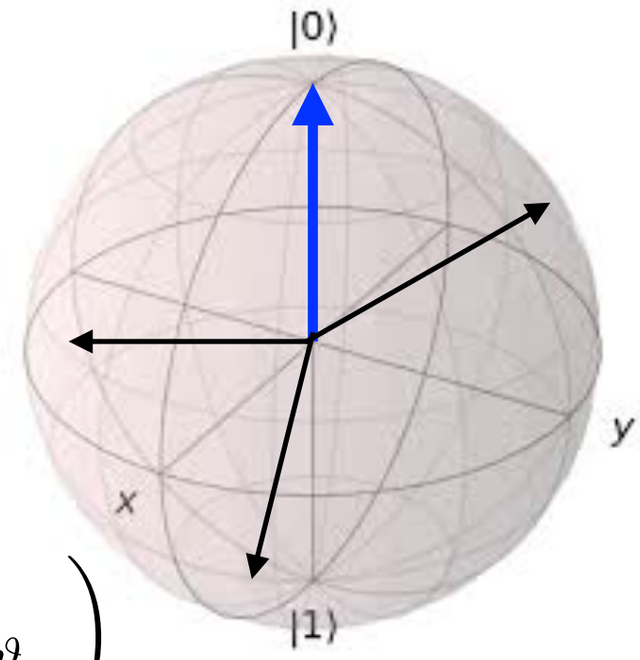

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RL state space: $\mathcal{S} = \{(\vartheta, \varphi) | \vartheta \in [0, \pi],\ \varphi \in [0, 2\pi)\}$

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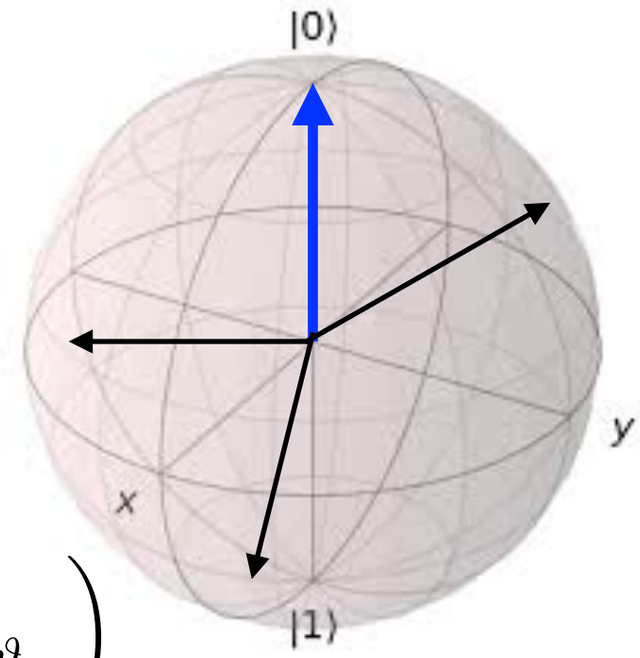

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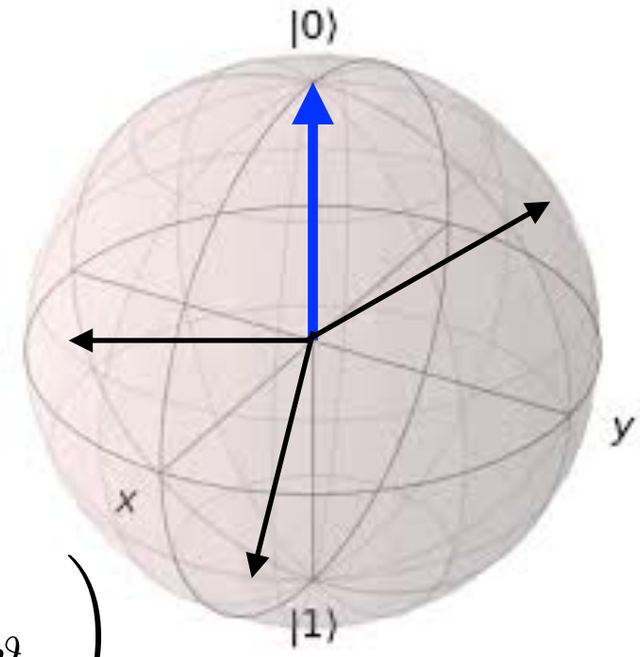

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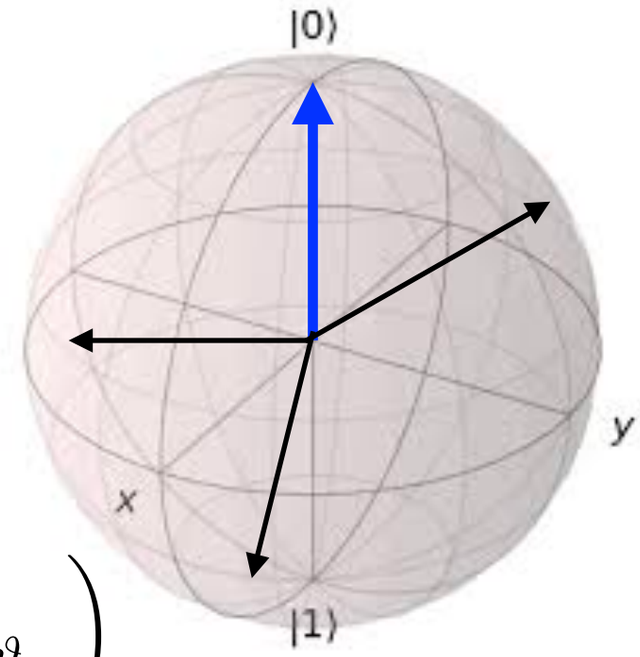

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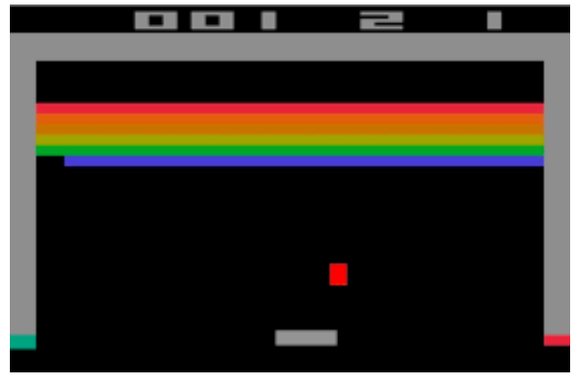
- define reward: $r_t = |\langle 0|\psi_t\rangle|^2$
- choose **RL algorithm:** policy gradient

simulate trial trajectories τ_j

$$\nabla_\theta J(\theta) \approx \frac{1}{N_{\mathrm{MC}}}\sum_{j=1}^{N_{\mathrm{MC}}} \nabla_\theta \log \pi_\theta(\tau_j) \sum_t R_t(\tau_j)$$

Value Function Algorithms



→ Value iteration methods

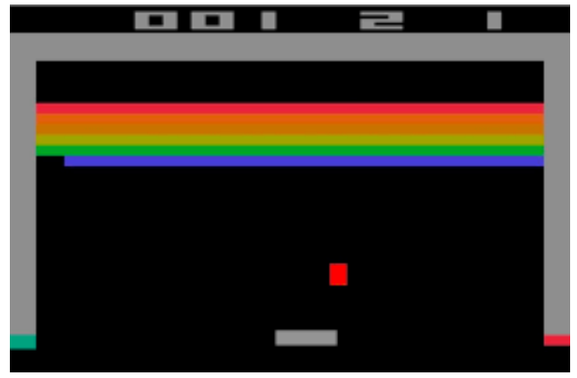
- value function: ***expected*** total return under the policy $\pi(a|s)$ from state s

$$v_\pi(s) = \mathbb{E}_{a\sim\pi(a|s)}[G_t|S_t = s] \qquad G_t = R_{t+1} + R_{t+2} + \dots$$

$$= R_{t+1} + G_{t+1}$$

	$v_\pi(s)$
S_1	1.3
S_2	2.1
S_3	1.5

Value Function Algorithms



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problem: cannot reconstruct policy from value function

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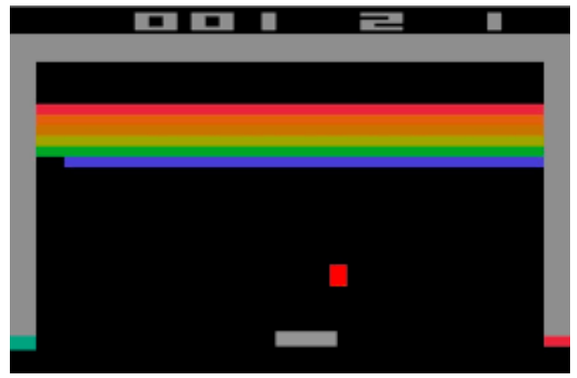
Value Function Algorithms



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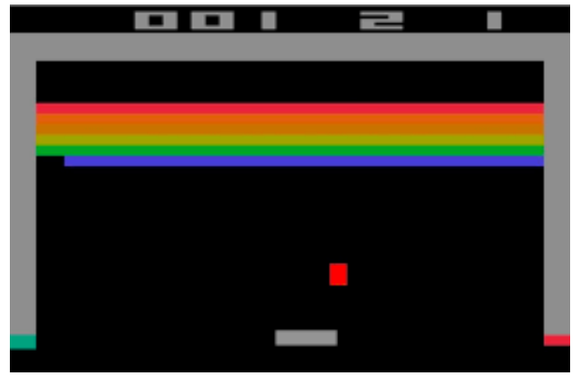
- action-value (or Q-) function: ***expected*** total return under the policy $\pi(a|s)$ starting from state s and taking action a:

$$Q_\pi(s,a) = \mathbb{E}_{a\sim\pi(a|s)}[G_t|S_t = s, A_t = a]$$

	$v_\pi(s)$
S_1	1.3
S_2	2.1
S_3	1.5

$Q(s,a)$	A_1	A_2	A_3
S_1	1.5	0.5	2.1
S_2	1.3	4.4	0.2
S_3	0.9	0.9	3.3

Value Function Algorithms



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$$v_\pi(s) = \sum_a \pi(a|s) Q_\pi(s,a)$$

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Q-Learning

- optimal action-value function: $Q_*(s,a) = \max_\pi Q_\pi(s,a)$
- optimal value function: $v_*(s) = \max_a Q_*(s,a)$
- optimal policy: $\pi_*(a|s) = \text{argmax}_{a'} Q_*(s,a')$

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Bellman's equation: $Q_*(s,a) = \sum_{s'} p(s'|s,a) \left[r(s,s',a) + \max_{a'} Q_*(s',a') \right]$

appears on both sides of equation; compute recursively

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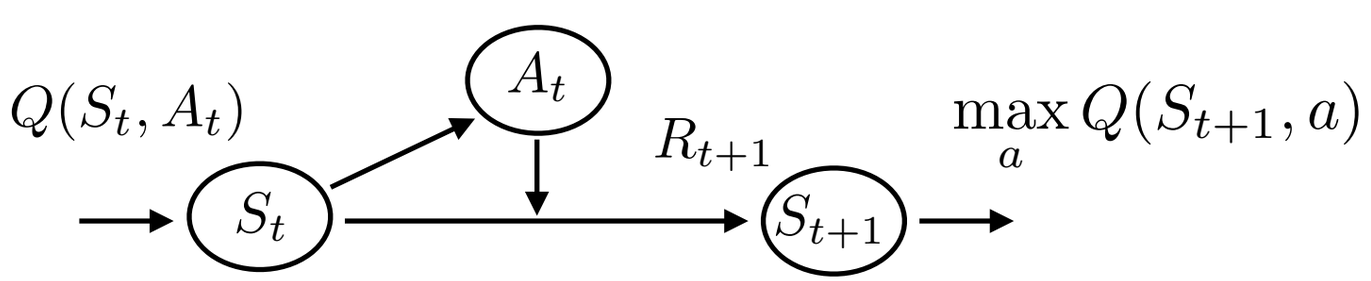
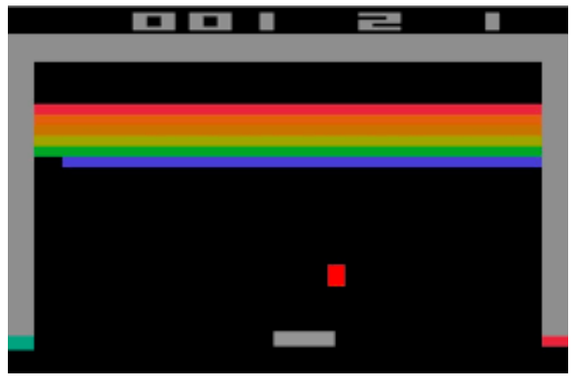
appears on both sides of equation; compute recursively

→ Q-learning: iterate following two steps until convergence

1. error according to definition $\delta_t = Q(S_t,A_t) + R_{t+1} - \max_a Q(S_{t+1},a)$
2. update current function $Q_{\text{new}} = Q_{\text{old}} + \alpha\delta_t \qquad \alpha \in [0,1)$



Q-Learning



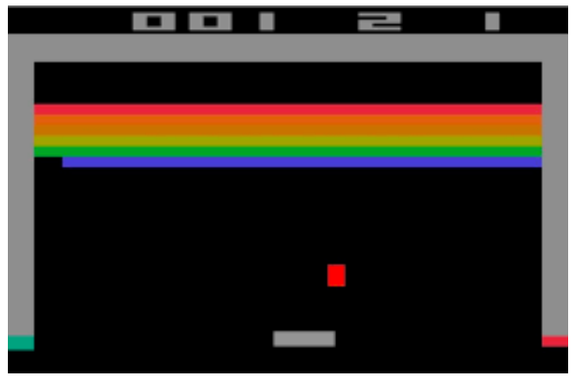
→ improve policy using current Q-function

- take action which maximizes the Q-value at each step

iteration 1

$Q(s,a)$	A_1	A_2	A_3
S_1	1.5	0.5	2.1
S_2	0.3	4.4	0.7
S_3	0.9	0.9	1.3

Q-Learning



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$$\pi(S_1) = A_3$$

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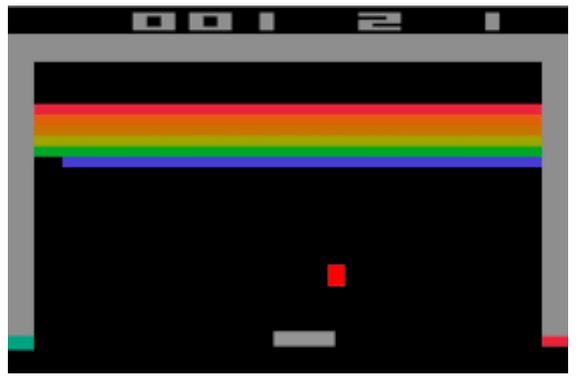
Q-Learning



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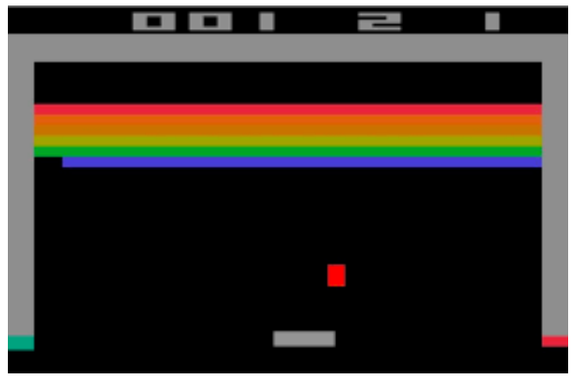
Q-Learning



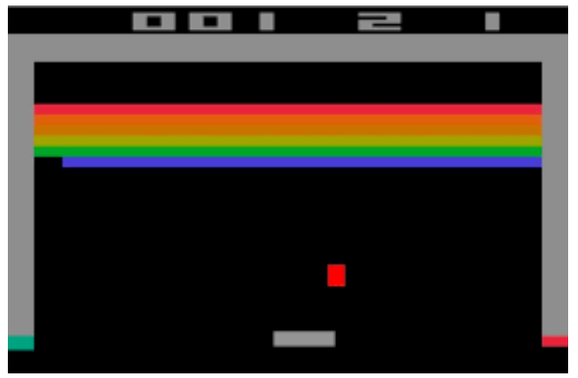
→ improve policy using current Q-function

- take action which maximizes the Q-value at each step

iteration 2

$Q(s,a)$	A_1	A_2	A_3
S_1	1.6	0.4	1.8
S_2	0.6	2.8	0.1
S_3	0.6	1.1	1.0

Q-Learning



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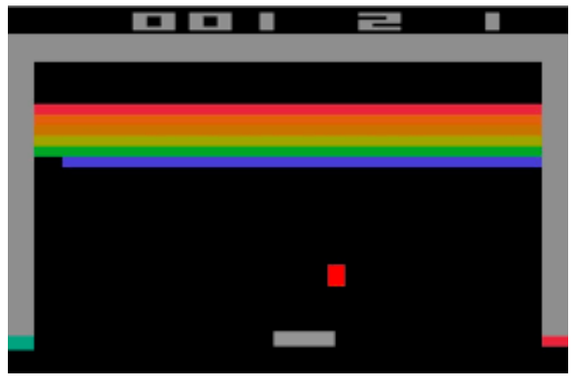
Q-Learning



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S_2	0.6	2.8	0.1
S_3	0.6	1.1	1.0

$$A = \text{argmax}_a Q(S, a)$$

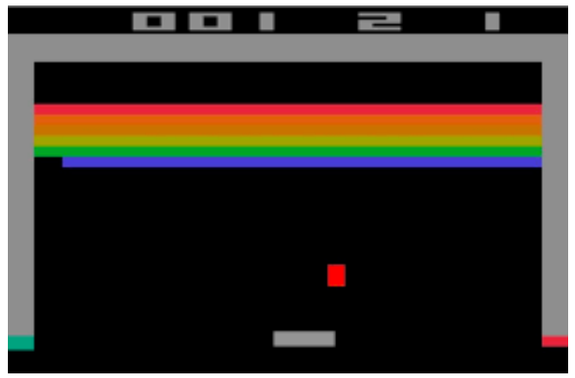
$$\pi(S_1) = A_3$$

$$\pi(S_2) = A_2$$

$$\pi(S_3) = A_2$$

1. error according to definition $\delta_t = Q(S_t, A_t) + R_{t+1} - \max_a Q(S_{t+1}, a)$
2. update current function $Q_{\text{new}} = Q_{\text{old}} + \alpha\delta_t \qquad \alpha \in [0, 1)$

Q-Learning



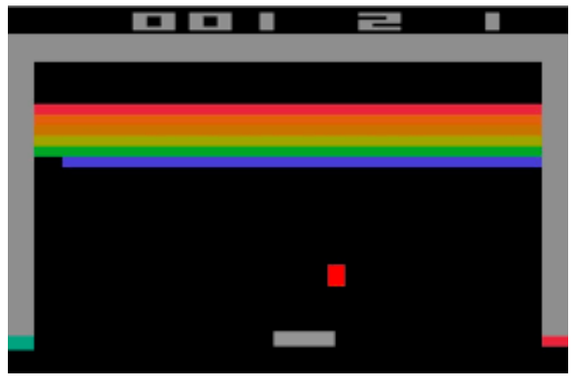
→ improve policy using current Q-function

- take action which maximizes the Q-value at each step

iteration 100

$Q(s,a)$	A_1	A_2	A_3
S_1	0.6	1.3	0.6
S_2	1.6	0.8	0.9
S_3	0.8	1.7	0.5

Q-Learning



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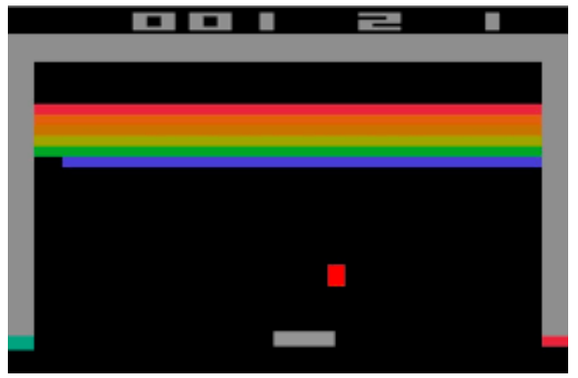
Q-Learning



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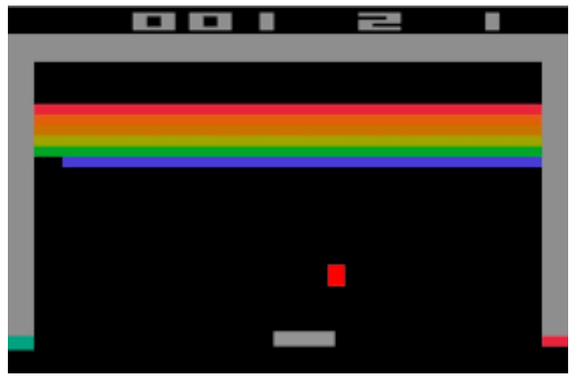
$$\delta_t = Q(S_t, A_t) + R_{t+1} - \max_a Q(S_{t+1}, a) = 0$$

Q-Learning



→ improve policy using current Q-function

- take action which maximizes the Q-value at each step

iteration 100

converged

$Q(s,a)$	A_1	A_2	A_3
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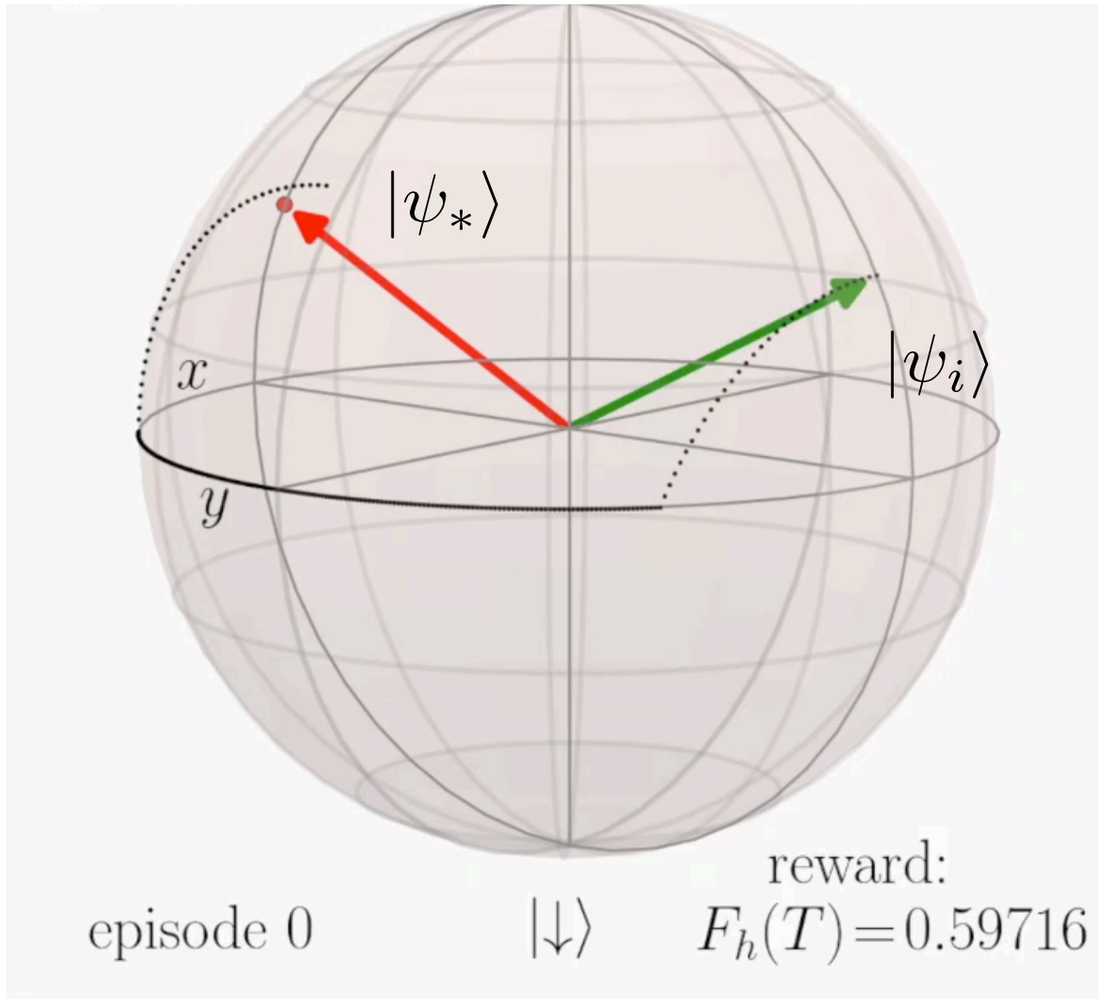
RL Applied to Quantum State Preparation

$$H(t) = -S^z - h_x(t) S^x$$

$$S^x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$S^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$



state preparation = fidelity optimization

$$F_h(t) = |\langle\psi_*|\psi(t)\rangle|^2$$

$$|\psi(t)\rangle = \mathcal{T} \mathrm{e}^{-i\int_0^t \mathrm{d}t' H(t')} |\psi_i\rangle$$

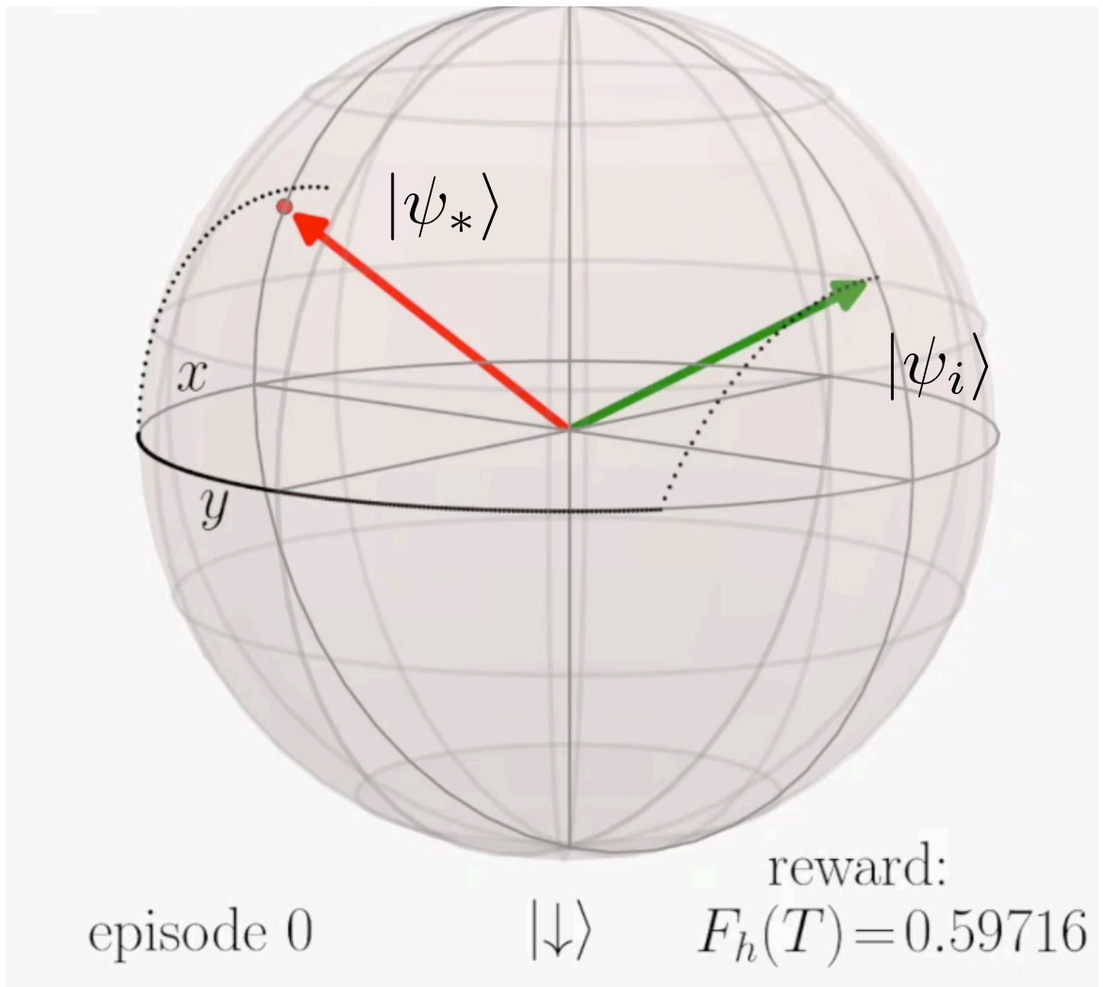
RL Applied to Quantum State Preparation

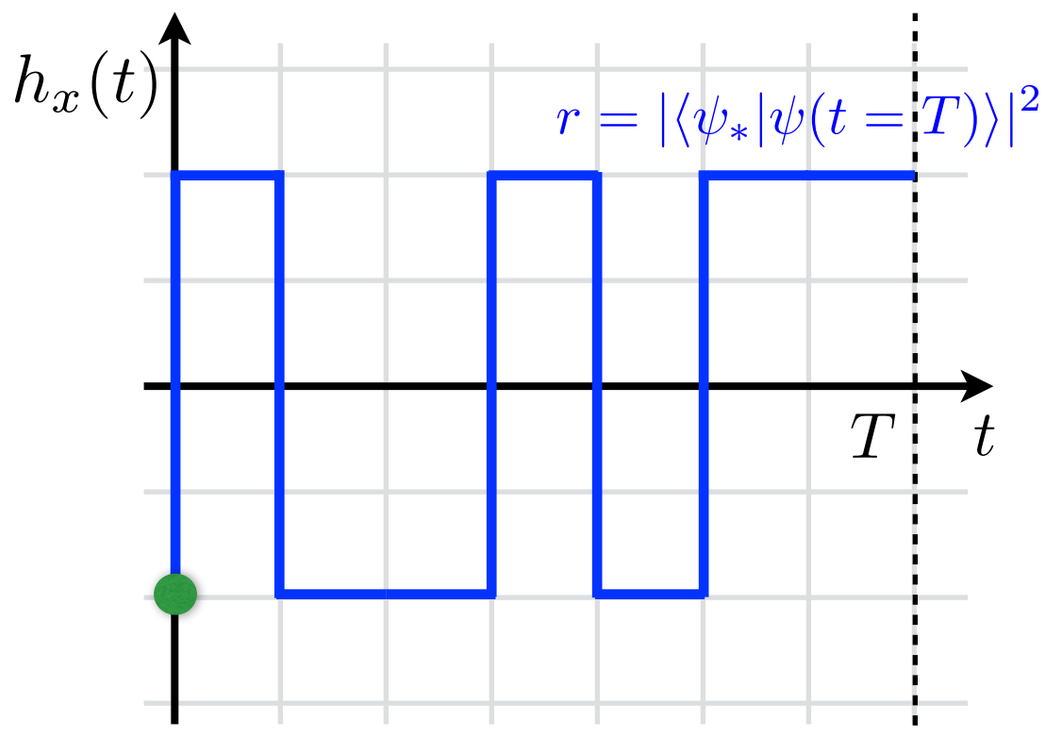
$$H(t) = -S^z - h_x(t) S^x$$

$$S^x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$F_h(t) = |\langle \psi_* | \psi(t) \rangle|^2$$

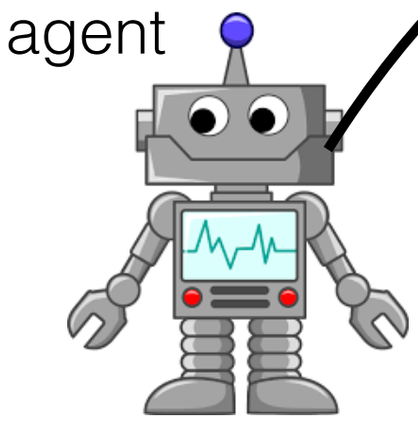
task: find optimal field within family of bang-bang protocols $h \in \{\pm 4\}$





episode completed

RL Applied to Quantum State Preparation



1

feedback loop,
updates RL agent

3

ENVIRONMENT

2

$$H(t) = H_0 + H_{\text{ctrl}}(t)$$

$|\psi_i\rangle$: GS of H_0

$|\psi_*\rangle$: target state

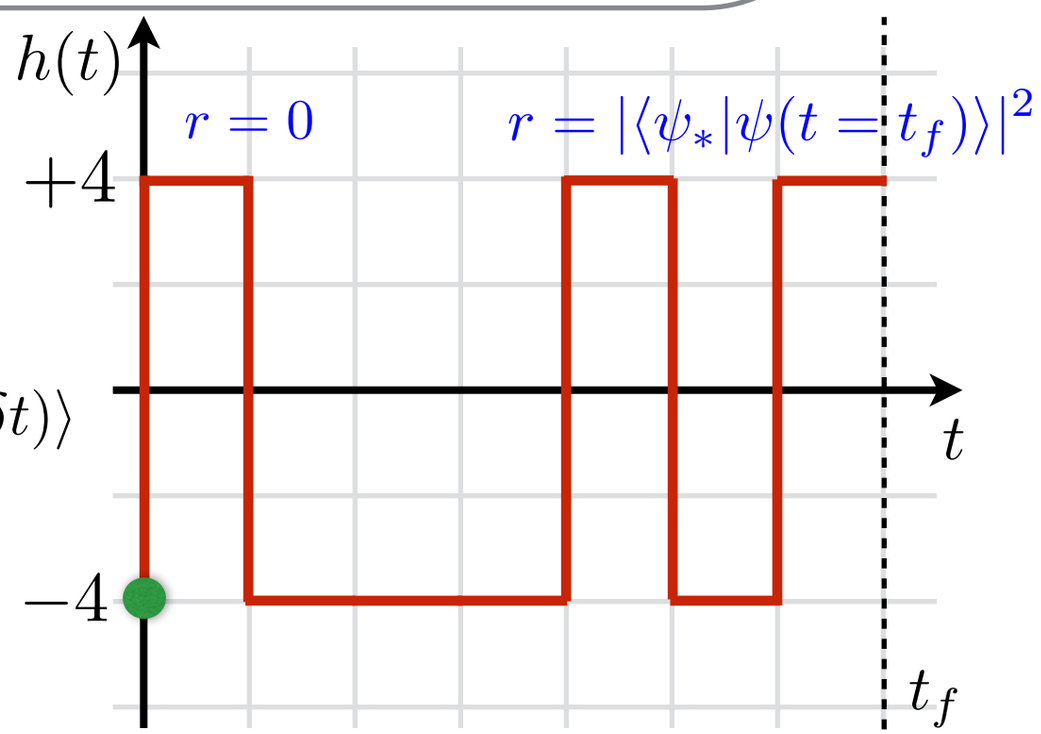
$$i\partial_t|\psi(t)\rangle = H(t)|\psi(t)\rangle \; t \in [0, t_f]$$

reward $r = \begin{cases} 0 & , 0 \le t < t_f \\ |\langle\psi_*|\psi(t=t_f)\rangle|^2 & , t = t_f \end{cases}$

1 start from state $s_0 = [h(0)] = [-4]$
take action $a_0 : \delta h = +8$
go to state $s_1 = [h(0), h(\delta t)] = [-4, +4]$

2 solve Schrödinger Eq. and obtain the QM state $|\psi(\delta t)\rangle$

3 calculate reward r
and use it to update $Q(s, a)$
which in turn is used to choose subsequent actions



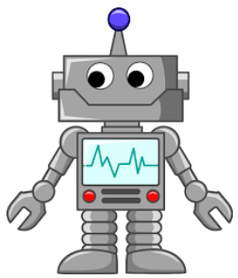
episode completed

MB et al, PRX 8 031086 (2018)

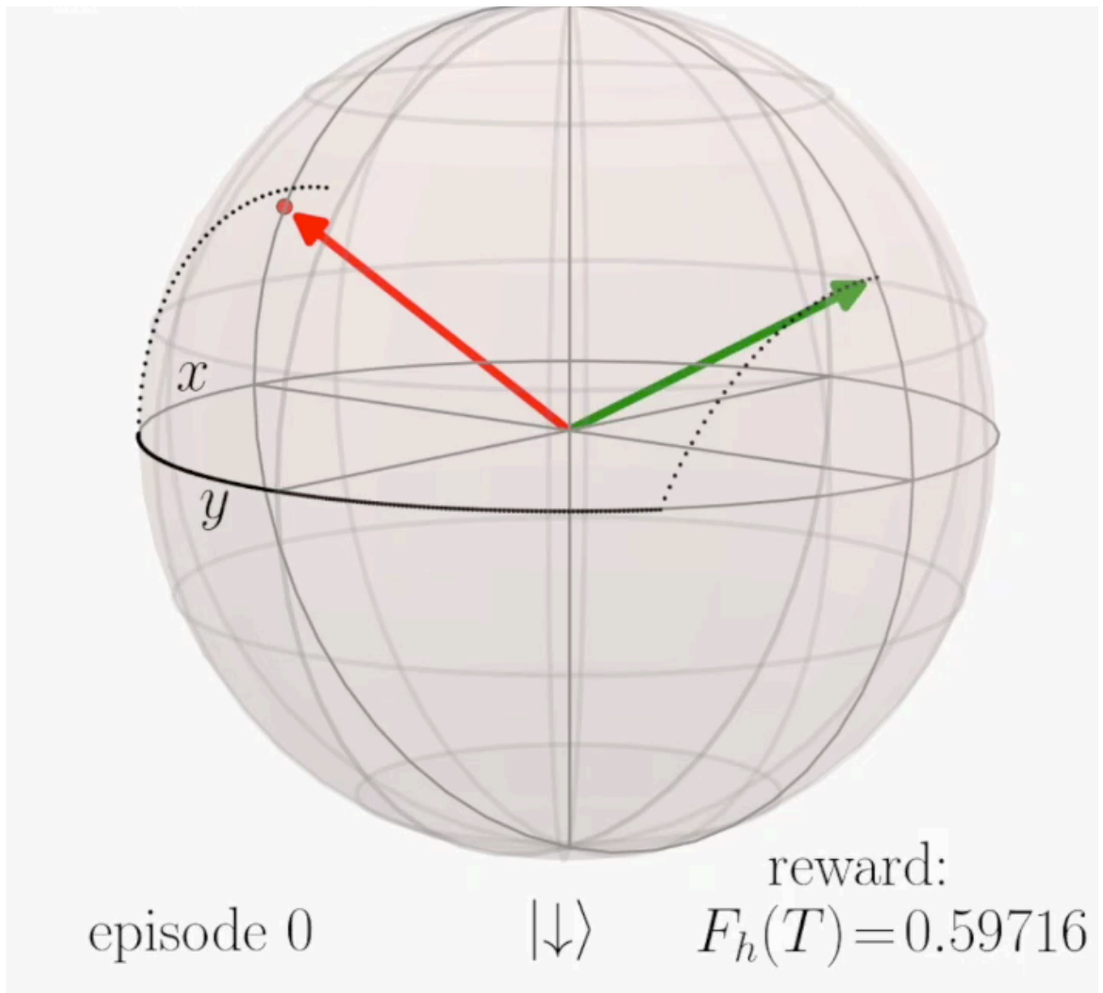
RL Applied to Quantum State Preparation

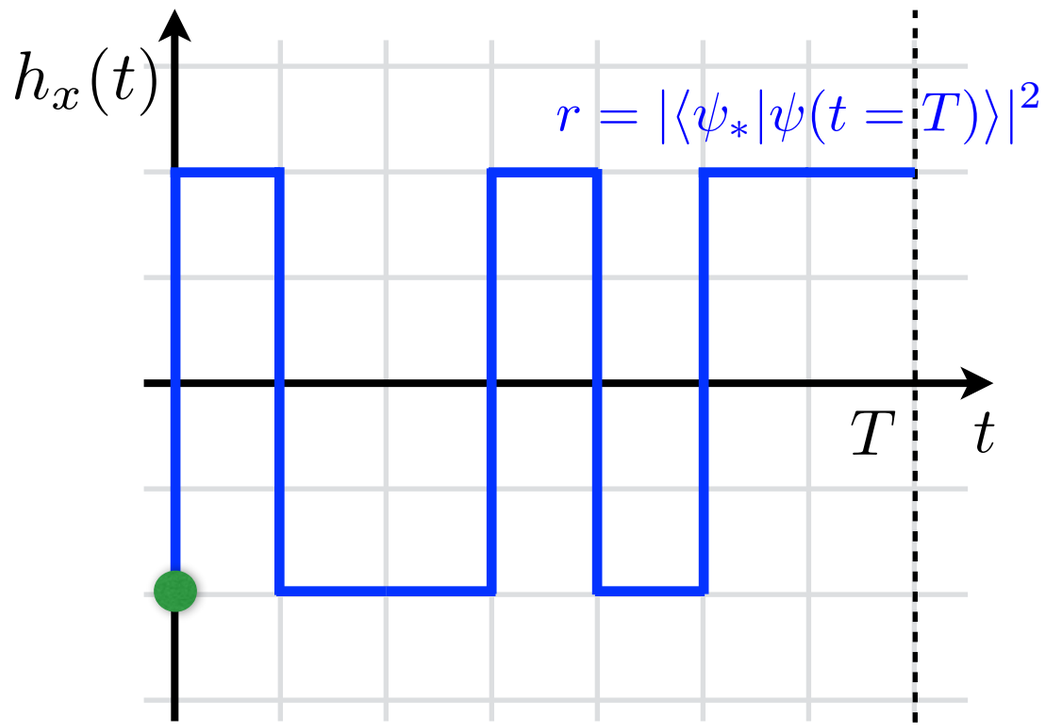
$$H(t) = -S^z - h_x(t) S^x$$

$h \in \{\pm 4\}$ bang-bang protocols



movie of the learning process

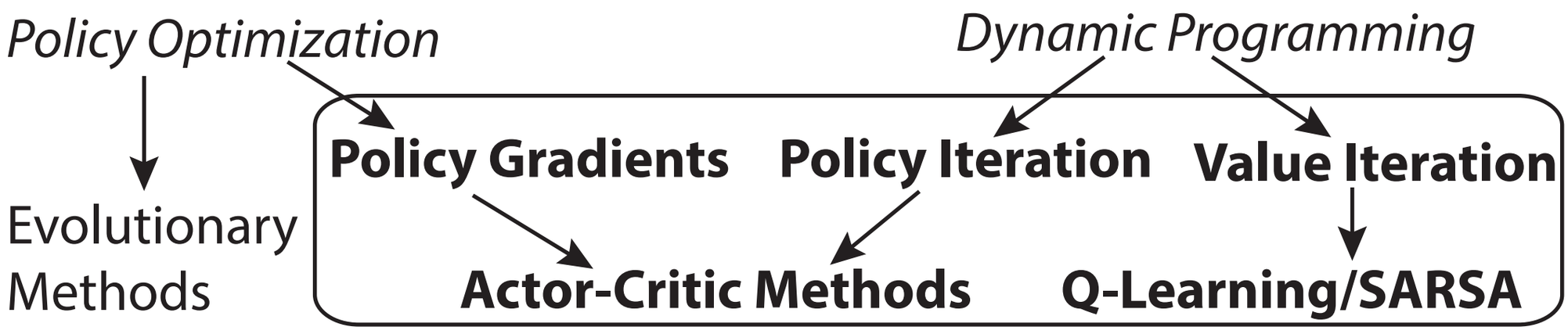




episode completed

Overview of RL Algorithms

→ overview of RL algorithms



Overview of RL Algorithms

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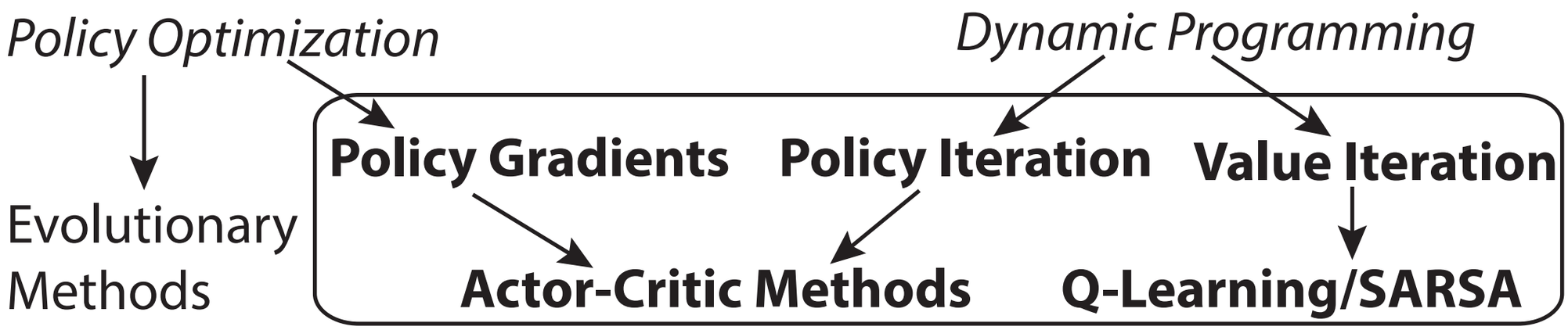
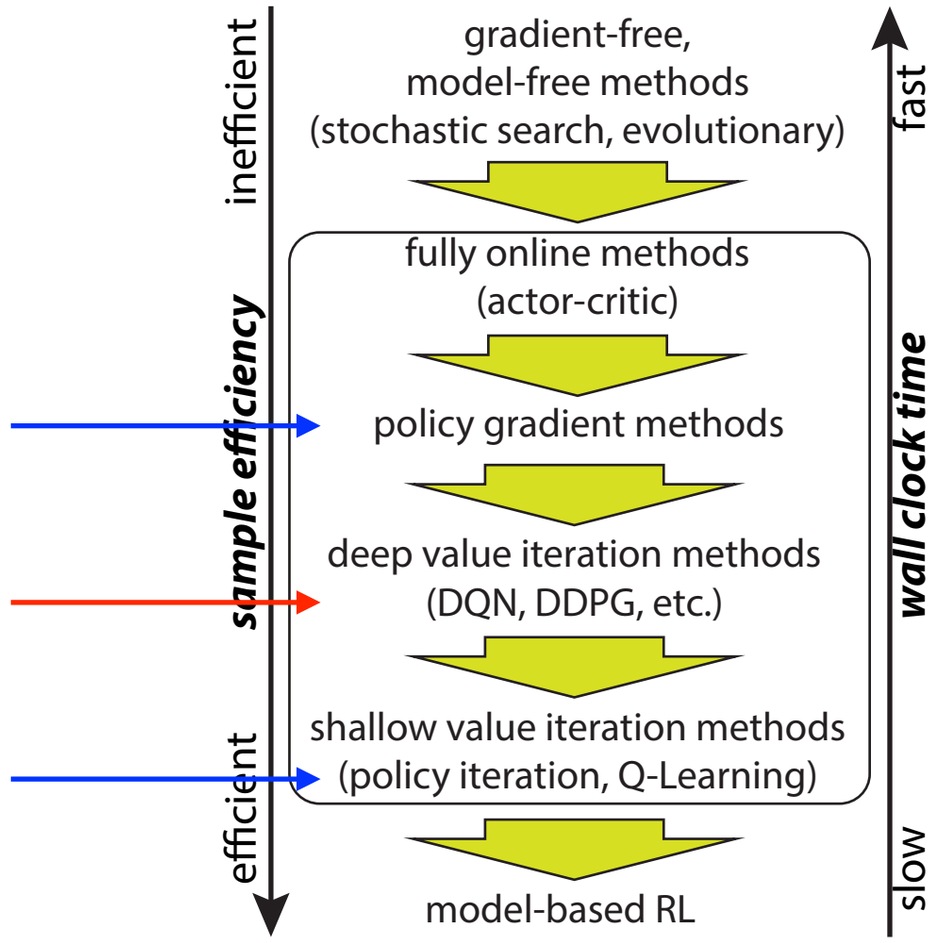
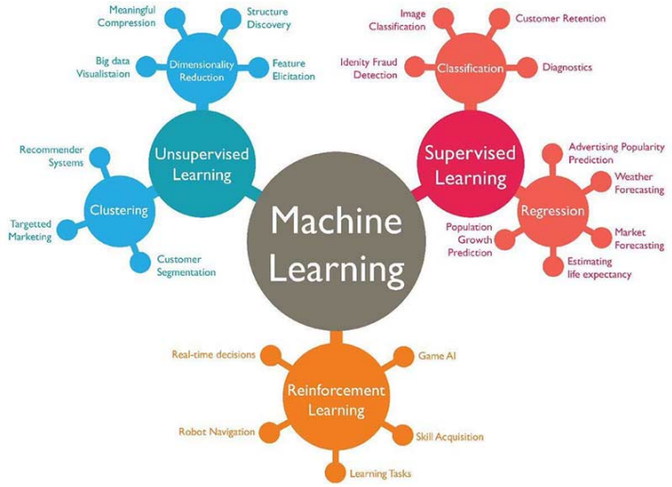


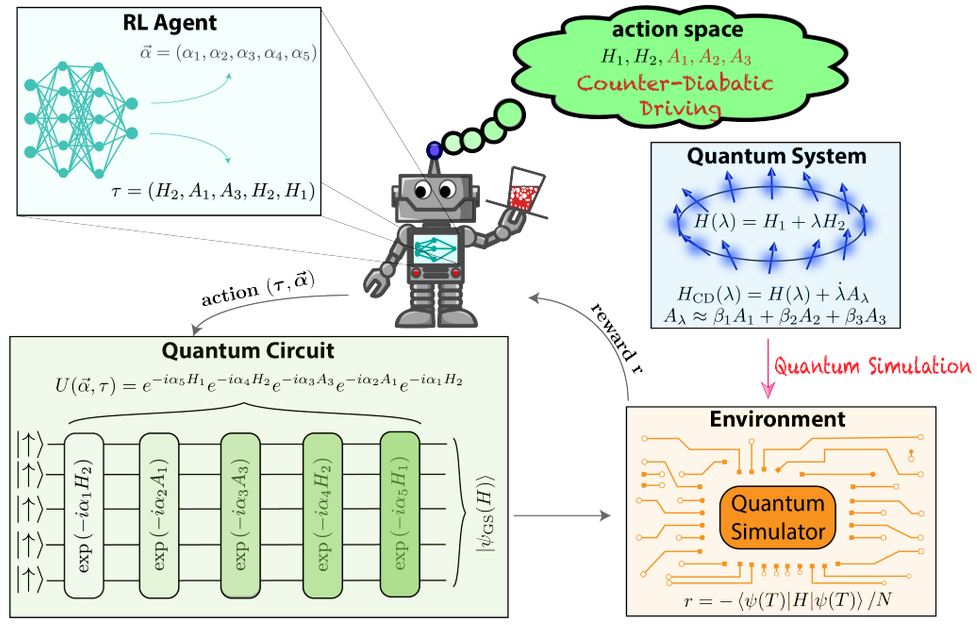
→ which algorithm to use?



Overview

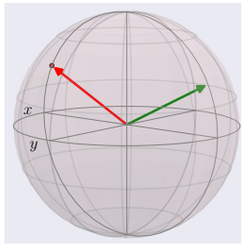


- What is Reinforcement Learning (RL)?
- RL framework in a nutshell
- RL algorithms
- Applications of RL in quantum physics



Applications of RL in Quantum Physics

→ **quantum control**



MB et al, PRX 8 031086 (2018)
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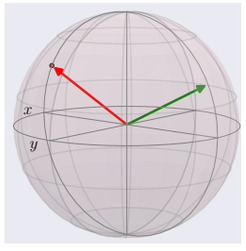
Porotti, Comm Phys 2 (2019)

+ many more

Applications of RL in Quantum Physics

→ **quantum control**



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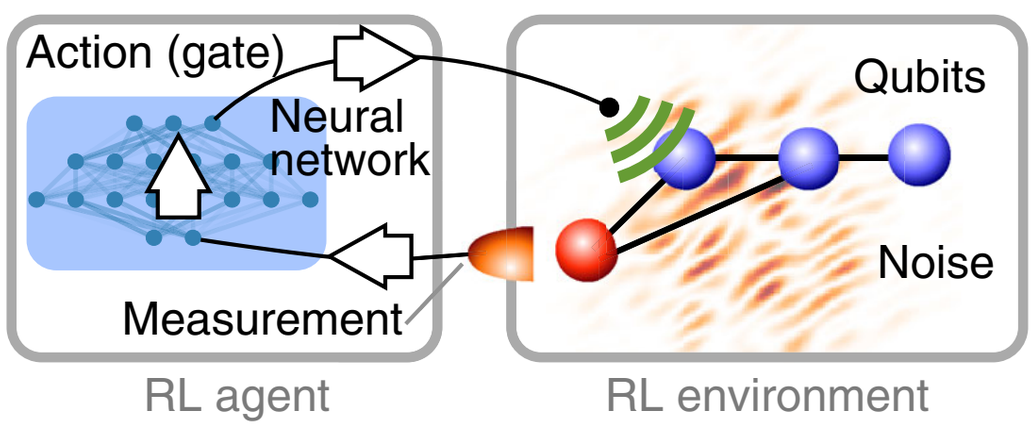
+ many more

→ **quantum error correction**

- **task:** find error correcting code that protects qubits from decoherence



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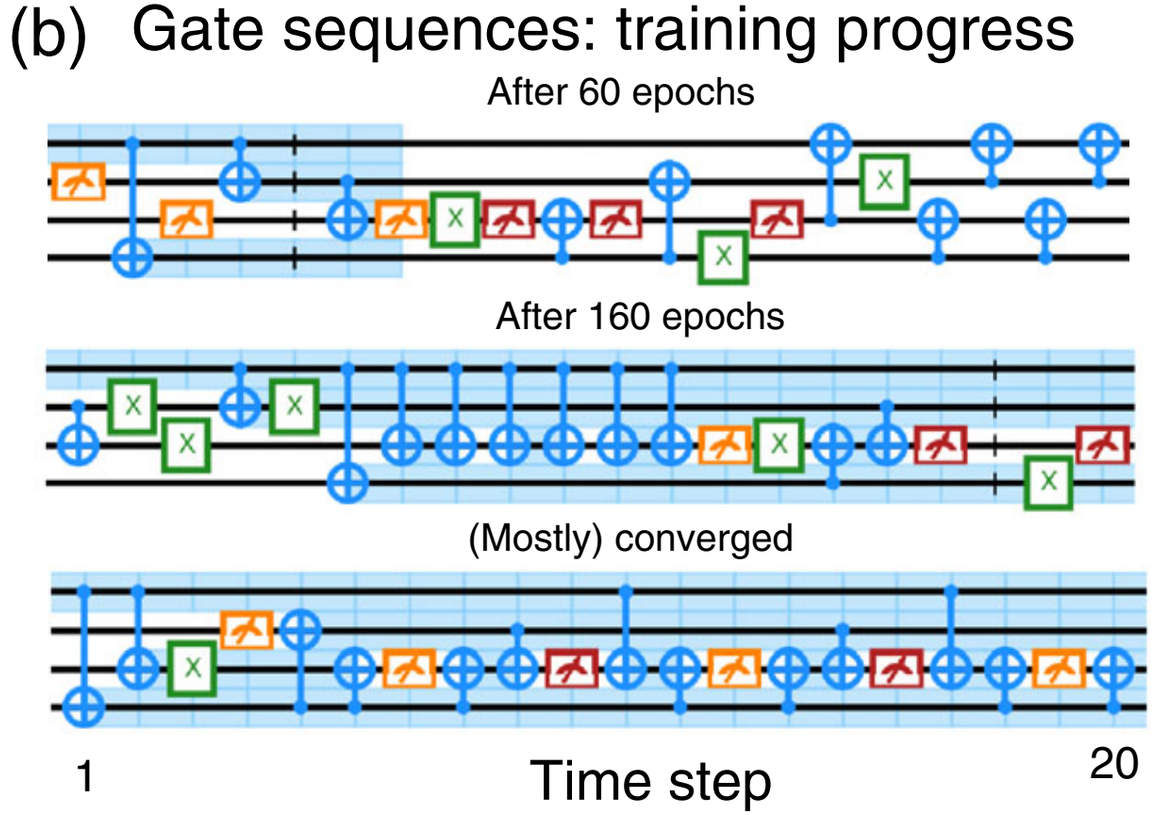
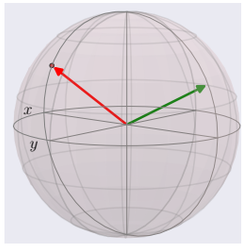


Applications of RL in Quantum Physics

→ quantum control



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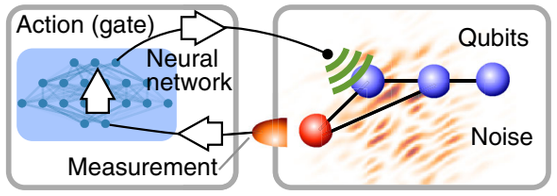

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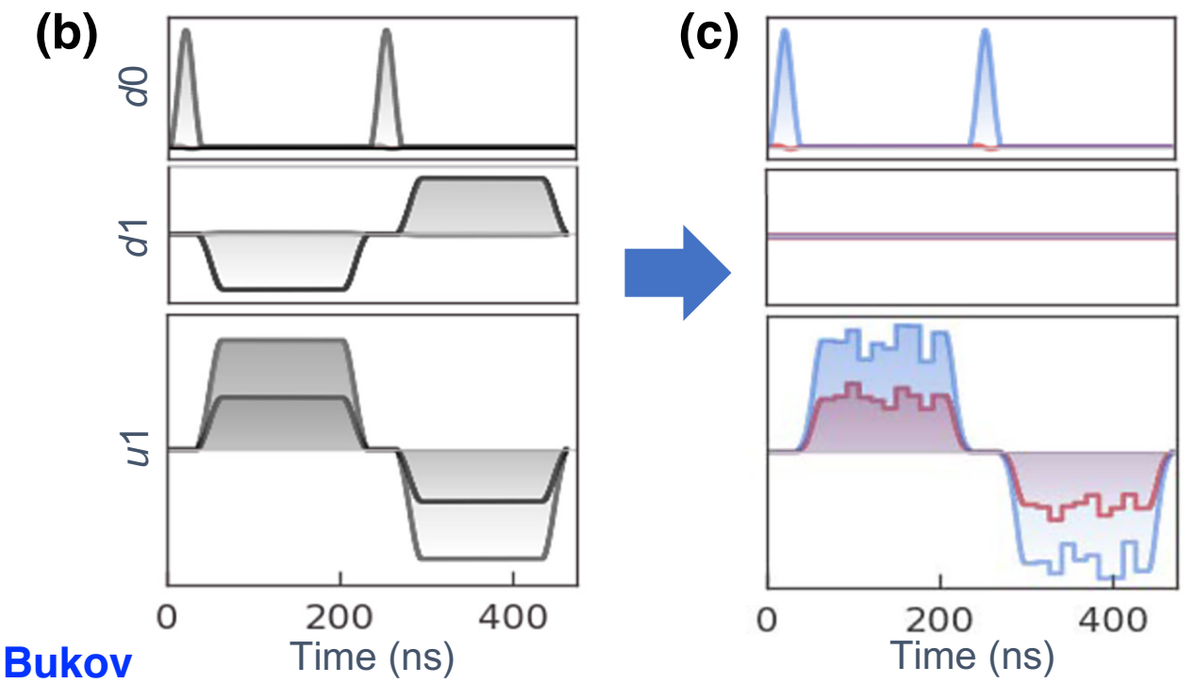
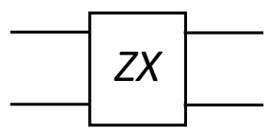
Andreasson et al, Quantum 3 183 (2019)
Sweke et al, ML Sci Tech 2 025005 (2020)

→ quantum gates design

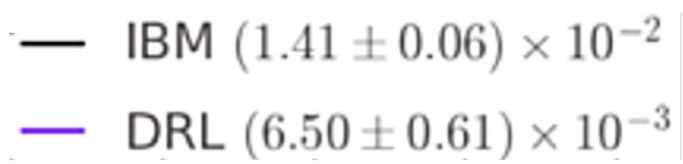
- **task:** find high-fidelity pulses that emulate gates on a quantum computer



Baum et al, PRX Quantum 2, 040324 (2021)



cross resonance gate



infidelity / error rate

Applications of RL in Quantum Physics

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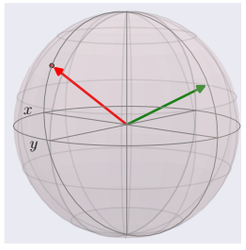

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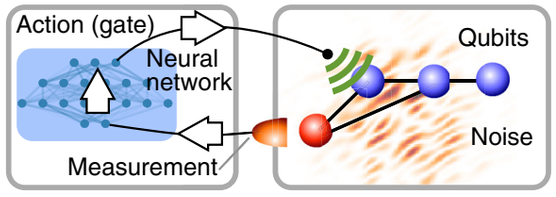
→ quantum error correction



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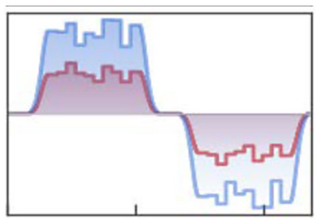
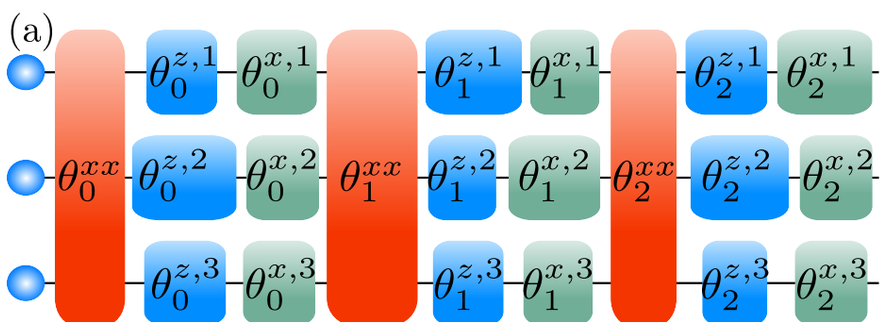
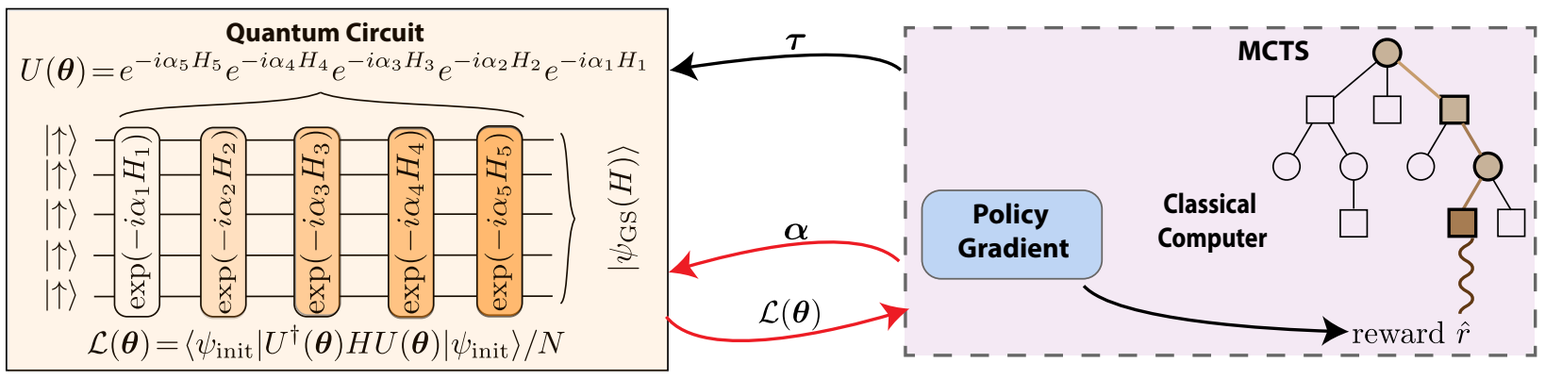


Baum et al, PRX Quantum 2, 040324 (2021)

→ variational quantum circuit design

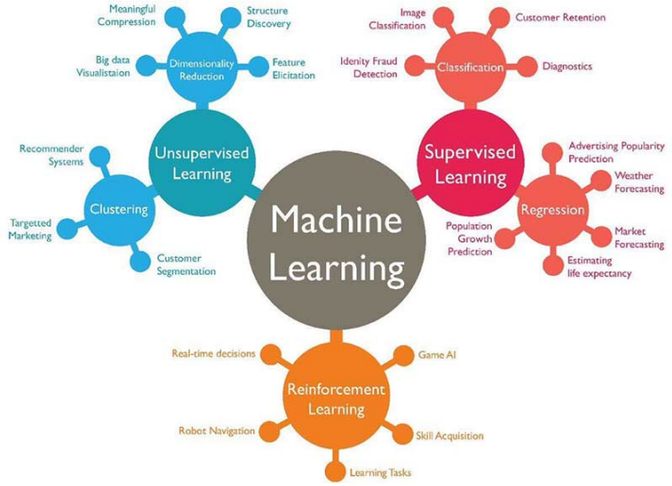


Bolens et al, PRL 2021



Yao et al, MSML 2019, 2021, 2022

Overview



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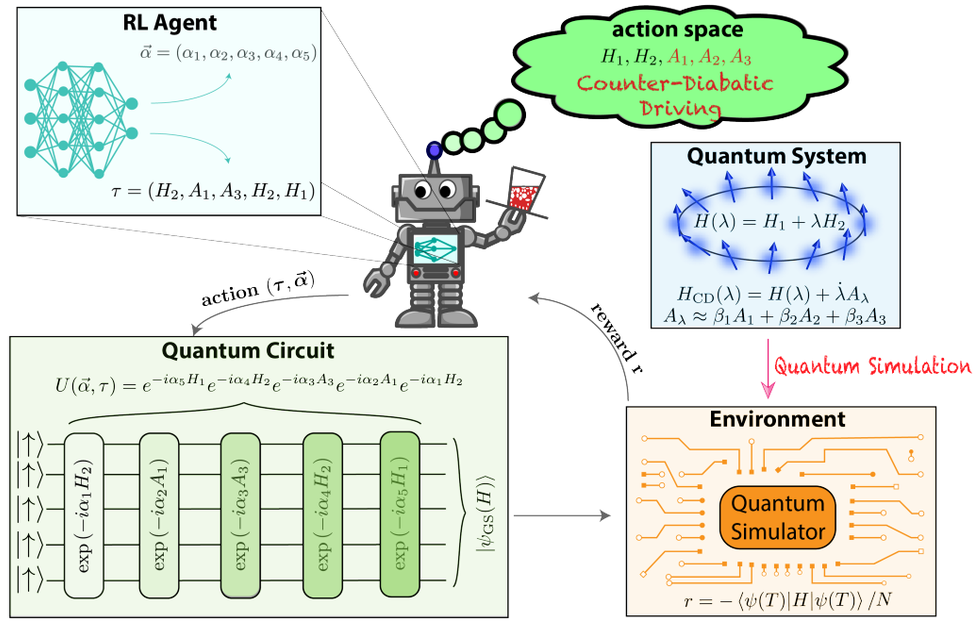
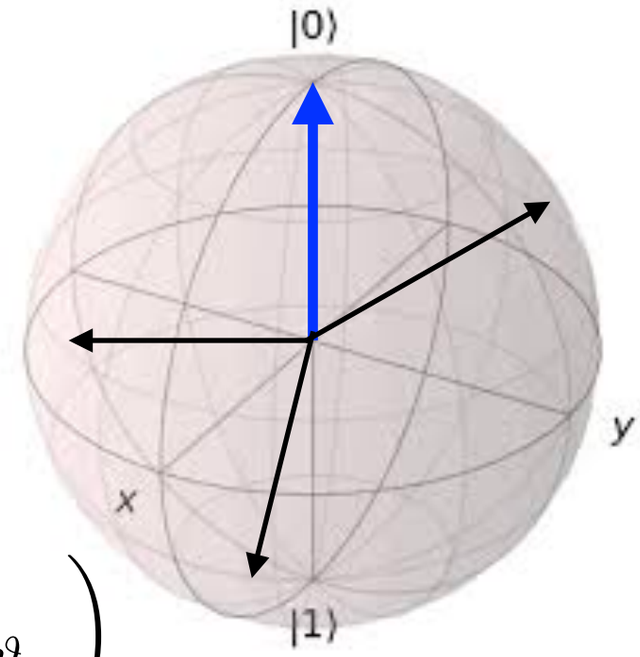


RL for Quantum State Initialization

Bloch sphere



→ **quantum control:** two-level system

- **task:** prepare $|0\rangle$ using infinitesimal rotations

$$U_\alpha = \exp\left(-i\frac{\delta t}{2}\sigma^\alpha\right) \qquad \alpha = x, y, z$$

- define **RL states**:

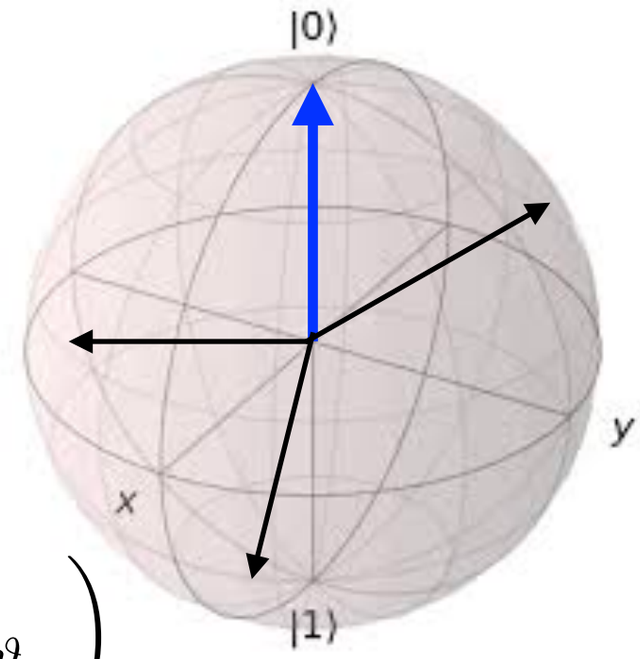
parametrization of state of system: $|\psi\rangle = \begin{pmatrix} \cos\frac{\vartheta}{2} \\ e^{i\varphi}\sin\frac{\vartheta}{2} \end{pmatrix}$

RL state space: $\mathcal{S} = \{(\vartheta, \varphi)|\vartheta \in [0, \pi],\ \varphi \in [0, 2\pi)\}$

- define **RL actions**: $\mathcal{A} = \{I, U_\alpha|\alpha = x, y, z\}$ $\qquad |\psi'\rangle = U_\alpha|\psi\rangle$ $\qquad s \mapsto s'$
- define reward: $r_t = |\langle 0|\psi_t\rangle|^2$

RL for Quantum State Initialization

Bloch sphere



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problem: *continuous* state space has infinitely many configurations

RL with Function Approximation

→ **problem:** state space has exponentially many configurations $|\mathcal{A}|^{N_T}$

- can we estimate values of not yet encountered states?

RL with Function Approximation

→ **problem:** state space has exponentially many configurations $|\mathcal{A}|^{N_T}$

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→ YES, via inter- & extrapolation: parametrize the Q-function/policy

$$Q(s,a) \to Q_\theta(s,a) \qquad \pi(a|s) \to \pi_\theta(a|s)$$

variational parameters θ

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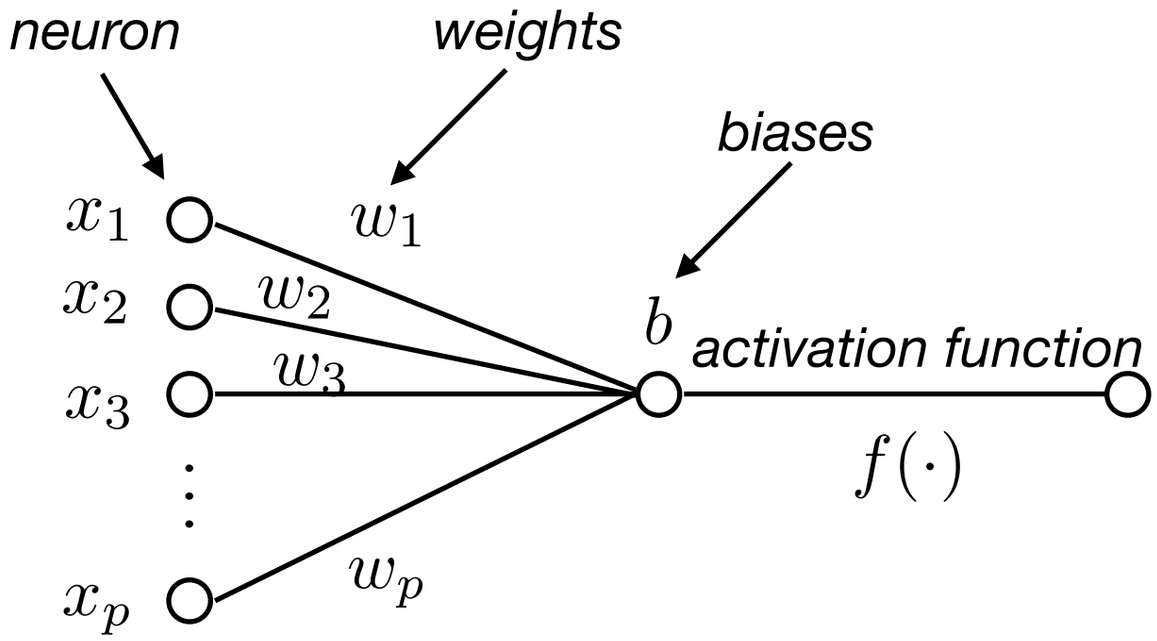
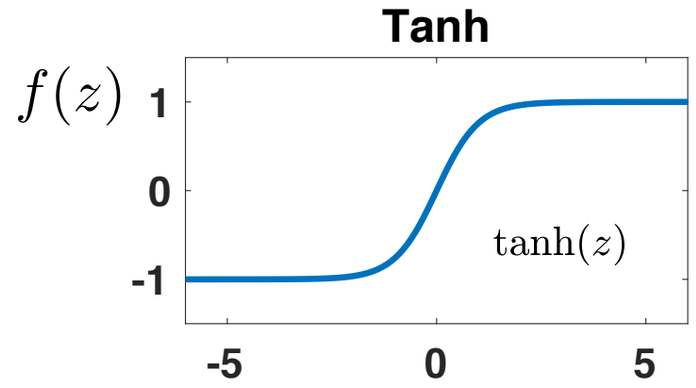
- typical approach: use deep neural network **(Deep RL)**



$$y = f(W \cdot x + b)$$



$$W = (w_1, w_2, \ldots, w_p) \qquad \theta = \{W, b\}$$

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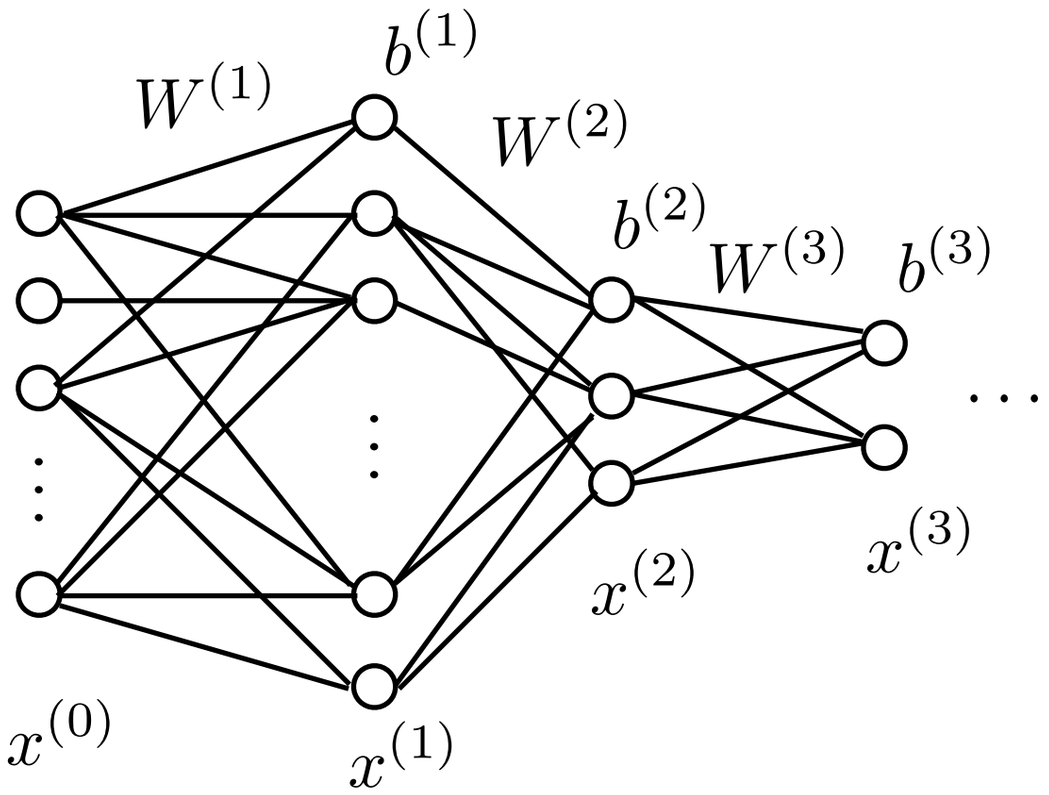


$$x^{(0)} \quad \text{input layer}$$

$$x_i^{(1)} = f^{(1)}\left(W_{ij}^{(1)} x_j^{(0)} + b_i^{(1)}\right)$$

$$x_i^{(2)} = f^{(2)}\left(W_{ij}^{(2)} x_j^{(1)} + b_i^{(2)}\right)$$

$b_i^{(l)}$: bias vector of layer l

$W_{ij}^{(l)}$: weight matrix of layer l

$f^{(l)}$: activation function of layer l

RL for Quantum State Initialization

→ **quantum control:** two-level system

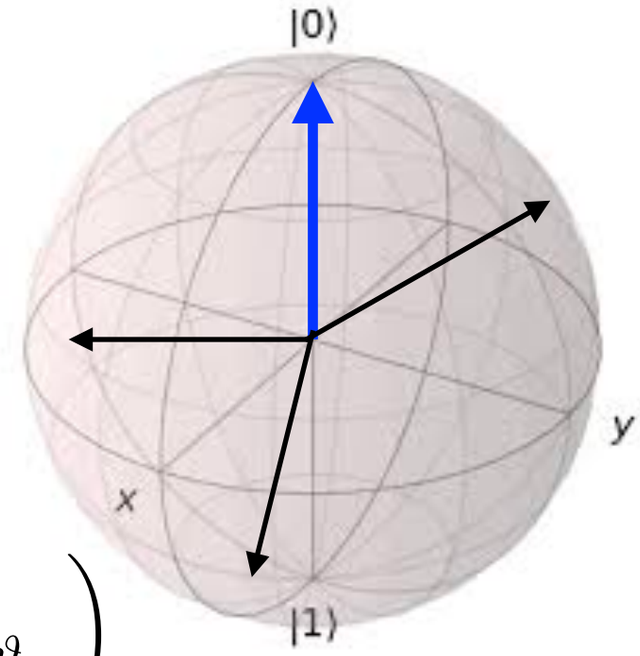
- **task:** prepare $|0\rangle$ using infinitesimal rotations

$$U_\alpha = \exp\left(-i\frac{\delta t}{2}\sigma^\alpha\right) \qquad \alpha = x, y, z$$

- define **RL states**:

parametrization of state of system: $|\psi\rangle = \begin{pmatrix} \cos\frac{\vartheta}{2} \\ e^{i\varphi}\sin\frac{\vartheta}{2} \end{pmatrix}$

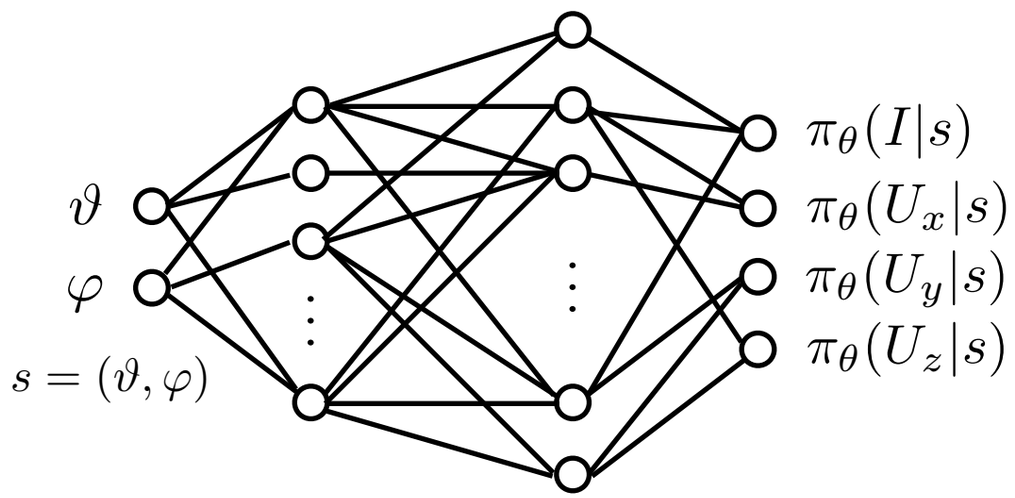
Bloch sphere



RL state space: $\mathcal{S} = \{(\vartheta, \varphi)|\vartheta \in [0, \pi],\ \varphi \in [0, 2\pi)\}$

- define **RL actions**: $\mathcal{A} = \{I, U_\alpha|\alpha = x, y, z\}$
- define reward: $r_t = |\langle 0|\psi_t\rangle|^2$
- choose **RL algorithm:** policy gradient

$$\pi_\theta(a|s)$$



RL for Quantum State Initialization

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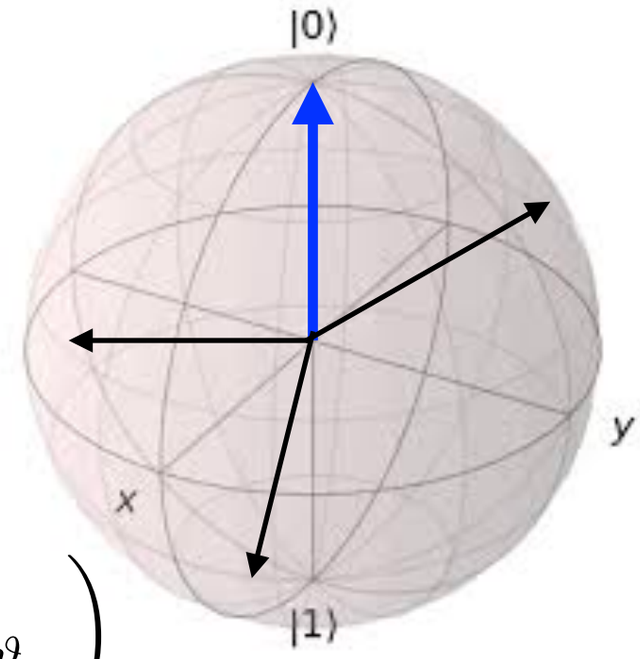

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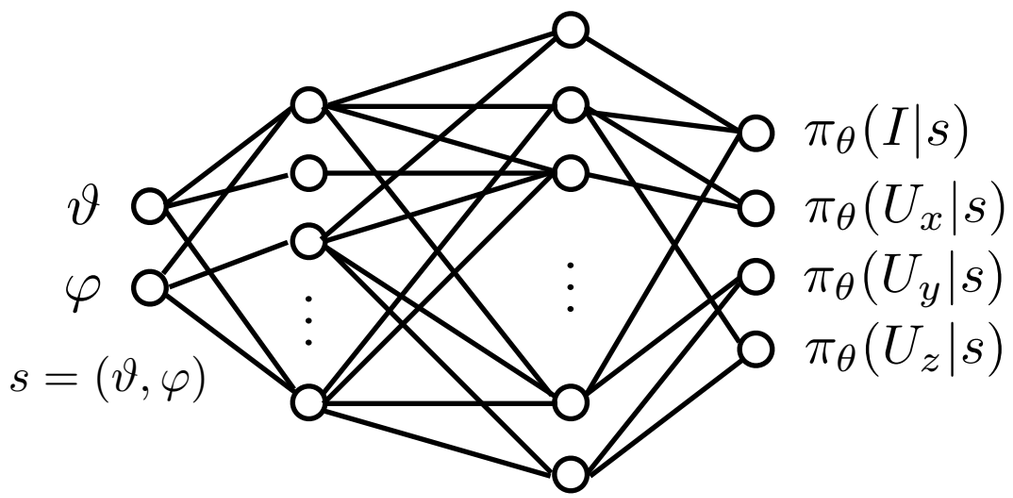
simulate trial trajectories τ_j

$$\nabla_\theta J(\theta) \approx \frac{1}{N_{\mathrm{MC}}}\sum_{j=1}^{N_{\mathrm{MC}}} \nabla_\theta \log \pi_\theta(\tau_j) \sum_t R_t(\tau_j)$$



RL for Quantum State Initialization

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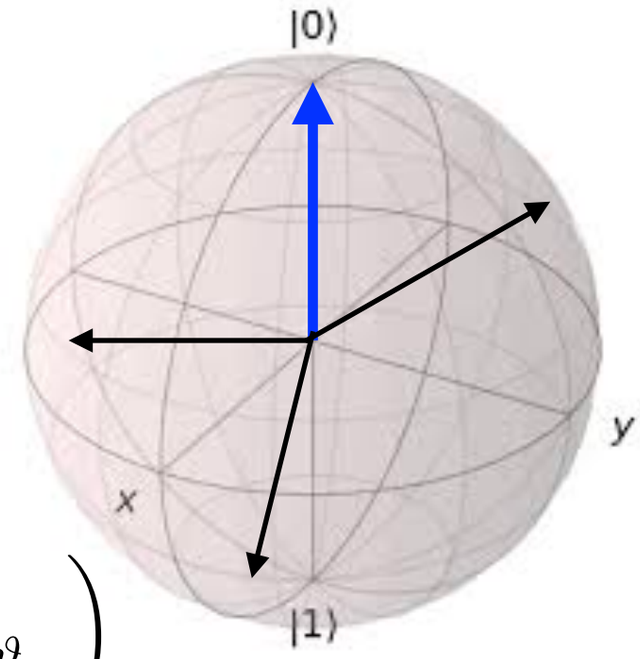

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Check out Jupyter notebook for how this works in practice!

https://github.com/mgbukov/quant22_notebooks

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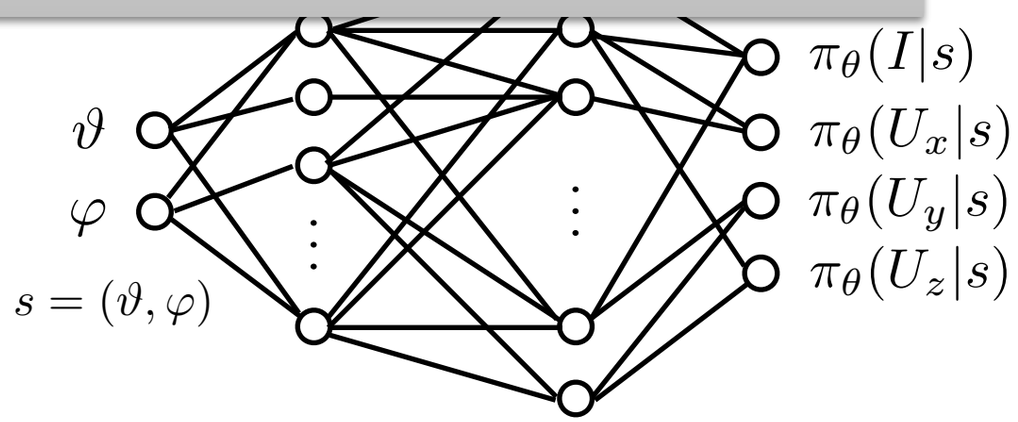

Thanks for your attention!

→ Useful Literature

M. Nielsen, *Neural Networks and Deep Learning* (online book)

Sutton and Barto, *Reinforcement Learning: an Introduction*, MIT press

S. Levine, *You Tube*, UC Berkeley (videos of lecture course)

M. Bukov, *lecture course,* Sofia University

http://quantum-dynamics.phys.uni-sofia.bg/teaching/WiSe_2020_RL_class/

€€€
European Commission
Horizon 2020
European Union funding
for Research & Innovation

Check out Jupyter notebook for how this works in practice!

https://github.com/mgbukov/quant22_notebooks

Marin Bukov

web: *www.pks.mpg.de/nqd*