A Tutorial on Optimal Control and Reinforcement Learning methods for Quantum Technologies

arXiv:2112.07453

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[5]INFN, Sez. Catania.

Pgi-controlclub, 2022-03-11

motivation

Quantum control is central to most quantum technologies (computing, simulation, metrology, ...)

Quantum Optimal Control is a widely used tool for the development of quantum technologies

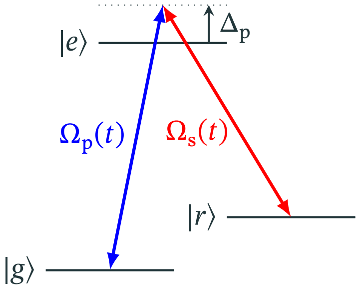
Reinforcement Learning has huge success in robotics and games, and offers a direct approach to control problems

outline

1. population transfer in three-level systems and STIRAP
2. “super” *very* <u>short</u> mention of **Optimal Control** and application to 3LS
3. “brief” idea of **Reinforcement Learning** and application to 3LS
4. discussion and conclusions

population transfer in three-level systems and STIRAP

population transfer in a three-level system



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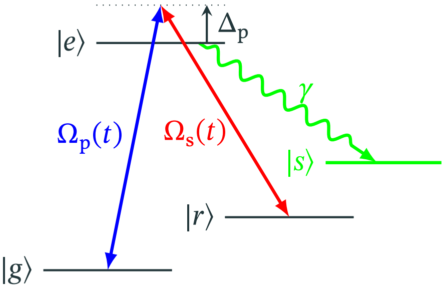

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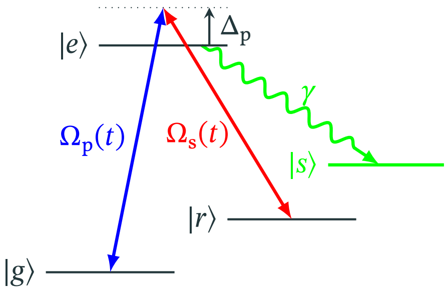

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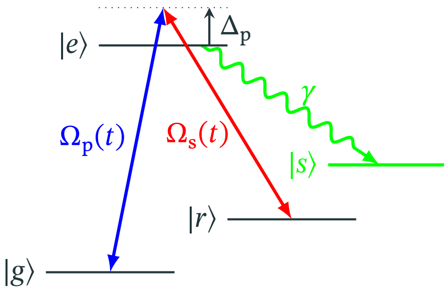

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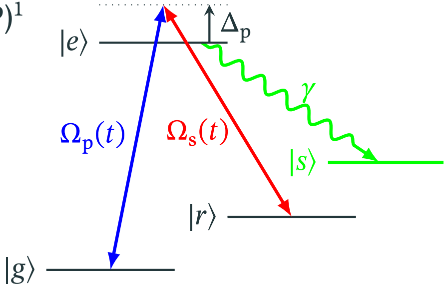
fidelity

$$\mathcal{F} = \mathrm{Tr}\{\rho(T)|r\rangle\langle r|\}$$

population transfer in a three-level system - STIRAP

STimulated Raman Adiabatic Passage (STIRAP)[1]

- adiabatic protocol
- population of the lossy state $|e\rangle$ low
- $\mathcal{F} \approx 1$



[1] J. R. Kuklinski, U. Gaubatz, F. T. Hioe, K. Bergmann, Phys. Rev. A 40 (11) (1989),
K. Bergmann, H. Theuer, B. Shore, Reviews of Modern Physics 70 (3) (1998),
N. V. Vitanov, A. A. Rangelov, B. W. Shore, K. Bergmann, Reviews of Modern Physics 89 (1) (2017).

Adiabatic Theorem

Given a time dependent Hamiltonian $H_0(t)$ and its instantaneous eigenstates $|n(t)\rangle$

$$H_0(t)|n(t)\rangle = E_n(t)|n(t)\rangle,$$

[2] $\hbar|\langle n(t)|\partial_t m(t)\rangle| \ll |E_n(t) - E_m(t)|, \forall m \neq n.$

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in general is $|\psi(t)\rangle = \sum_n c_n(t)|n(t)\rangle, \quad \sum_n |c_n(t)|^2 = 1.$

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If $H_0(t)$ is slowly varying[2] and the initial state is an eigenstate, ie $|\psi(t_\mathrm{i})\rangle = |m(t_\mathrm{i})\rangle$, then

$$|\psi(t)\rangle \simeq \mathrm{e}^{\mathrm{i}\alpha_m(t)}|m(t)\rangle, \quad \forall t$$
$$\text{i.e. } c_n(t) \simeq \mathrm{e}^{\mathrm{i}\alpha_m(t)}\delta_{mn}.$$

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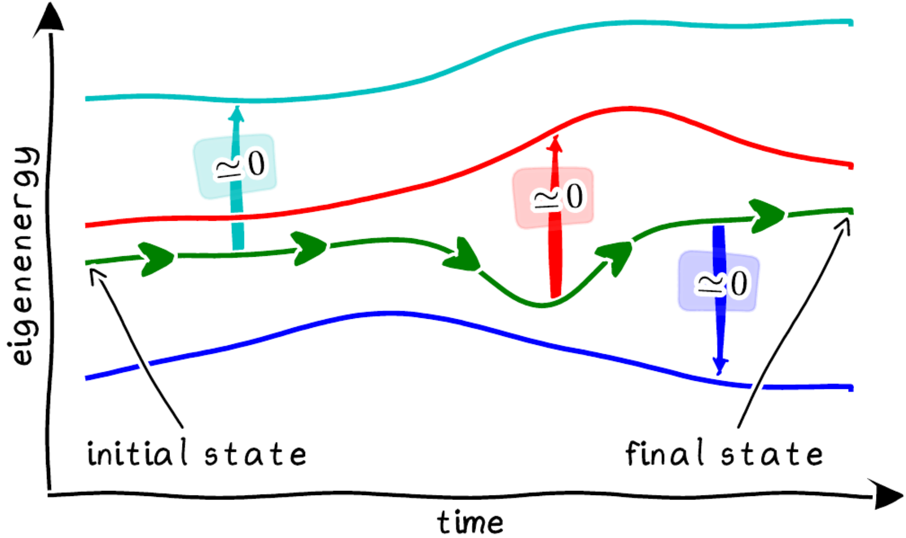
adiabatic following of an instantaneous eigenstate



population transfer in a three-level system - STIRAP

the three-level Hamiltonian we consider is $\frac{H(t)}{\hbar} = \frac{1}{2}\begin{pmatrix} 0 & \Omega_{\mathrm{p}}(t) & 0 \\ \Omega_{\mathrm{p}}(t) & 2\Delta_{\mathrm{p}} & \Omega_{\mathrm{s}}(t) \\ 0 & \Omega_{\mathrm{s}}(t) & 0 \end{pmatrix}$

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and its instantaneous eigenstates are

$$|a_0(t)\rangle = \begin{pmatrix} \cos\theta \\ 0 \\ -\sin\theta \end{pmatrix} \quad |a_-(t)\rangle = \begin{pmatrix} \sin\theta\cos\phi \\ -\sin\phi \\ \cos\theta\cos\phi \end{pmatrix} \quad |a_+(t)\rangle = \begin{pmatrix} \sin\theta\sin\phi \\ \cos\phi \\ \cos\theta\sin\phi \end{pmatrix}$$

with

$$\tan\theta(t) = \frac{\Omega_p(t)}{\Omega_s(t)} \qquad \tan\phi(t) = \frac{\sqrt{\Omega_p(t)^2 + \Omega_s(t)^2}}{\Delta_p + \sqrt{\Delta_p^2 + \Omega_p(t)^2 + \Omega_s(t)^2}}$$

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consider the instantaneous eigenstate $|a_0(t)\rangle$ (the *dark state*)

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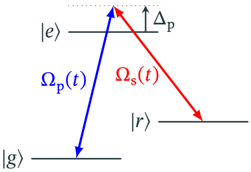

if the pulses are counterintuitively ordered

$$\lim_{t\to t_\mathrm{i}} \frac{\Omega_p(t)}{\Omega_s(t)} = 0, \quad \lim_{t\to t_\mathrm{f}} \frac{\Omega_s(t)}{\Omega_p(t)} = 0 \quad \Longrightarrow \quad \lim_{t\to t_\mathrm{i}} \theta(t) = 0, \quad \lim_{t\to t_\mathrm{f}} \theta(t) = \frac{\pi}{2}$$

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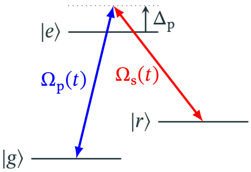

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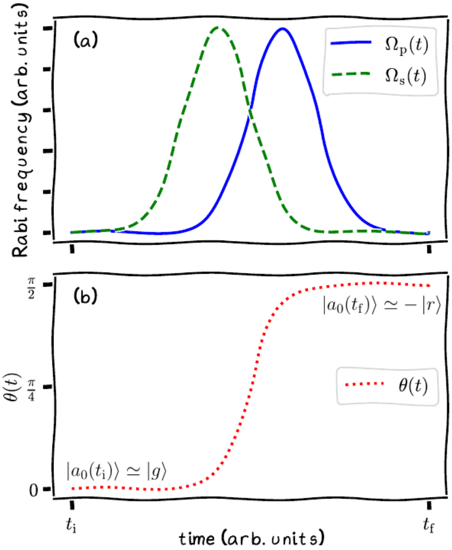
then

$$|a_0(t_i)\rangle = |g\rangle \quad \text{and} \quad |a_0(t_f)\rangle = -|r\rangle$$

population transfer in a three-level system - STIRAP



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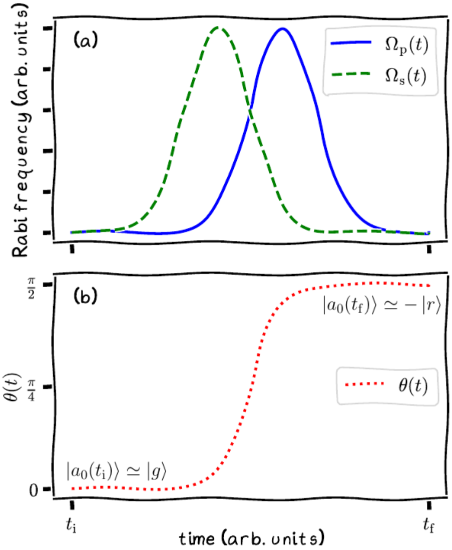

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adiabaticity condition

“area of the pulses and their overlap $\gtrsim$ 10”

population transfer in a three-level system - STIRAP

to remember

STIRAP:

- allows for efficient population transfer in a three-level system
- is characterized by the counterintuitive order of the pulses
- is an adiabatic process (area of the pulses should be *large* and they should overlap)

“super” *very short* mention of Optimal Control

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system described by the set of differential equations

$$\dot{\rho}(t) = f(\rho(t), \boldsymbol{u}(t), t), \quad t \in [0, T],$$

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- $\boldsymbol{u}(t) = (u_1(t), u_2(t), \dots, u_M(t))$ are controls

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introduce a cost functional whose minimization corresponds to the desired dynamics

$$\mathcal{J}(\rho(t), \boldsymbol{u}(t), T) = 1 - \mathcal{F} = 1 - \mathrm{Tr}\left\{\rho_{\mathrm{targ}}^{\dagger}\rho(T)\right\}$$

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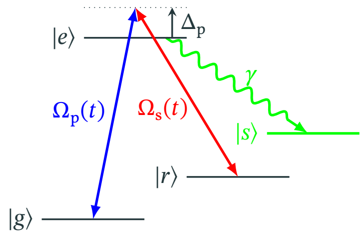
$\boxed{\text{find } \boldsymbol{u}(t) \text{ which minimize } \mathcal{J}}$

Optimal Control of population transfer in three-level system



set of differential equations (master equation)

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with Hamiltonian

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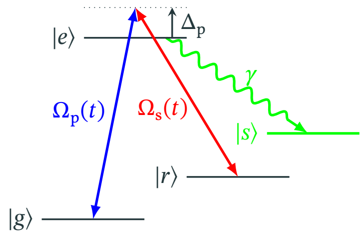
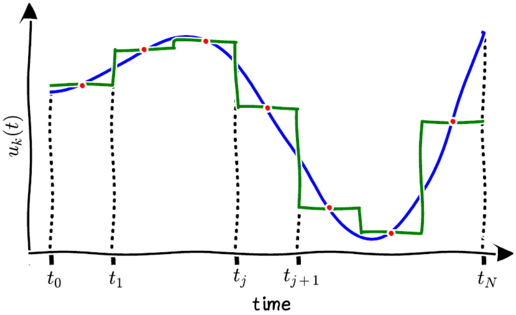


the controls are $\Omega_\mathrm{p}(t)$ and $\Omega_\mathrm{s}(t)$

Optimal Control of population transfer in three-level system

$\Omega_\mathrm{p}(t)$ and $\Omega_\mathrm{s}(t)$ *step functions* $\longrightarrow$ each pulse parametrized by N real numbers



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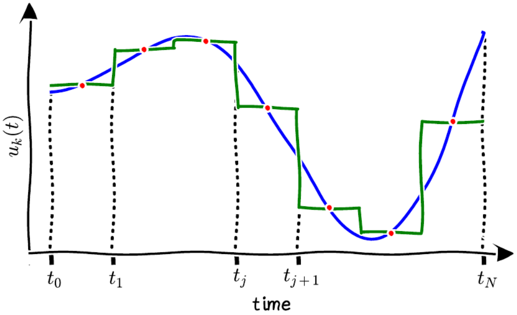
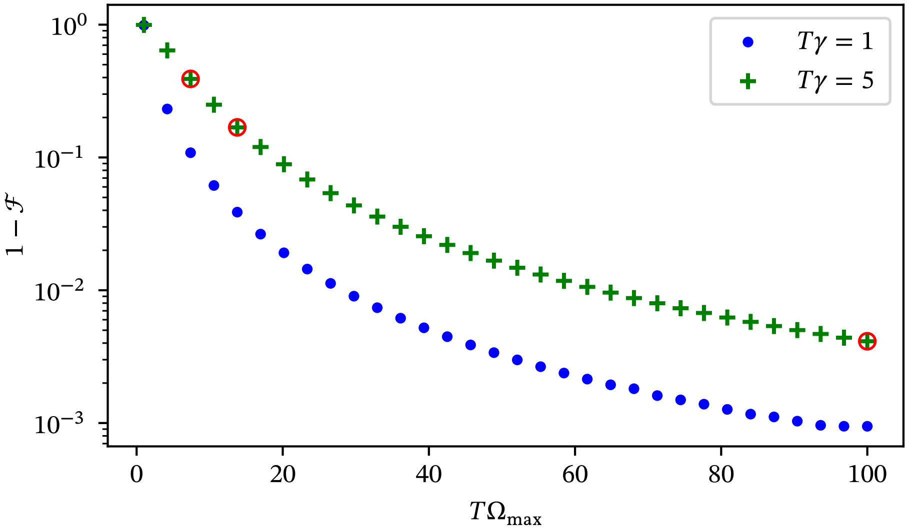


minimize the cost function $\mathcal{J}(\rho(t), \bar{\boldsymbol{u}}, T) = 1 - \mathrm{Tr}\{|r\rangle\langle r|\rho(T)\}$

with respect to $\bar{\boldsymbol{u}} = \left(\Omega_\mathrm{p}(t_0), \Omega_\mathrm{p}(t_1), \ldots, \Omega_\mathrm{p}(t_{N-1}), \Omega_\mathrm{s}(t_0), \Omega_\mathrm{s}(t_1), \ldots, \Omega_\mathrm{s}(t_{N-1})\right)$

Optimal Control of population transfer in three-level system



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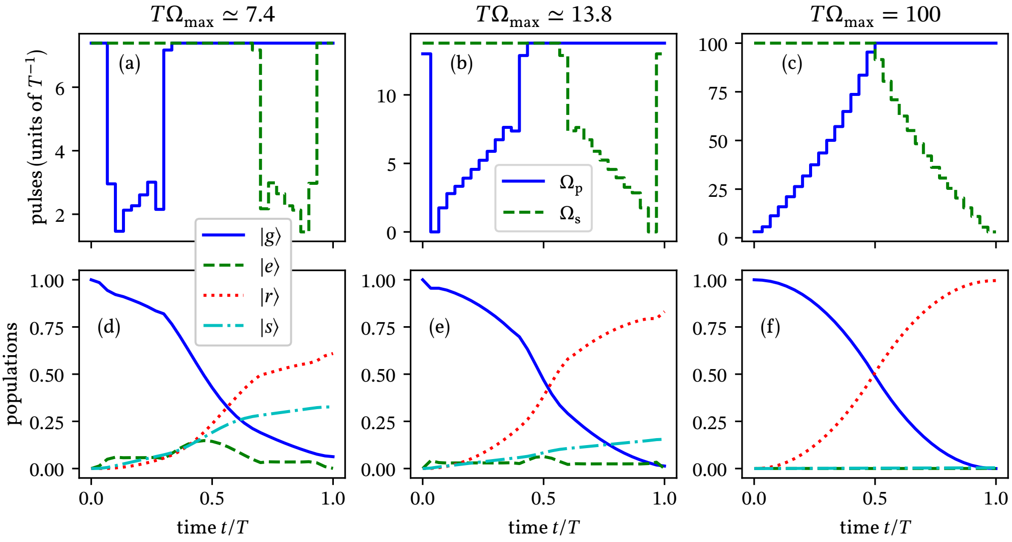

"brief" idea of **Reinforcement Learning**[3]

- Markov Decision Processes (MDPs)
  - policies
  - goals, rewards and returns
  - value functions
- policy gradient and REINFORCE

[3] R. S. Sutton, A. G. Barto, Reinforcement Learning: An Introduction, MIT press, 2018

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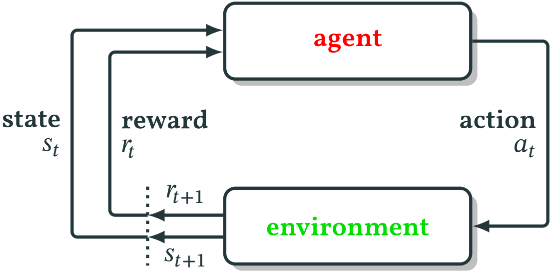
i will not be rigorous

there will be some *small* imprecision

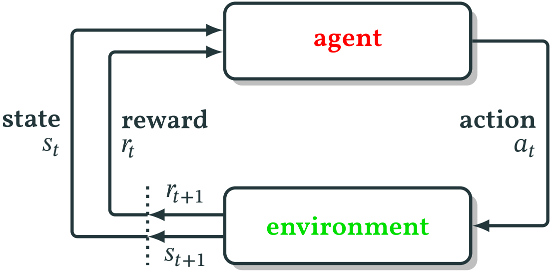
agent-environment interface



agent the learner and the decision maker

environment the thing interacting with the agent, everything outside the agent

agent-environment interface



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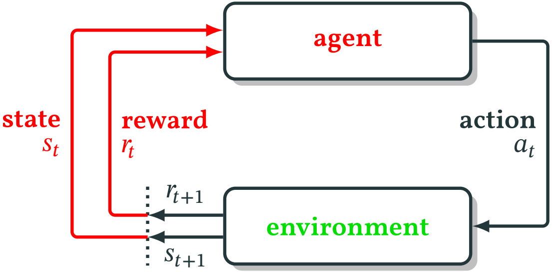

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- the agent receives $(r_t, s_t) = \begin{cases} s_t \in \mathcal{S} & \text{is a repr. of the environment's } \textit{state} \\ r_t \in \mathcal{R} \in \mathbb{R} & \text{is a } \textit{reward} \end{cases}$

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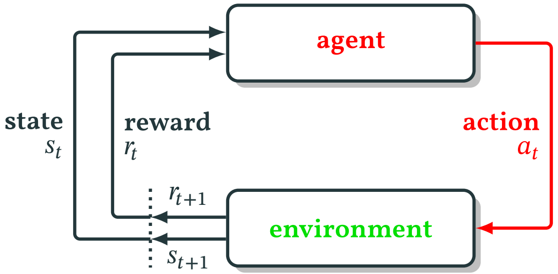

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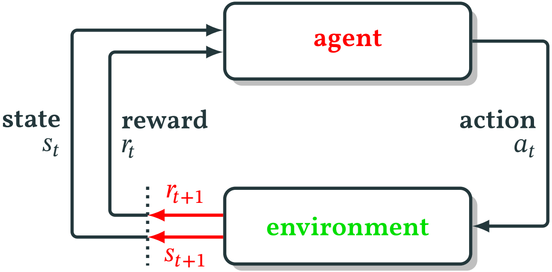

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- the agent selects an *action* $a_t \in \mathcal{A}(s_t)$ $\longrightarrow$ environment
- the environment reaches the new state s_{t+1} and produces the reward r_{t+1}

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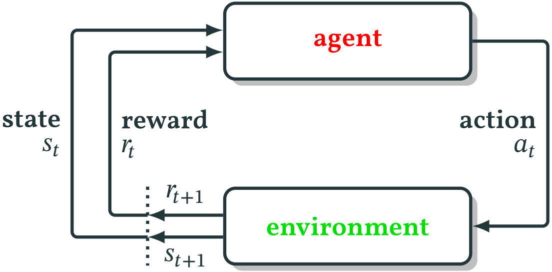

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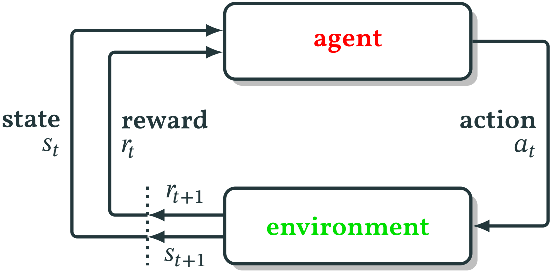
the agent, the environment and their interaction give rise to a *trajectory*

$$\cancel{r_0 = 0}, s_0, a_0, r_1, s_1, a_1, \dots, r_t, s_t, a_t, \dots, r_N, s_N, a_N$$

agent-environment interface



agent the learner and the decision maker

environment the thing interacting with the agent, everything outside the agent

the agent, the environment and their interaction give rise to a *trajectory*

$$\cancel{r_0 = 0}, s_0, a_0, r_1, s_1, a_1, \ldots, r_t, s_t, a_t, \ldots, r_N, s_N, a_N$$

episodic task

- *termination step* $N < \infty$
- after each episode the environment is reset to an initial state

dynamics function

the environment's dynamics is completely characterized by

dynamics function $p : \mathcal{S} \times \mathcal{R} \times \mathcal{S} \times \mathcal{A} \rightarrow [0, 1]$

$$p(s', r|s, a) = \Pr\{s_t = s', r_t = r|s_{t-1} = s, a_{t-1} = a\}$$

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not a *restriction* on the dynamics or the decision process, but a ***requirement*** on the representation of the state

MDP framework - to remember

the MDP framework is an abstraction of the problem of *goal-directed learning from interaction*

three signals passing back and forth between an agent and its environment:

- the choices made by the agent (the actions)
- the basis on which the choices are made (the states)
- definition of the agent's goal (the rewards)

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the **actions** are what one learns

environment dynamics function

three-level population transfer as an MDP

- the environment is the three-level system and its evolution
- the agent *chooses* which pulses to apply on the system

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$s_i = \rho(t_i) = \rho^{(i)}$

actions

$a_i = (\Omega_{\mathrm{p}}^{(i)}, \Omega_{\mathrm{s}}^{(i)})$

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evolution of the quantum system:

$$\rho^{(i+1)} = \exp\Big(\mathcal{L}(\Omega_\mathrm{p}^{(i)}, \Omega_\mathrm{s}^{(i)})\Delta t\Big)\rho^{(i)} \longrightarrow s_{i+1} = \exp[\mathcal{L}(a_i)\Delta t]s_i$$

what about r_{i+1}?

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$$r_1 = r_2 = \cdots = r_{N-1} = 0, \quad r_N = \mathrm{Tr}\Big\{|r\rangle\langle r|\rho^{(N)}\Big\}$$

what's missing?

how the agent chooses the actions?

how the agent learns the actions that will achieve our goal?

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what is the agent?

policies

the agent chooses the actions using a policy function

a **policy** π is a mapping from *states* to *probabilities of selecting actions*

- agent following policy π at time t:
  in state s, the agent chooses action a with probability $\pi(a|s)$
- $\pi(a|s)$ is a probability distribution over $a \in \mathcal{A}(s)$ for each $s \in \mathcal{S}$

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Reinforcement Learning methods specify how the agent's policy is changed as a result of its interaction with the environment in order to achieve our goal

goals and rewards

reward hypothesis

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reward for three-level population transfer

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return

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discounted return

$$G_t = r_{t+1} + \gamma r_{t+2} + \gamma^2 r_{t+3} \cdots + \gamma^{T-t-1} r_T$$

- $0 \leq \gamma \leq 1$ *discount rate*,
- r_k reward at step k,
- $T \leq \infty$ *termination step*

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myopic agent	***farsighted*** agent
$\gamma = 0$	$\gamma \lesssim 1$

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value functions

state-value function for policy π: *value of state s under policy π*

expected return when starting in s and following π thereafter

$$v_\pi(s) = \mathbb{E}_\pi[G_t | s_t = s]$$

action-value function for policy π: *value of taking action a in state s under policy π*

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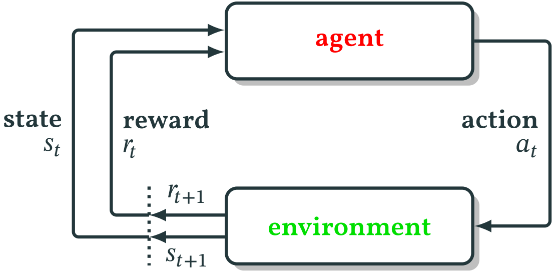
The value functions v_π and q_π can be estimated from experience

MDP framework - to remember



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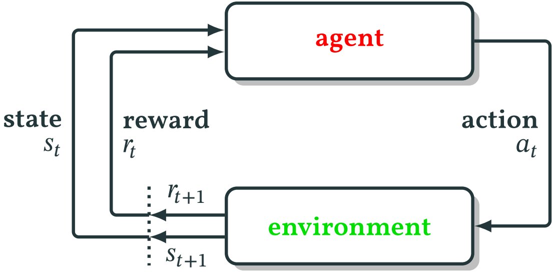

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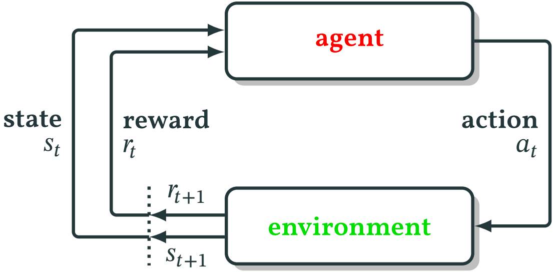

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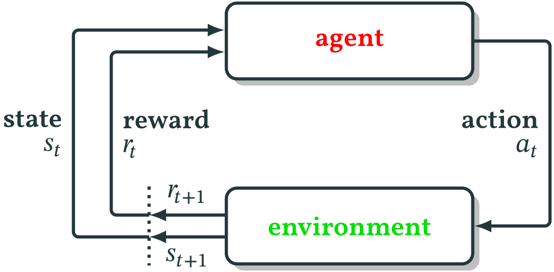

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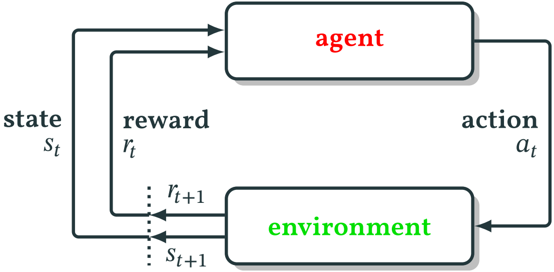

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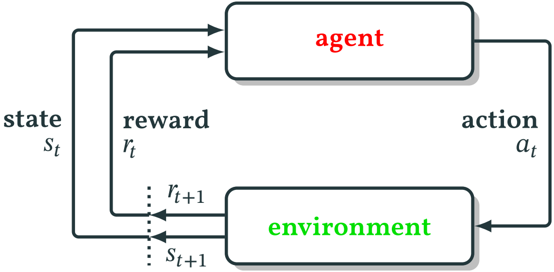

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policy gradient methods and REINFORCE

policy gradient methods

- parameterize the policy with vector $\theta \in \mathbb{R}^d$

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methods that follow this general schema are called *policy gradient* methods

REINFORCE: monte carlo policy gradient

the performance is the state-value of the initial state

$$J(\theta) = v_{\pi_\theta}(s_0)$$

and obtain the following estimate for the gradient[4]

$$\nabla J(\theta) \propto \mathbb{E}_{\pi_\theta}\left[G_t \frac{\nabla \pi_\theta(a_t|s_t)}{\pi_\theta(a_t|s_t)} \right] = \mathbb{E}_{\pi_\theta}[G_t \nabla \ln \pi_\theta(a_t|s_t)]$$

REINFORCE update

$$\theta_{t+1} = \theta_t + \alpha G_t \nabla \ln \pi_{\theta_t}(a_t|s_t)$$

[4]using the *policy gradient theorem*

REINFORCE algorithm

we have a policy π_θ parametrized by θ

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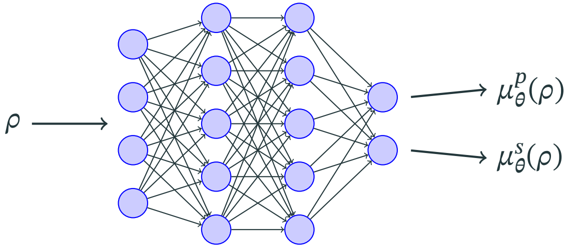
after "convergence"

agent following the policy π_θ will maximize $J(\theta) = v_{\pi_\theta}(s_0)$

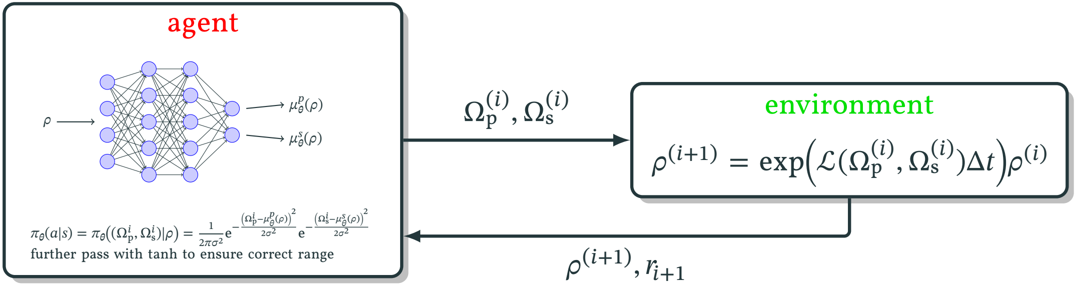
policy for population transfer in three-level systems



$$\pi_\theta(a|s) = \pi_\theta\Big((\Omega_\mathrm{p}^{(i)}, \Omega_\mathrm{s}^{(i)})|\rho\Big) = \frac{1}{2\pi\sigma^2}\mathrm{e}^{-\frac{\left(\Omega_\mathrm{p}^{(i)}-\mu_\theta^p(\rho)\right)^2}{2\sigma^2}}\,\mathrm{e}^{-\frac{\left(\Omega_\mathrm{s}^{(i)}-\mu_\theta^s(\rho)\right)^2}{2\sigma^2}}$$

further pass with tanh to ensure correct range

policy for population transfer in three-level systems



policy for population transfer in three-level systems

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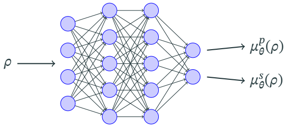

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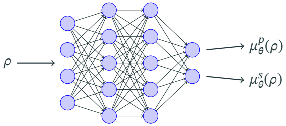

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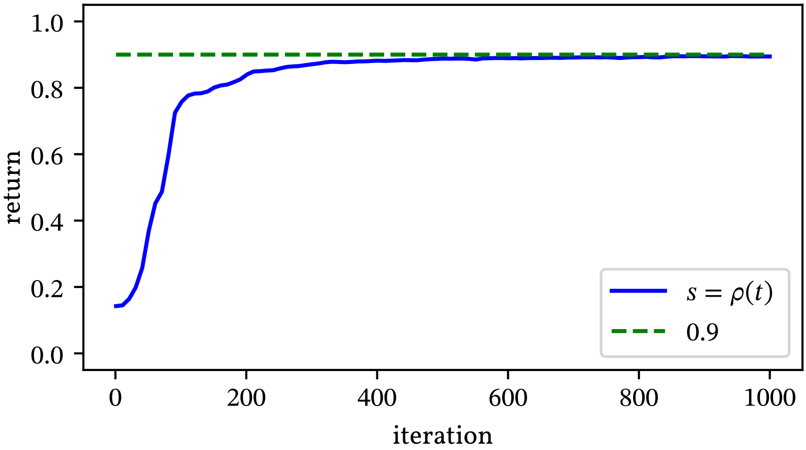
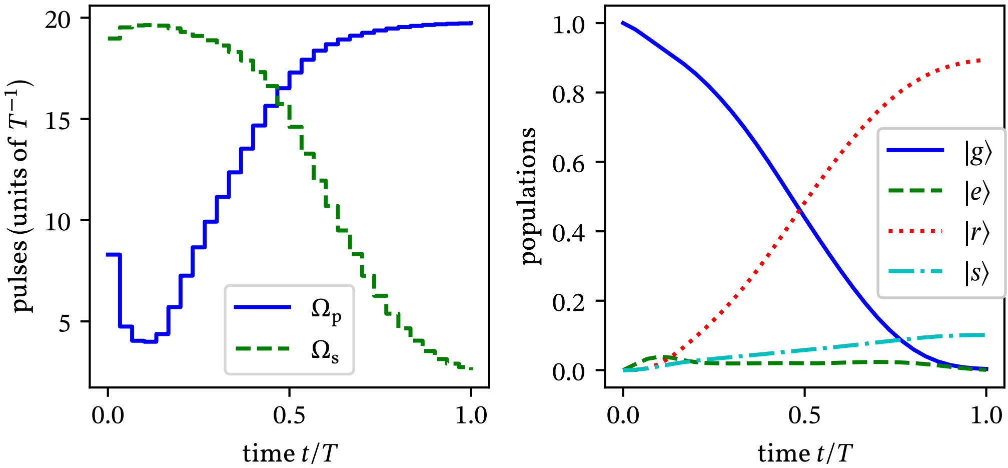
use **REINFORCE** to search for optimal policy $\pi(a, s)$

RL results



$$T\Omega_{\max} = 20, \quad T\gamma = 5$$

RL results



20
15
10
5
pulses (units of T^{-1})
0.0
0.5
1.0
time t/T
Ω_p
Ω_s
1.0
0.8
0.6
0.4
0.2
0.0
populations
0.0
0.5
1.0
time t/T
$|g\rangle$
$|e\rangle$
$|r\rangle$
$|s\rangle$

discussion and conclusions

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  - free parameters for OCT are 60, for RL are 7644

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https://www.github.com/luigiannelli/threeLS_populationTransfer


this is the end