Introduction to Machine Learning for Science

Workshop @ Casimir PhD School

Evert van Nieuwenburg, Leiden University

Plan for workshop

Aiming for hands-on participation!

Quick intro and setup (5’)

Examples!

Note!

This workshop aims at showing a few basics to give you an idea of possibilities. For in-depth explanations, it is best to either find online tutorials (or ask chatGPT for one?) or join a class at your university.

Have fun, and have an open mind to look for applications of ML in your own research!

Machine Learning is easy to get started with

And the best way to get better at it, like fitting curves, is to use it

https://github.com/condensedAI/casimir2023

- Easiest way to install python + editors etc: **Anaconda**
- Alternative: cloud-based python (Google Colab)

I will switch back&forth between code and these slides

Machine Learning may be useful for you, too

Let's look at some examples

Unsupervised learning

Given

$$\{X\} = (\vec{x}_1, \vec{x}_2, \ldots)$$

Learn

$$p(x)$$

Clustering,
Dimensionality Reduction

(generative)

Supervised learning

Given

$$\{X, Y\} = \Big((\vec{x}_1, \vec{y}_1), (\vec{x}_2, \vec{y}_2), \ldots\Big)$$

Learn

$$p(y \mid x)$$

Classification

Reinforcement learning

Given

State $\vec{S}$ of environment/system

Learn

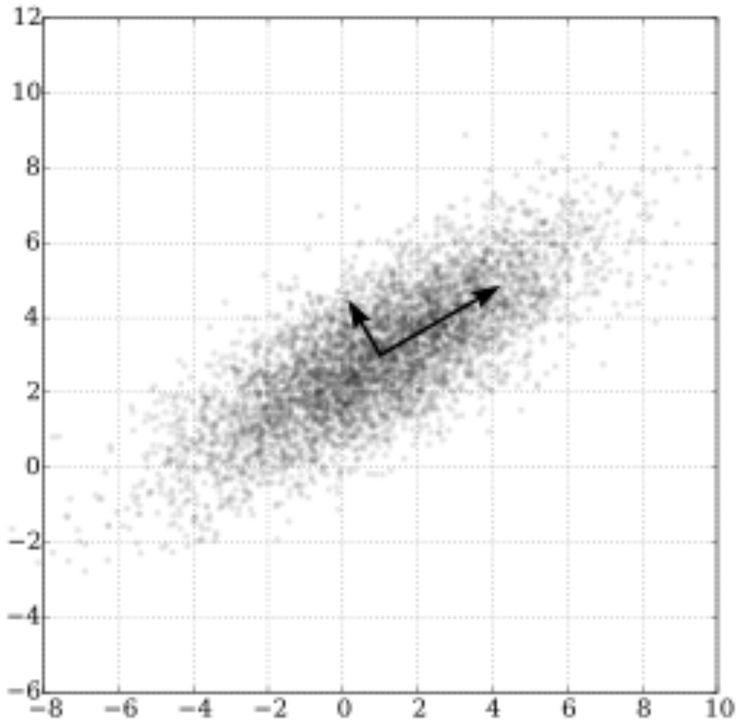
$$\pi(a \mid s)$$

Action

Planning / Control

Principal Component Analysis

“Machine Learning” essentials (i.e. try this first)



"In a high-dimensional dataset, find axis along which variance is largest”

Scikit-learn

Supervised learning is intuitive

Here is an example to train your own brain on

- (2, 8, 24, 16) = 0
- (8, 6, 10, 12) = 0
- (122, 32, 2, 4) = 0
- (6, 34, 42, 10) = 0
- (46, 32, 18, 12) = 0

- (3, 7, 13, 121) = 1
- (9, 1, 57, 67) = 1
- (15, 17, 27, 45) = 1
- (45, 29, 19, 9) = 1
- (7, 89, 71, 1) = 1

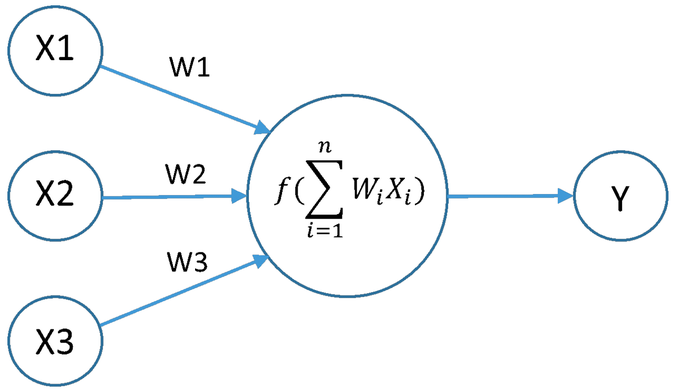
- (42, 18, 6, 2) = ?

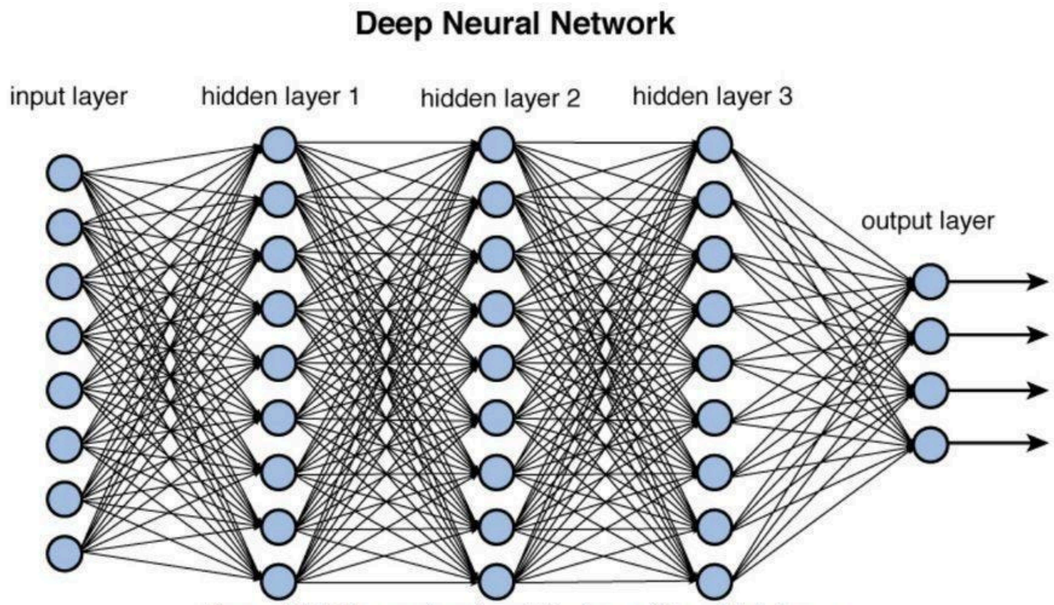
P(0 | (2,8,24,16)) = 1

- p(0 | (18, 5, 71, 2)) = ??

Nowadays, ML ~ (deep) neural networks

NNs can in theory fit anything (universal), and in practice still quite a lot

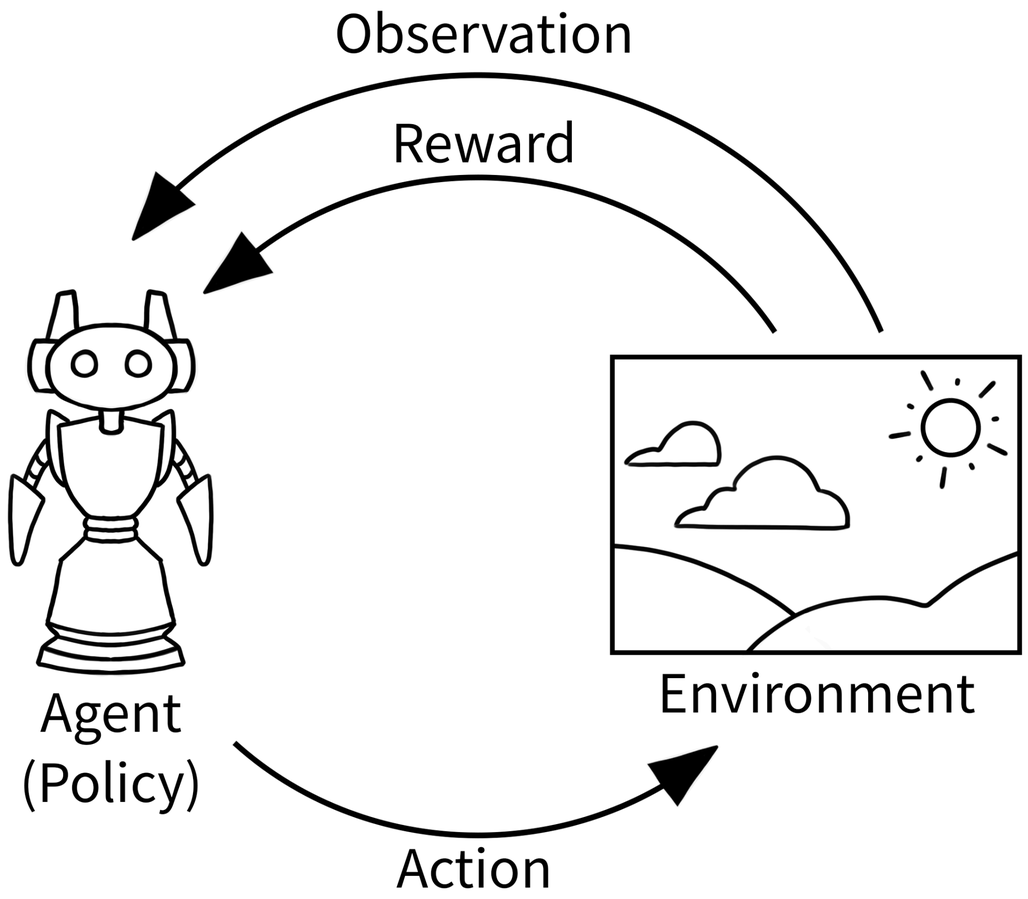




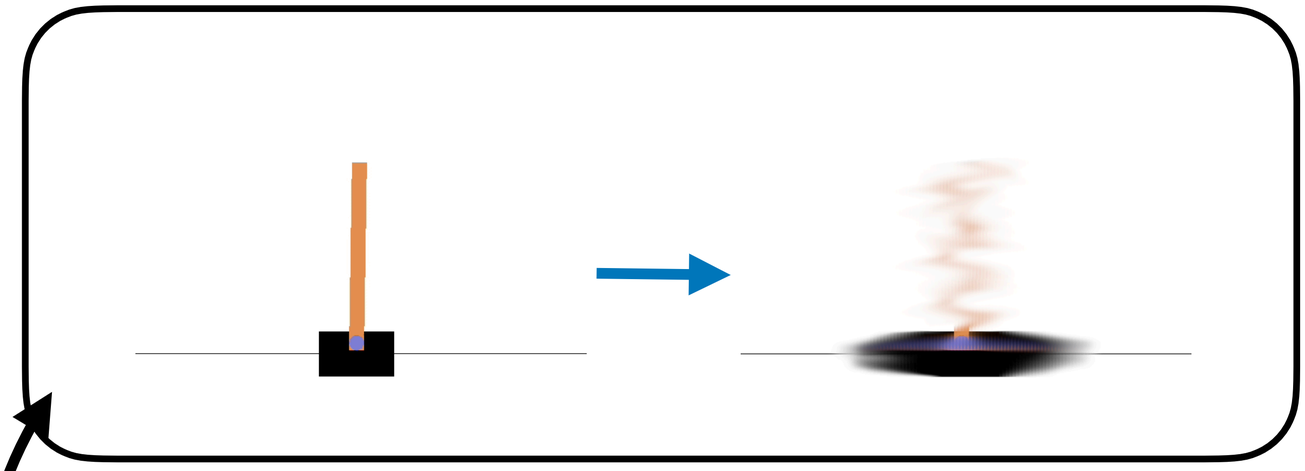
Idea: keep adjusting the weights until error on all examples is smallest!

Reinforcement Learning

Control problem

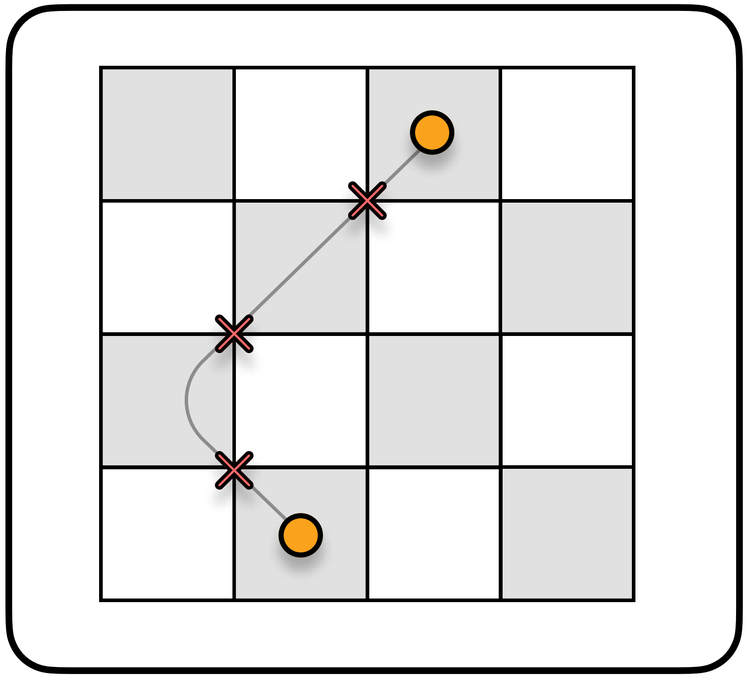


Quantum Control



Controlling quantum systems

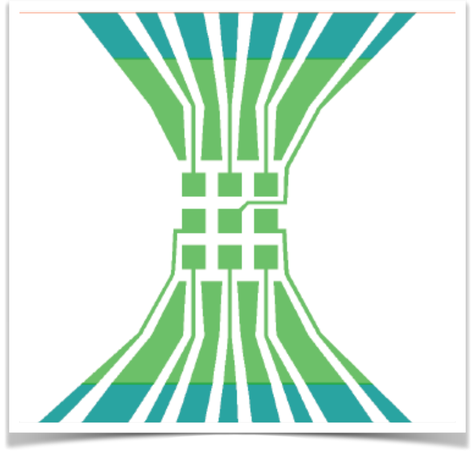
Qs: Can RL control quantum systems?
Fundamental difference between
quantum and ‘classical stochastic’?

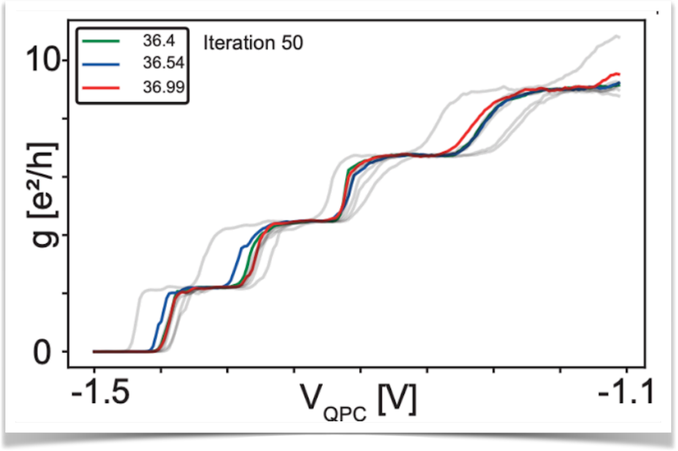


Quantum Error Correction
Single player game (against environment)!

Q: Worst-case by replacing
environment
with AI opponent?

Physics “labs of the future”

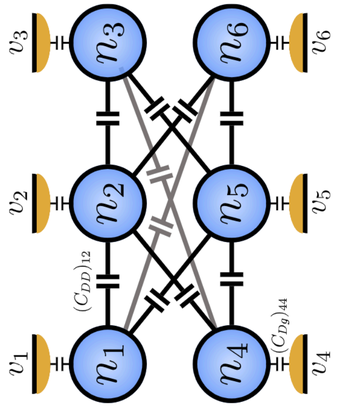


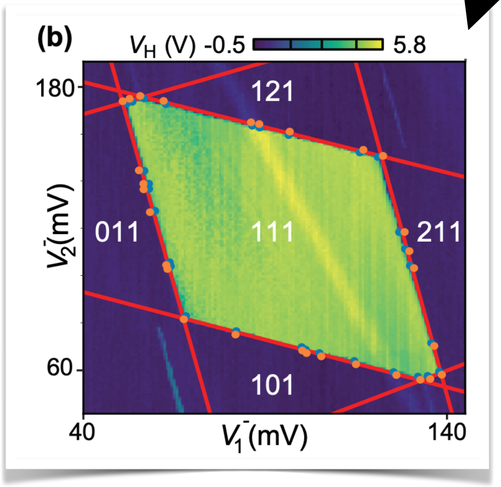


Design (+optimise) quantum experiments

Black box optimisation of handful of variables
Goal and constraints: physics!
(Gradient free, safe, adaptive, …)

Mapping high-dimensional polytopes
(“Good morning routine”, few runs, …)





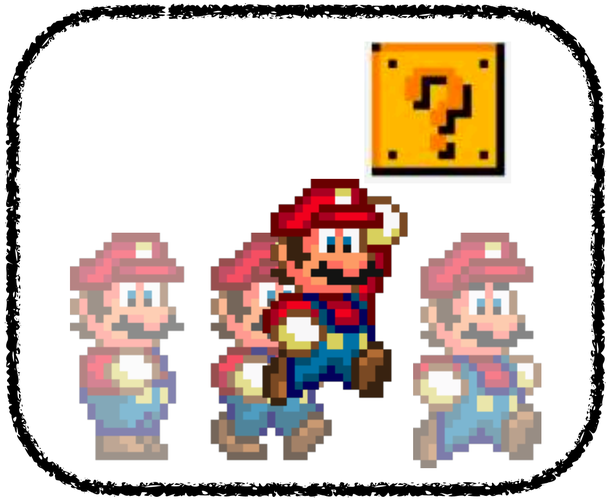
Automated tuning of quantum systems

Quantum Games

https://github.com/quantumlib/unitary

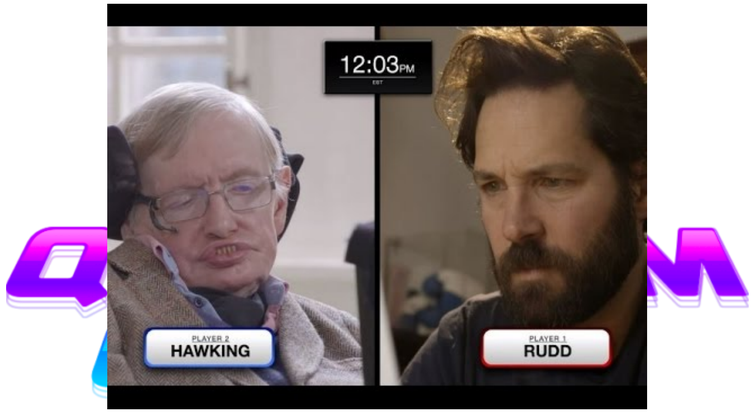
tiqtaqtoe

“Fox in a hole”



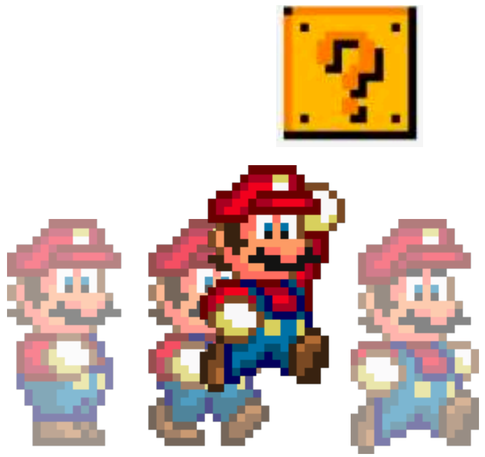
Contribute!
Quantum Mario
Quantum Wordle
Quantum 2048
…

quantumchess.net



Research

- How does an AI system internally represent a quantum system?
- Should the AI system itself be quantum?



Please reach out!

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