UCLA QCBio Collaboratory

Machine Learning with Python

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2023 Spring

Thanks Dr. Seyoon Ko for some code materials

Notation of the slides

- `Code or Pseudo-Code chunk` starts with "➢", e.g.
  - ➢ `print("Hello world!")`

- Link is underlined

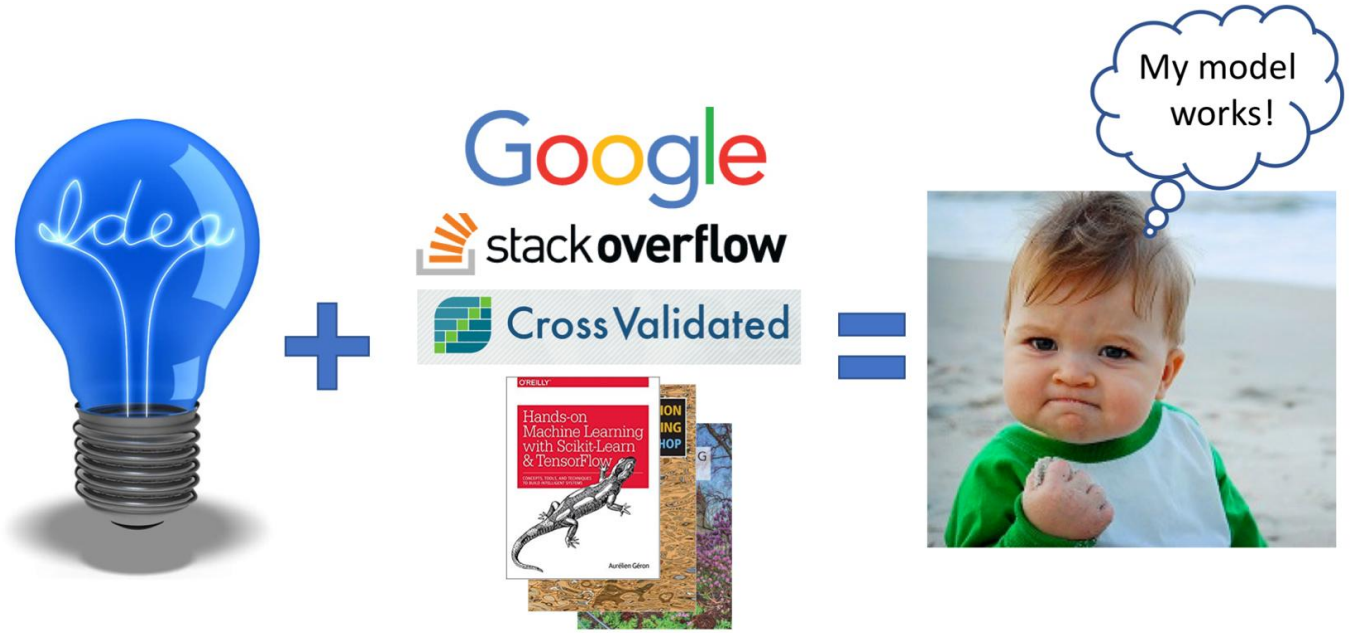
- Important terminology is in **bold** font

Workshop goals

- Understand the rationales behind machine learning algorithms
- Know the advantages/limitations of some machine learning algorithms
- Apply machine learning algorithms to solve problems, and make the models perform better

Workshop goals

- Use online resources to transform your idea into a model!



Workshop goals

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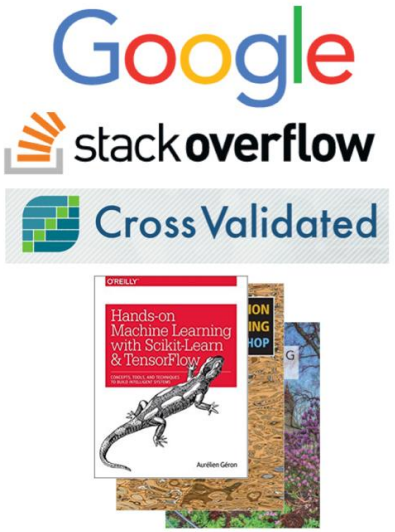
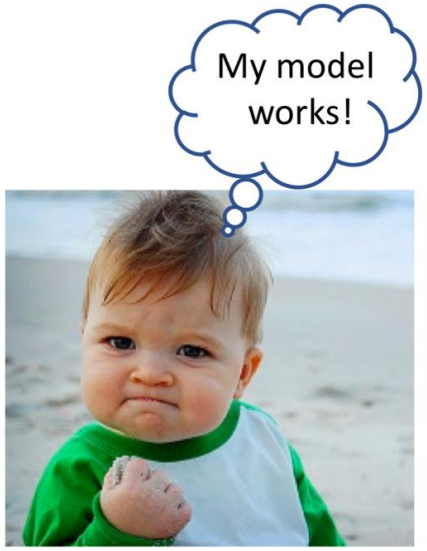
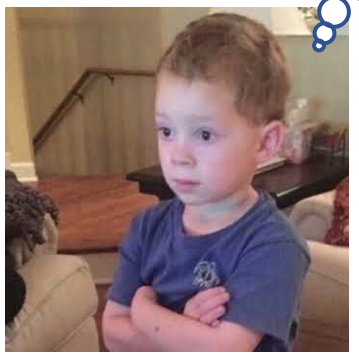




Tune parameters



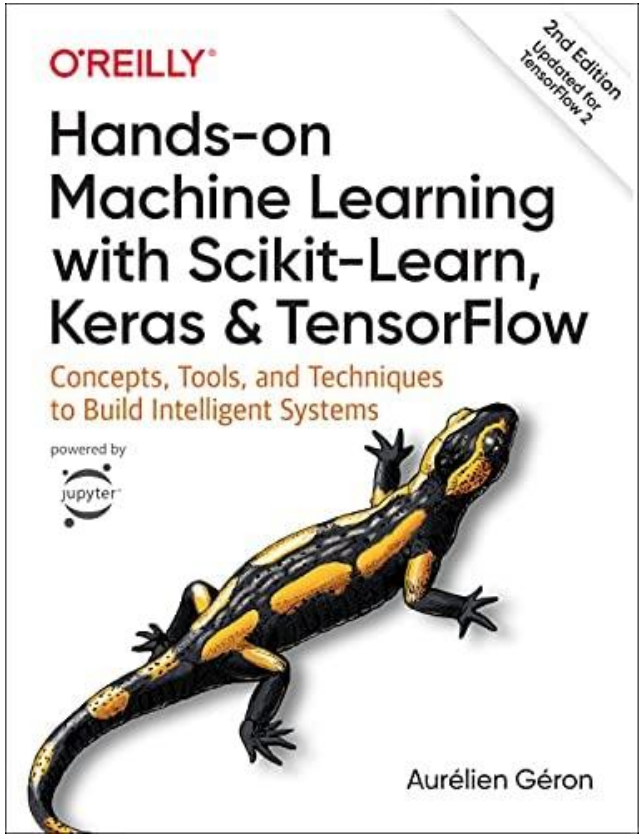
Agenda

- Day 1: Introduction to machine learning
  - Some key concepts in machine learning
  - Jupyter notebook and some packages usage

- Day 2: Supervised learning
  - Classification
  - Regression
  - Regularization

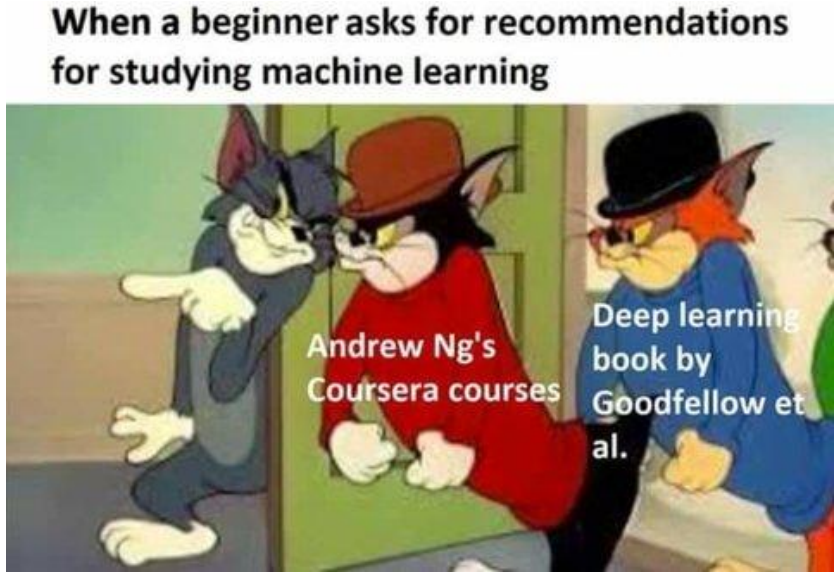
- Day 3: Unsupervised learning
  - Dimension reduction
  - Clustering

References



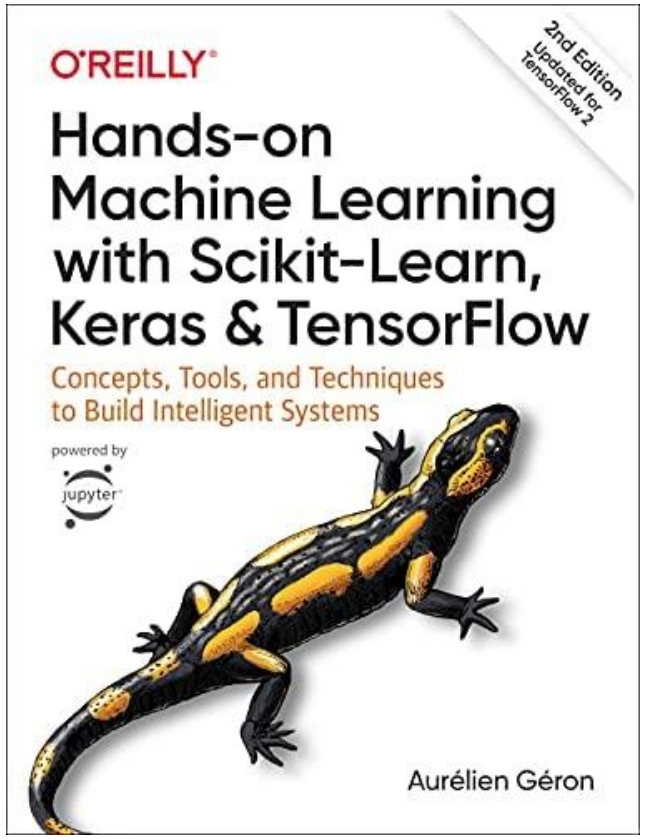
link

- Other useful reference



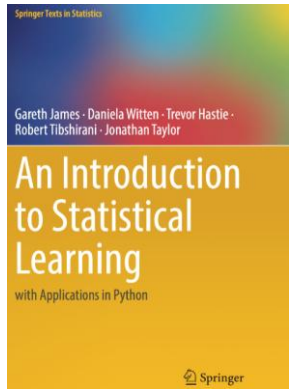
- Write down questions to this Google doc

References



link

- Other useful reference
  - An introduction to statistical learning
  - Machine learning: a probabilistic perspective
  - Deep learning



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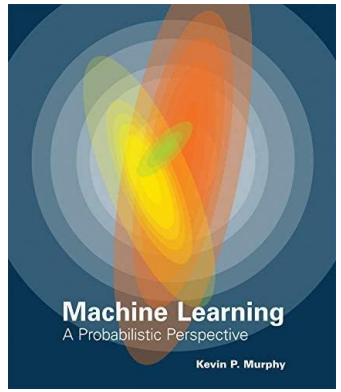

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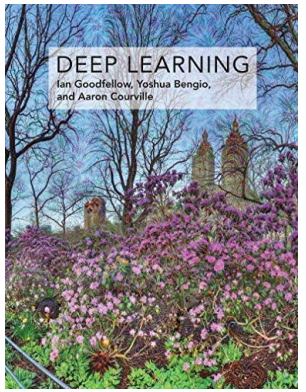

link

- Write down questions to this Google doc

UCLA QCBio Collaboratory

Day 1: Introduction to Machine Learning

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2023 Spring

Overview

Time

- 3-hour workshop (45min + 45min + 30min + practice/Q&A)

Topics

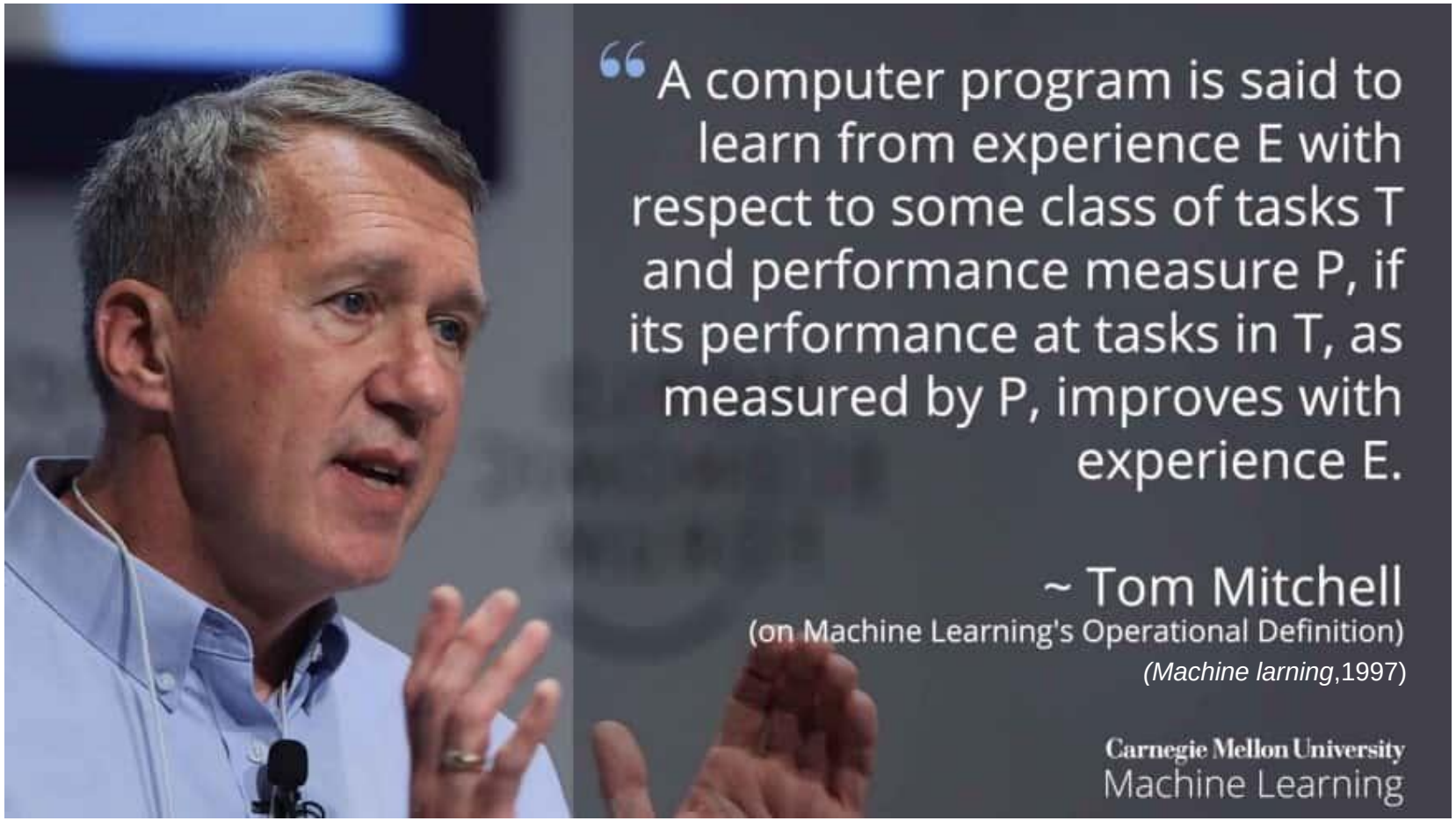
- ❑ Introduction to machine learning
  - What's machine learning?
  - Types of machine learning
  - Machine learning applications
- ❑ Some key concepts in machine learning
- ❑ Recap of useful tools and packages
  - Jupyter notebook
  - NumPy, Matplotlib
- ❑ Examples and practices

What is machine learning?

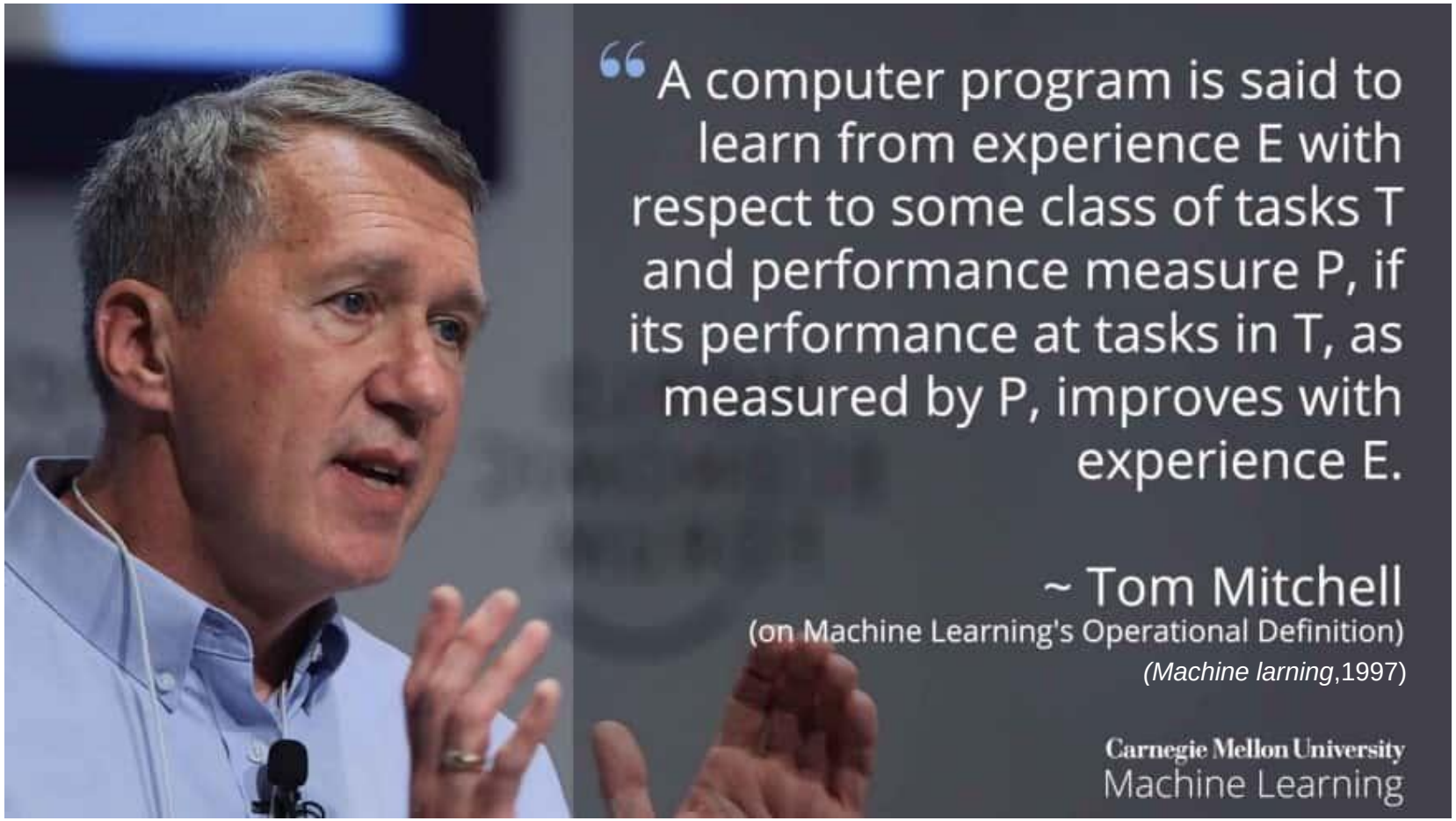
Arthur Lee Samuel *(1959)*

Machine Learning *the "field of study that gives computers the ability to learn without being explicitly programmed".*

What is machine learning?



What is machine learning?



Experience

- Data

Task

- Classification
- Regression
- Clustering
- Dimension reduction

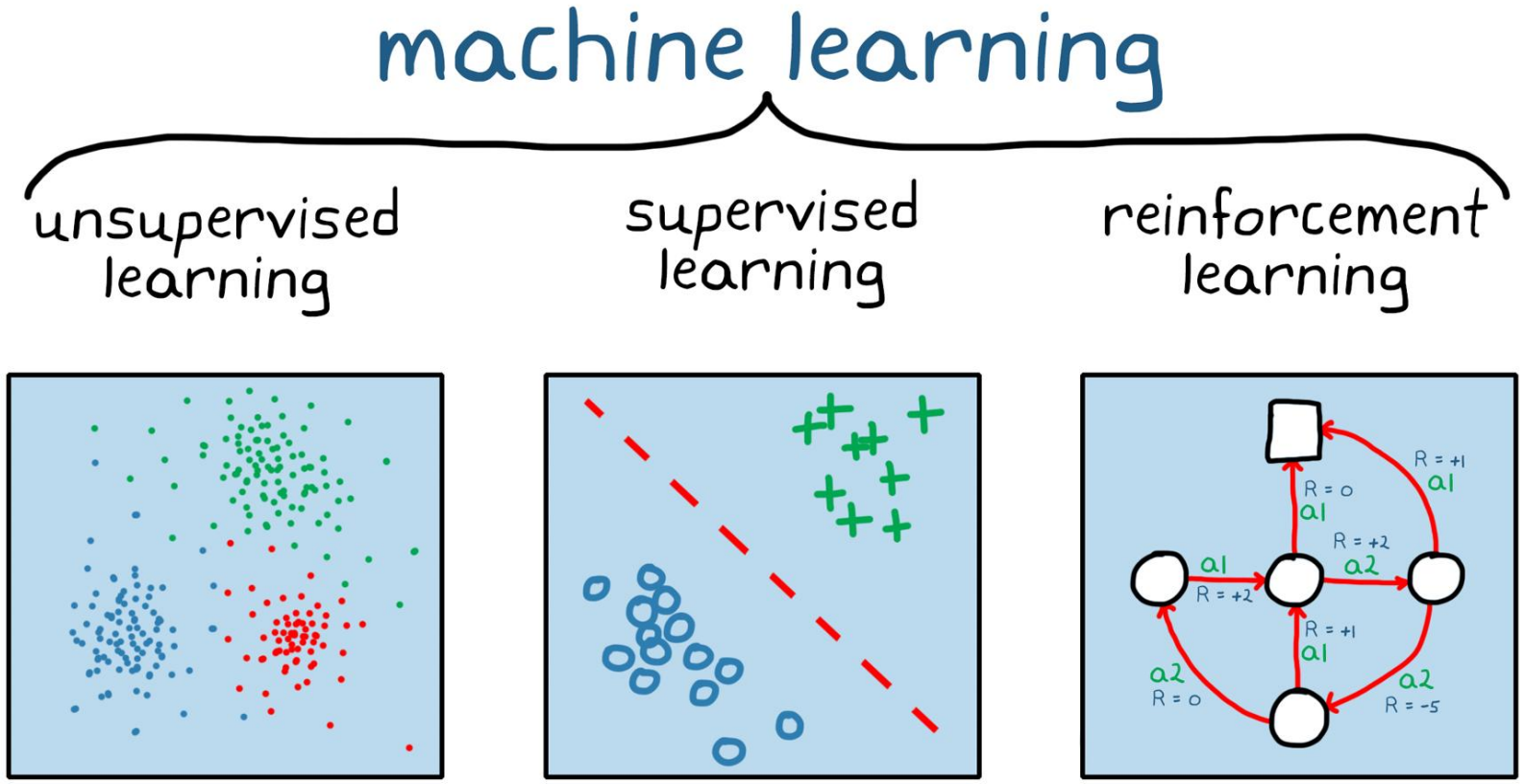
…

Performance

- Entropy loss
- Mean squared error
- Reconstruction error

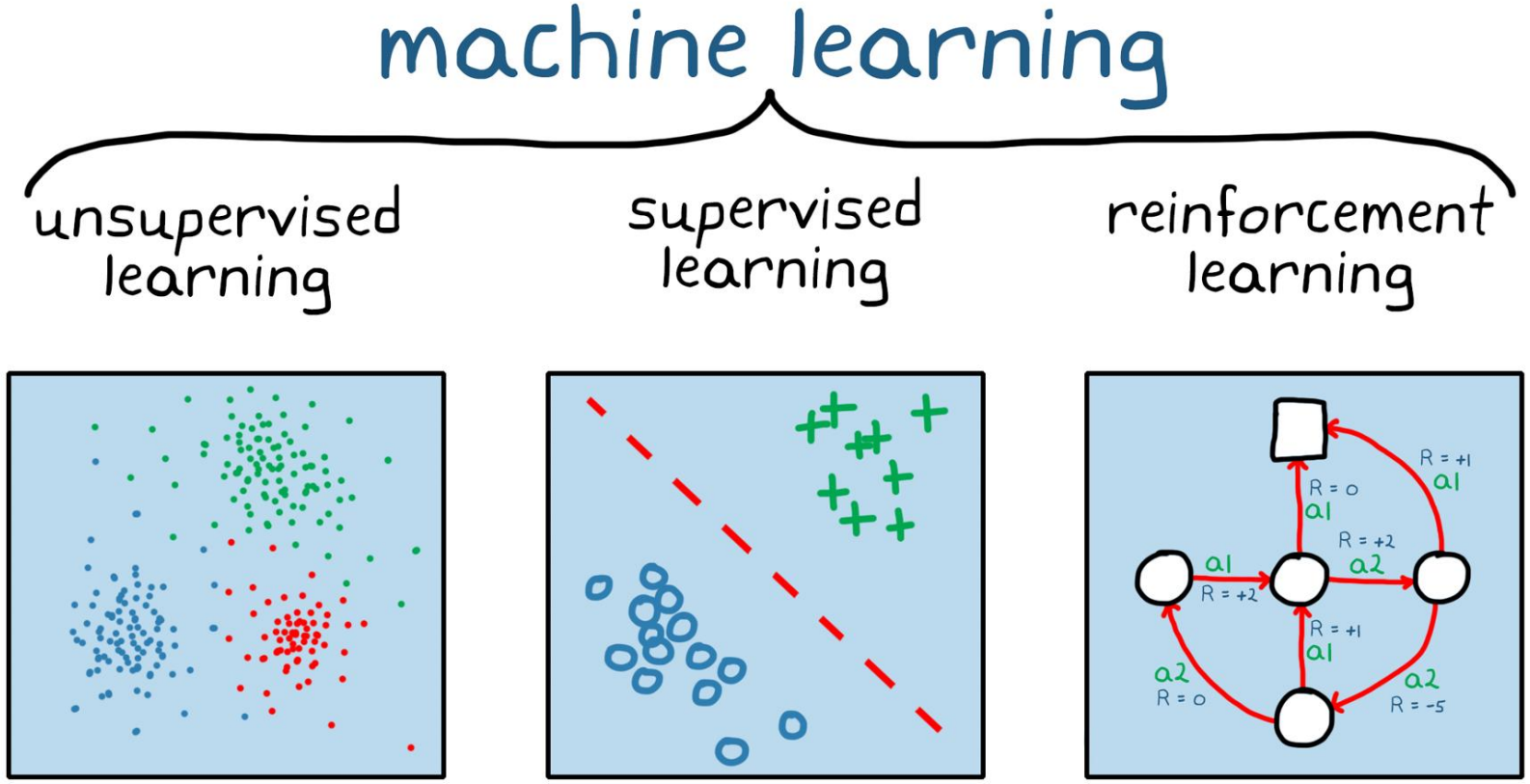
…

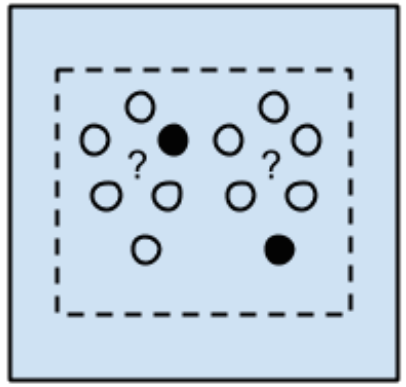
Types of machine learning



https://www.mathworks.com/discovery/reinforcement-learning.html

Types of machine learning





Semi-supervised Learning Algorithms

Self-supervised Learning

Other category types

- Batch learning vs Online-learning
  - **Batch learning**: system is trained using all available data
  - **Online learning**: system is trained incrementally by feeding data sequentially, data can be on the fly

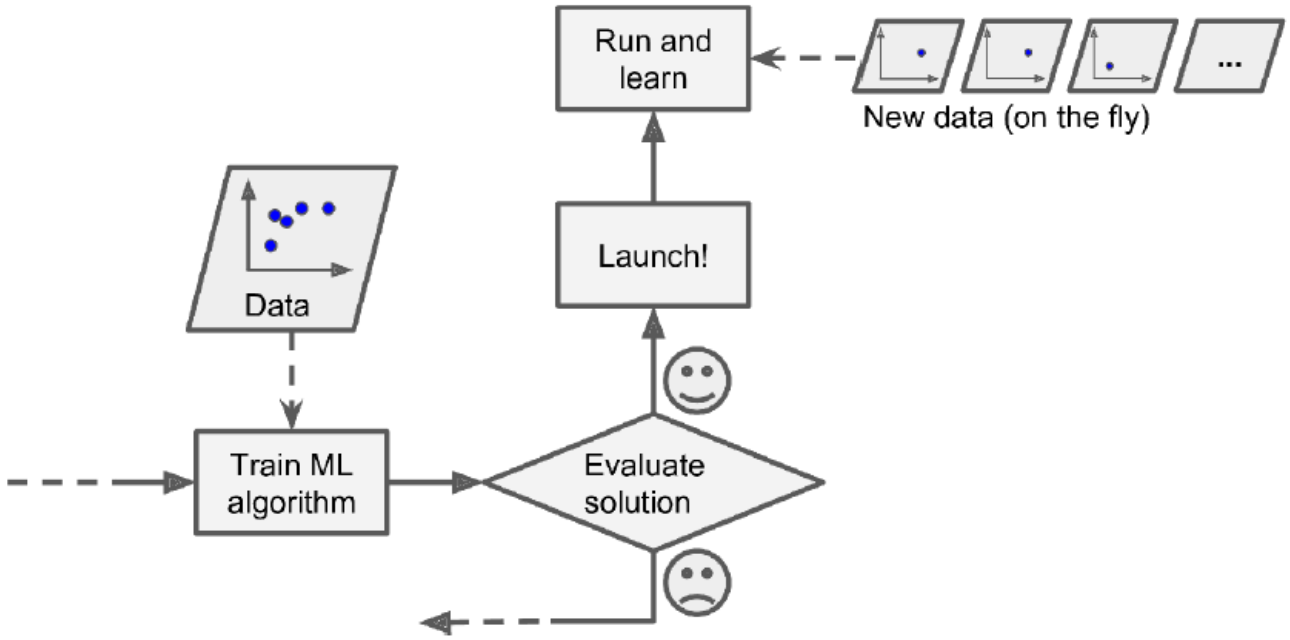


Figure 1-13. In online learning, a model is trained and launched into production, and then it keeps learning as new data comes in

Other category types

- Batch learning vs Online-learning
  - **Batch learning**: system is trained using all available data
  - **Online learning**: system is trained incrementally by feeding data sequentially, data can be on the fly

- Instance-based learning vs model-based learning
  - **Instance-based learning**: the system learns the example by heart, then generalizes to new cases by using a similarity measure
  - **Model-based learning**: build a model from existing examples, and use the model to make predictions

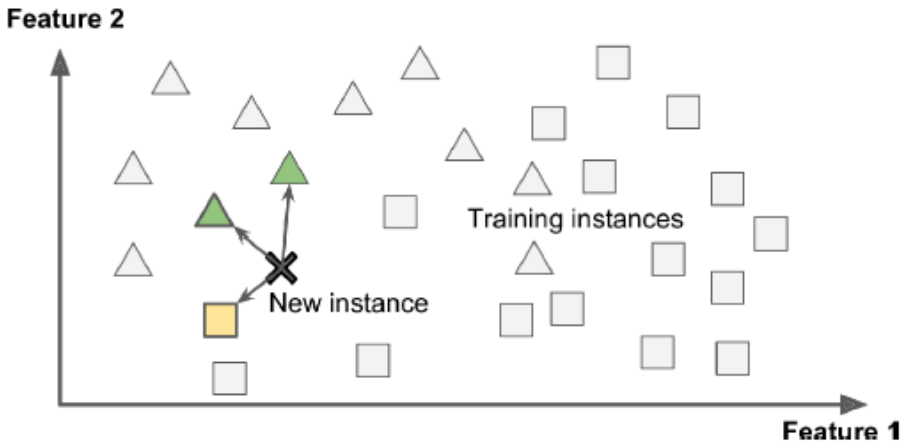


Figure 1-15. Instance-based learning

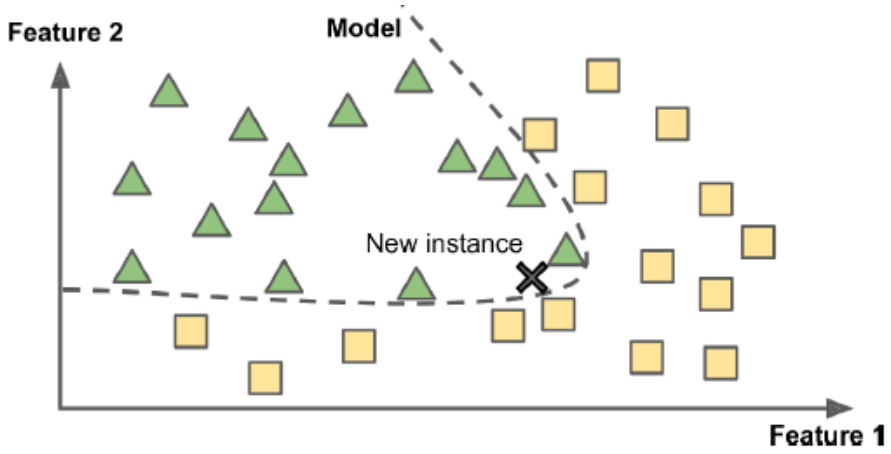


Figure 1-16. Model-based learning

Supervised learning

- Training data with n ***samples*** of ***features*** **x** and ***labels*** y
- Learn a function class f(**x**) to describe y based on **x**

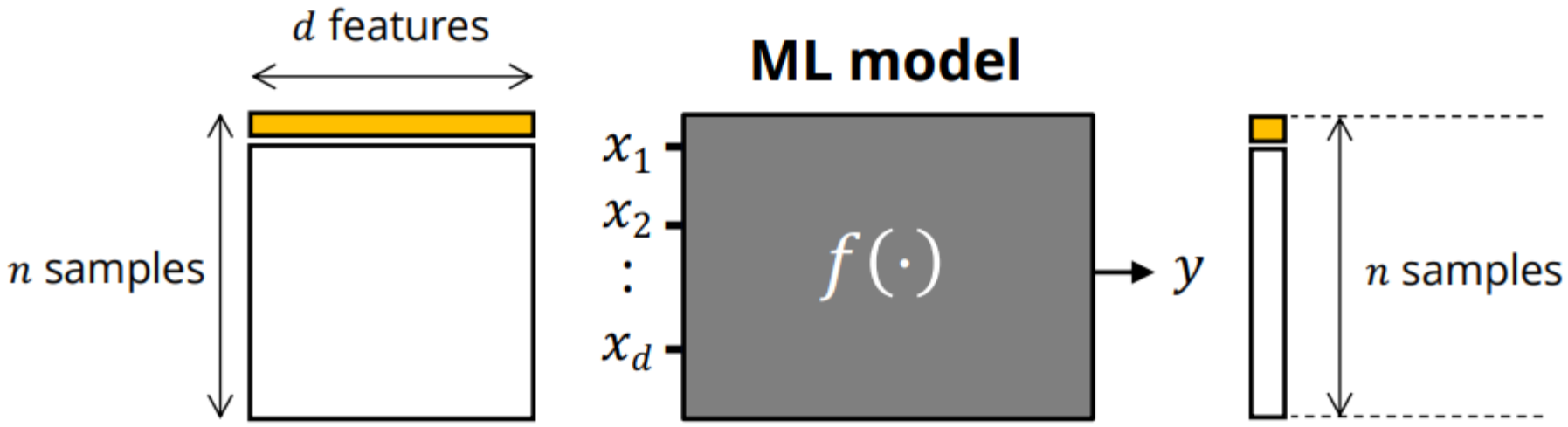
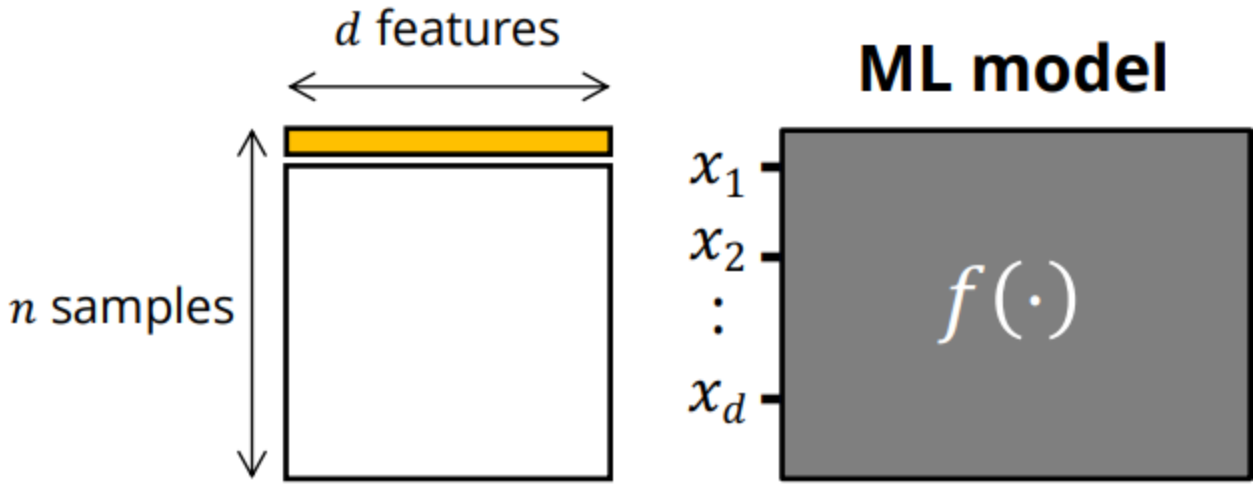
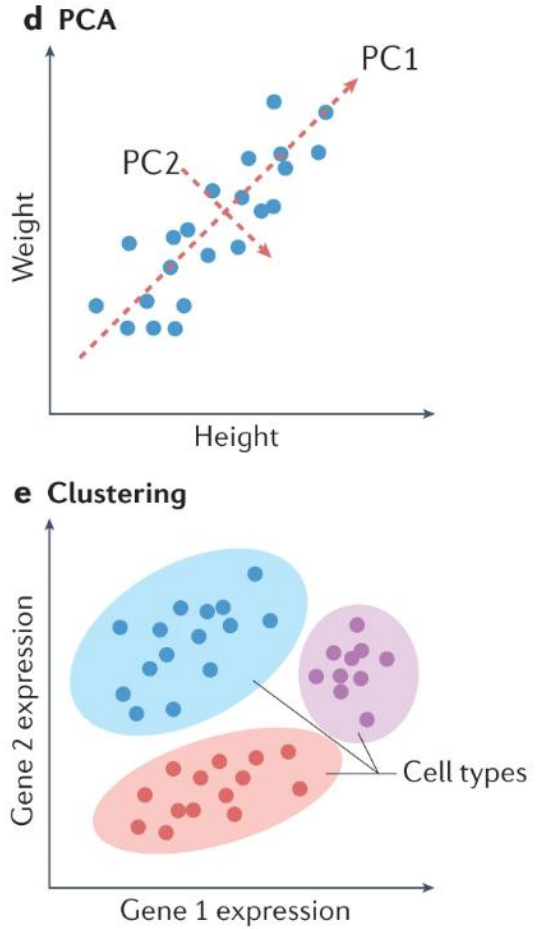


Figure adopted from CSEP 590B Explainable AI

Unsupervised learning

- Training data with n ***samples*** of ***features*** **x, no label**
- Identify underlying patterns in unlabeled data

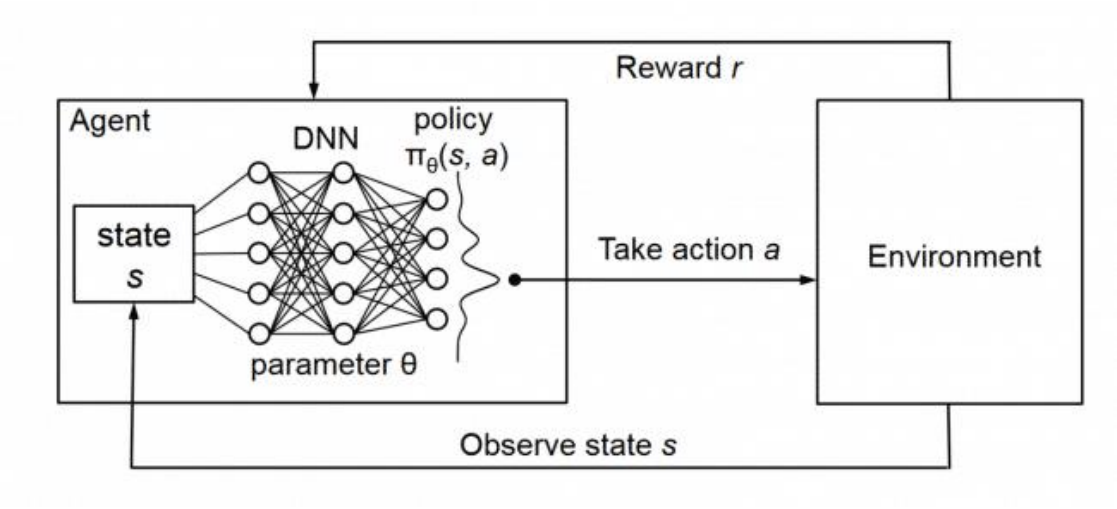


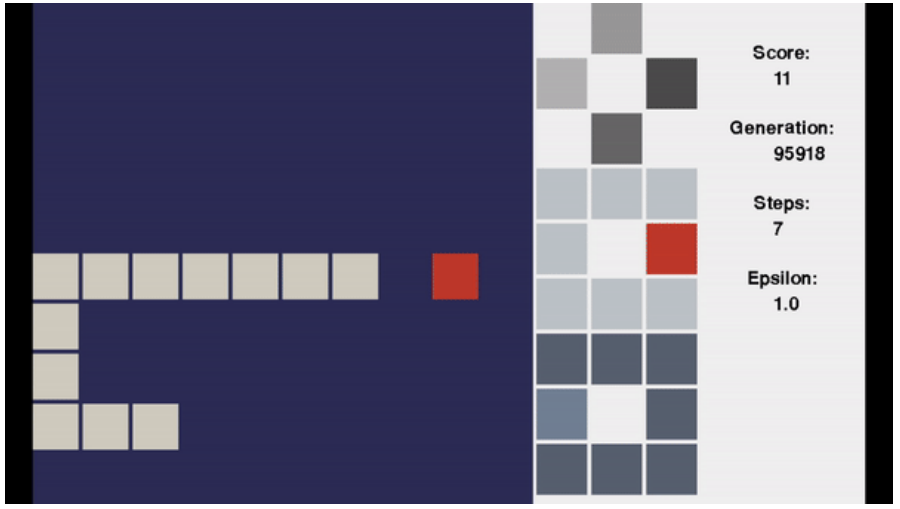


Greener et.al, Nature reviews molecular cell biology (2021)

Reinforcement learning

- Learning system (agent) observe the *environment*, select and perform *actions*, and get *rewards* in return
- Learn by itself what is the best strategy (*policy*), to get the most reward over time





https://www.novatec-gmbh.de/en/blog/deep-q-networks/
https://github.com/ludius0/SnakeQ

What can machine learning do?

- Face/Speech recognition
- Recommendation system
- Machine translation
- Self-driving system
- Stock market prediction
- Create images/songs/paintings/stories

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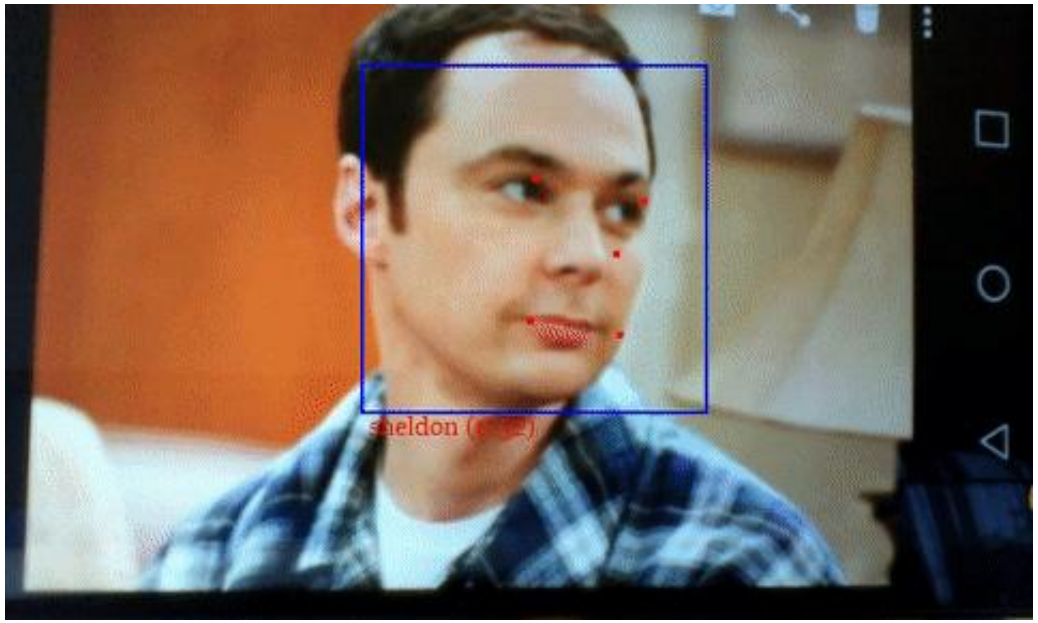
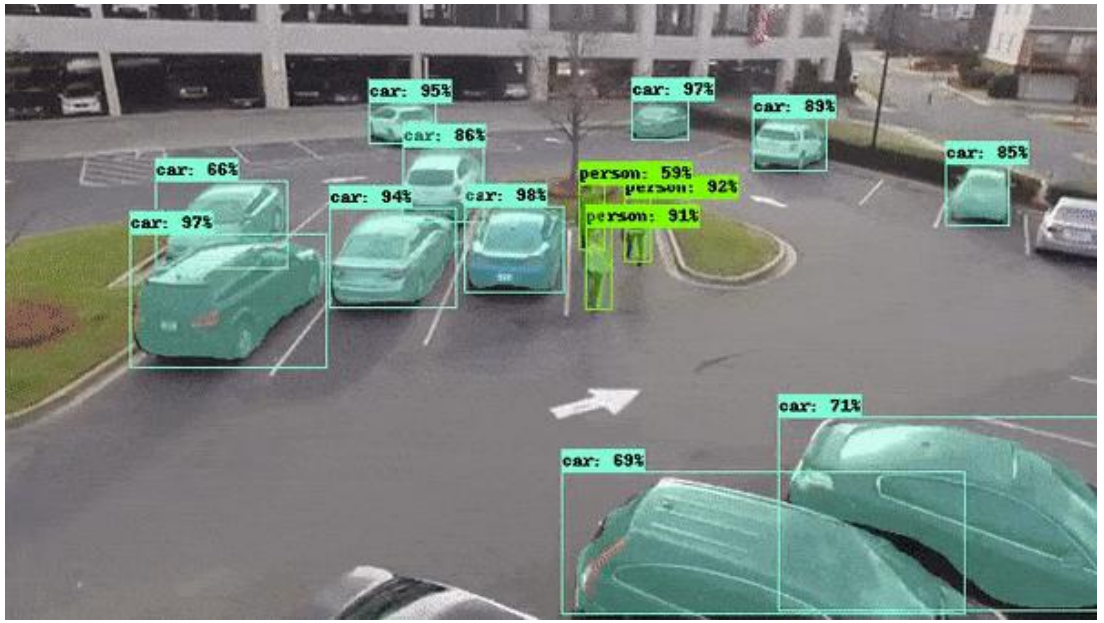
Figures from internet and STATS231A

More examples

- Object segmentation and recognition





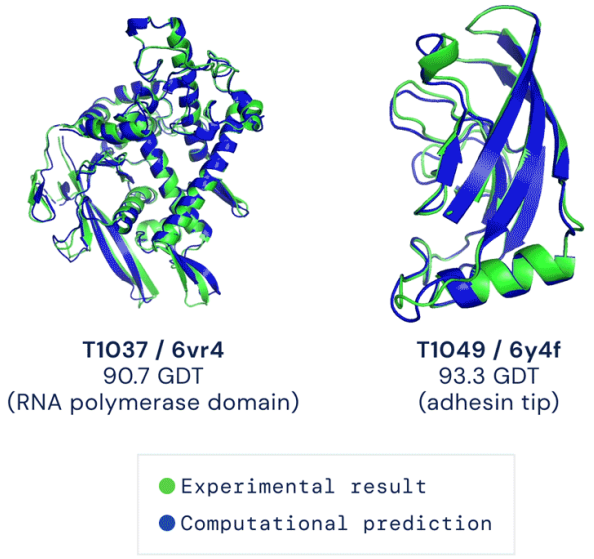
Figures from internet and STATS231A

More examples

AlphaGo (2016)

Monte Carlo tree search

AlphaFold (2021)



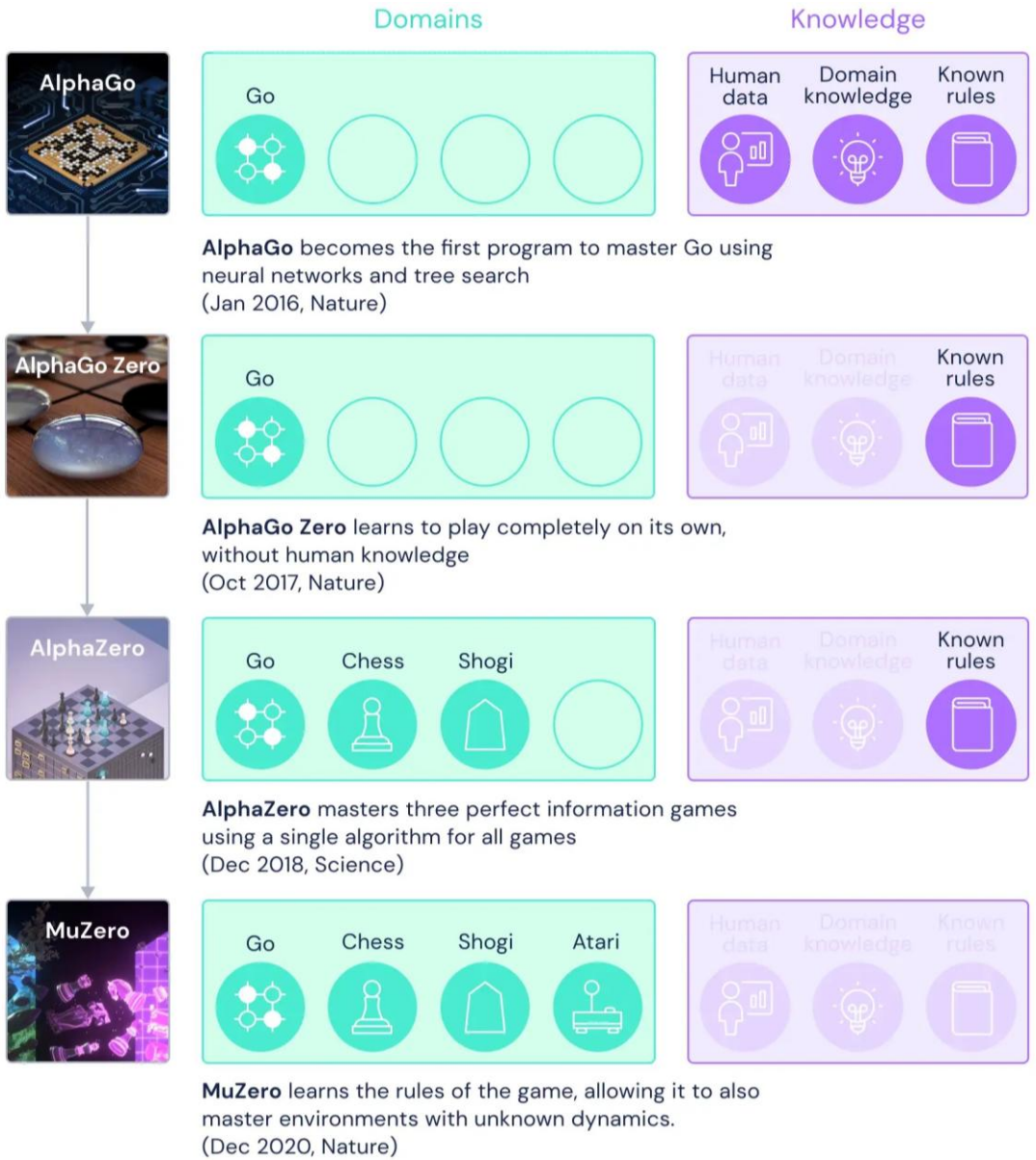
Transformer (self-attention)

AlphaTensor (2022)

Reinforcement learning

Images from internet

AlphaGo keeps evolving



https://www.deepmind.com/

Machine learning in biomedical research

- Imaging/sequencing processing
- Protein 3D structure prediction
- Genetic risk assessment
- Disease diagnosis
- Drug design

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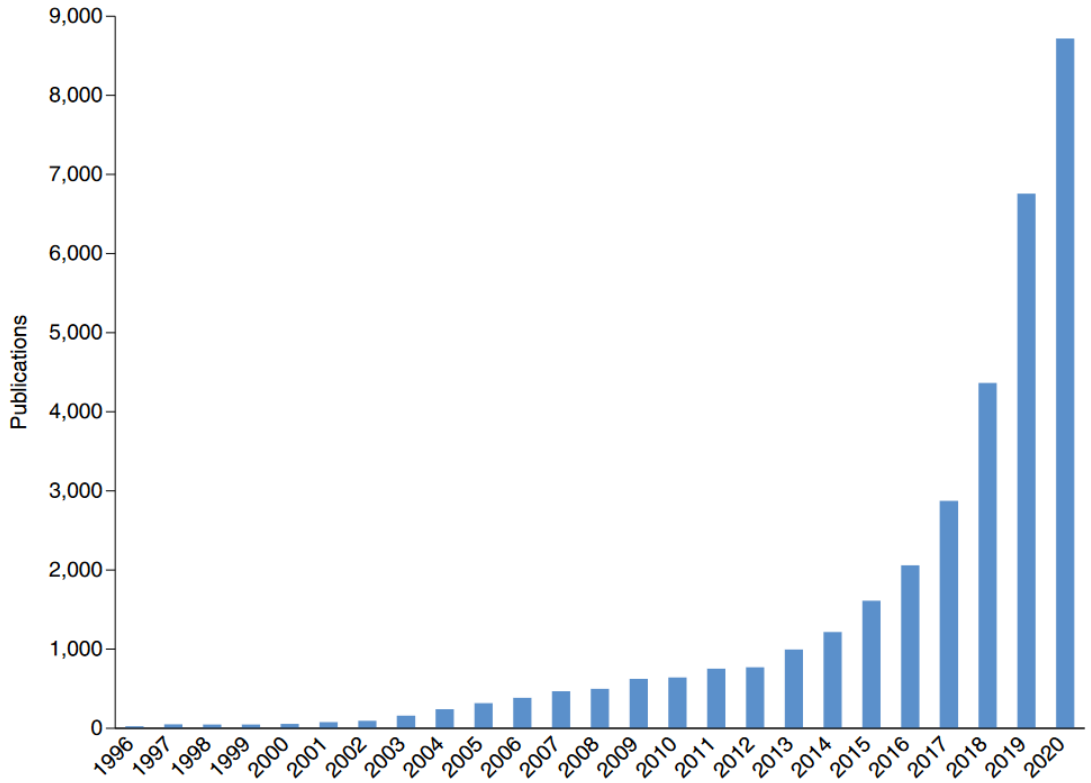


Fig. 1 | Exponential increase of ML publications in biology. The number of ML publications per year is based on Web of Science from 1996 onwards using the topic category for "machine learning" in combination with each of the following terms: "biolog*", "medicine", "genom*", "prote*", "cell*", "post translational", "metabolic" and "clinical".

Walsh et.al, Nat Methods (2021)

Train a machine learning model: a big picture

Train a machine learning model: a big picture

- Frame the problem
  - Supervised or unsupervised?
  - Classification or regression?

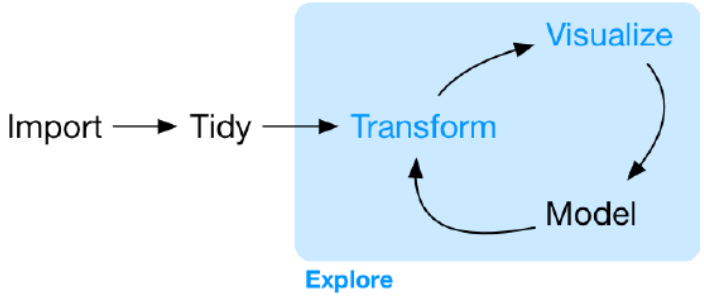
    …
- Select the performance measure (loss function):
  - Regression: RMSE, MAE
  - Classification: cross entropy
  - Dimension reduction: reconstruction error

    …
- **Cost / loss function** measures how *bad* your model fits the data

Train a machine learning model: a big picture

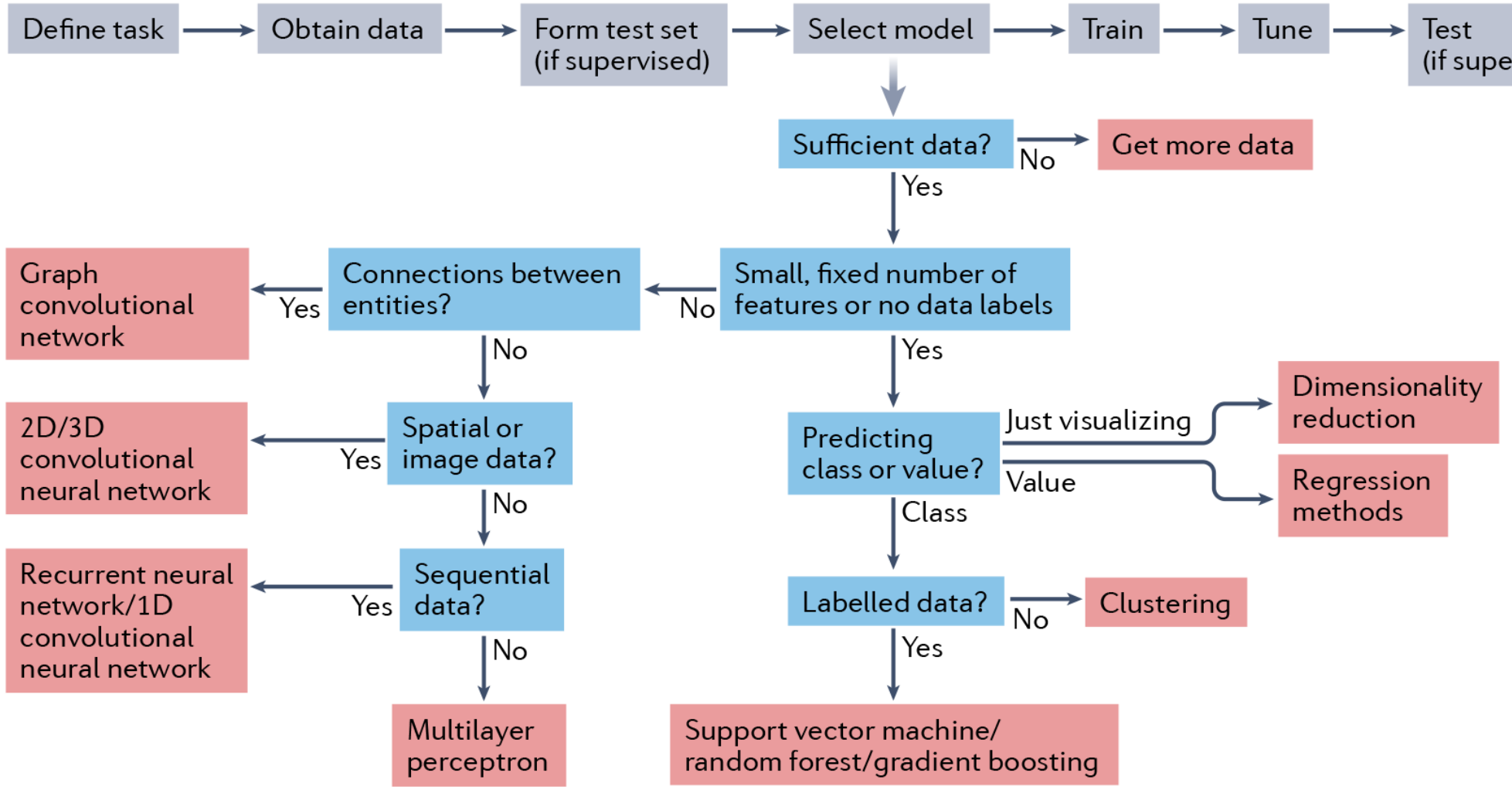
- Prepare the data
  - Download / gather data
  - Explore the data structure (descriptive analysis)
  - Perform data cleansing, processing, feature engineering

    …



- Create a test set (for supervised learning)
  - The only way to know how well a model will generalize to new cases is to actually try it out on new cases
  - Split the data into training and test set
    - Training set: train your models
    - Test set: evaluate the model (estimate the generalization error)
    - usually use 80% samples for training, holdout 20% samples for test

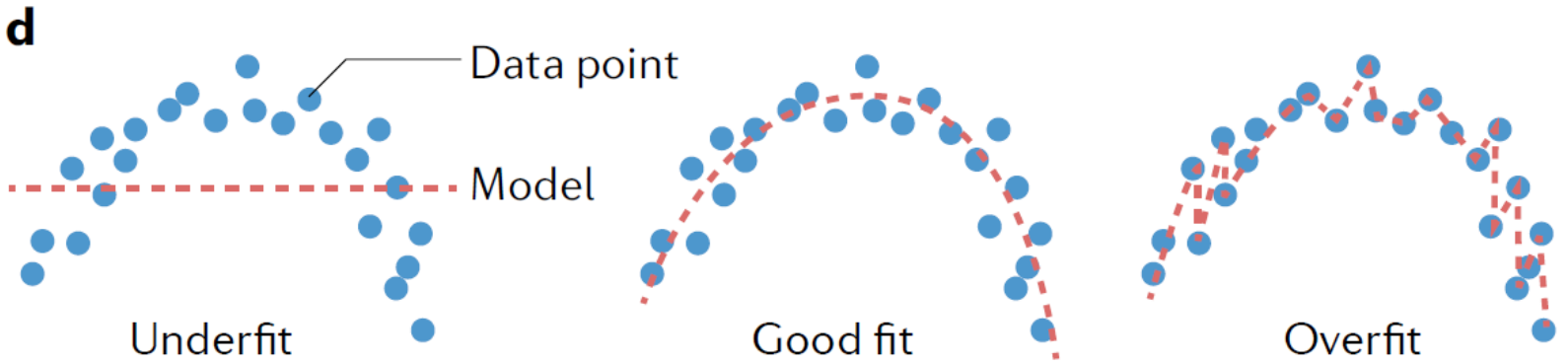
Train a machine learning model: a big picture



Greener et.al, *Nature reviews molecular cell biology* (2021)

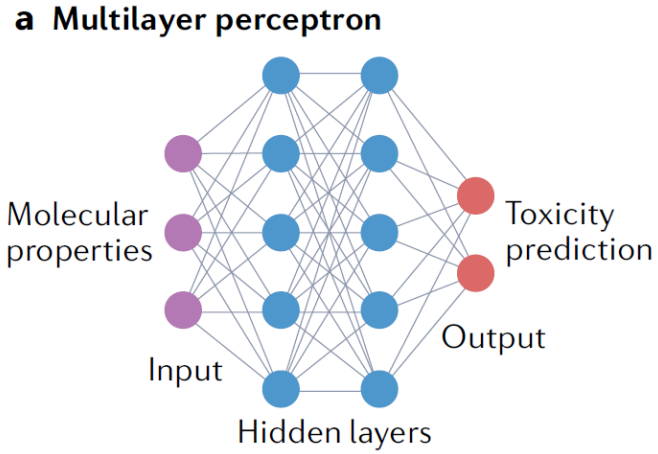
Train a machine learning model: a big picture

- Train a model:
  - Run an algorithm to find the model parameters that fits the training data the best (and hopefully make good predictions on new data)



Train a machine learning model: a big picture

- Tune hyperparameters:
  - **Hyperparameters** are parameters of a learning algorithm (not of the model)
  - Unlike model parameters, hyperparameters are not updated during training (although they are adjustable)



Example of hyperparameters:
- Number of neurons per layer
- Number of hidden layers

…

Train a machine learning model: a big picture

- Consider you have a set of hyperparameters/models to try
  - For each of them, you trained the model on training dataset, and then evaluate it on the test dataset, then you pick out the model with the best performance
  - Any problem?

Train a machine learning model: a big picture

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  - You measured the generalization error multiple times on the test set, and you adapted the model and hyperparameters to produce the best model *for that particular set*

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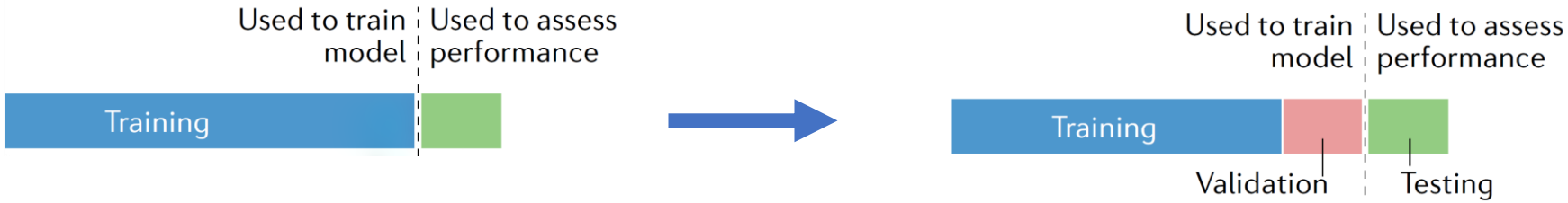
  - Solution: *holdout validation*



Train a machine learning model: a big picture

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  - Any problem?
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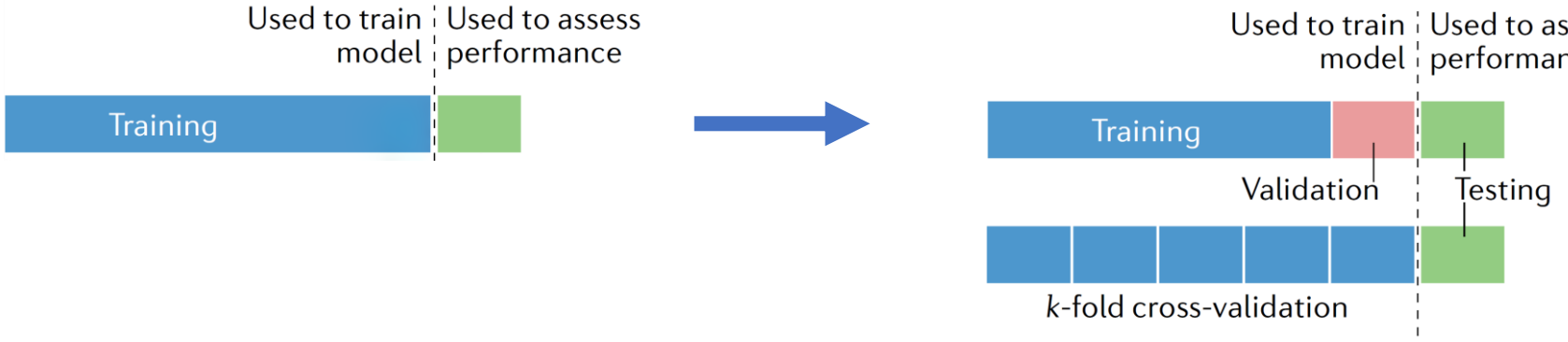
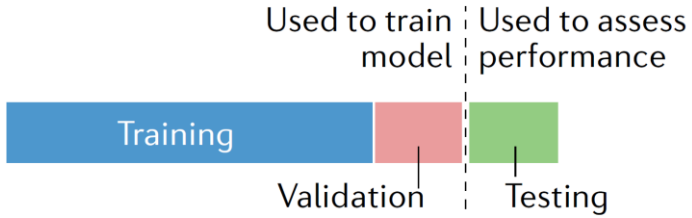
  - Solution: *holdout validation*, typically use cross validation when validation set is small



Train a machine learning model: a big picture

- Tune hyperparameters
  - Train multiple models with various hyperparameters on the reduced training set
  - Select the model that performs best on the validation set (or repeated cross validation)
  - Train the best model on the full training set (including the validation set), this gives you the final model
  - Lastly, evaluate this final model on the test set to get an estimate of the generalization error



Main challenges for machine learning

The system will not perform well if your training set is too small, or if the data is not representative, is noisy, or is polluted with irrelevant features

- Insufficient data
  - It takes a lot of data for many Machine Learning algorithms to work properly
  - but small- and medium-sized datasets are still very common in biological research
- Nonrepresentative data
  - Use a training set that is representative of the cases you want to generalize to

Main challenges for machine learning

The system will not perform well if your training set is too small, or if the data is not representative, is noisy, or is polluted with irrelevant features

- Insufficient data
  - It takes a lot of data for many Machine Learning algorithms to work properly
  - but small- and medium-sized datasets are still very common in biological research
- Nonrepresentative data
  - Use a training set that is representative of the cases you want to generalize to
- Poor quality data (garbage in, garbage out)
  - Spend time cleaning up your training data
  - Remove clear outliers
- Irrelevant features
  - Feature selection: selecting the most useful features
  - Feature extraction: combing existing features to produce a more useful one
  - Creating new features

Summary: what we have learned so far

Key concepts in machine learning:

- ❑ Definition of machine learning
- ❑ 3 types of machine learning
- ❑ The big picture of training a machine learning model

More details about:

- ❑ Training/test set
- ❑ Loss function
- ❑ Overfitting/underfitting
- ❑ Hyperparameters tunning (model selection)
- ❑ Cross validation
- ❑ Challenges in machine learning

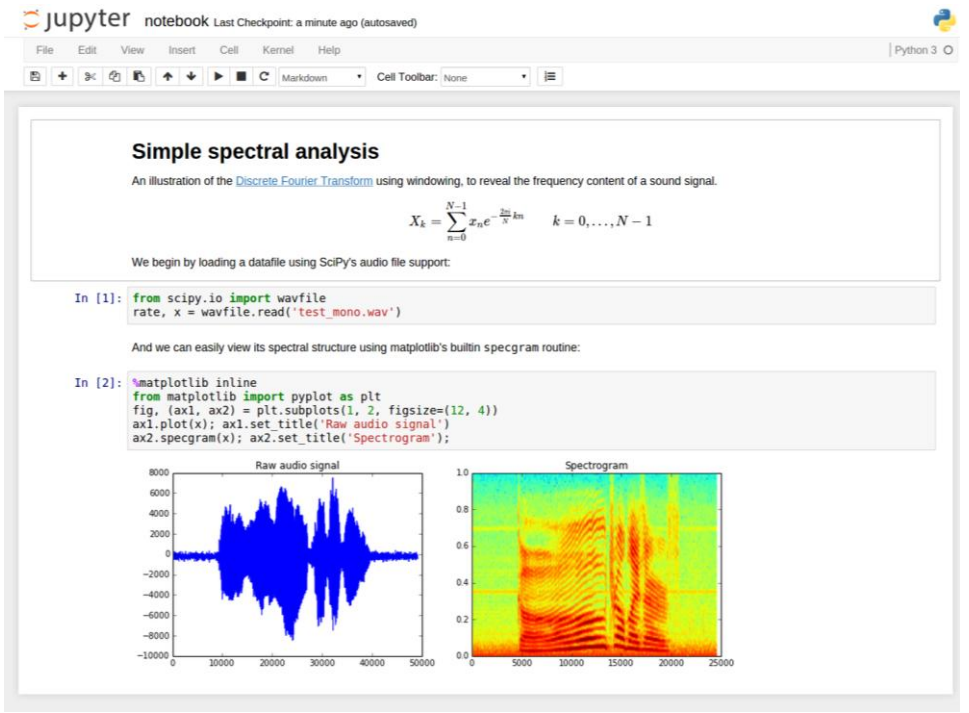
Enough theory, let’s play!

- Jupyter notebook
- Usage of some popular packages
- A toy example in machine learning

Jupyter notebook

- An open-source, web-based interactive computing platform
  - Suitable for exploration, and prototyping
  - Convenient in sharing, documentation and making plots, powerful for data analysis

- Similar applications:
  - JupyterLab (an extension of Jupyter notebook)
  - R markdown Notebook (R)
  - Matlab Live Script (Matlab)



Fun fact: Jupyter stands for **Ju**lia, **Pyt**hon, **R**.

Preparation: Install Jupyter notebook

- Install on your local computer: link

Install the classic Jupyter Notebook with:

```
pip install notebook
```

To run the notebook:

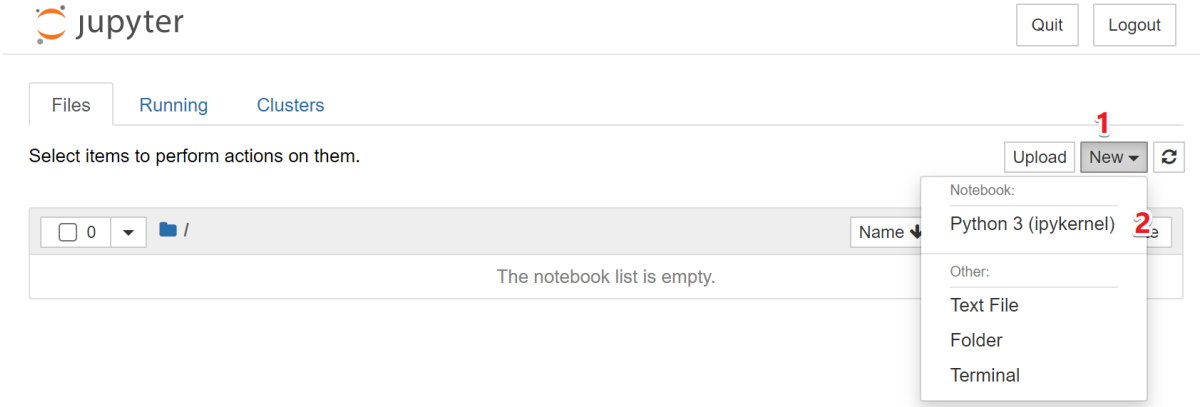
```
jupyter notebook
```

- If you are on Hoffman2: link
  - `wget https://raw.githubusercontent.com/rdauria/jupyter-notebook/main/h2jupynb`
  - `chmod u+x h2jupynb`
  - `./h2jupynb --help`
  - `./h2jupynb -u your_username -t 4 -m 8 –v 3.9.6`

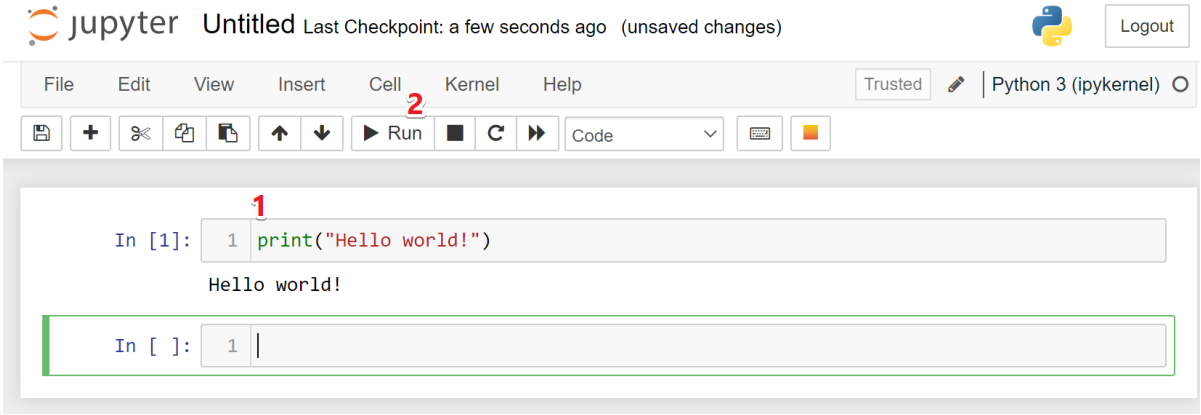
- Alternatively, you can use Google colab

Preparation: Create a new notebook

- Create a new notebook



- Say “Hello world!”

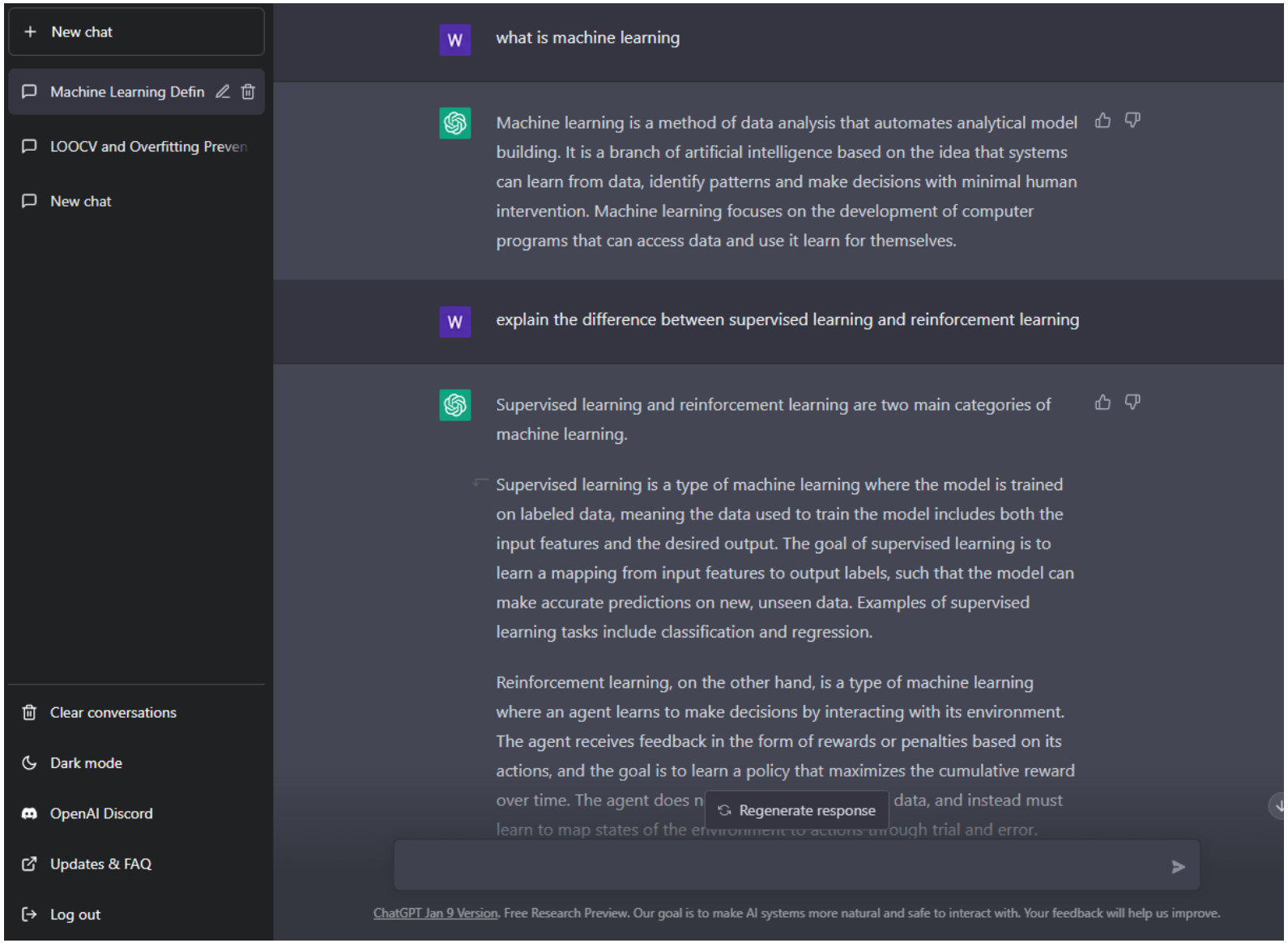


- Now let’s move to the Jupyter notebook tutorial
  - `git clone https://github.com/wbvguo/qcbio-ML_w_Python.git`

Where to get help?

- https://www.google.com
- https://stackoverflow.com
- https://stats.stackexchange.com/
- https://towardsdatascience.com/
- https://openai.com/blog/chatgpt/

ChatGPT


New chat
Machine Learning Defin
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what is machine learning
Machine learning is a method of data analysis that automates analytical model building. It is a branch of artificial intelligence based on the idea that systems can learn from data, identify patterns and make decisions with minimal human intervention. Machine learning focuses on the development of computer programs that can access data and use it learn for themselves.
explain the difference between supervised learning and reinforcement learning
Supervised learning and reinforcement learning are two main categories of machine learning.
Supervised learning is a type of machine learning where the model is trained on labeled data, meaning the data used to train the model includes both the input features and the desired output. The goal of supervised learning is to learn a mapping from input features to output labels, such that the model can make accurate predictions on new, unseen data. Examples of supervised learning tasks include classification and regression.
Reinforcement learning, on the other hand, is a type of machine learning where an agent learns to make decisions by interacting with its environment. The agent receives feedback in the form of rewards or penalties based on its actions, and the goal is to learn a policy that maximizes the cumulative reward over time. The agent does n
Regenerate response
data, and instead must
learn to map states of the environment to actions through trial and error.
ChatGPT Jan 9 Version. Free Research Preview. Our goal is to make AI systems more natural and safe to interact with. Your feedback will help us improve.

Q&A

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