Machine Learning for Physics and Astronomy

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Lecture 5, 28/09/2020

Today's lecture

- Pattern recognition and classification with Convolutional Neural Networks
- Bayesian Neural Networks
- Reinforcement Learning (pre-recorded)
- Guest lecture by **Dr. Christoph Weniger** on applications of ML for astroparticle physics

Convolutional Neural Networks

Supervised learning and classification

The goal is to **predict a class label** from a pre-defined list of possibilities

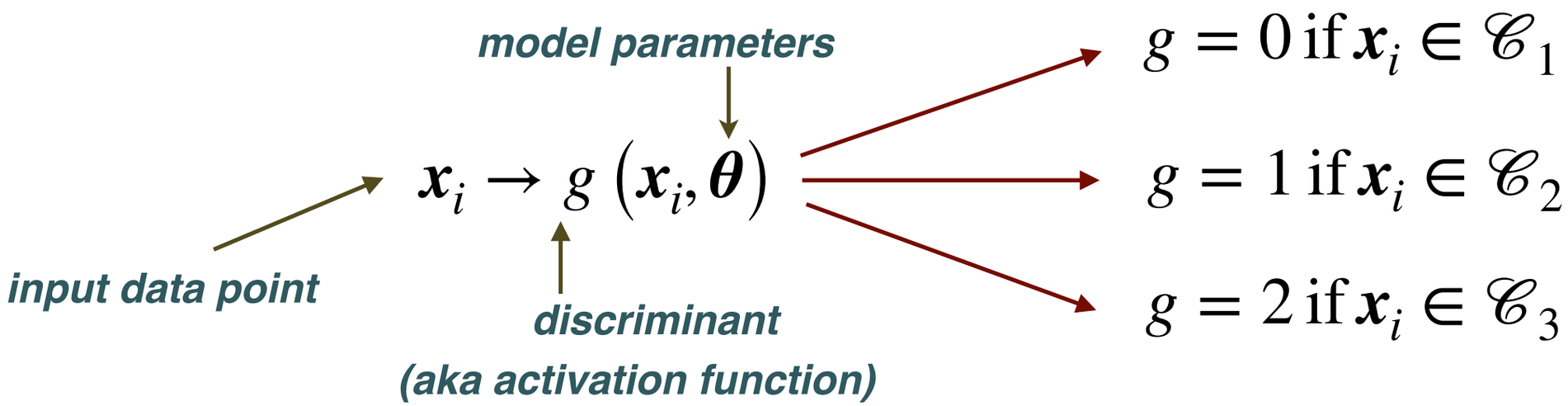
the simplest type of problem is **binary classification** (yes/no problems)

e.g. should I put this email in the spam folder?

but in general one considers **multiclass classification** (> 2 categories)

e.g. which type of bird is the one I just photographed?

In the context of ML applications there exist a large number of approaches to classifications tasks. The most basic one is based on assembling a **discriminant function** that maps each input data point to its specific class



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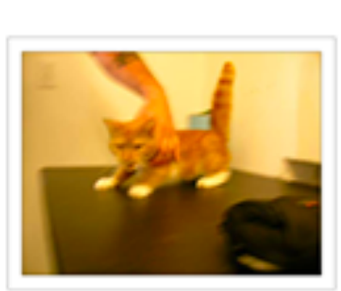
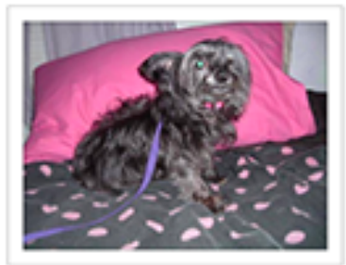


cat or dog?



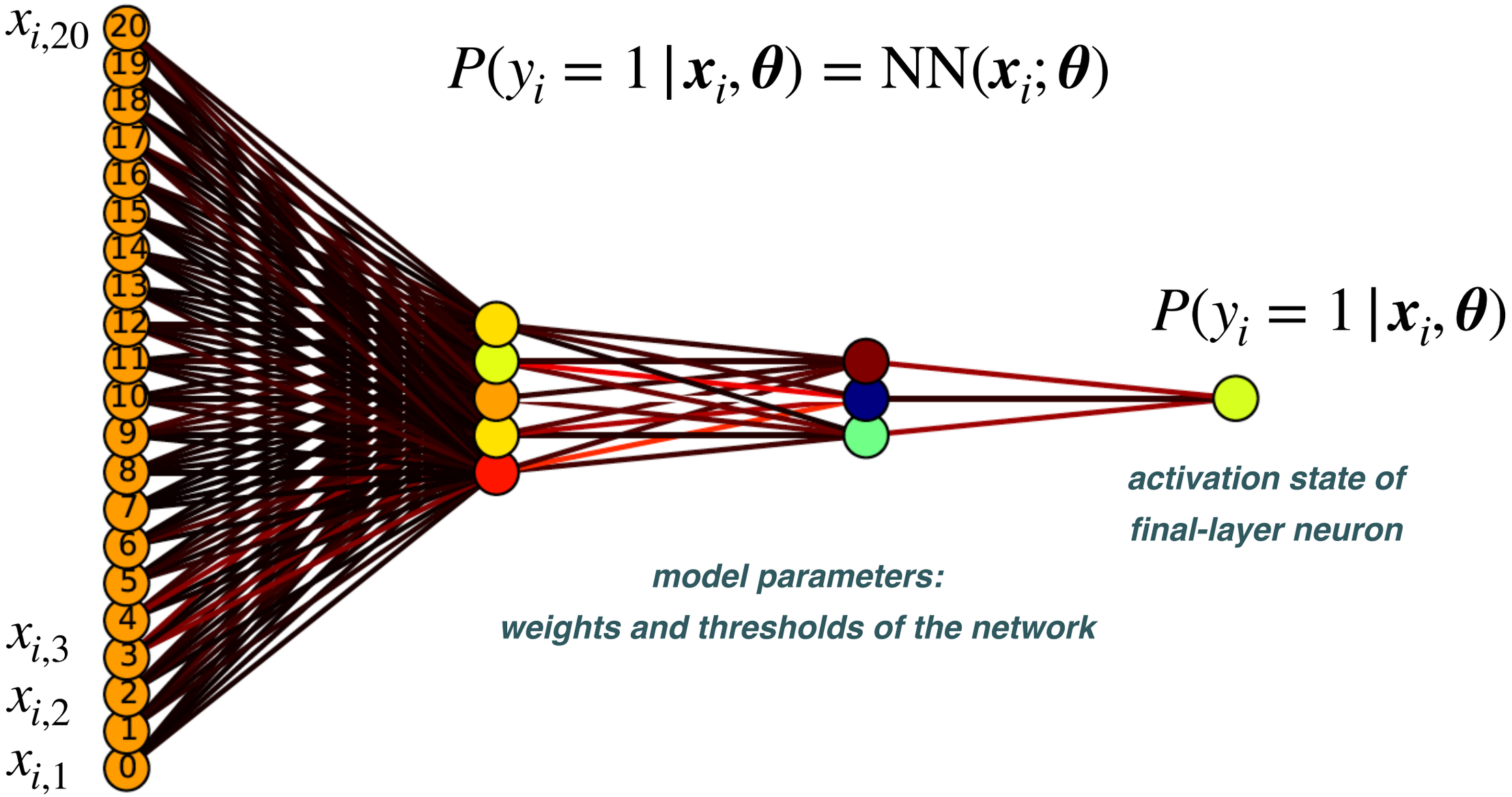
Supervised learning and classification

instead of modelling the classification probability by a **simple logistic function**

$$P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \frac{1}{1 + e^{-\boldsymbol{x}_i^T \boldsymbol{\theta}}}$$

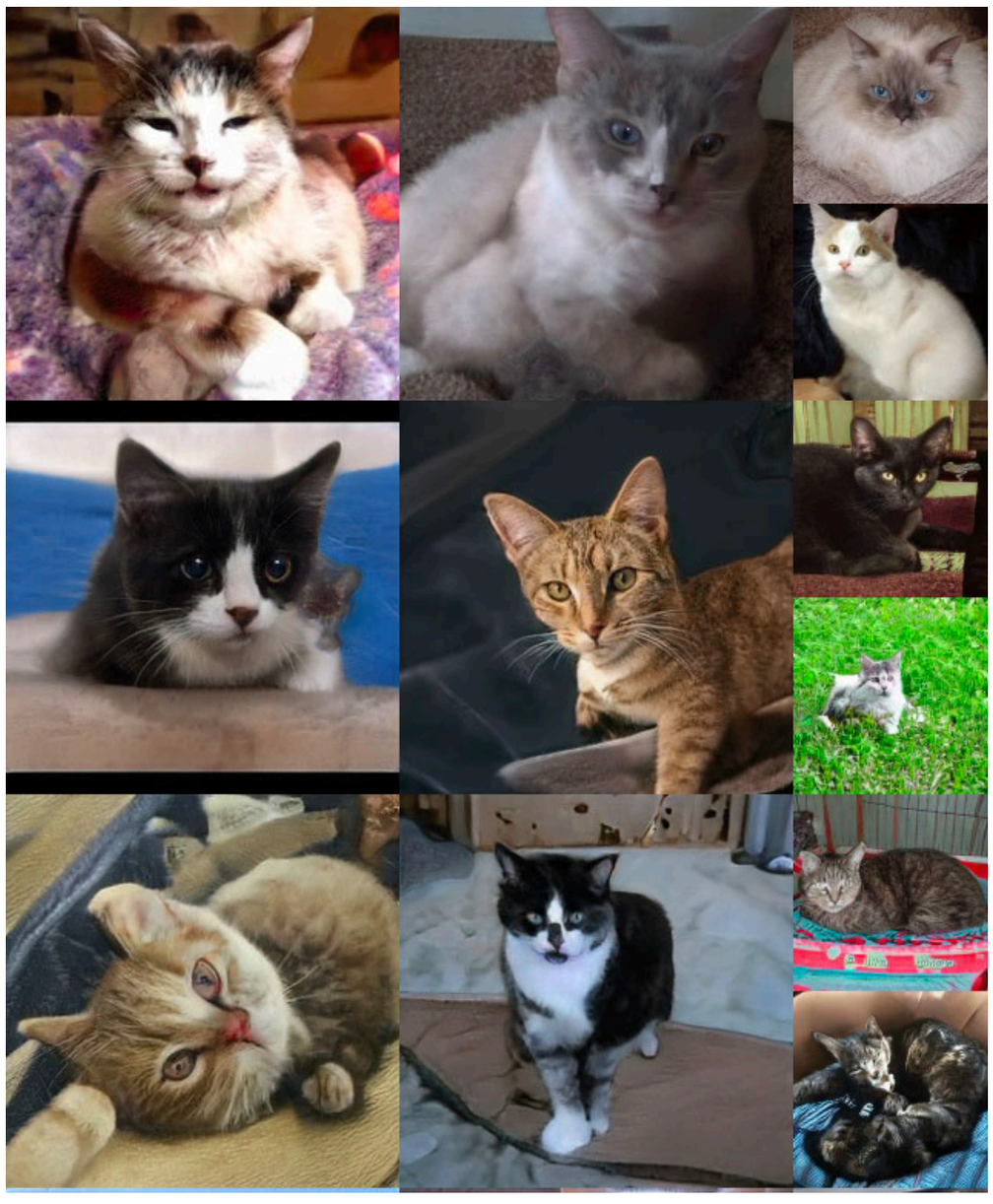
one can adopt more complex models, such as deep neural networks

$$P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \mathrm{NN}(\boldsymbol{x}_i; \boldsymbol{\theta})$$



Learning with symmetry

Like physical systems, many datasets and supervised learning tasks also possess additional **symmetries and structure** what can (and should) be exploited



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- *Cats can be anywhere in the image: **translational invariance***

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O***ur classifier should exhibit all these high-level features***

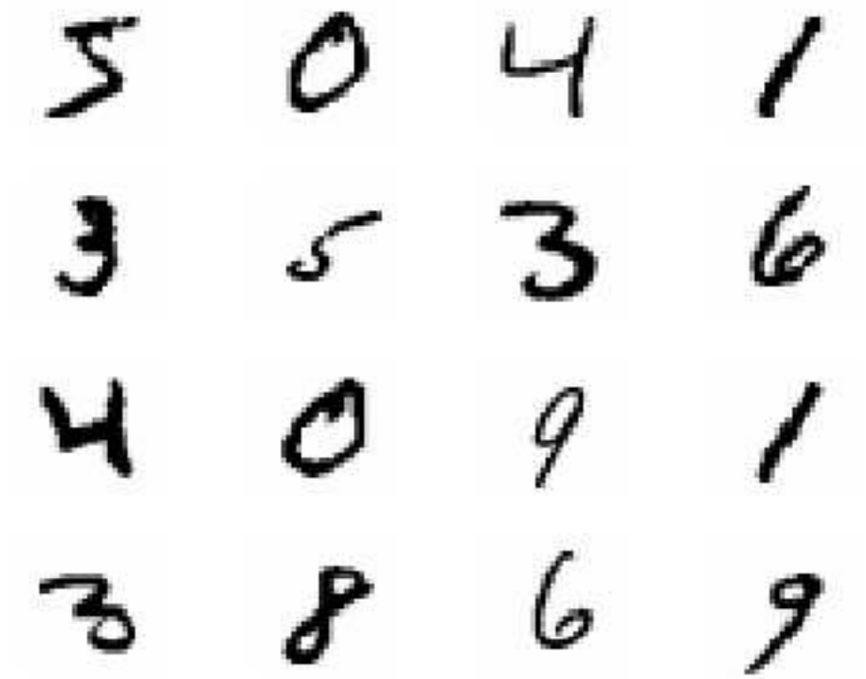
Learning with symmetry

our goal is to create models which are **invariant** wrt certain transformations of the inputs

CNNs hard-code these invariance properties into the **structure of the network**

extensively used for applications in **pattern recognition**

e.g. classify handwritten digits



Inputs: set of pixel intensity values of each image

Output: posterior probability distribution over the 10 digit classes

what kind of **symmetries** must we built-in in our ML classifier model?

Learning with symmetry

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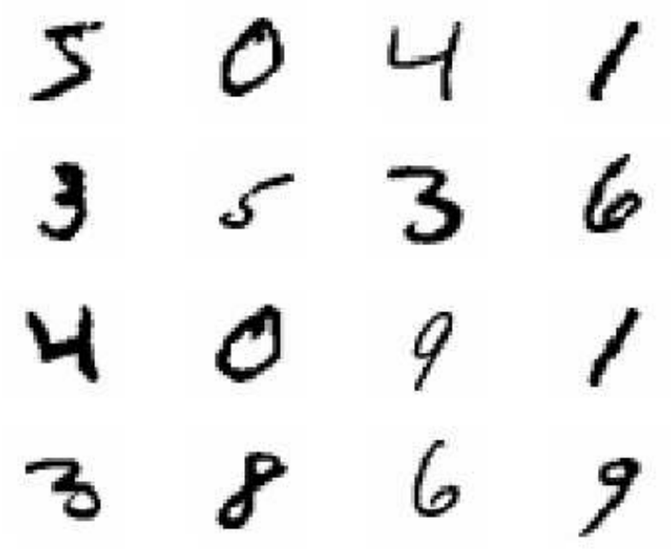
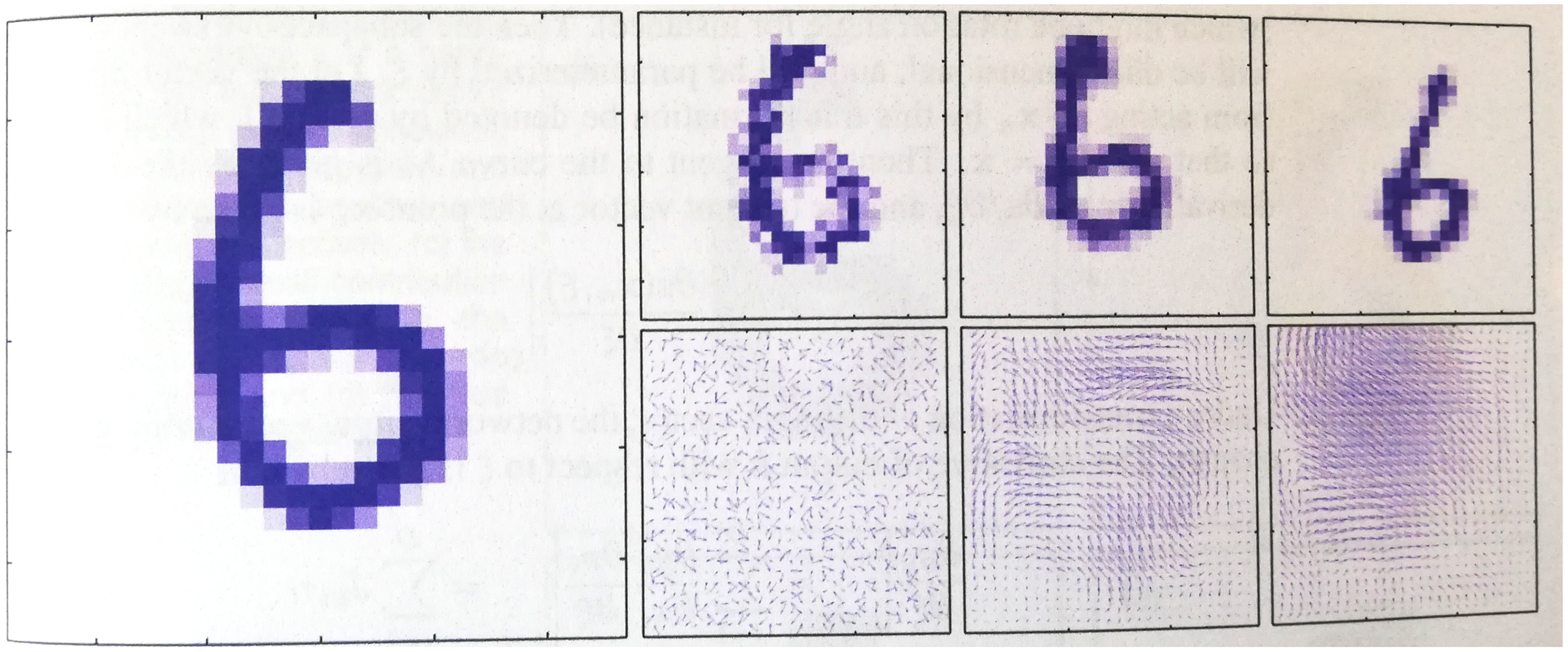


some are obvious choices ...

- Invariance under **translations**
- Invariance under **scaling**



Learning with symmetry

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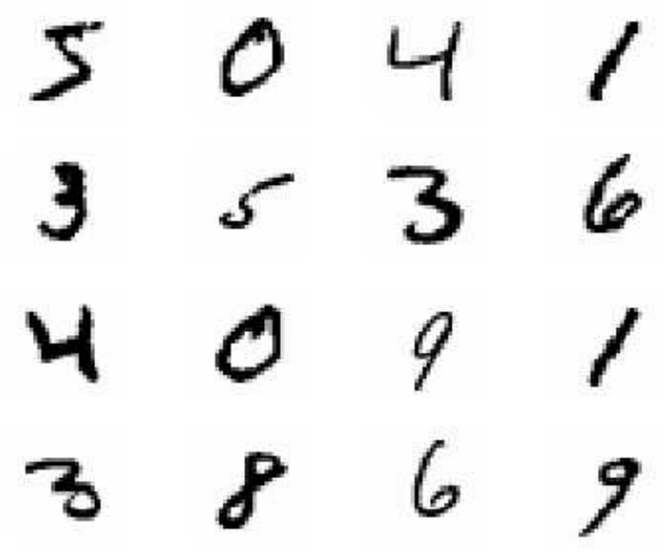
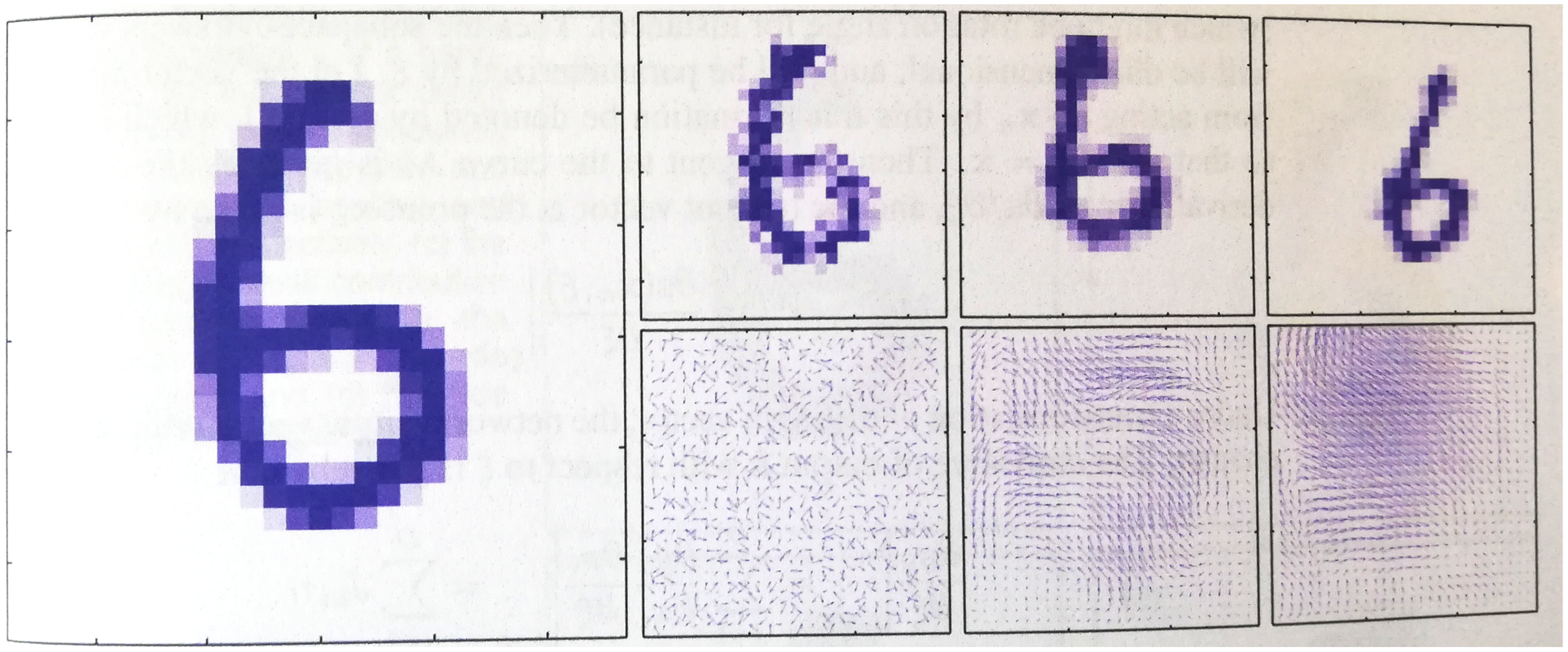


- Invariance under **translations**
- Invariance under **scaling**
- Invariance under **small rotations**
- Invariance under **smearing**
- Invariance under **elastic deformations**

but others are more non-trivial!



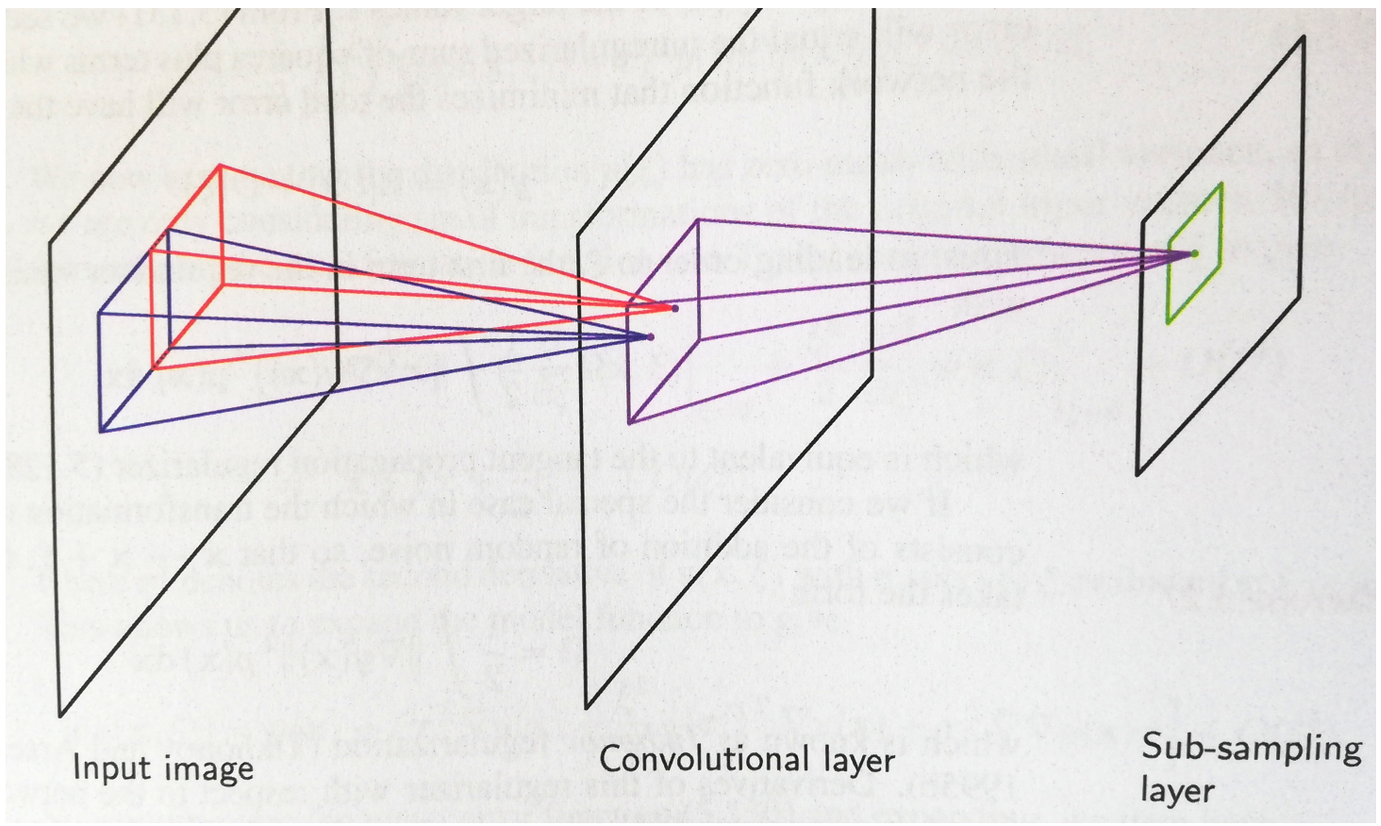
Convolutional Neural Networks

the simplest approach would be to input the images to a **fully connected NN** which given enough training data (and time) would **learn the symmetries by example**

however this way a crucial property is ignored: **nearby pixels are strongly correlated**
we should aim instead first to **identify local features** that depend on small subregions

afterwards such local features can be combined into **higher-level ones**

Convolutional Neural Networks (CNNs) are architectures that take **advantage of this additional high-level structures** that all-to-all coupled networks fail to exploit



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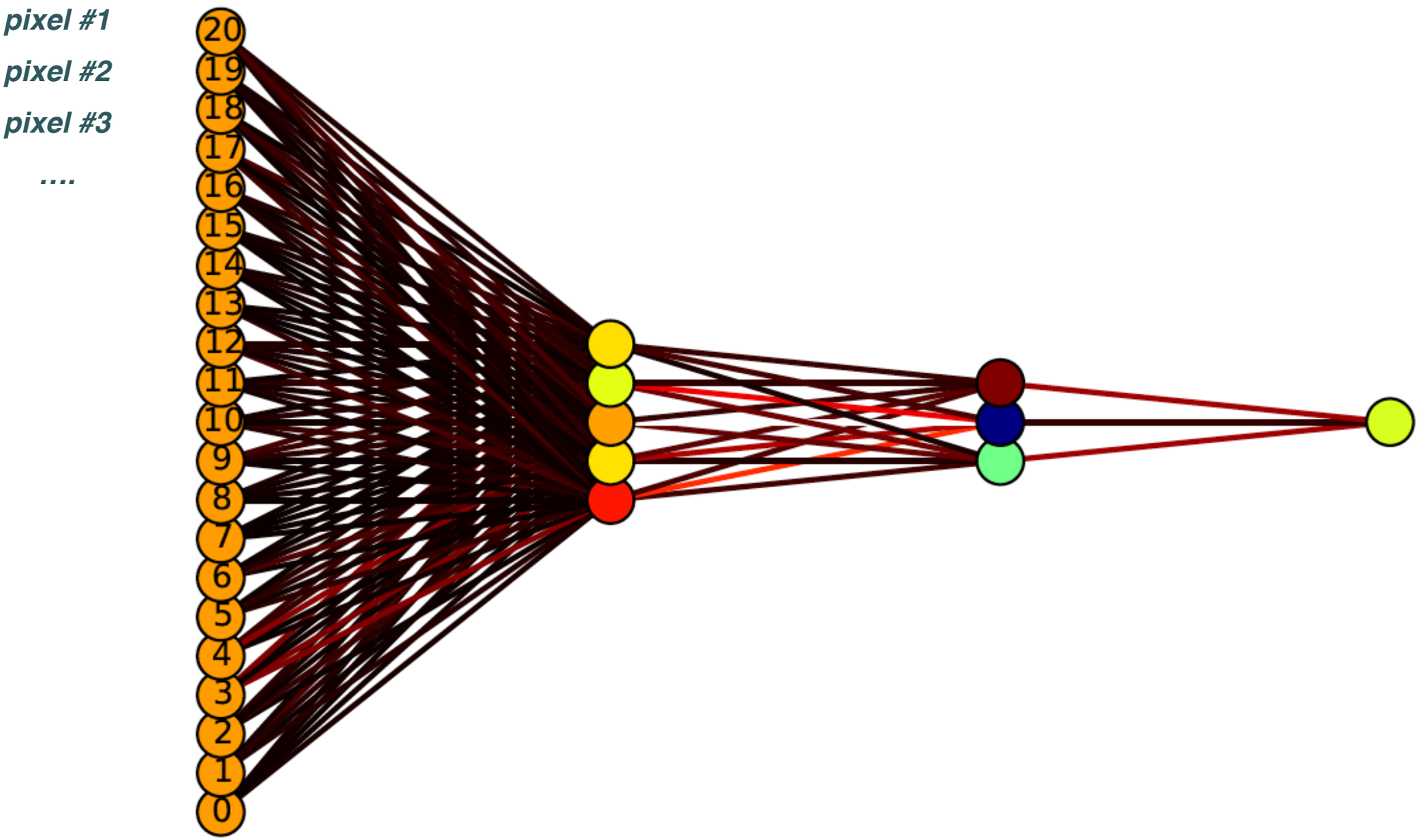
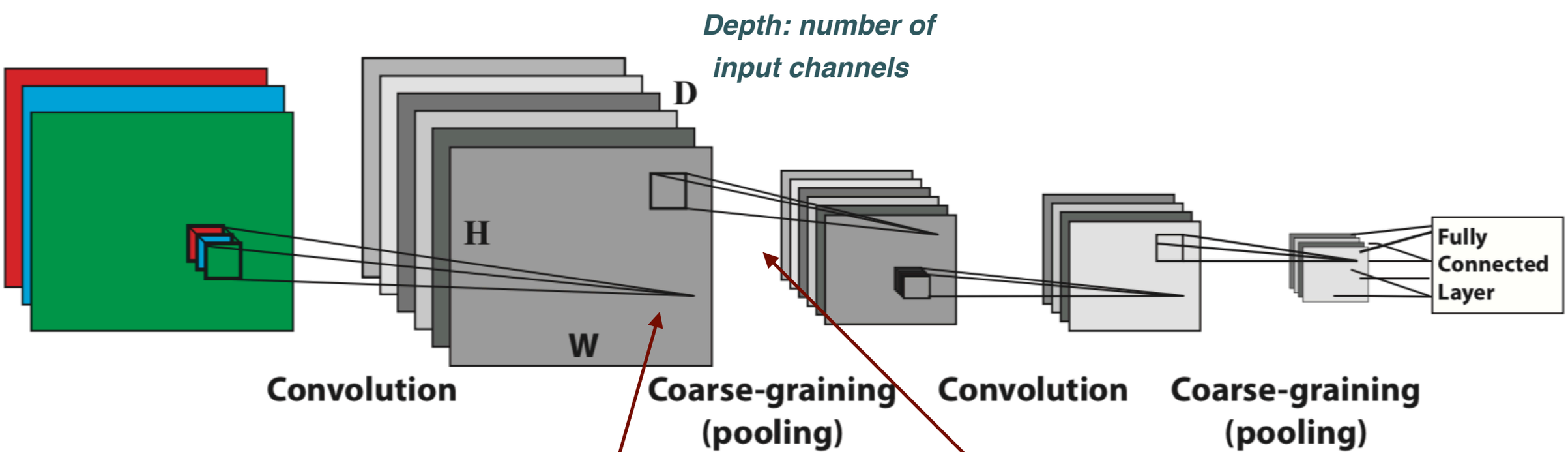


Convolutional Neural Networks

A CNN is a translationally invariant neural network that respects locality of the input data



D=3 for RGB images
Height (H) and Width (W) determined by number of pixels

neuron activation state: convolution with local spatial filter (eg 3 x 3 pixel grid)

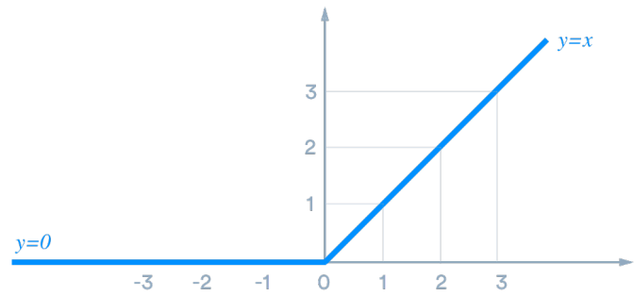
pooling layers reduce H, W while preserving D

Convolutional Neural Networks

CNNs are composed by

two kinds of layers

Convolution of input with **filters**



size-3 Filter

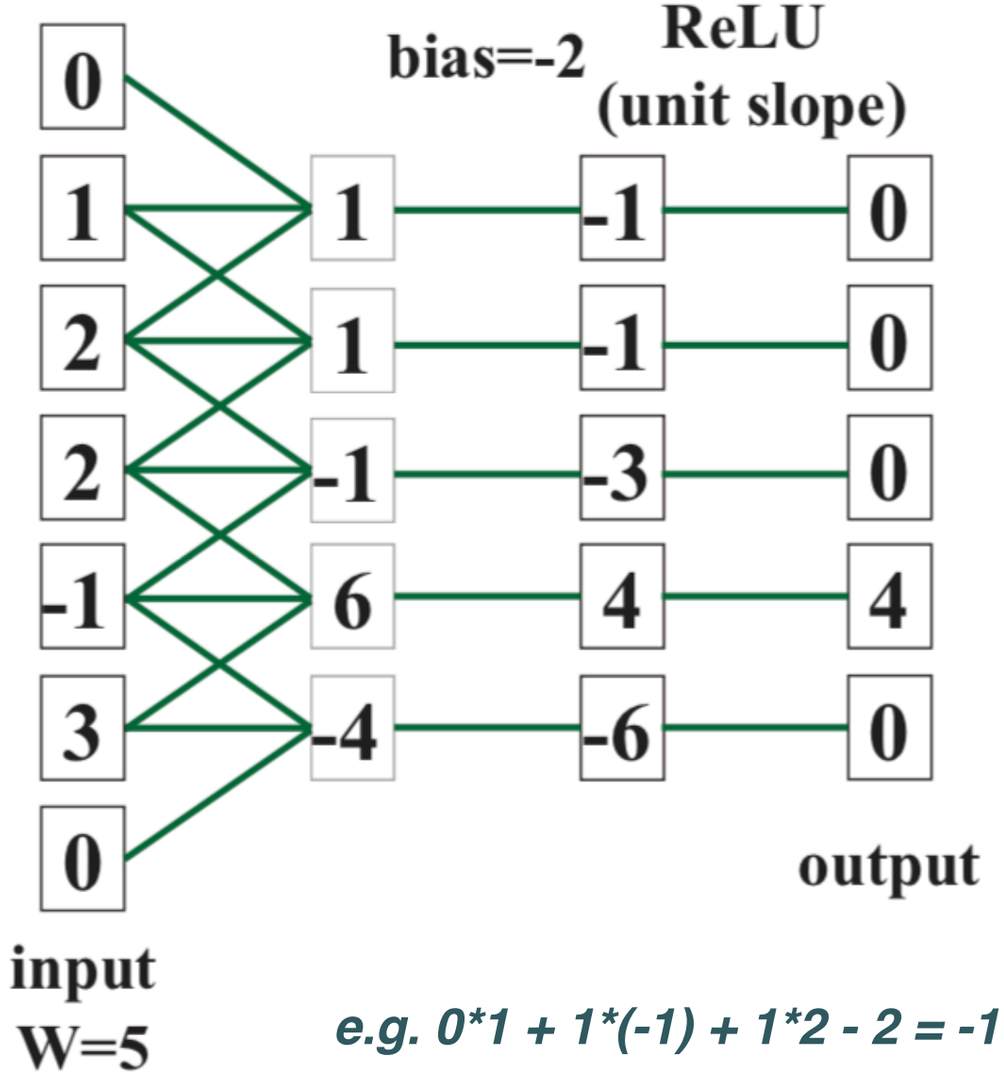
F=3

weight=[1,-1,1]

bias=-2

ReLU

(unit slope)



example of

convolutional layer

note that convolution changes the depth,

but not the height and width of the network

e.g. 0*1 + 1*(-1) + 1*2 - 2 = -1

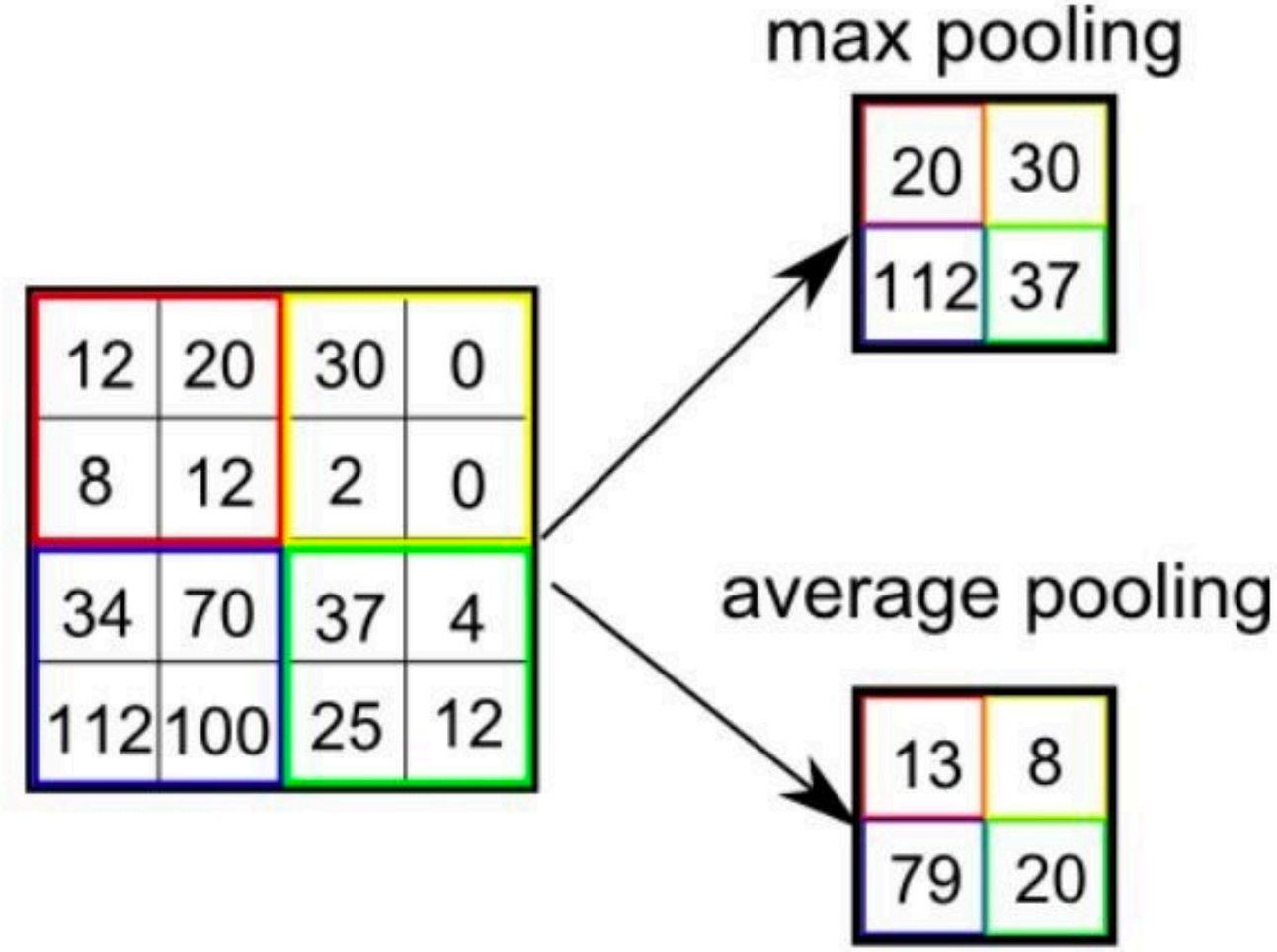
Convolutional Neural Networks

CNNs are composed by two kinds of layers

- Convolution layer of input with **filters**
- **Pooling** layer that coarse-grains the input while maintaining locality and spatial structure

e.g. **MaxPool**, the spatial dimensions are coarse-grained by replacing a small region by single neuron whose output is maximum value of the output in the region

in average pooling, one averages over output in region



Convolutional Neural Networks

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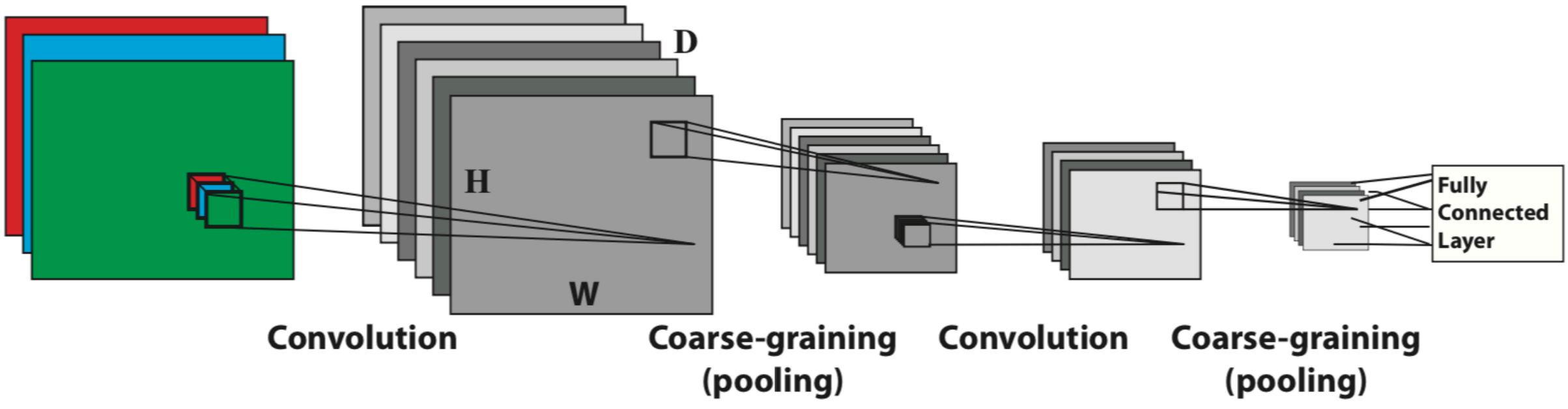
the convolution and max-pool layers are followed by an **all-to-all connected layer and a high-level classifier**, so that one can train CNNs using the standard backpropagation algorithm



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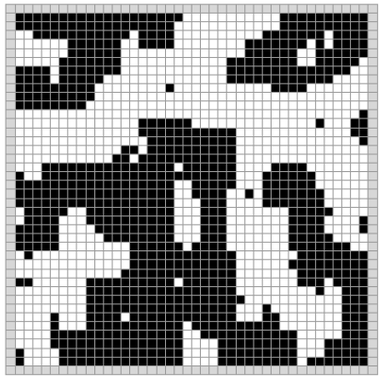
note that only problems characterised by a **spatial locality** are amenable to CNNs:
for example the 2D Ising dataset can be studied with CNNs, but not the SUSY dataset

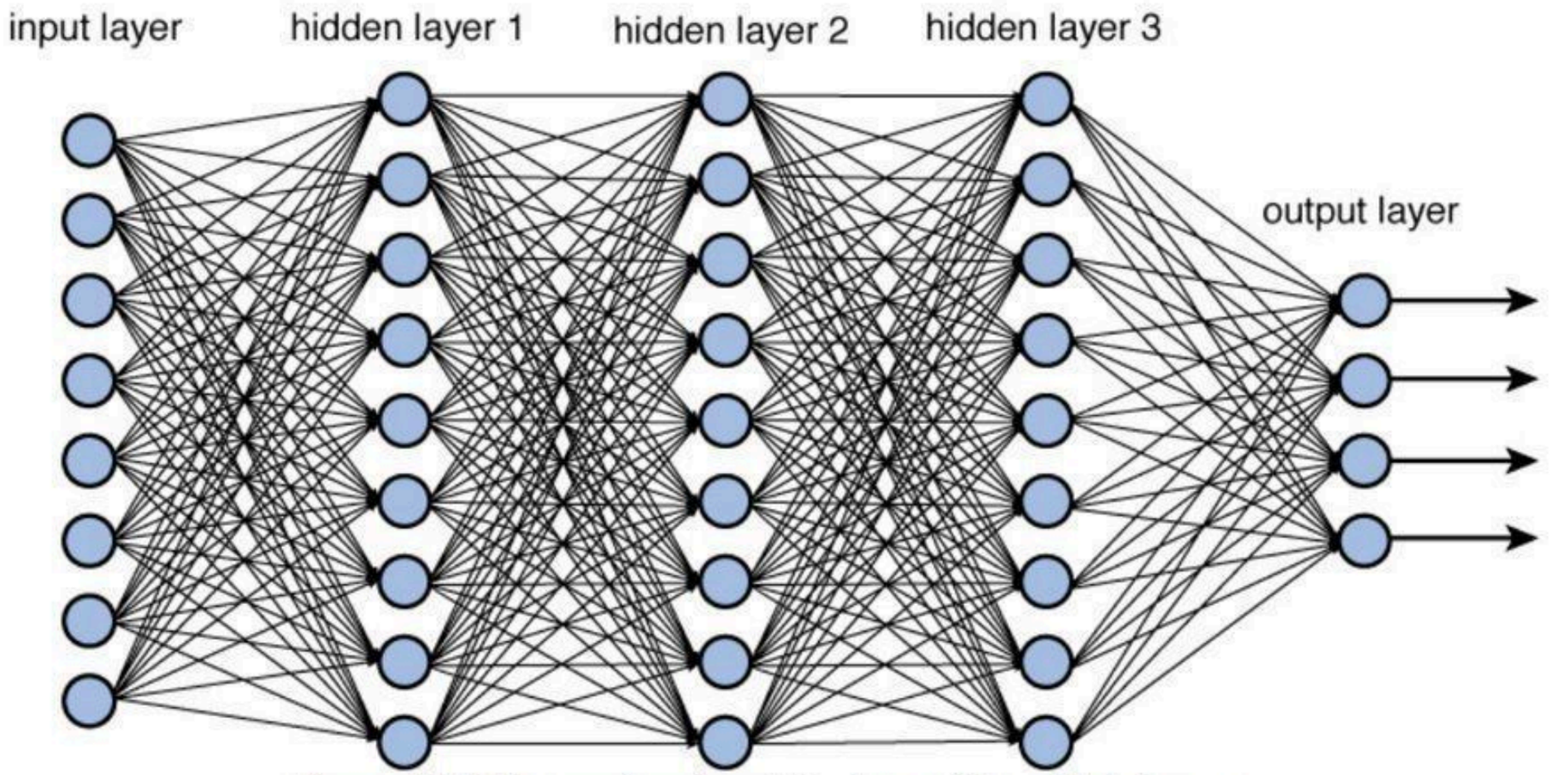


How CNNs work

Bayesian Neural Networks

A probability distribution for NNs

up to here when considering neural networks our goal was to use maximum likelihood to determine the **best values of its model parameters**



$$E(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\left(\mathscr{F}_i^{(\mathrm{dat})} - \mathscr{F}_i^{(\mathrm{model})}(\hat{\boldsymbol{y}};\boldsymbol{\theta})\right)^2 \qquad \frac{\partial E(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = 0 \;\rightarrow \boldsymbol{\theta}_{\mathrm{opt}}$$

plus cross-validation etc

However for many applications we'd like a probabilistic interpretation of the NN output!

A probability distribution for NNs

up to here when considering neural networks our goal was to use maximum likelihood to determine the **best values of its model parameters**

for many applications we'd like to know the **full posterior distribution** of the model

consider the problem of predicting a single continuous target variable t from vector of inputs $\boldsymbol{x}$ by means of a multi-layer feed-forward neural network. Assume the **conditional probability** is

$$p\left(t\,|\,\boldsymbol{x},\boldsymbol{\theta},\beta\right) = \mathcal{N}\left(t\,|\,y(\boldsymbol{x},\boldsymbol{\theta}),\beta^{-1}\right)$$

α, β are the model hyperparameters

conditional probability — *Gaussian Distribution* — *mean: NN output* — *variance*

and we also assume a prior distribution over the model parameters to be Gaussian

prior probability →

$$p(\boldsymbol{\theta}) = \mathcal{N}\left(\boldsymbol{\theta}\,|\,\mathbf{0},\alpha^{-1}\mathbf{1}\right)$$

the key to determine the probability distribution of our ML model is **Bayes' Theorem**

Bayesian Inference

Bayesian inference a method of statistical inference in which **Bayes' theorem** is used to **update the probability for an hypothesis** as more information becomes available

in Bayesian statistics there are two main ingredients:

conditional probability

likelihood function

$$p(\boldsymbol{X} \mid \boldsymbol{\theta})$$

probability of observing the dataset ***X*** given model parameters ***θ***

prior distribution

$$p(\boldsymbol{\theta})$$

prior probability

knowledge of model parameters before we see the data **X**

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which are used to compute the **posterior distribution** using **Bayes' Theorem**

posterior probability

$$p(\boldsymbol{\theta}\,|\,\boldsymbol{X}) = \frac{p(\boldsymbol{X}\,|\,\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int d\boldsymbol{\theta}' p(\boldsymbol{X}\,|\,\boldsymbol{\theta}')p(\boldsymbol{\theta}')}$$

probability of the model parameters ***θ*** after observing the dataset ***X***

Bayesian Inference for Neural Nets

back to our model, given *N* observations, the **likelihood** will just the product of the (independent) conditional probabilities

conditional probability

$$p\left(\mathscr{D}\,|\,\boldsymbol{\theta},\beta\right)=\prod_{n=1}^{N}\mathcal{N}\left(t_n\,|\,y(\boldsymbol{x}_n,\boldsymbol{\theta}),\beta^{-1}\right)$$

dataset

and using Bayes' Theorem, the **posterior probability for the NN parameters** is

posterior probability

$$p\left(\boldsymbol{\theta}\,|\,\mathscr{D},\alpha,\beta\right)\propto p\left(\mathscr{D}\,|\,\boldsymbol{\theta},\beta\right)p\left(\boldsymbol{\theta}\,|\,\alpha\right)$$

which will be **non-gaussian** since the neural-net output depends non-linearly on its params

one can construct a Gaussian approximation to the posterior based on the **Laplace approximation** once we have found a local maximum

$$\ln p\left(\boldsymbol{\theta}\,|\,\mathscr{D},\alpha,\beta\right)=-\frac{\alpha}{2}\boldsymbol{\theta}^T\boldsymbol{\theta}-\frac{\beta}{2}\sum_{n=1}^{N}\left(y(\boldsymbol{x}_n,\boldsymbol{\theta})-t_n\right)^2+\text{const}$$

log-likelihood

from prior

for fixed α,β one can find a local minimum with standard algorithms such as SGD with backpropagation

Bayesian Inference for Neural Nets

having found a local maximum of the posterior distributions, we can construct its Gaussian approximation by means of the **Hessian matrix** (matrix of second derivatives)

$$\boldsymbol{A} = -\nabla^2 \ln p\left(\boldsymbol{\theta} \,|\, \mathscr{D}, \alpha, \beta\right) = \alpha \boldsymbol{I} + \beta \boldsymbol{H}$$

$$H_{ij} = \frac{\partial^2}{\partial \theta_i \partial \theta_j} \left(\frac{1}{2} \sum_{n=1}^{N} \left(y(\boldsymbol{x}_n, \boldsymbol{\theta}) - t_n \right)^2 \right)$$

and thus the **gaussian approximation to the posterior** is

$$p\left(\boldsymbol{\theta} \,|\, \mathscr{D}, \alpha, \beta\right) \simeq q\left(\boldsymbol{\theta} \,|\, \mathscr{D}, \alpha, \beta\right) = \mathcal{N}\left(\boldsymbol{\theta} \,|\, \boldsymbol{\theta}_{\mathrm{MAP}}, \boldsymbol{A}^{-1}\right)$$

full posterior — *gaussian approx* — *local max of posterior*

finally we are able to evaluate the sought-for **predictive distribution** by marginalising

$$p(t \,|\, \boldsymbol{x}, \mathscr{D}) = \int p(t \,|\, \boldsymbol{x}, \boldsymbol{\theta}, \beta)\, q\left(\boldsymbol{\theta} \,|\, \mathscr{D}, \alpha, \beta\right)$$

probability to observe an output t given 1) a new input vector x and 2) the training dataset D

conditional probability, depends on NN function output

probability dist of the model parameters given training dataset

Bayesian Inference for Neural Nets

now we can evaluate **the full probability distribution** associated to our ML model!

$$p(t\,|\,\boldsymbol{x},\mathscr{D}) = \int p(t\,|\,\boldsymbol{x},\boldsymbol{\theta},\beta)\, q\left(\boldsymbol{\theta}\,|\,\mathscr{D},\alpha,\beta\right)$$

unfortunately the integral is still very complicated given the non-linear nature of the NN output

we can simply this expression with the assumption that the (Gaussian) **posterior distribution varies slowly** as compared to the NN output

$$p(t\,|\,\boldsymbol{x},\mathscr{D},\alpha,\beta) = \mathcal{N}\left(t\,|\,y(\boldsymbol{x},\boldsymbol{\theta}_{\mathrm{MAP}}),\sigma^2(\boldsymbol{x})\right)$$

where the input dependent variance of this gaussian distribution is given by

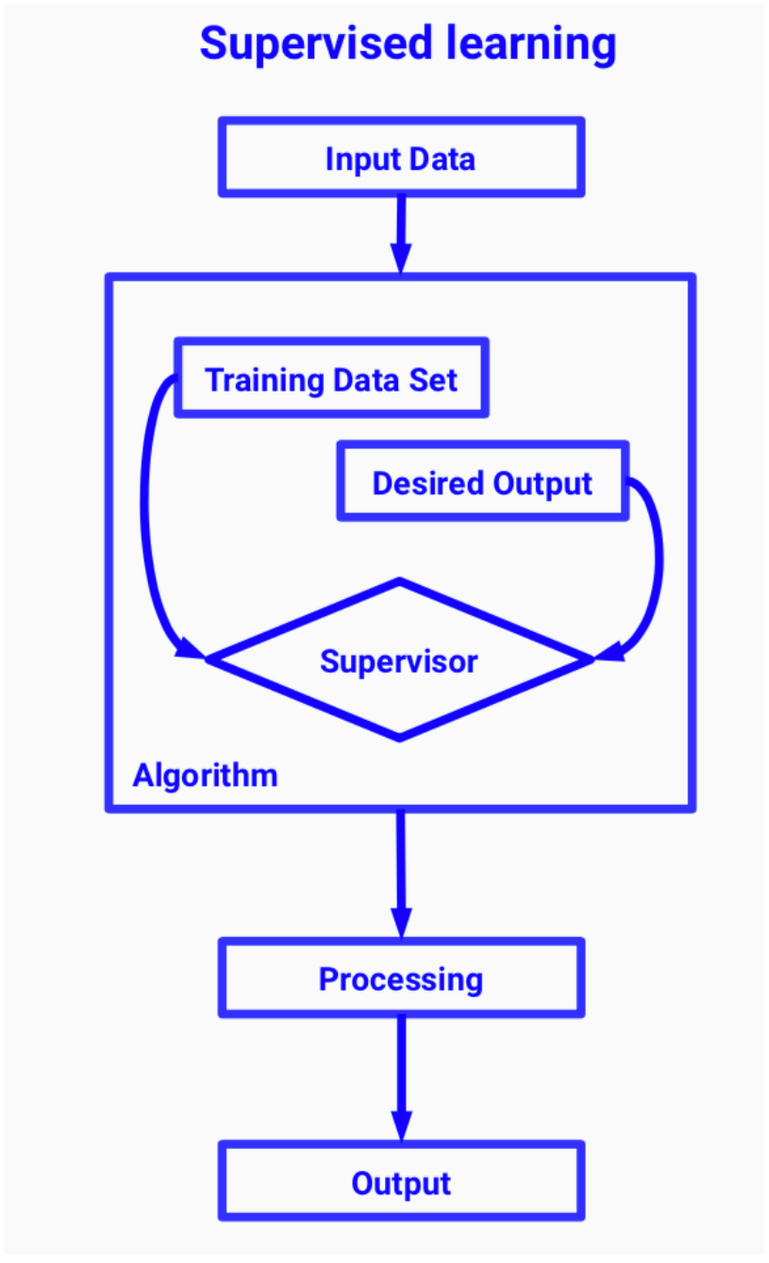
$$\sigma^2(\boldsymbol{x}) = \beta^{-1} + \boldsymbol{g}^T\boldsymbol{A}^{-1}\boldsymbol{g}$$

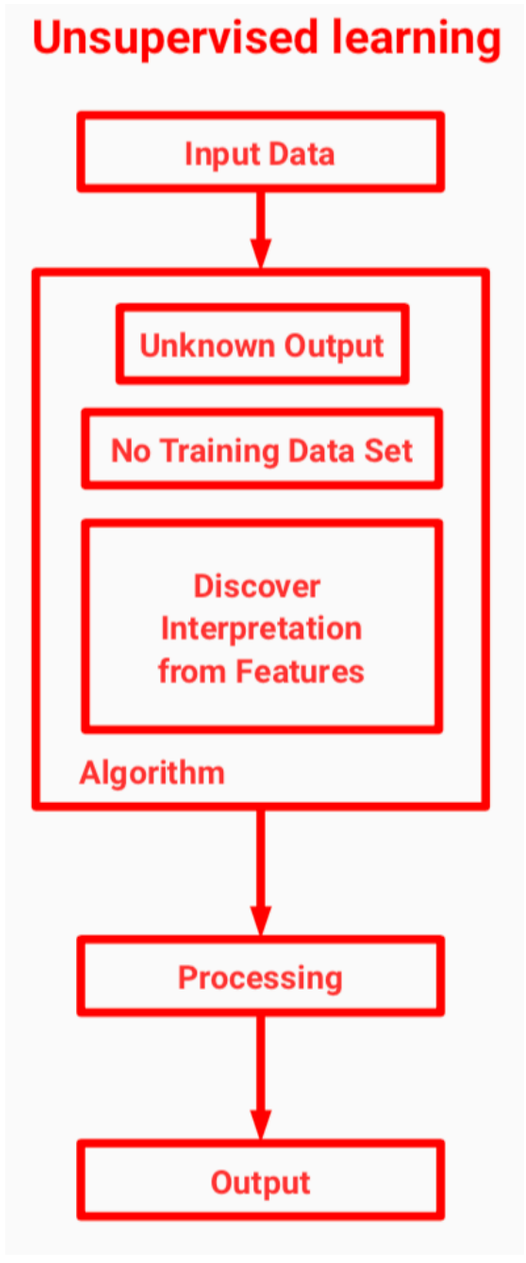
$$y\left(\boldsymbol{x},\boldsymbol{\theta}\right) \simeq y\left(\boldsymbol{x},\boldsymbol{\theta}_{\mathrm{MAP}}\right) + \boldsymbol{g}^T(\boldsymbol{\theta}-\boldsymbol{\theta}_{\mathrm{MAP}})$$

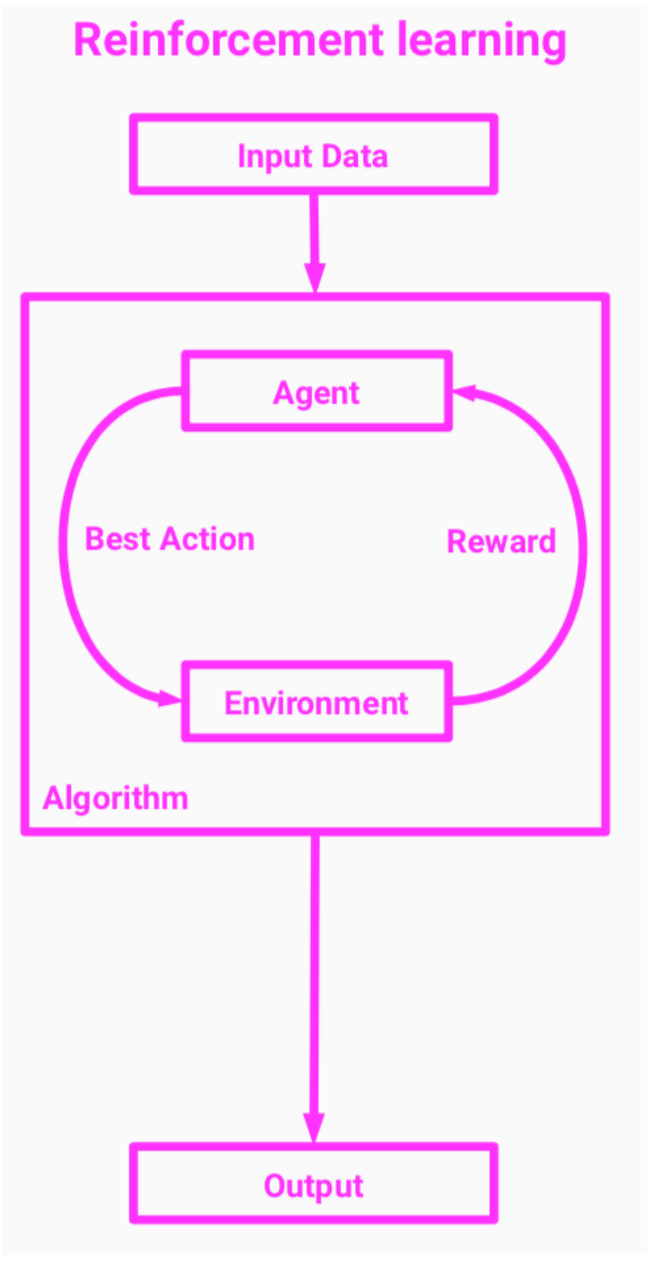
finally the hyperparameters of the model can be determined by means of the **evidence framework**

Reinforcement Learning

Supervised vs Unsupervised Learning







Reinforcement Learning

So far we have considered **two main paradigms** in Machine Learning problems

Supervised Learning: starting from a training dataset with **labelled examples,** $\{x_i, y_i\}_{i=1,N}$, produce a **model f(x)** that predicts and generalises the info in the training sample.
The labels y_i can be continuous (underlying law is function) or discrete (classification)

Unsupervised Learning: starting from a training dataset with **unlabelled examples,** $\{x_i\}_{i=1,N}$, produce a **model** that takes a sample as input and as output produces the solution of a practical problem, such as **clustering**, **dimensional reduction**, or **outlier detection**

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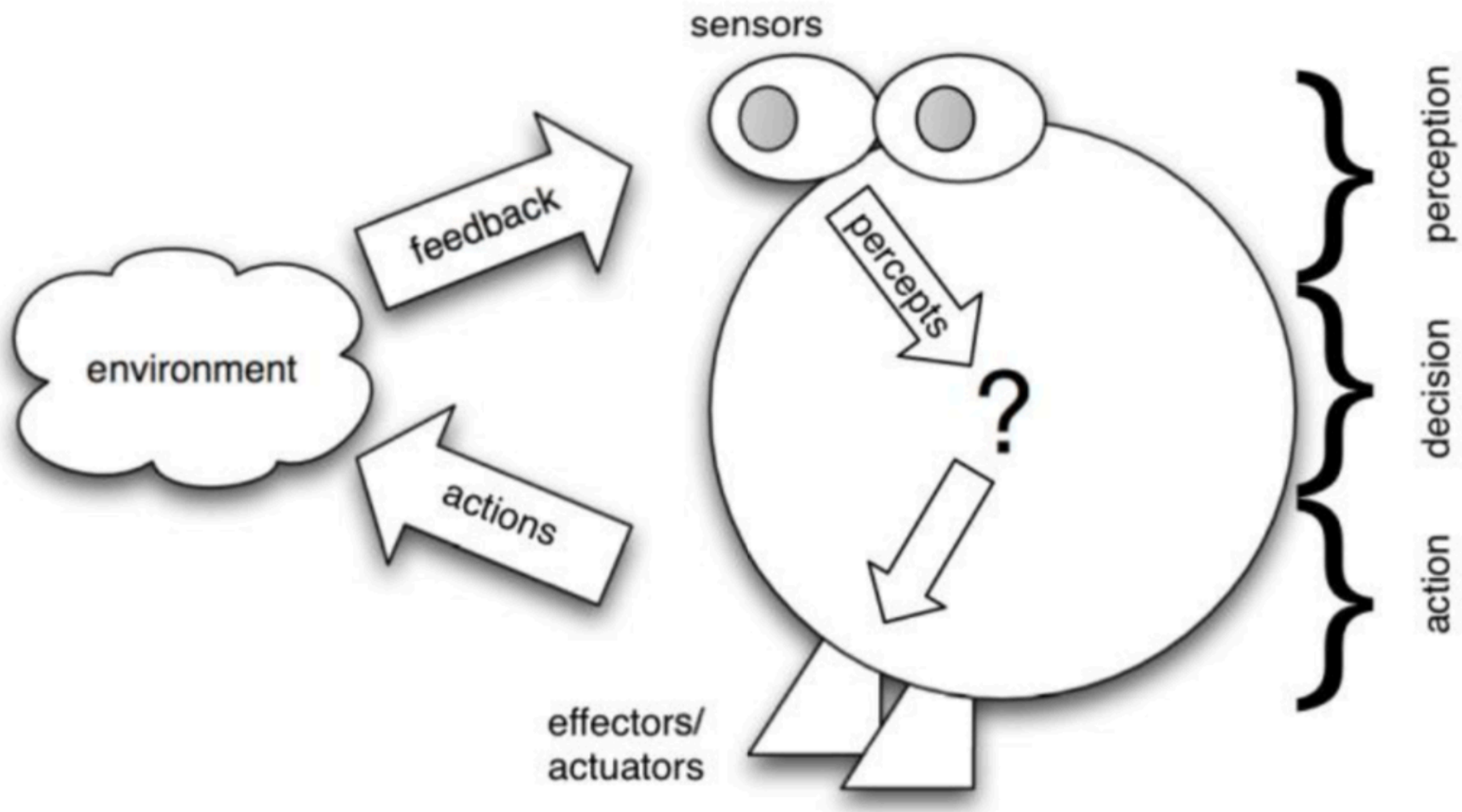
now we want to discuss a **third ML paradigm**

Reinforcement Learning: given a complex task in a complex environment (dynamic, non deterministic, only partly accessible) train an **agent** that carry out **autonomous action** in this environment and complete the requested task

Agents in Reinforcement Learning

In the context of **Reinforcement Learning,** an **agent** is a computer system capable **autonomous action** in some environment, in order to achieve its delegated goals



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Can you think of trivial ``agents''?

Agents in Reinforcement Learning

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trivial agents: thermostat, e-mail daemons, alarms, ….

Agents in Reinforcement Learning

In the context of **Reinforcement Learning,** an **agent** is a computer system capable **autonomous action** in some environment, in order to achieve its delegated goals

non-trivial agents should exhibit the following properties:

- ***Reactive*:** interact with environment and react its changes
- ***Proactive***: recognise opportunities and take initiative
- ***Social*:** cooperate with other agents (and humans!) via cooperation, negotiation, coordination
- ***Rational:*** the agent will always act to fulfil its goals
- ***Adaptability:*** the agent is able to improve its performance over time

Agents in Reinforcement Learning

Environments in RL can exhibit the following features:

- ***Accessible or Inaccessible*:** can the agent obtain updated and accurate information about the state of the environment?

- ***Deterministic or non-deterministic*** : has each action that the agent perform always associated the same effect?

- ***Static vs dynamics*:** is the environment stable expect for the action of the agent?

- ***Discrete vs continuous:*** are there a finite or infinite number of actions possible?

A Reinforcement Learning system

The ultimate goal of **Reinforcement Learning** is to

design an agent that **performs complex tasks** and **takes autonomous action** to fulfil its design goals, in an environment that is: partly inaccessible, non-deterministic, non-episodic, dynamic and continuous (*i.e.* the real world!).

☑ The agent receives the state of the environment as a **vector of features** (inputs)

☑ The agent can execute actions in every state, with different actions bringing **different** rewards

☑ Goal: **learn a policy**, i.e. a function that maps the features of an state vector to an optimal action to be taken in that stage

☑ An action is optimal if it **maximizes the expected average reward**

☑ In RL **decision making is sequential and the goal is long-term** (i.e. game playing, robotics, resource management, ...)

Agents in Reinforcement Learning

The ultimate goal of **Reinforcement Learning** is to

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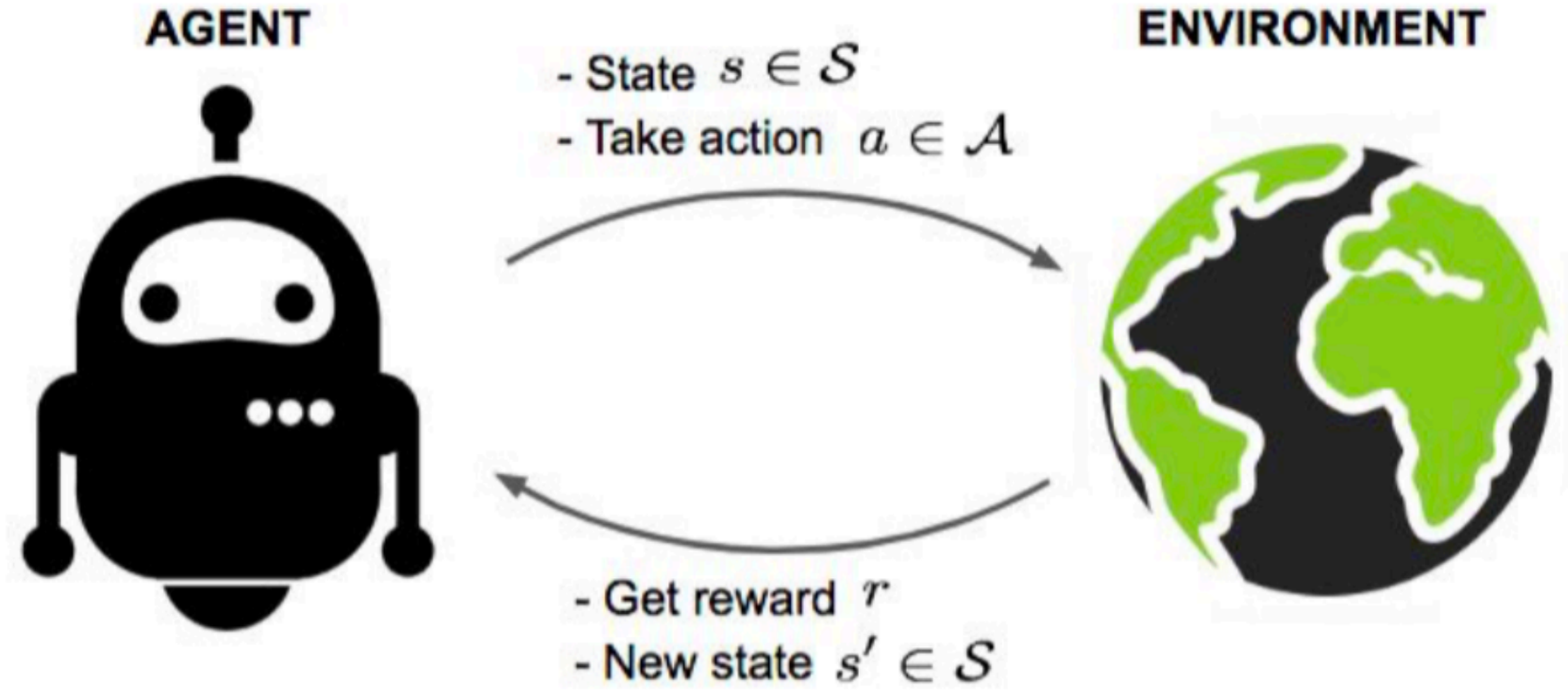
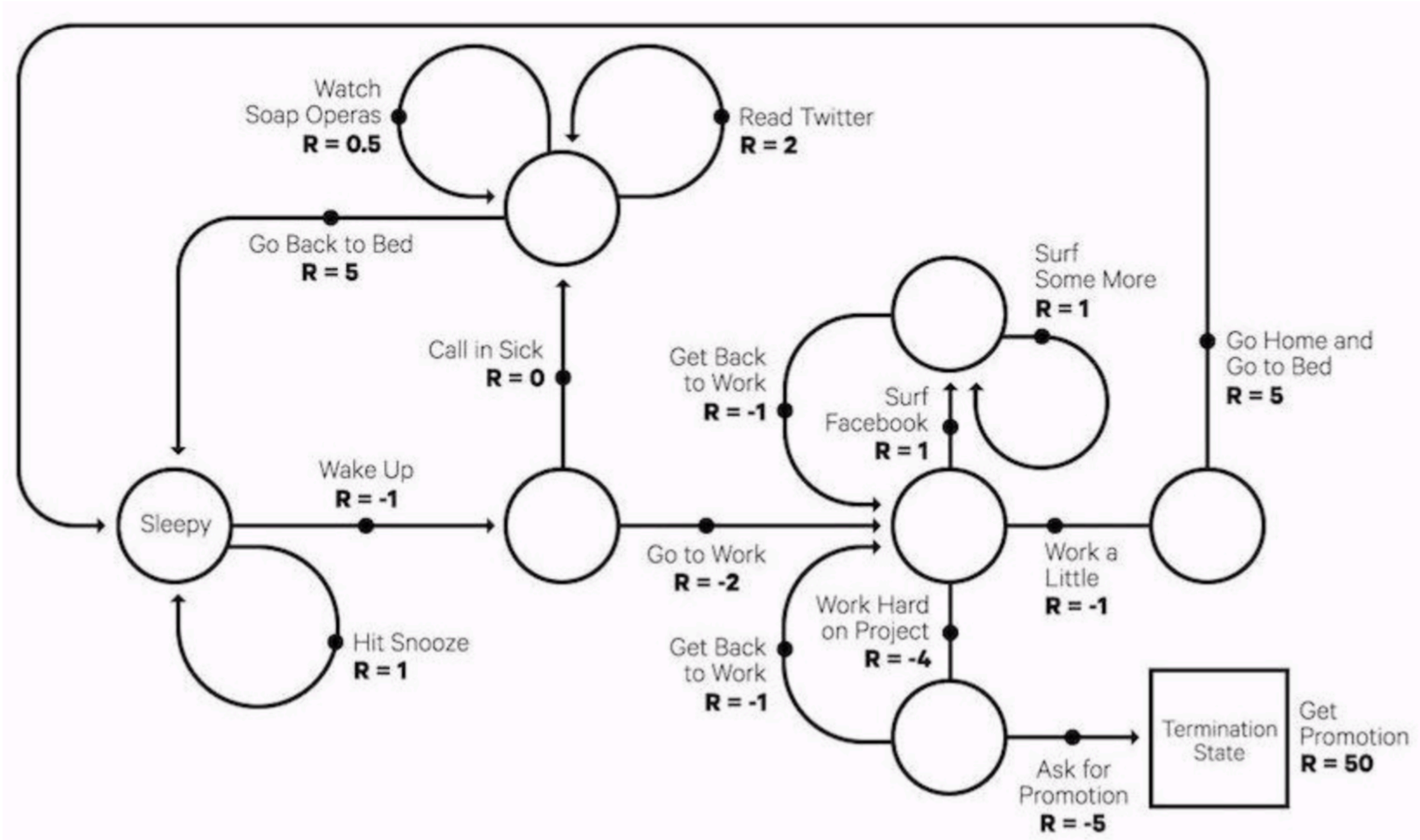


A Reinforcement Learning system

use **Reinforcement Learning** is to determine the actions that will get us a promotion at work!

the goal of RL is **maximise the total reward**: need to explore all possible options to determine the best policy for each action that it might need to carry

A Reinforcement Learning system



explore all possible options to determine the best policy for each action that it might need to carry

Reinforcement Learning for Games

AlphaGo: using machine learning to master the ancient game of Go

BLOG POST
RESEARCH

04 DEC 2018

AlphaZero: Shedding new light on chess, shogi, and Go

BLOG POST
RESEARCH

24 JAN 2019

AlphaStar: Mastering the Real-Time Strategy Game StarCraft II

In late 2017 we introduced AlphaZero, a single system that taught itself from scratch how to master the games of chess, shogi (Japanese chess), and Go, beating a world-champion program in each case. We were excited by the preliminary results and thrilled to see the response from members of the chess community, who saw in AlphaZero's games a ground-breaking, highly dynamic and "unconventional" style of play that differed from any chess playing engine that came before it.

Reinforcement Learning for Games

DeepMind AlphaStar: AI breakthrough or pushing the limits of reinforcement learning?

By **Ben Dickson** - November 4, 2019

4 min read

DeepMind's AI program AlphaStar managed to defeat 99.8 percent of StarCraft II players.

Reinforcement Learning for Games

Q-learning

Q-learning is a **model-free reinforcement learning algorithm,** which aims to learn a **policy** about what actions should the agent carry out for different circumstances

no model of the environment need: the agent learns to maximise its future reward by repeatedly interacting with the environment

In Q-learning, the weight for a step into the future is calculated by the **discount factor**

$$0 \leq \gamma^{\Delta t} \leq 1$$

earlier rewards valued higher than later ones

analog of cost function in Supervised Learning is the **quality of state-action combination**

$$Q : S \times A \rightarrow \mathbb{R}$$

quality function — *state* — *action*

the goal of Q-learning is to determine the actions that the agent should take for each state in order to **maximise the total reward**

Q-learning

Schematically, at **each iteration of the Q-learning** algorithm the following steps take place:

- The agent selects an **action** a_t
- As a consequence of this action, the agent observes a **reward** r_t
- The agent then then enters into a **new state** s_t
- The quality function (cost function) Q is updated

$$Q^{\text{new}}(s_t, a_t) \leftarrow (1 - \alpha) \times Q^{\text{old}}(s_t, a_t) + \alpha \left(r_t + \gamma \times \max_a Q(s_{t+1}, a) \right)$$

reward

learning rate

discount factor

(estimate of) future optimal value

After training, **the agent has a policy** Q which tells it how to act for each circumstance

Deep Q-Networks

the model for the **policy function** (which action to take as function of the state) can be parametrised using Deep Neural Networks, in this case called Q-Networks