UNIVERSITY OF TECHNOLOGY
IN THE EUROPEAN CAPITAL OF CULTURE
CHEMNITZ

Deep Reinforcement Learning

Deep learning

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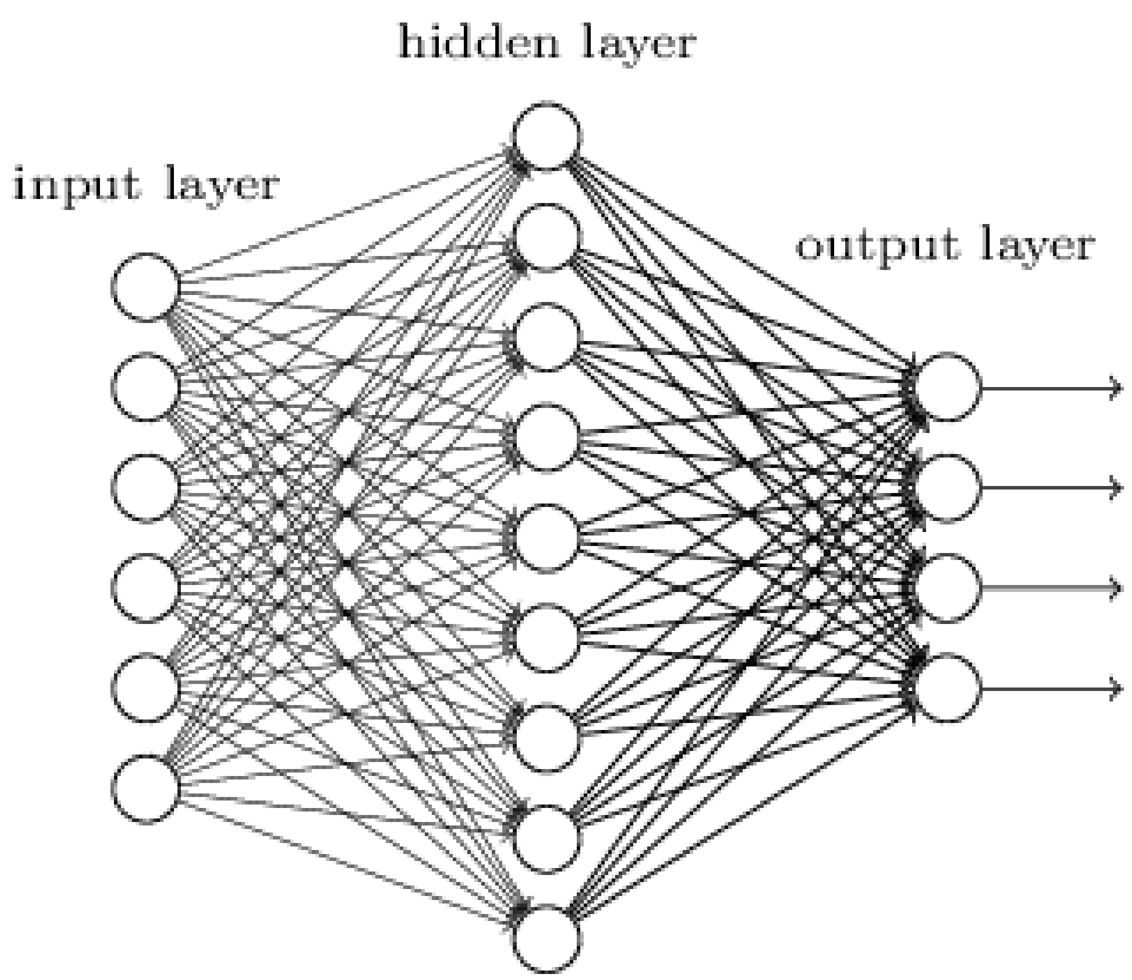
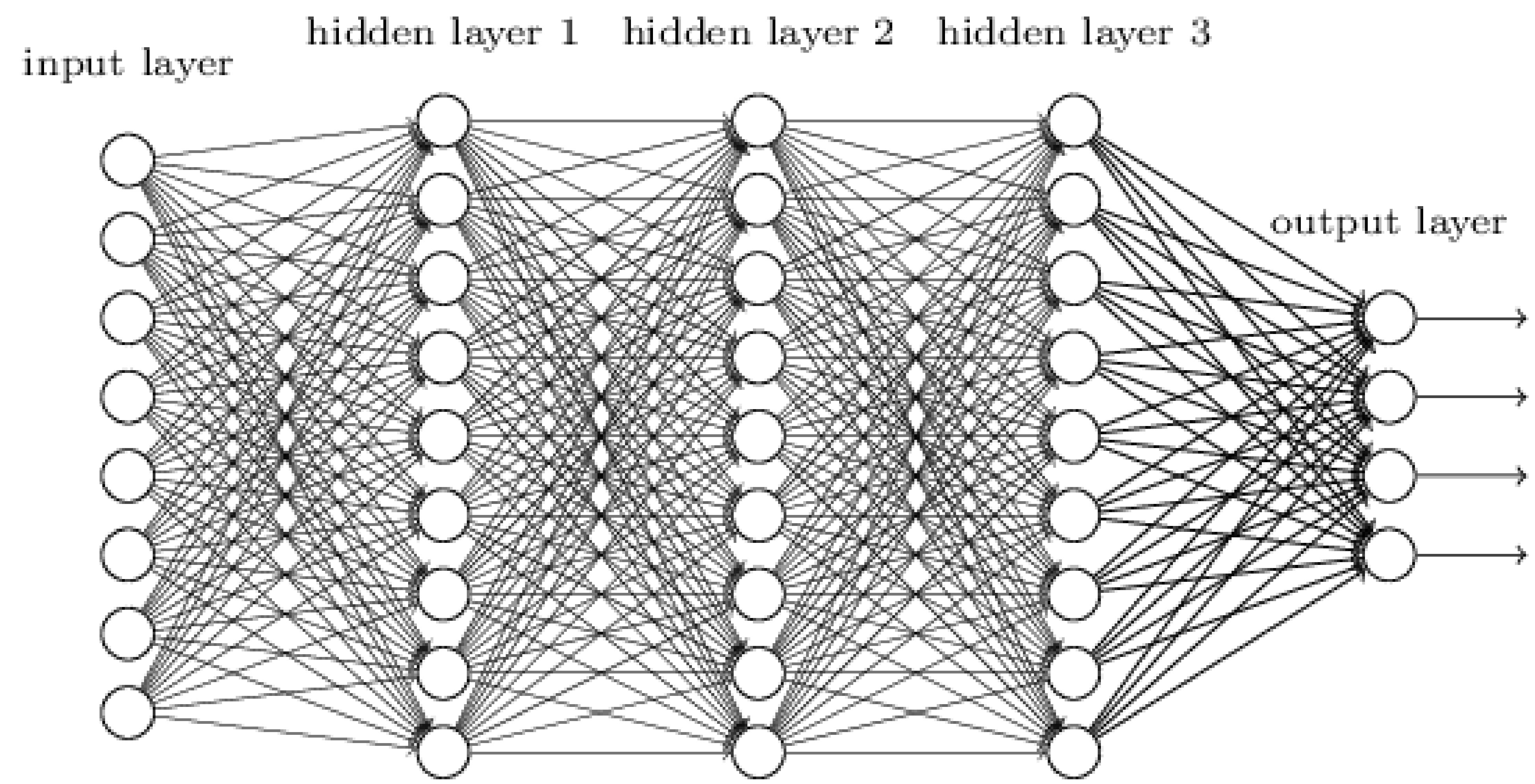
1 - Artificial neural networks

Artificial neural networks

- An **artificial neural network** (ANN) is a cascade of **fully-connected** (FC) layers of artificial neurons.





- Each layer k transforms an input vector $\mathbf{h}_{k-1}$ into an output vector $\mathbf{h}_k$ using a weight matrix W_k, a bias vector $\mathbf{b}_k$ and an activation function $f()$.

$$\mathbf{h}_k = f(W_k \times \mathbf{h}_{k-1} + \mathbf{b}_k)$$

- Overall, ANNs are **non-linear parameterized function estimators** from the inputs $\mathbf{x}$ to the outputs $\mathbf{y}$ with parameters θ (all weight matrices and biases).

$$\mathbf{y} = F_\theta (\mathbf{x})$$

Loss functions

- ANNs can be used for both **regression** (continuous outputs) and **classification** (discrete outputs) tasks.
- In supervised learning, we have a fixed **training set** $\mathcal{D}$ of N samples $(\mathbf{x}_t, \mathbf{t}_i)$, where t_i is the **desired output** or **target**.
- **Regression:**
  - The output layer uses a **linear** activation function: $f(x) = x$
  - The network minimizes the **mean square error** (mse) of the model on the training set:

$$\mathcal{L}(\theta) = \mathbb{E}_{\mathbf{x}, \mathbf{t} \in \mathcal{D}}[||\mathbf{t} - \mathbf{y}||^2]$$

- **Classification:**
  - The output layer uses the **softmax** operator to produce a probability distribution: $y_j = \frac{e^{z_j}}{\sum_k e^{z_k}}$
  - The network minimizes the **cross-entropy** or **negative log-likelihood** of the model on the training set:

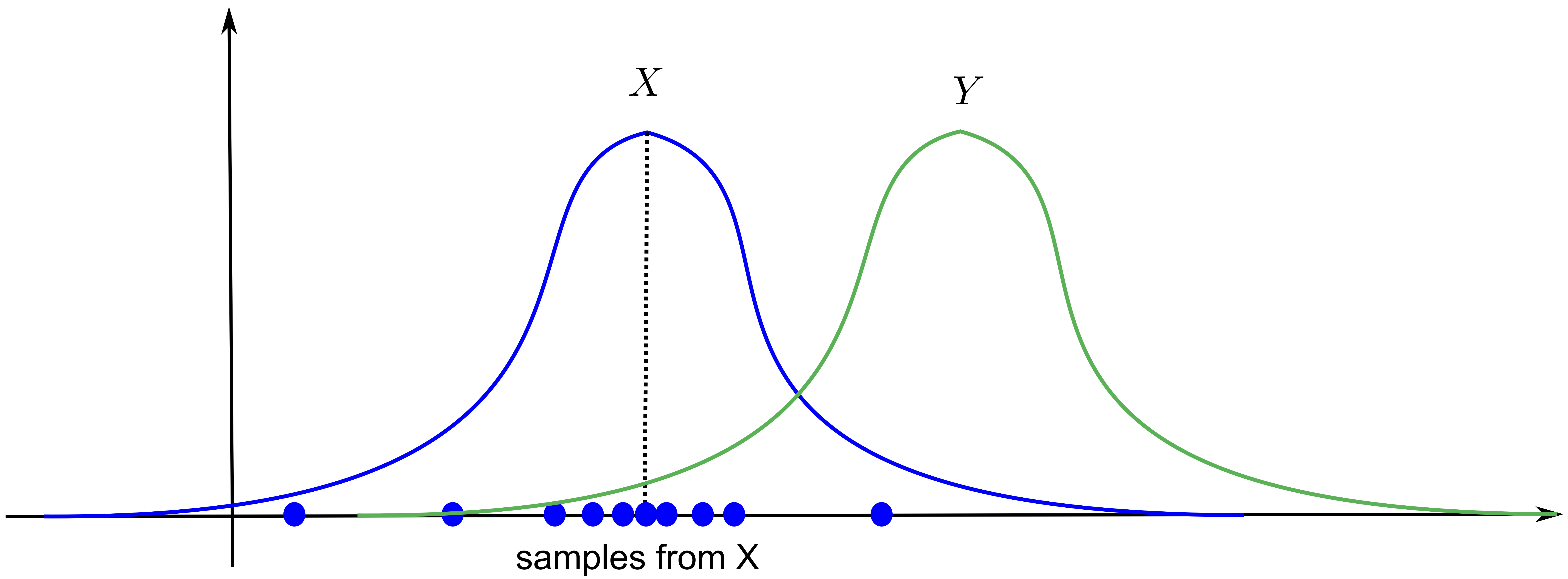
$$\mathcal{L}(\theta) = \mathbb{E}_{\mathbf{x}, \mathbf{t} \in \mathcal{D}}[- \mathbf{t} \, \log \mathbf{y}]$$

Cross-entropy

- The cross-entropy between two probability distributions X and Y measures their similarity:

$$H(X, Y) = \mathbb{E}_{x \sim X} [- \log P(Y = x)]$$

- Are samples from X likely under Y?
- Minimizing the cross-entropy makes the two distributions equal almost anywhere.



Cross-entropy

- In supervised learning, the targets $\mathbf{t}$ are fixed **one-hot encoded vectors**.

$$\mathcal{L}(\theta) = \mathbb{E}_{\mathbf{x}, \mathbf{t} \in \mathcal{D}}[- \sum_j t_j \, \log y_j]$$

- But it could be any target distribution.

Backpropagation

- In both cases, we want to minimize the loss function by applying **Stochastic Gradient Descent** (SGD) or a variant (Adam, RMSprop).

$$\Delta \theta = - \eta \, \nabla_\theta \mathcal{L}(\theta)$$

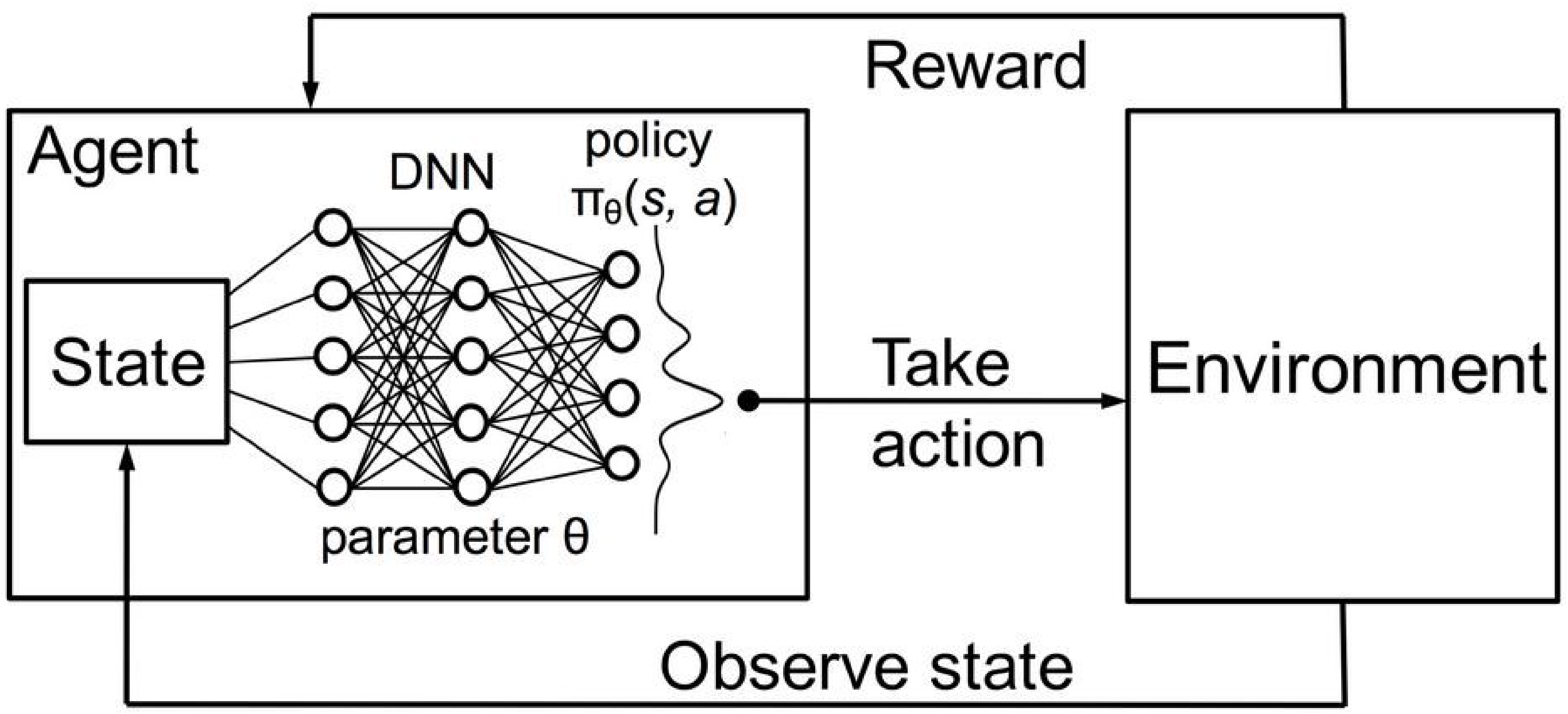
- The question is how to compute the **gradient of the loss function** w.r.t the parameters θ.
- For both the mse and cross-entropy loss functions, we have:

$$\nabla_\theta \mathcal{L}(\theta) = \mathbb{E}_\mathcal{D} [- (\mathbf{t} - \mathbf{y}) \, \nabla_\theta \, \mathbf{y}]$$

- There is an algorithm to compute efficiently the gradient of the output w.r.t the parameters: **backpropagation** (see Neurocomputing).
- In deep RL, we do not care about backprop: tensorflow or pytorch do it for us.

Rumelhart, Hinton, Williams (1986). “Learning representations by back-propagating errors”. Nature.

Components of neural networks



- There are three aspects to consider when building a neural network:

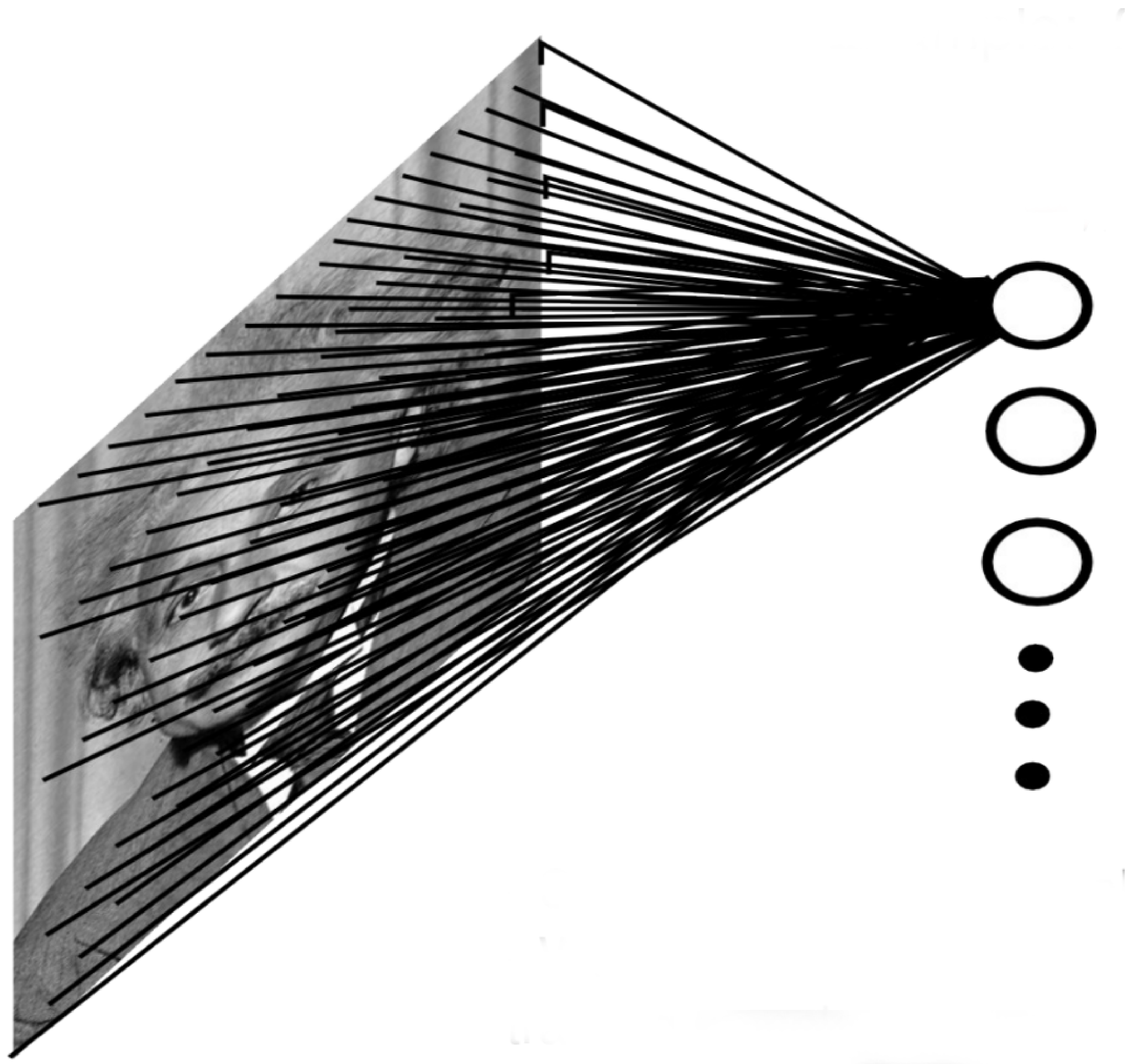
1. **Architecture:** how many layers, what type of layers, how many neurons, etc.
    - Task-dependent: each RL task will require a different architecture. Not our focus.
2. **Loss function:** what should the network do?
    - Central to deep RL!
3. **Update rule** how should we update the parameters θ to minimize the loss function? SGD, backprop.
    - Not really our problem, but see *natural gradients* later.

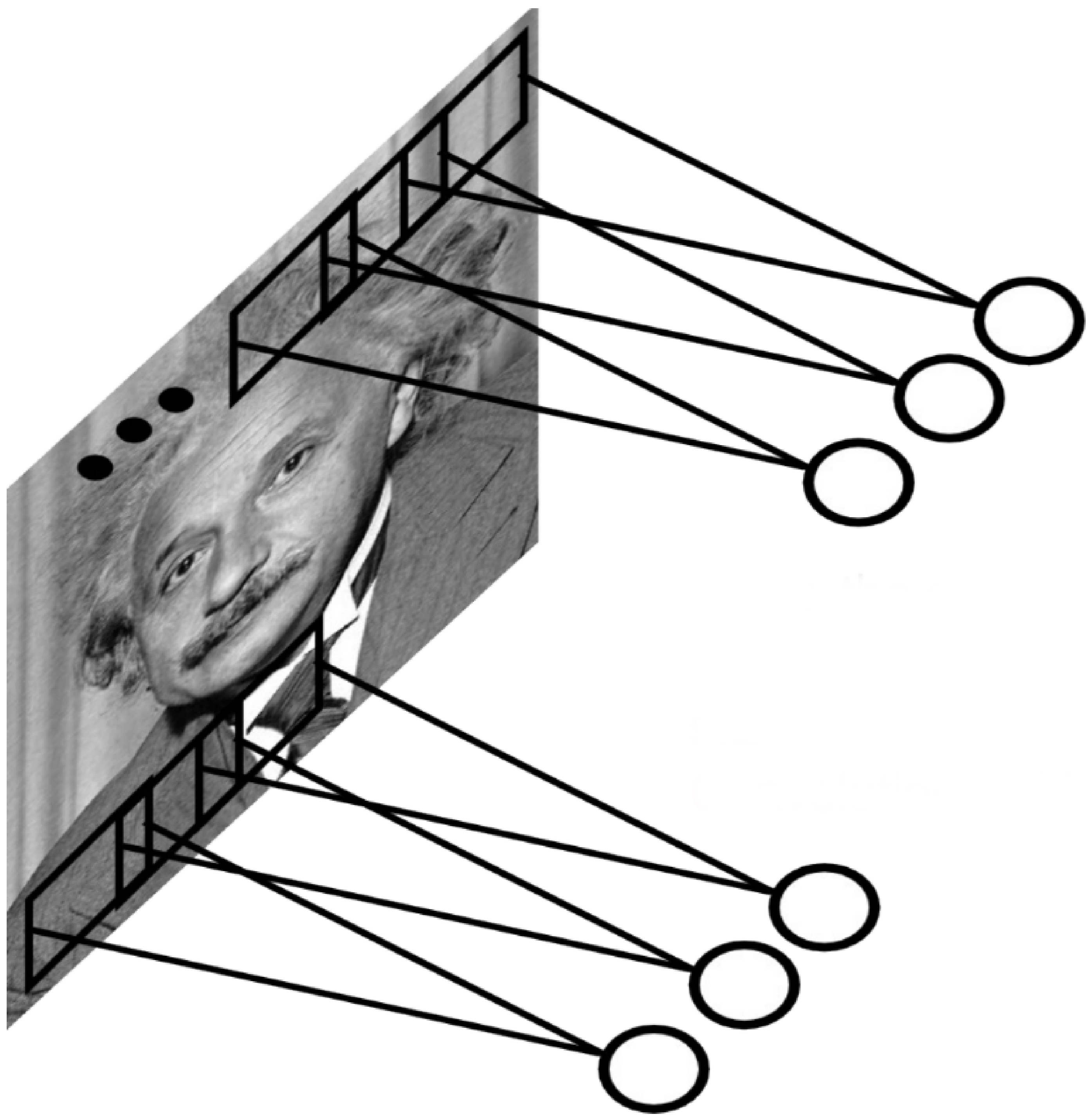
2 - Convolutional neural networks

Convolutional layers

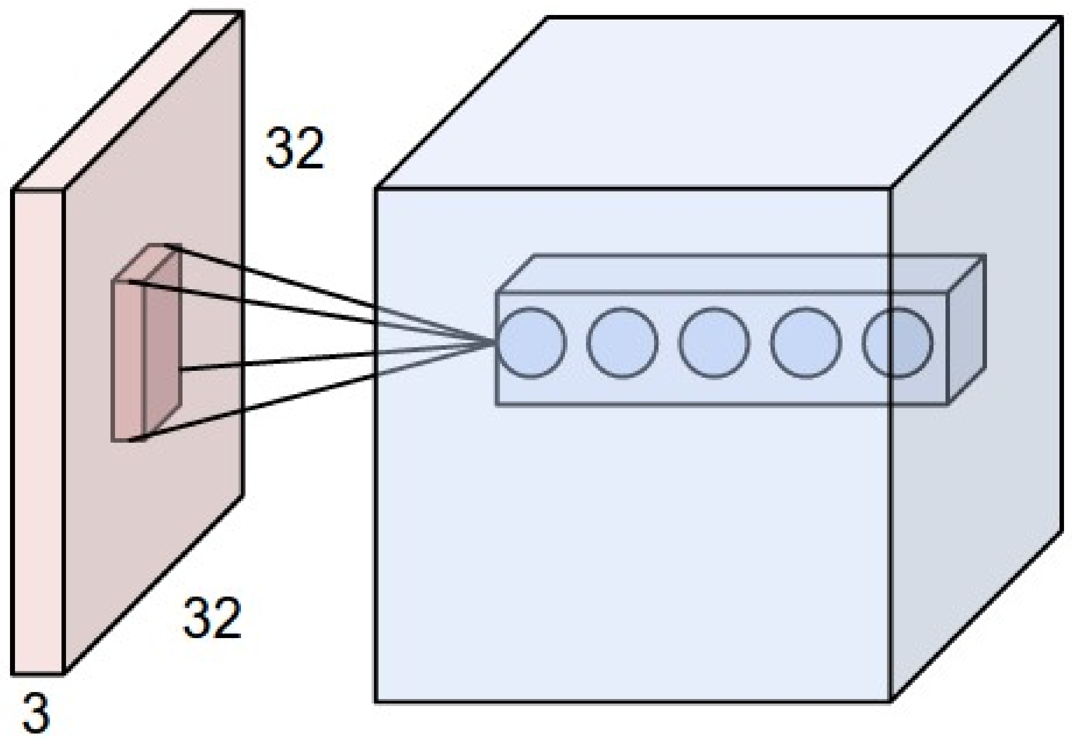
- When using images as inputs, **fully-connected networks** (FCN) would have too many weights:
  - Slow.
  - Overfitting.

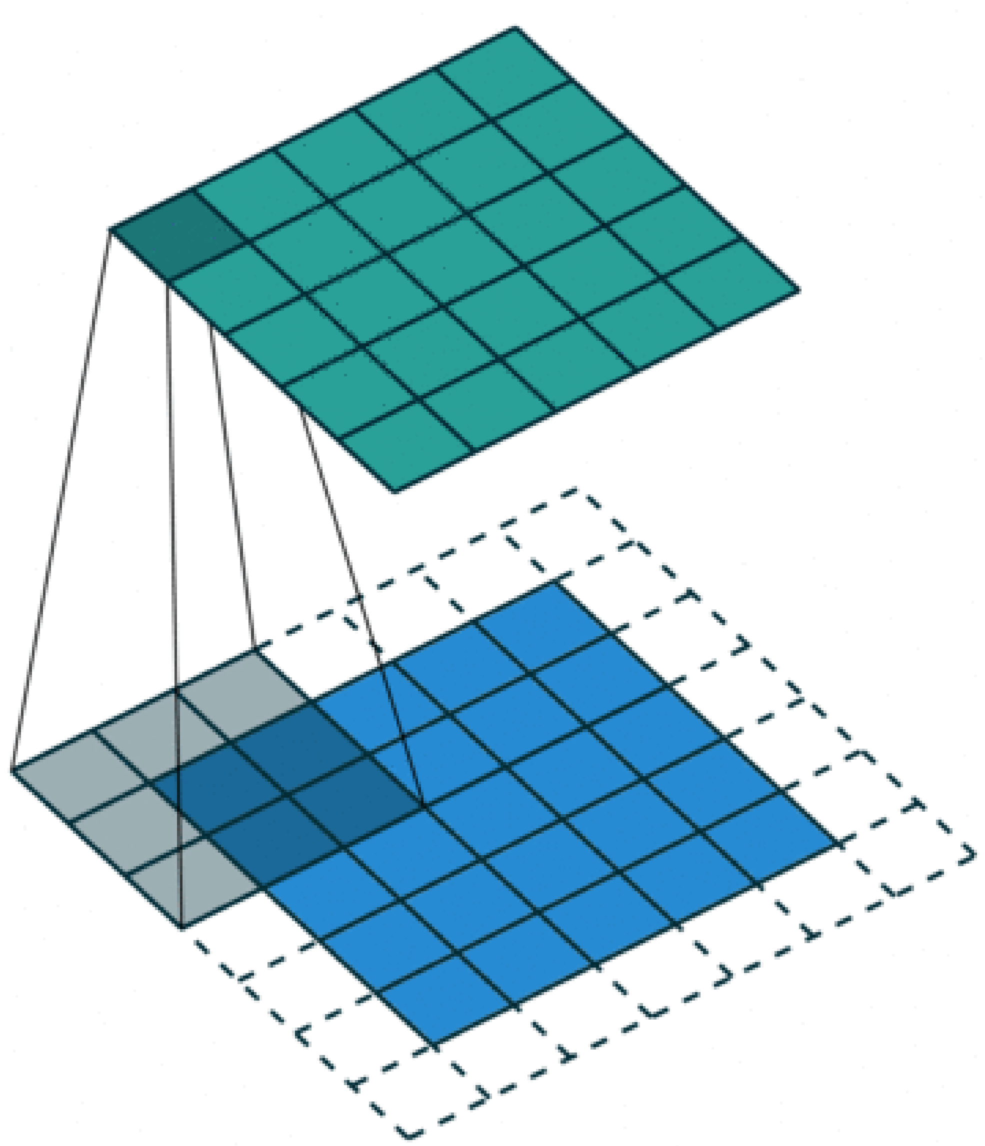
- **Convolutional layers** reduce the number of weights by **reusing** weights at different locations.
  - Principle of a convolution.
  - Fast and efficient.





Convolutional layers

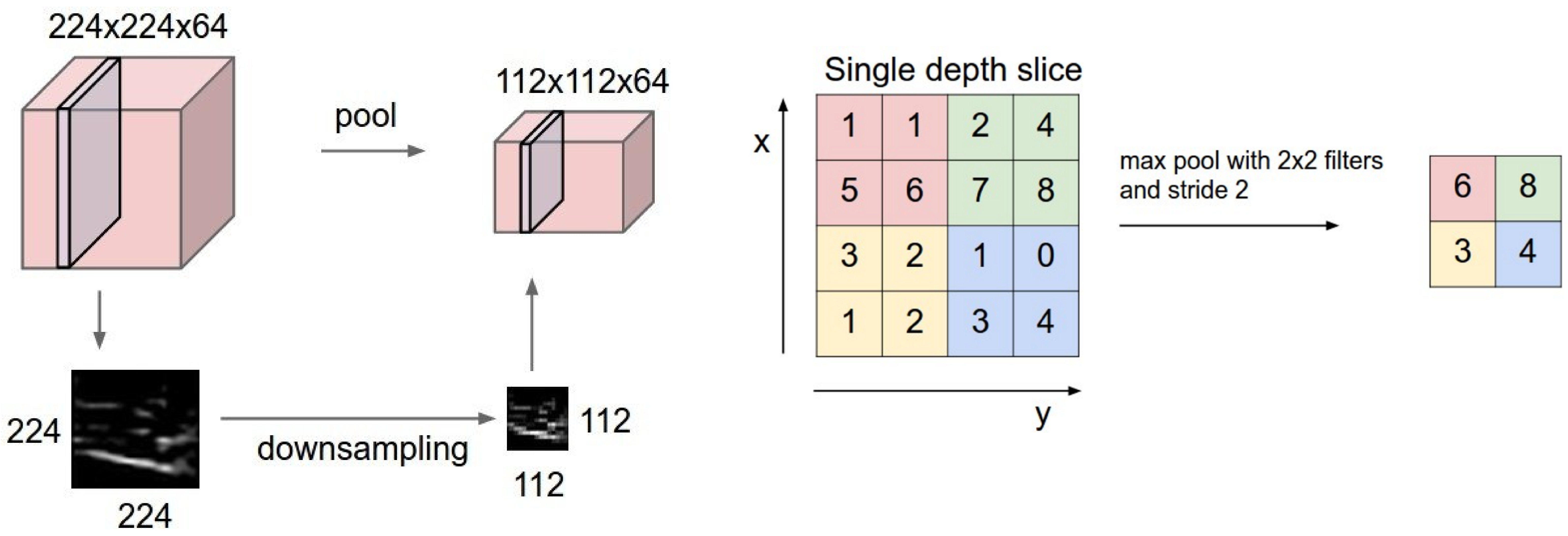




- A **convolutional layer** extracts **features** of its inputs.
- d filters are defined with very small sizes (3x3, 5x5...).
- Each filter is convoluted over the input image (or the previous layer) to create a **feature map**.
- The set of d feature maps becomes a new 3D structure: a **tensor**.
- If the input image is 32x32x3, the resulting tensor will be 32x32xd.
- The convolutional layer has only very few parameters: each feature map has 3x3 values in the filter and a bias, i.e. 10 parameters.
- The convolution operation is **differentiable**: backprop will work.

Source: https://github.com/vdumoulin/conv_arithmetic

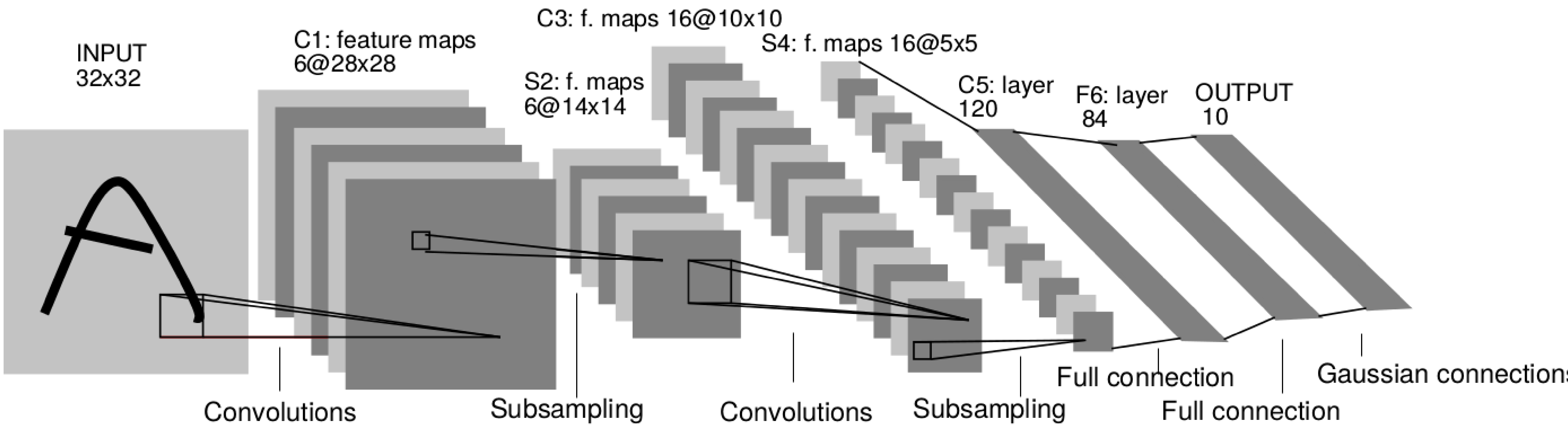
Max-pooling



Source: http://cs231n.github.io/convolutional-networks/

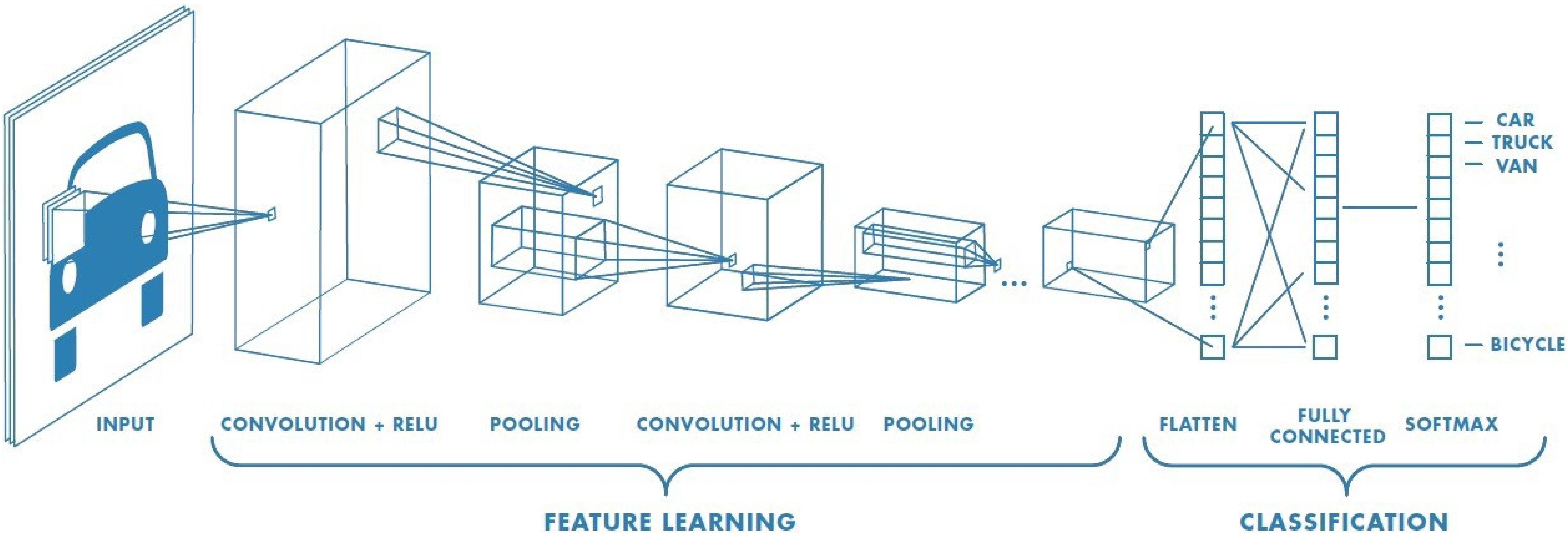
- The number of elements in a convolutional layer is still too high. We need to reduce the spatial dimension of a convolutional layer by **downsampling** it.
- For each feature, a **max-pooling** layer takes the maximum value of a feature for each subregion of the image (mostly 2x2).
- Pooling allows translation invariance: the same input pattern will be detected whatever its position in the input image.
- Max-pooling is also differentiable.

Convolutional neural networks



- A **convolutional neural network** (CNN) is a cascade of convolution and pooling operations, extracting layer by layer increasingly complex features.
- The spatial dimensions decrease after each pooling operation, but the number of extracted features increases after each convolution.
- One usually stops when the spatial dimensions are around 7x7.
- The last layers are fully connected. Can be used for regression and classification depending on the output layer and the loss function.
- Training a CNN uses backpropagation all along: the convolution and pooling operations are differentiable.

Convolutional neural networks



Source: https://towardsdatascience.com/a-comprehensive-guide-to-convolutional-neural-networks-the-eli5-way-3bd2b1164a53

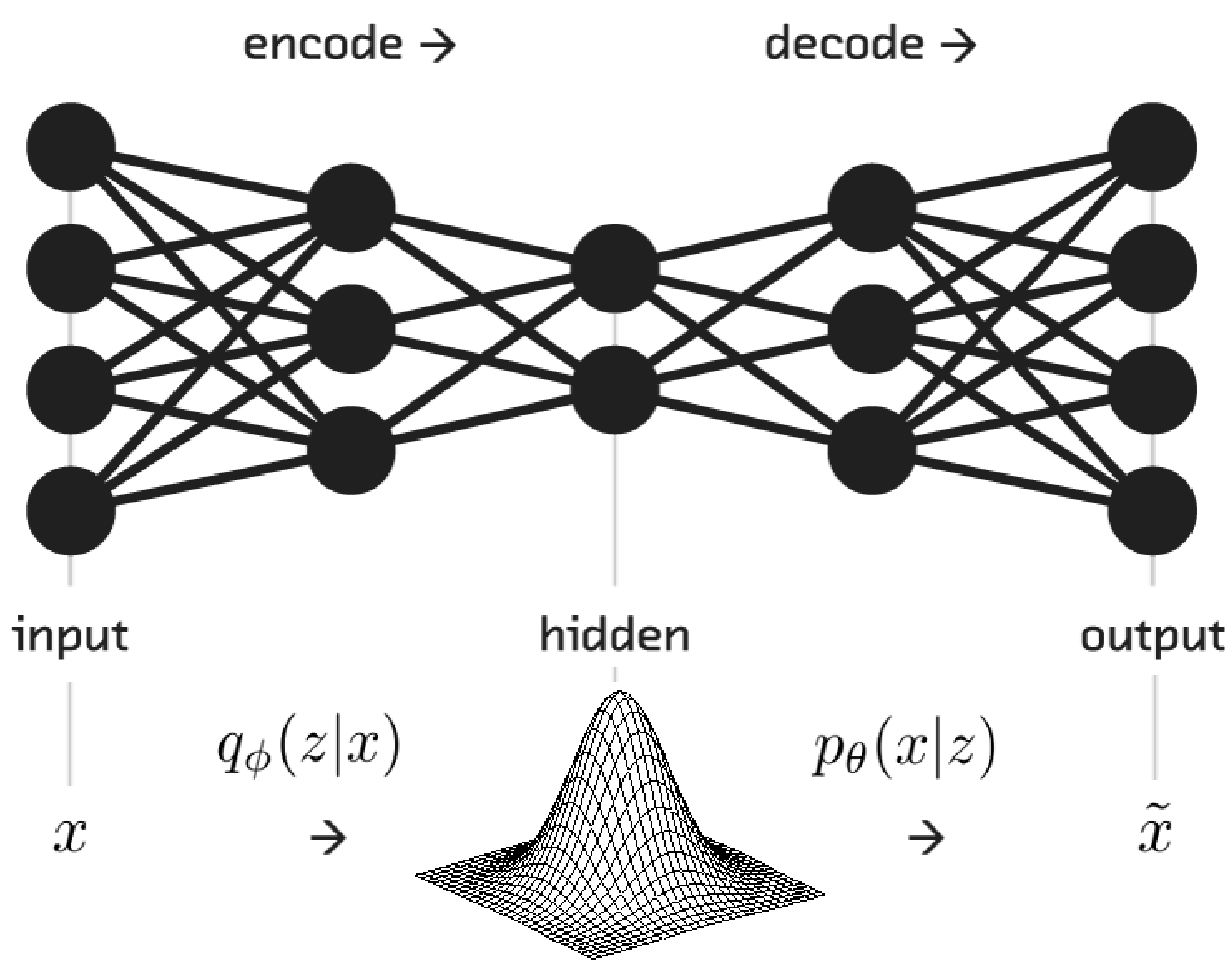
- The only thing we need to know is that CNNs are non-linear function approximators that work well with images.

$$\mathbf{y} = F_\theta(\mathbf{x})$$

- The conv layers **extract complex features** from the images through learning.
- The last FC layers allow to approximate values (regression) or probability distributions (classification).

3 - Autoencoders

Autoencoders



- The problem with FCN and CNN is that they **extract features** in supervised learning tasks.
    - Need for a lot of annotated data (image, label).
- **Autoencoders** allows **unsupervised learning**:
    - They only need inputs (images).
- Their task is to **reconstruct** the input:

$$\mathbf{y} = \tilde{\mathbf{x}} \approx \mathbf{x}$$

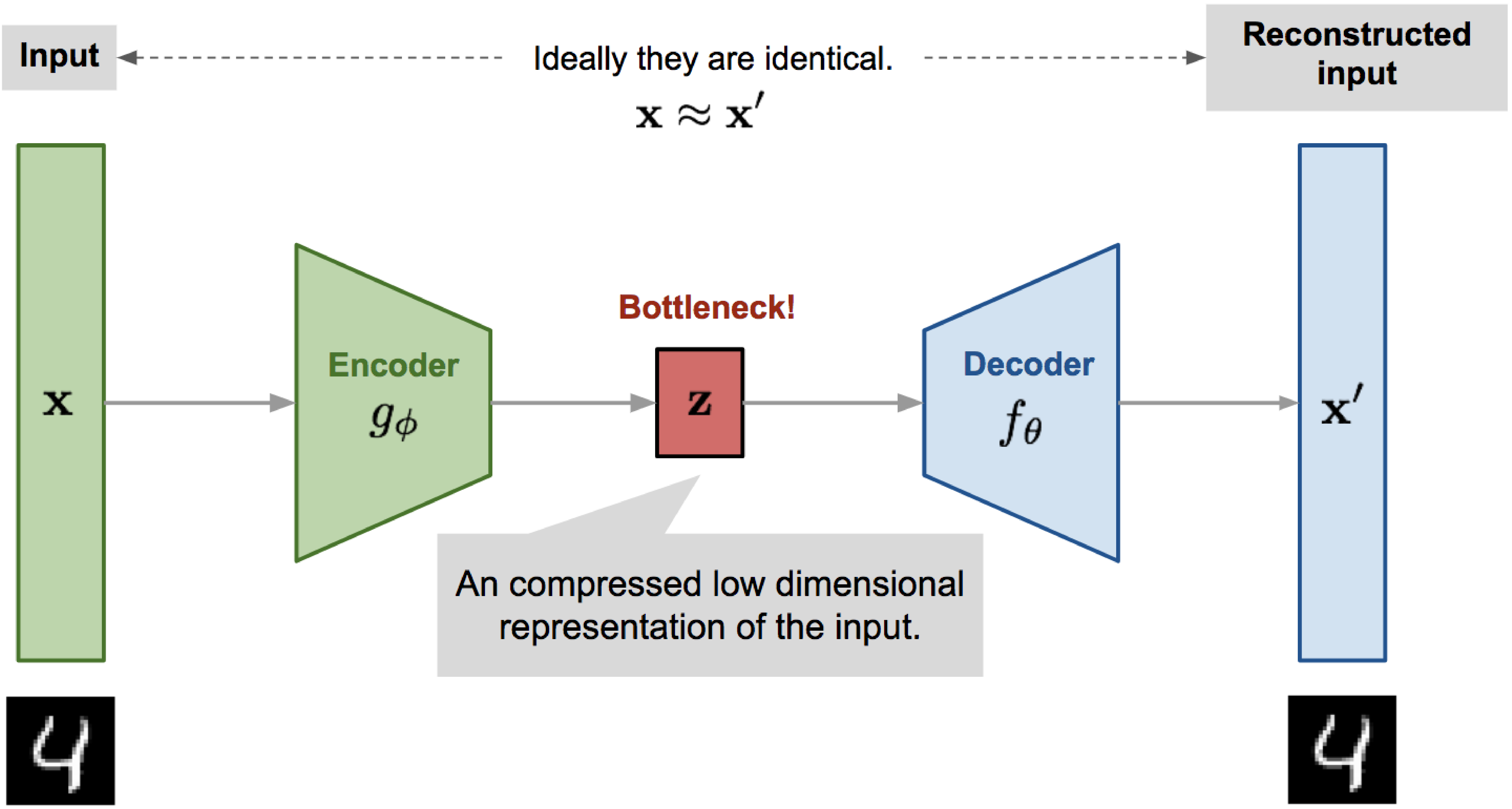
- The **reconstruction loss** is simply the **mse** between the input and its reconstruction.

$$\mathcal{L}_\text{autoencoder}(\theta) = \mathbb{E}_{\mathbf{x} \in \mathcal{D}} [||\tilde{\mathbf{x}} - \mathbf{x}||^2]$$

- Apart from the loss function, they are trained as regular NNs.

Autoencoders

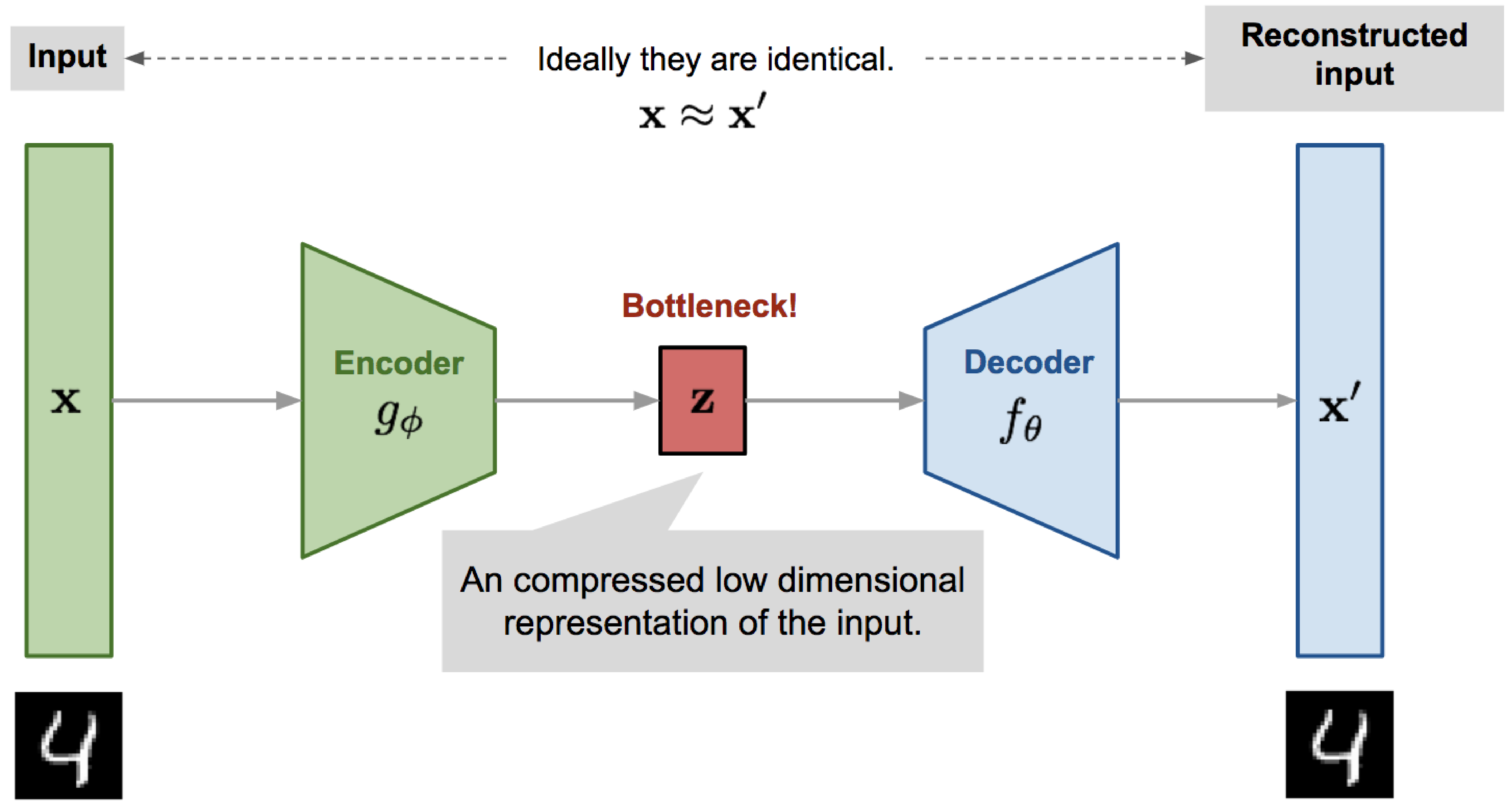
- Autoencoders consists of:
  - the **encoder**: from the input $\mathbf{x}$ to the **latent space** $\mathbf{z}$.
  - the **decoder**: from the latent space $\mathbf{z}$ to the reconstructed input $\tilde{\mathbf{x}}$.



Source: https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

Autoencoders

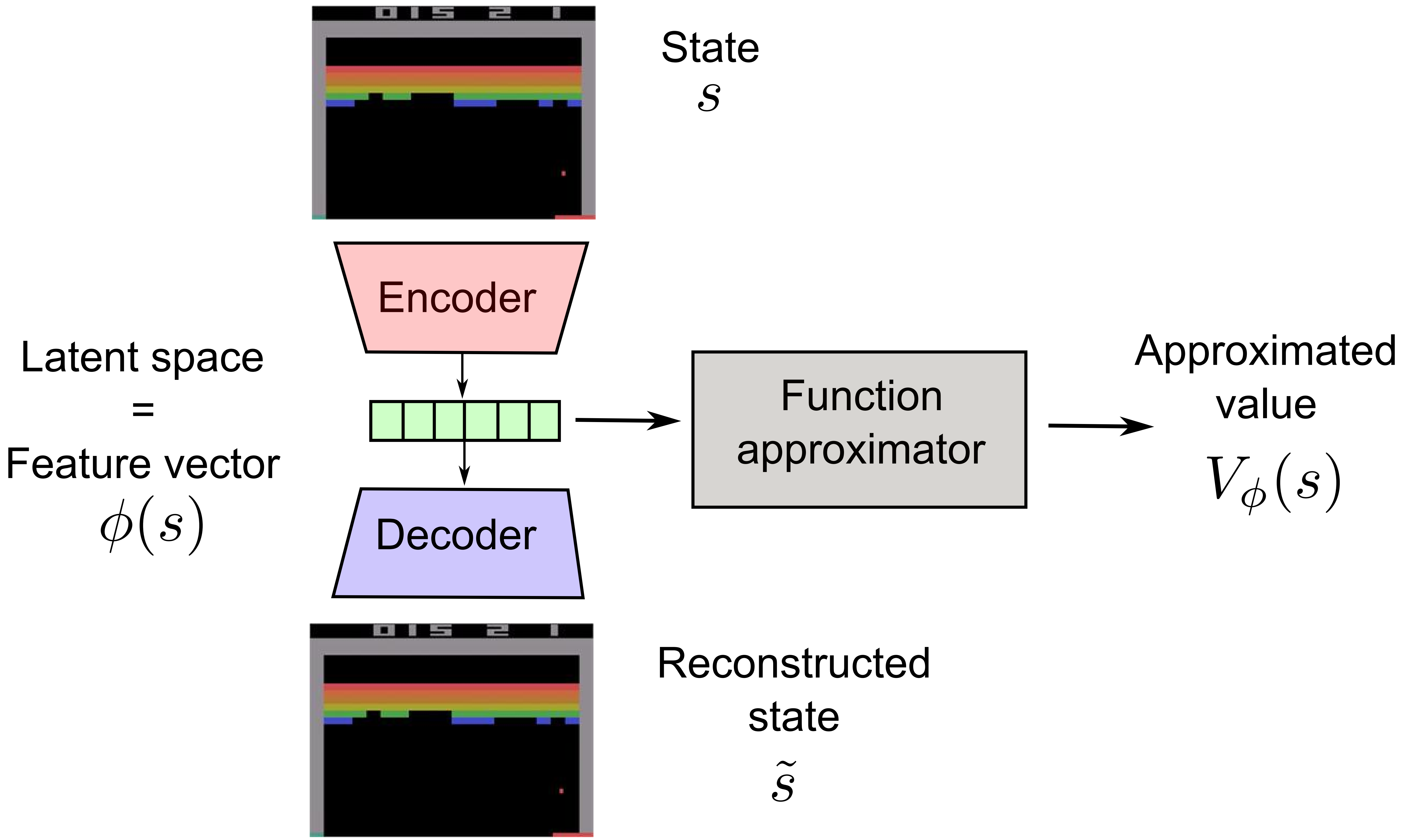
- The **latent space $\mathbf{z}$** is a **compressed representation** (bottleneck) of the inputs $\mathbf{x}$.
- It has to learn to compress efficiently the inputs without losing too much information, in order to reconstruct the inputs.
  - Dimensionality reduction.
  - Unsupervised feature extraction.



Source: https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

Autoencoders in deep RL

- In deep RL, we can construct the feature vector with an autoencoder.
- The autoencoder can be trained offline with a random agent or online with the current policy (auxiliary loss).



4 - Recurrent neural networks

Recurrent neural networks

- FCN, CNN and AE are **feedforward neural networks**: they transform an input $\mathbf{x}$ into an output $\mathbf{y}$:

$$\mathbf{y} = F_\theta(\mathbf{x})$$

- If you present a sequence of inputs $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_t$ to a feedforward network, the outputs will be independent from each other:

$$\mathbf{y}_0 = F_\theta(\mathbf{x}_0)$$

$$\mathbf{y}_1 = F_\theta(\mathbf{x}_1)$$

$$\dots$$

$$\mathbf{y}_t = F_\theta(\mathbf{x}_t)$$

- The output $\mathbf{y}_t$ does **not** depend on the history of inputs $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_{t-1}$.

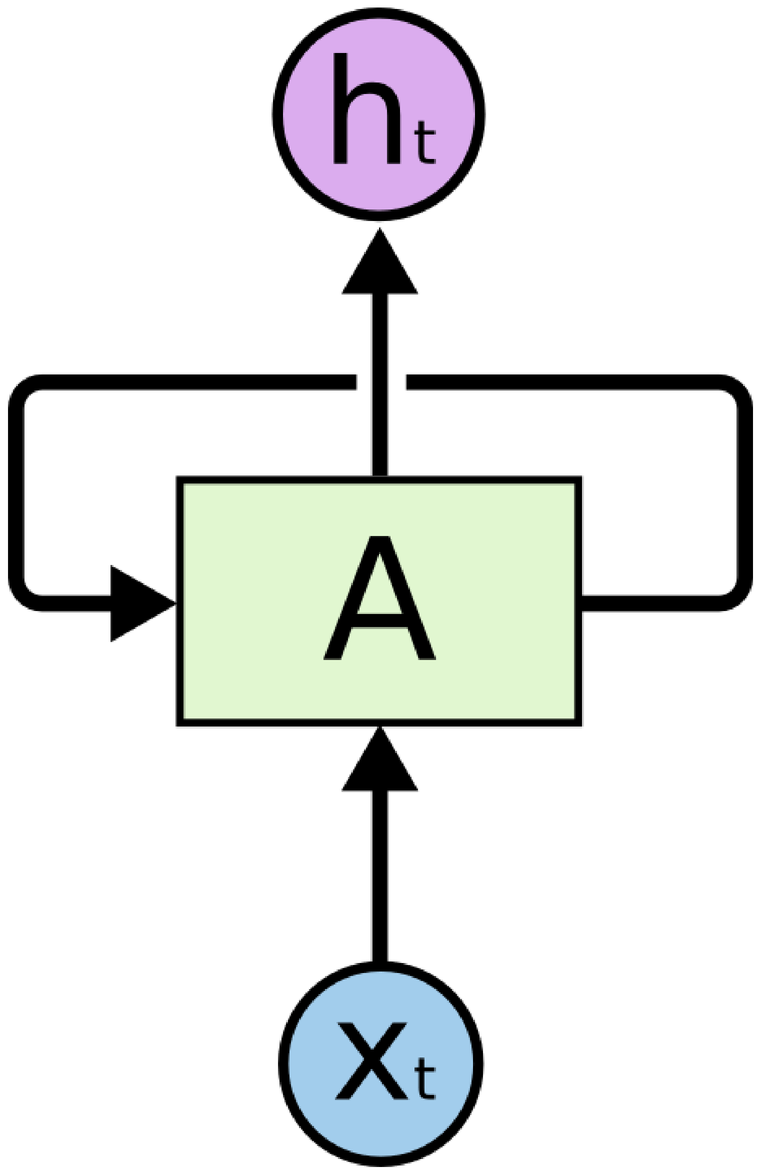
Recurrent neural networks

- This not always what you want.
- If your inputs are frames of a video, the correct response at time t might also depend on previous frames.

Source: https://srirangatarun.wordpress.com/2018/07/09/video-frame-prediction-with-keras/

- The task of the NN could be to explain what happens at each frame.
- As we saw, a single frame is often not enough to predict the future (**Markov property**).

Recurrent neural networks



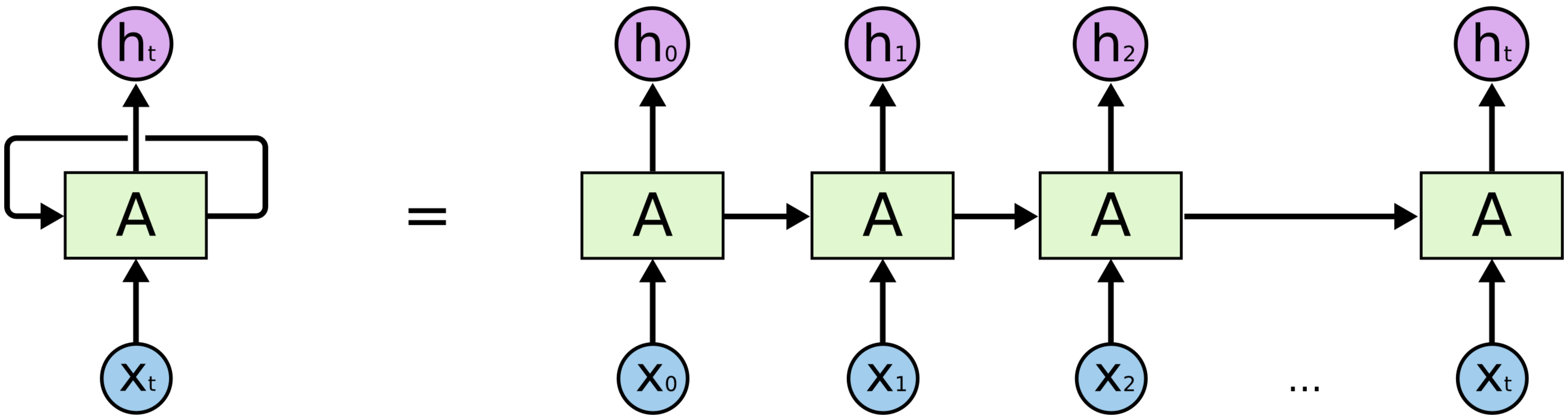
Source: C. Olah

- A **recurrent neural network** (RNN) uses it previous output as an additional input (*context*).
- All vectors have a time index t denoting the time at which this vector was computed.
- The input vector at time t is $\mathbf{x}_t$, the output vector is $\mathbf{h}_t$:

$$\mathbf{h}_t = f(W_x \times \mathbf{x}_t + W_h \times \mathbf{h}_{t-1} + \mathbf{b})$$

- The input $\mathbf{x}_t$ and previous output $\mathbf{h}_{t-1}$ are multiplied by **learnable weights**:
  - W_x is the input weight matrix.
  - W_h is the recurrent weight matrix.

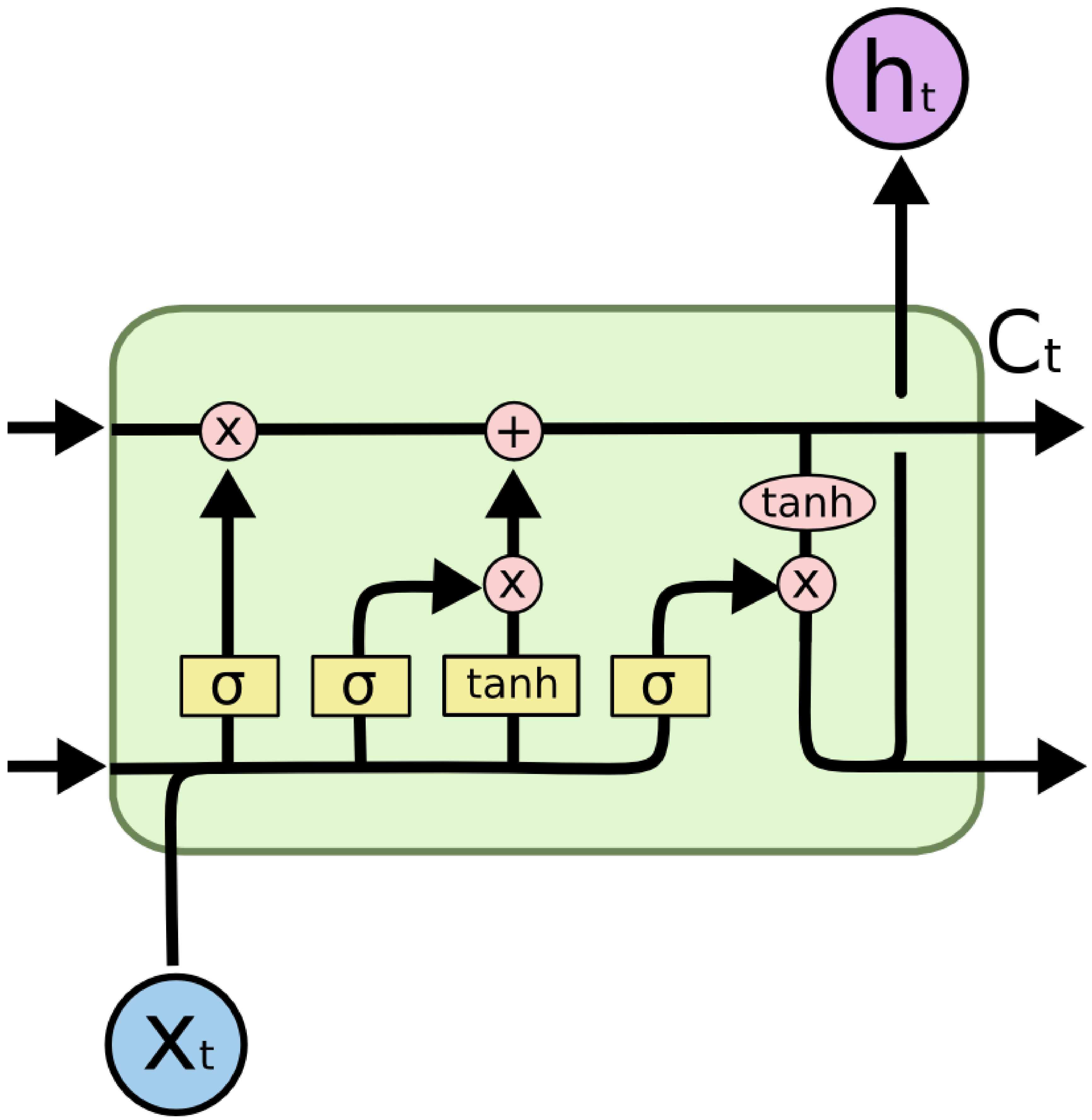
Recurrent neural networks



Source: C. Olah

- This is equivalent to a deep neural network taking the whole history $\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_t$ as inputs, but reusing weights between two time steps.
- The weights are trainable using **backpropagation through time** (BPTT).
- A RNN can learn the **temporal dependencies** between inputs.

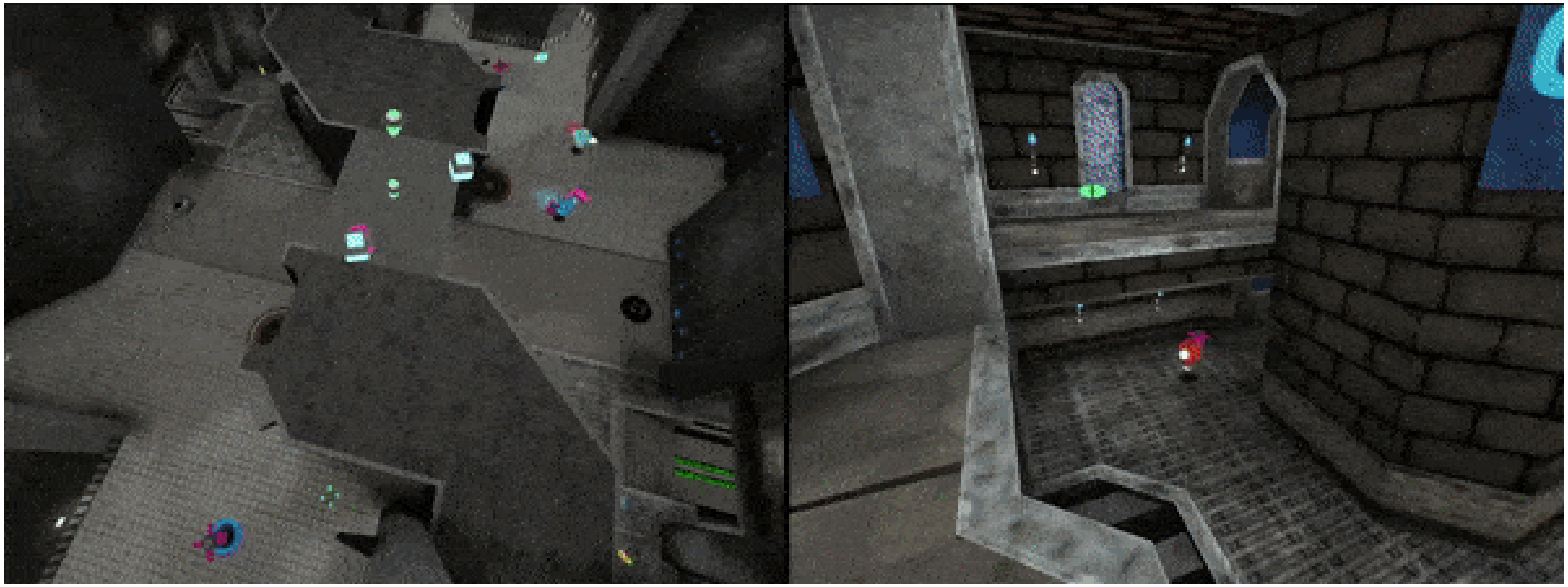
LSTM cell



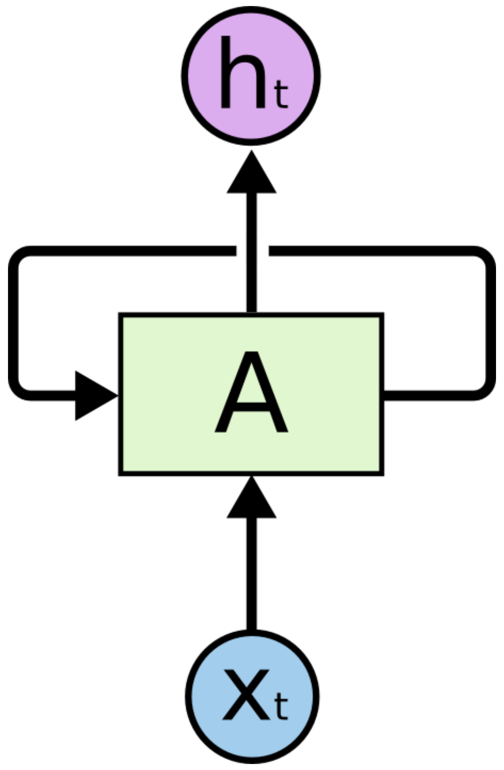
Source: C. Olah

- A popular variant of RNN is **LSTM** (long short-term memory).
- In addition to the input $\mathbf{x}_t$ and output $\mathbf{h}_t$, it also has a **state** (or **memory** or **context**) $\mathbf{C}_t$ which is maintained over time.
- It also contains three multiplicative **gates**:
  - The **input gate** controls which inputs should enter the memory.
  - The **forget gate** controls which memory should be forgotten.
  - The **output gate** controls which part of the memory should be used to produce the output.

RNN in RL



Source: https://deepmind.com/blog/article/capture-the-flag-science



- An obvious use case of RNNs in deep RL is for POMDP (partially observable MDP).
- If the individual states s_t do not have the Markov property, the output of a LSTM does:
  - The output of the RNN is a representation of the complete history $s_0, s_1, \dots, s_t$.
- We can apply RL on the output of a RNN and solve POMDPs for free!