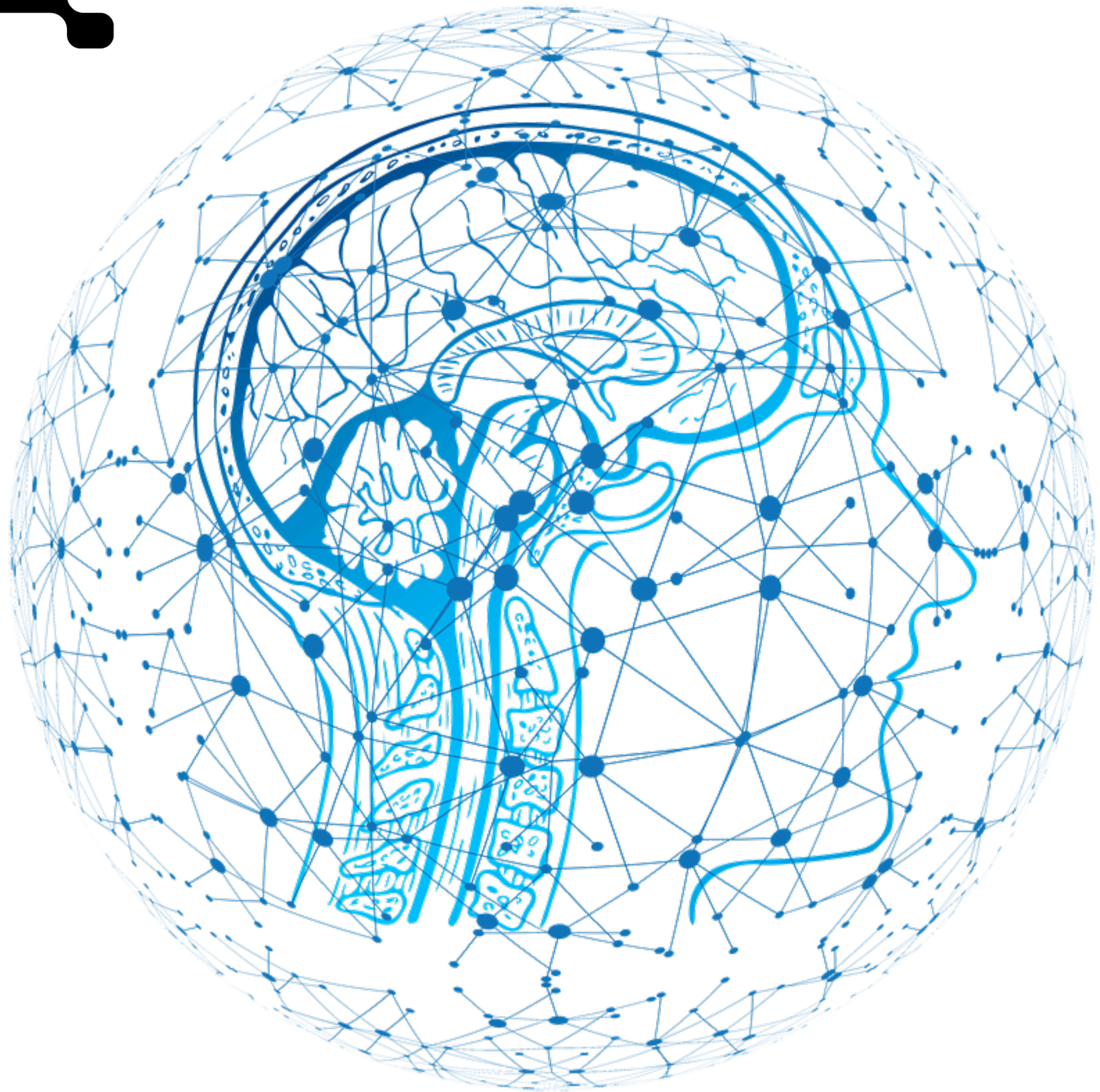


Introduction to High Performance Machine Learning

Convolutional Neural Networks
Recurrent Neural Networks
Generative Models

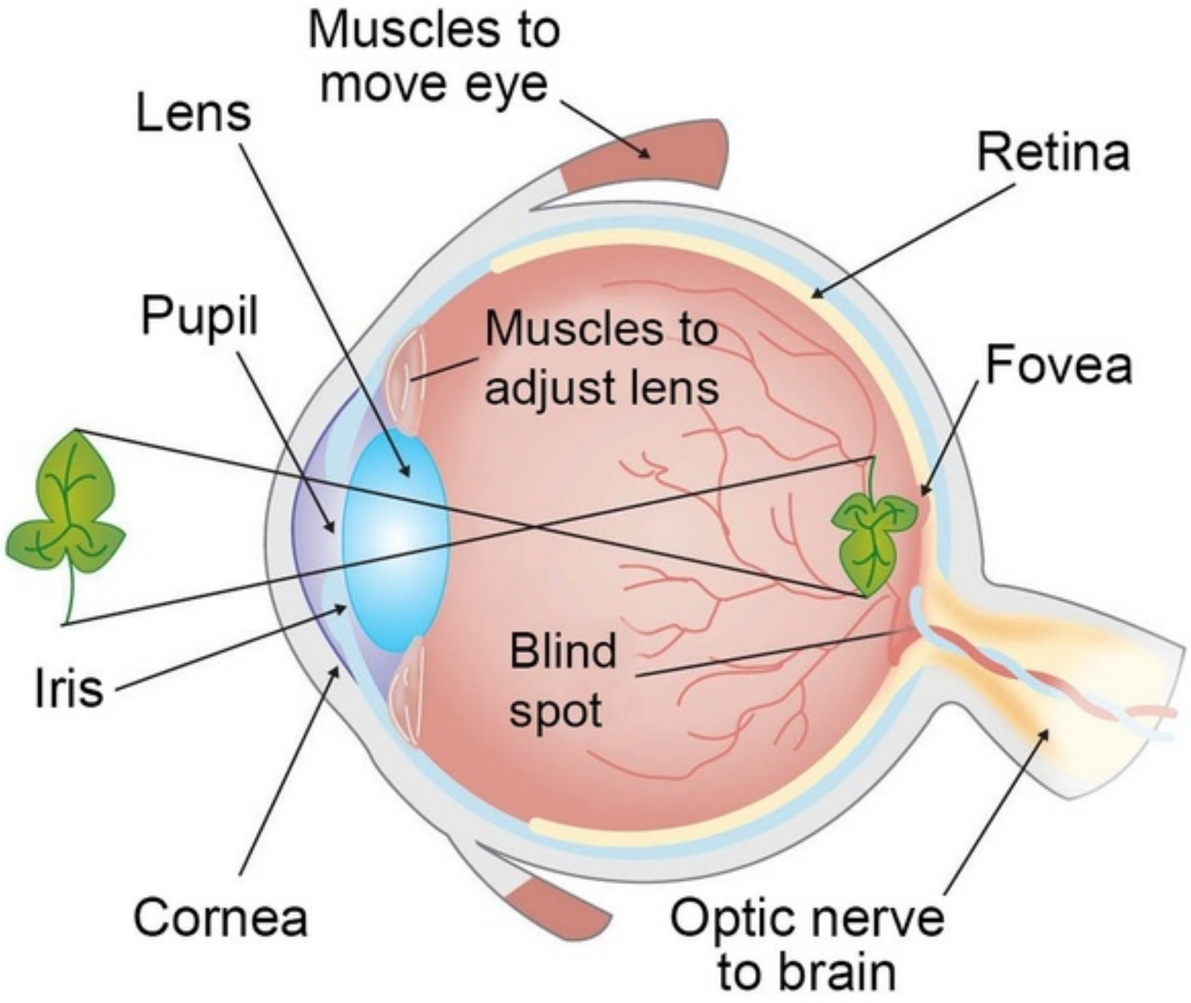
Maxwell Cai, PhD

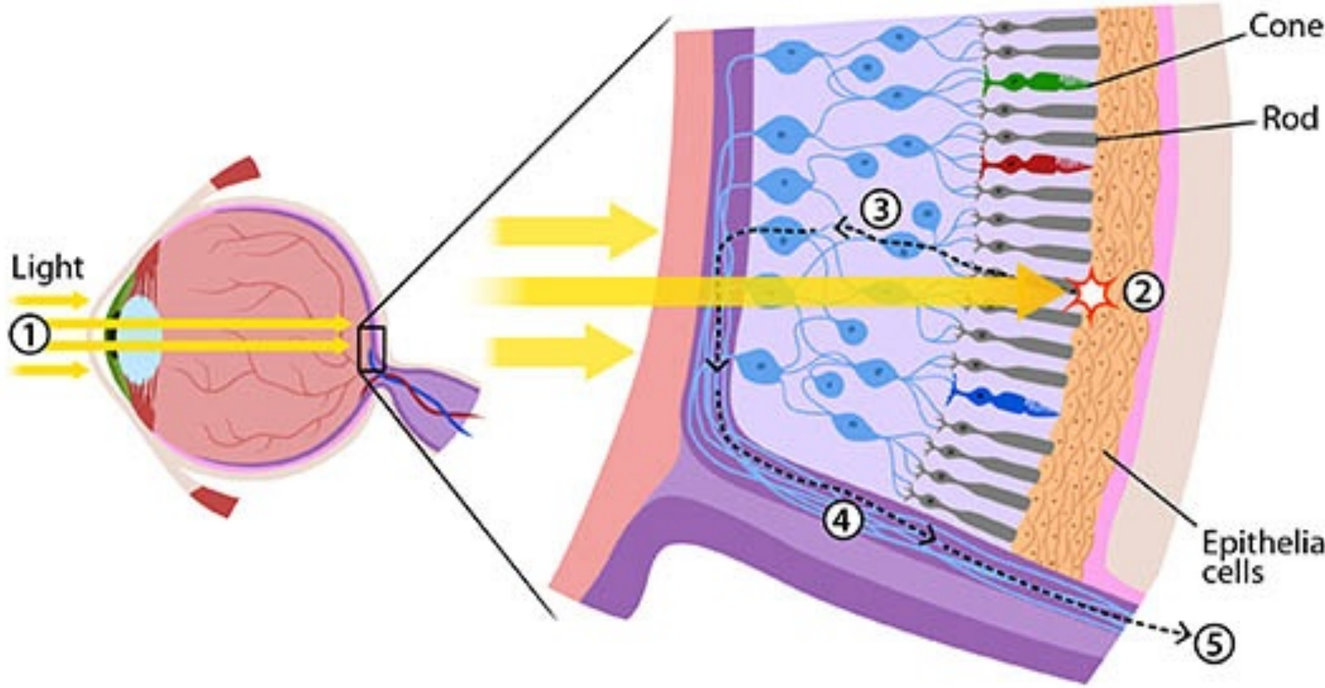
Welcome to the world of computer vision!

How do we let computers “see” something?

Ask ourselves first: How do we (humans) see something?

Human eyes

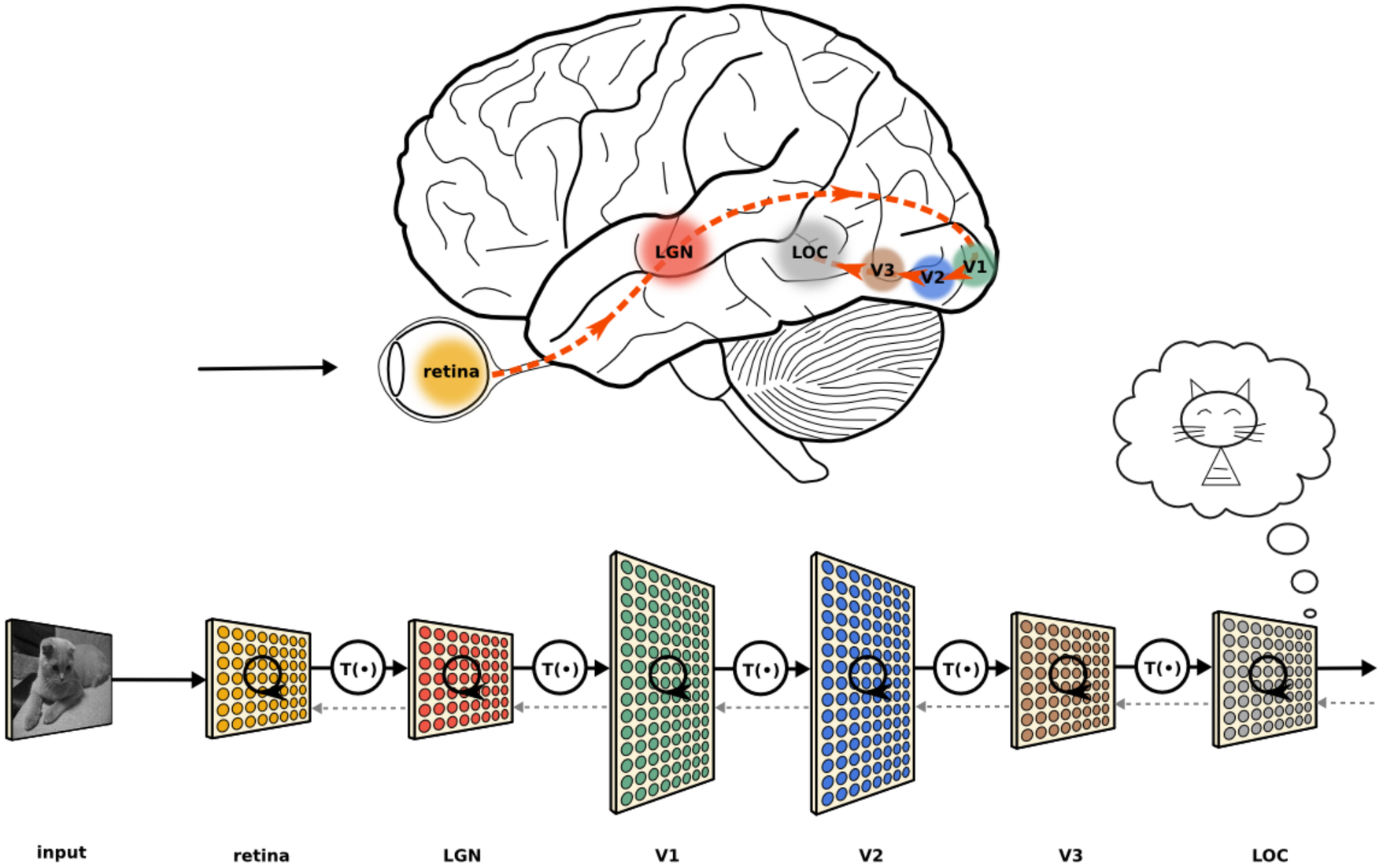




Source: Quora

Human brain: the (real) neural network

Source: arimaresearch.com



Representation of images in computers

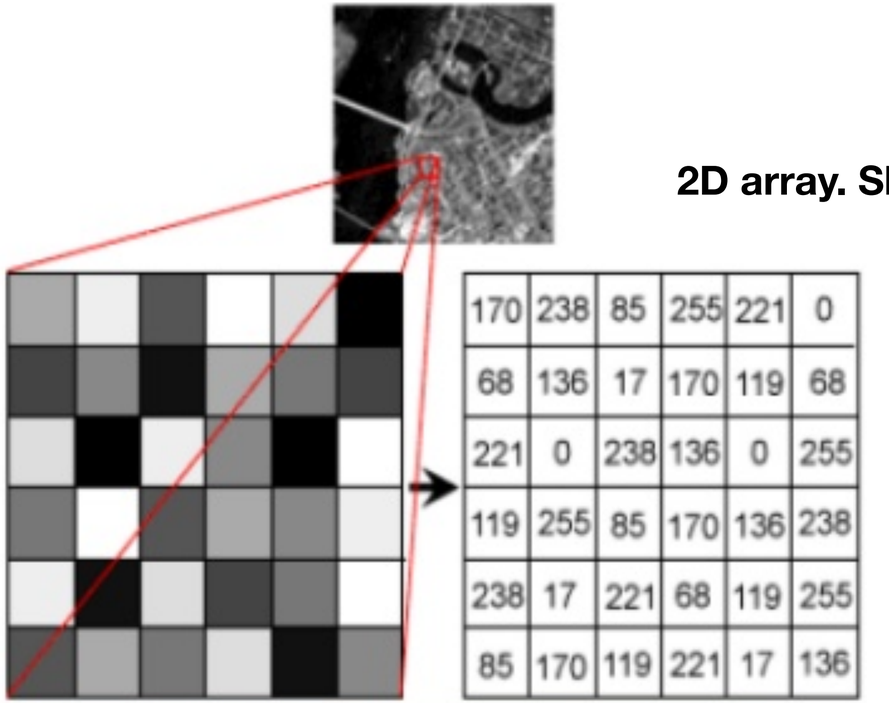
An image

… is a **matrix/array** of intensity values

… usually consists integers of [0, 255] or float points of [0, 1]

… each element of this matrix is called a **pixel**

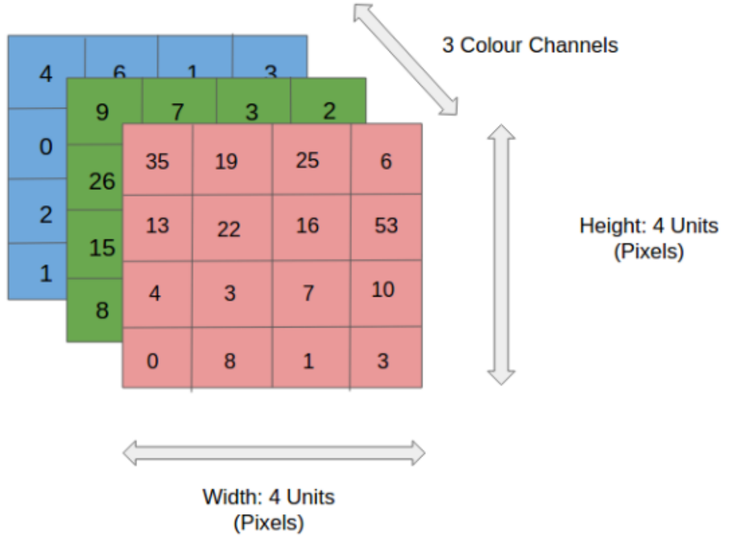
… can have 1 (greyscale) or multiple (color) **channels**



170	238	85	255	221	0
68	136	17	170	119	68
221	0	238	136	0	255
119	255	85	170	136	238
238	17	221	68	119	255
85	170	119	221	17	136

2D array. Shape: [width, height]

3D array. Shape: [width, height, channel]

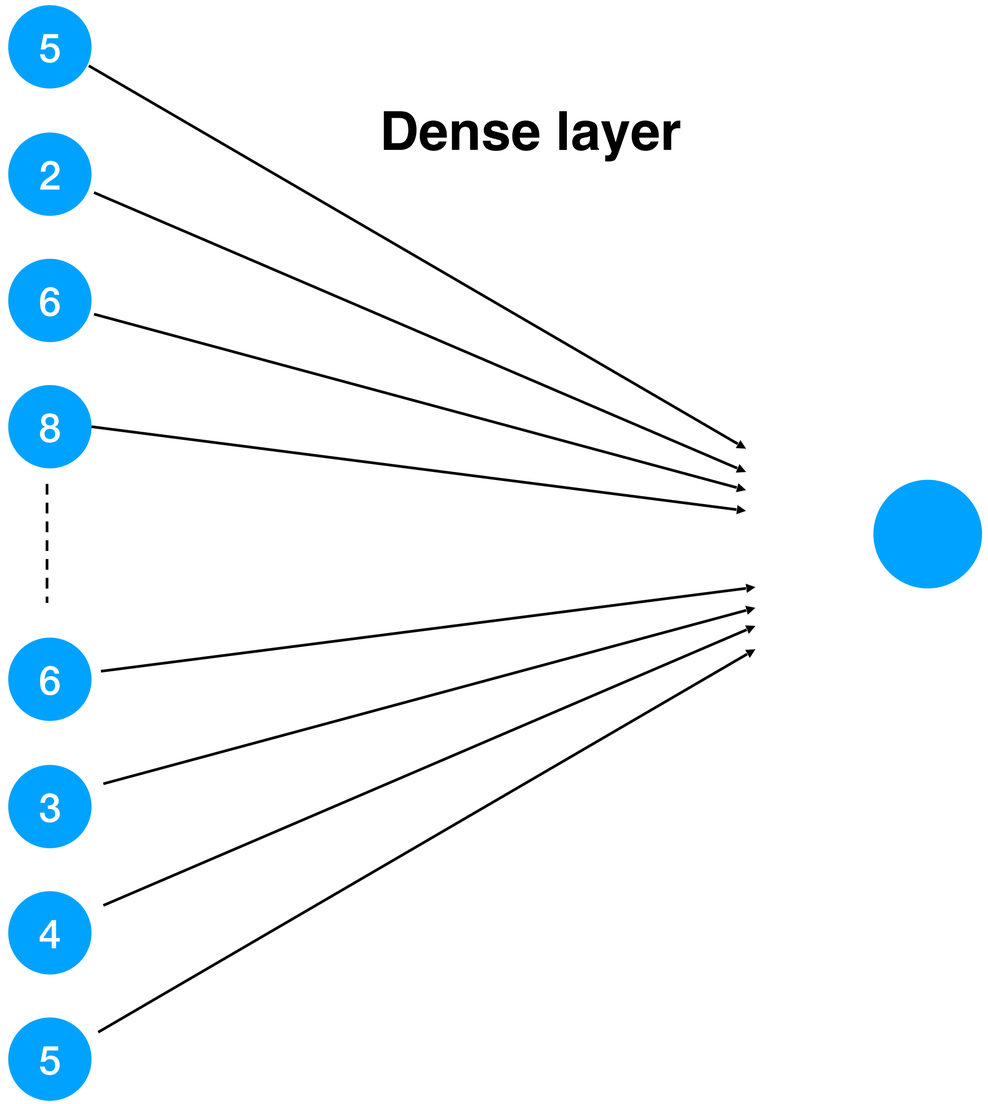


Dense network classifier (MLP)

So far, we have used multi-layer perceptions (MLP) to carry out some computer vision tasks (e.g., recognizing hand-written digits)…

5	2	6	8	2	0	1	2
4	3	4	5	1	9	6	3
3	9	2	4	7	7	6	9
1	3	4	6	8	2	2	1
8	4	6	2	3	1	8	8
5	8	9	0	1	0	2	3
9	2	6	6	3	6	2	1
9	8	8	2	6	3	4	5

Flatten layer



Problem:

- The resulting encoding is pixel location dependent.
- Spatial relationship is not preserved after flattening.

Filters in our daily lives

Forget about the commercial advertisements themselves…
Just think about the mathematical principles behind them…

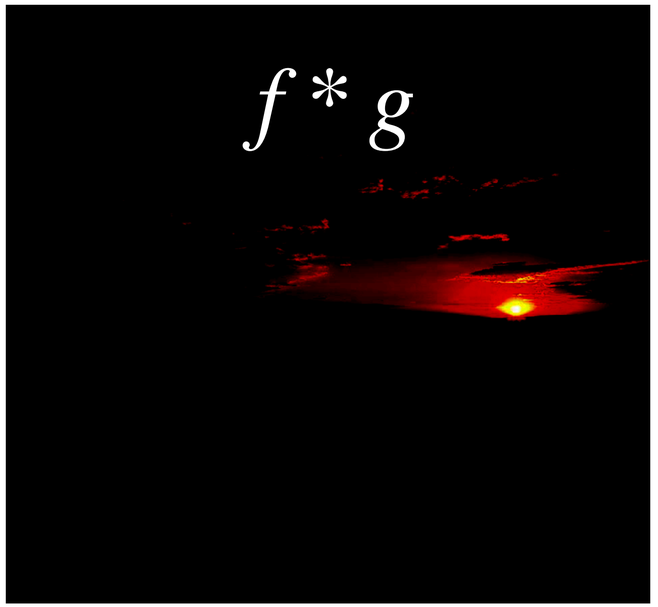
Filter in image processing

f

+

Filter
g

=



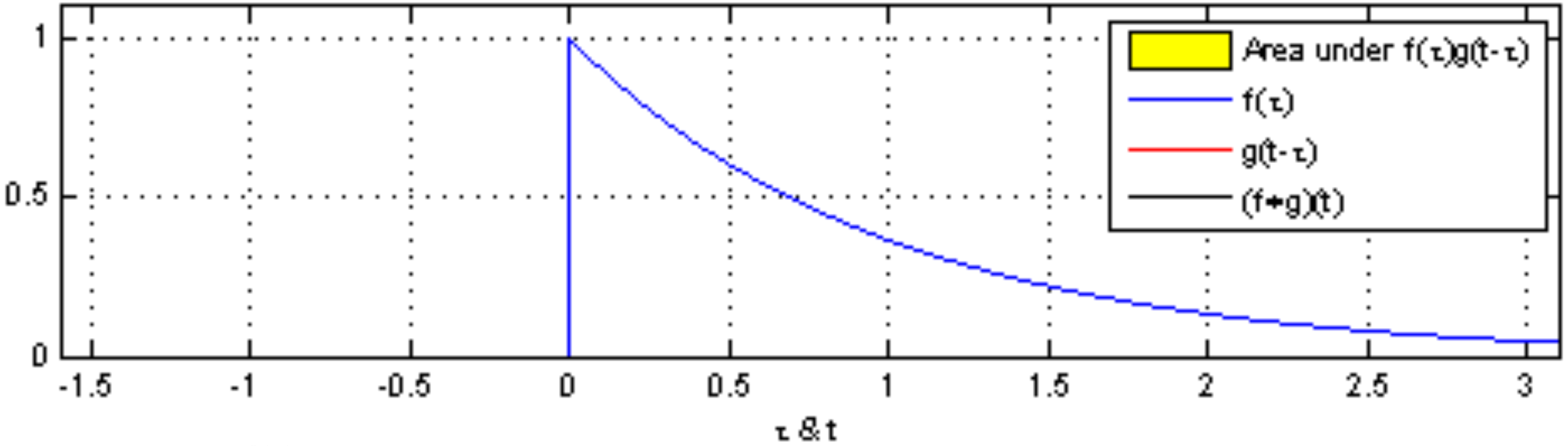
Filter
h

=

Using **different filters**, we can see the **same signal** in **different perspectives**.

Convolution

Typically, a filter applies a **convolution** operation upon the original signal.



Function: $f(t)$

Kernel: $g(t)$

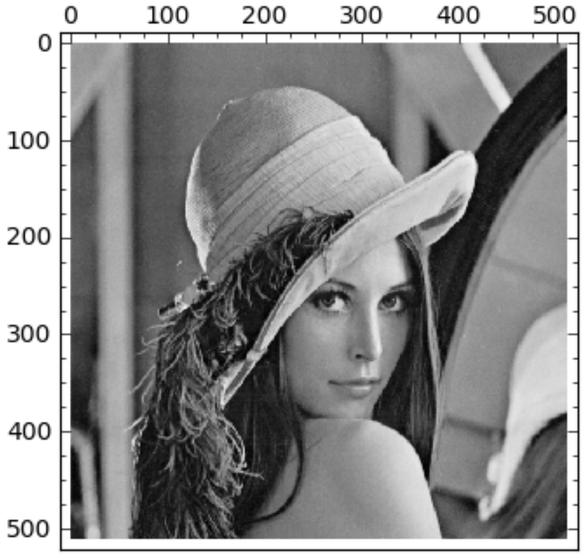
Convolution: $(f * g)(t)$

No signal → no response

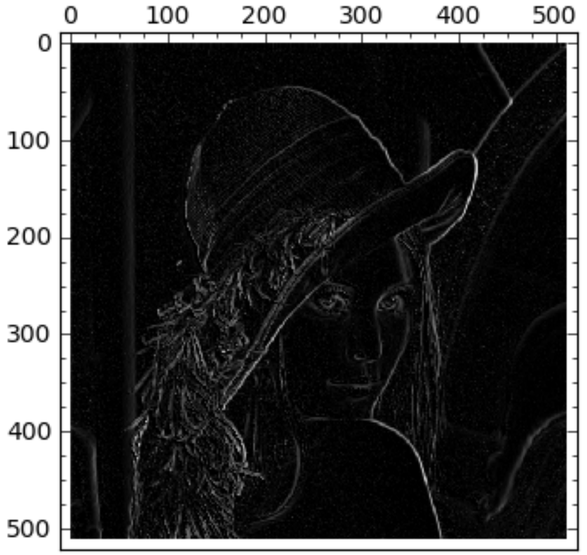
Strong signal → strong response

Filtering: a signal processing technique

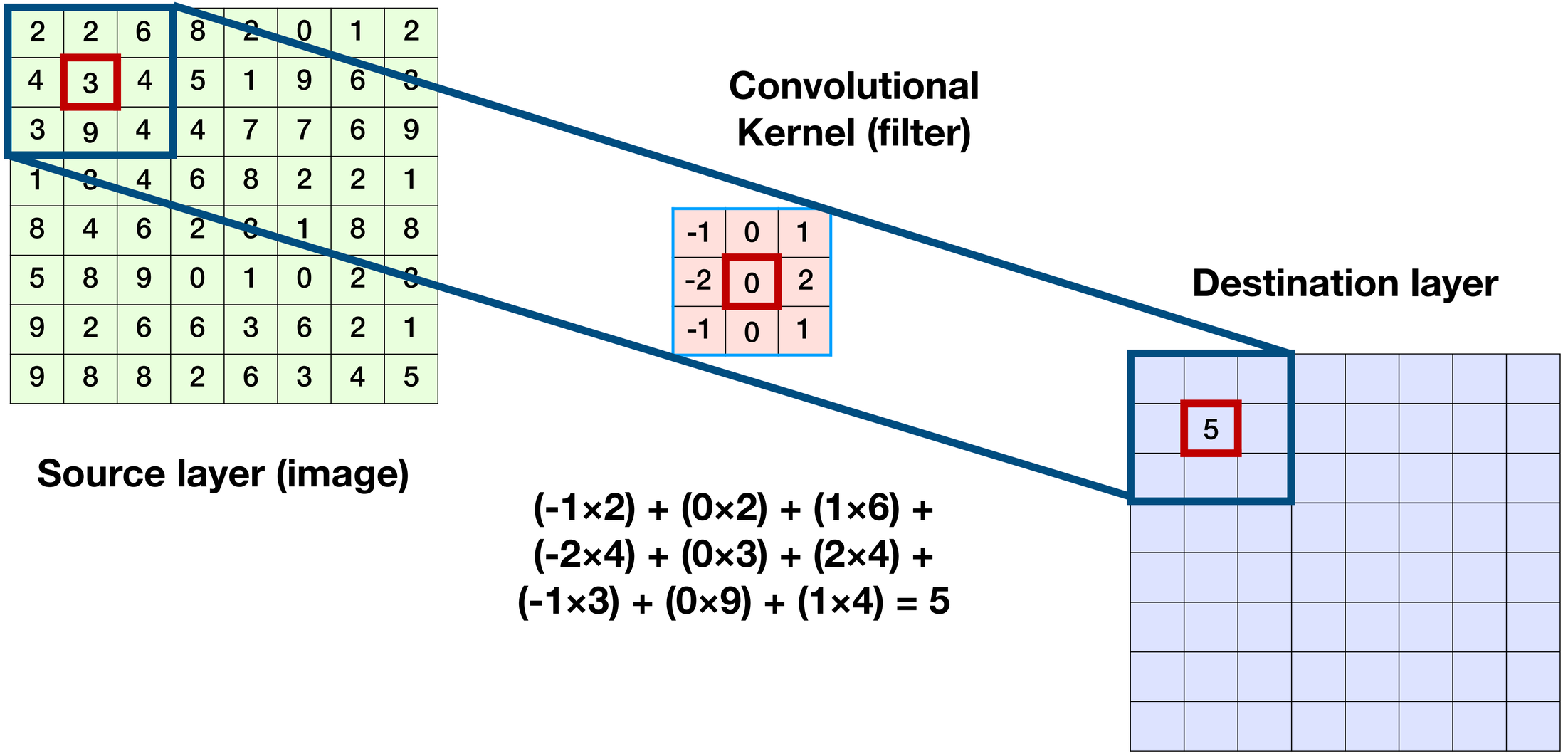
Convolution



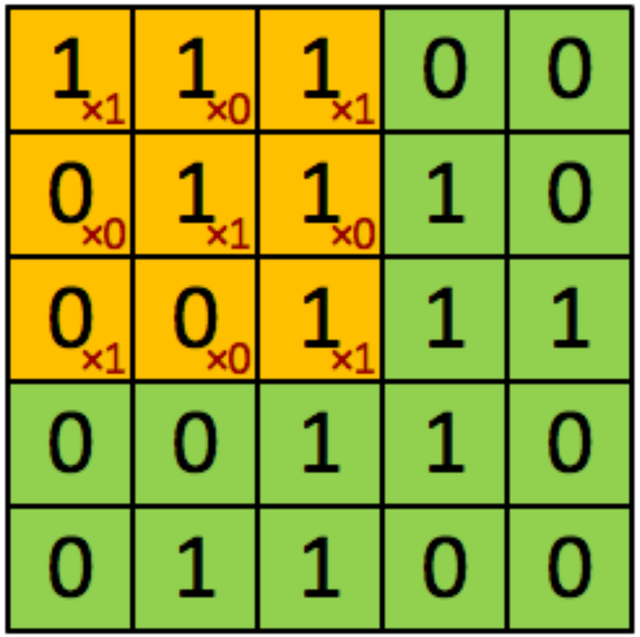
Convolution

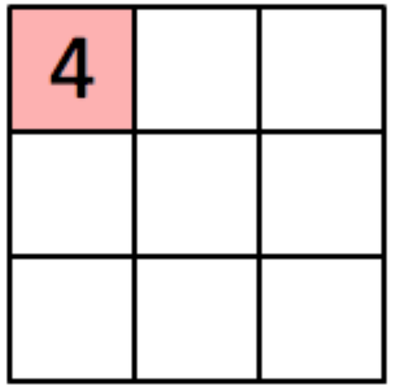


Convolution

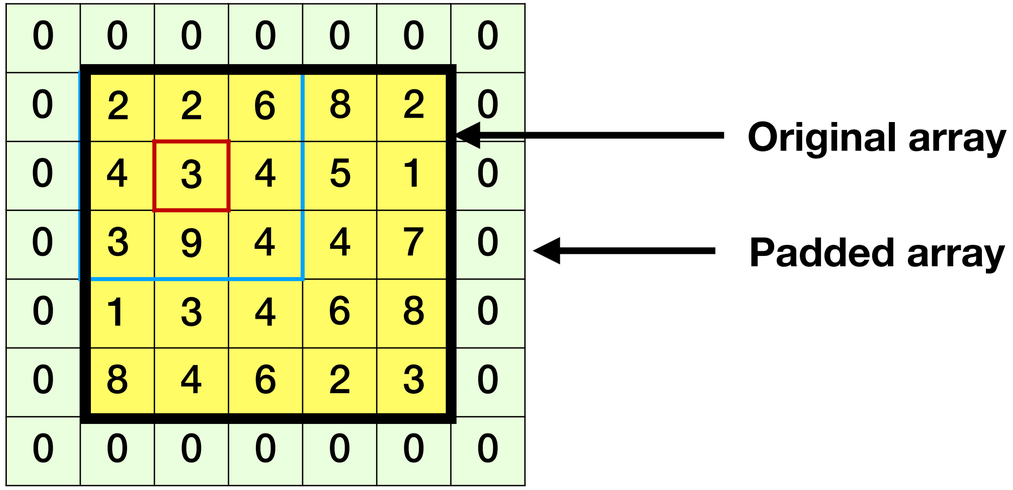


Convolution



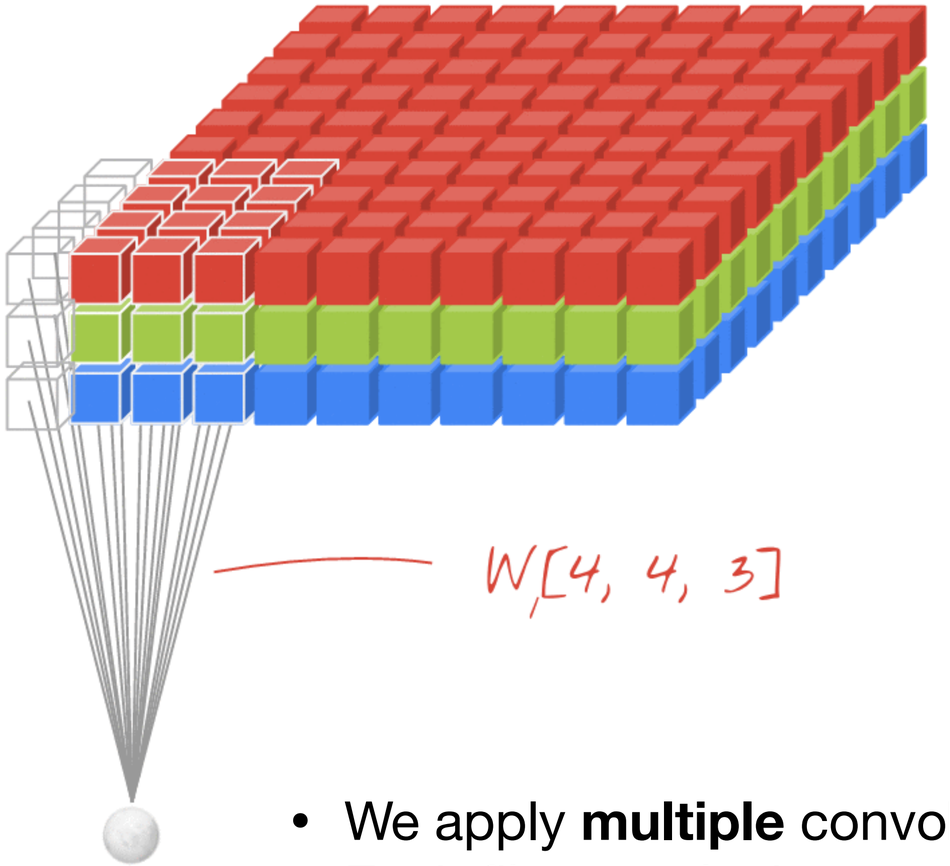


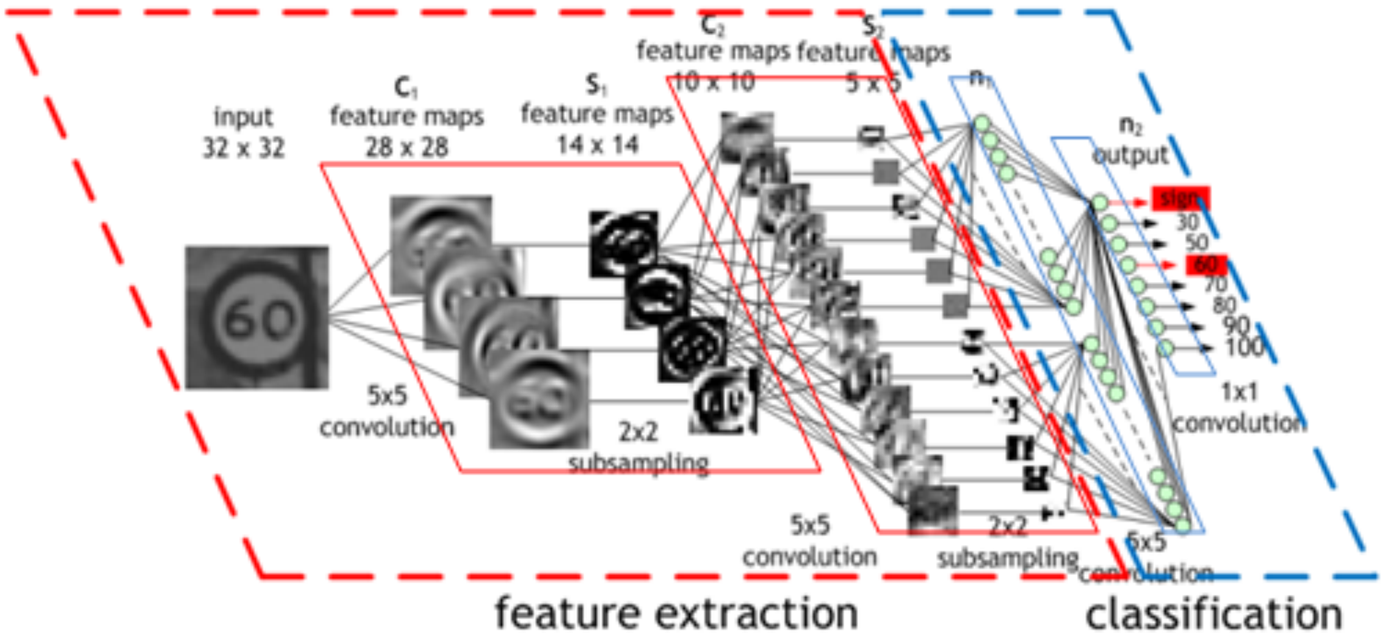
- The kernel is **shifted** over the image with a step size, and computes the output for each position.
- The step size is called **stride**.
- Output has **smaller** dimension than input:
  $\dim(\text{output}) = \dim(\text{input}) - (\dim(\text{kernel}) - 1)$
- **Padding** is used to solve this problem, which artificially make the image “bigger” by adding synthesis data (typically 0-padding)



Animation: Sumit Saha/Towards Data Science

Multiple convolutional channels





- We apply **multiple** convolutional **filters/kernels** to the **same** image.
- Each filter results in one convolutional **channel**.
- By learning the same image from different channels, one can detect complex patterns.

Animation: Martin Görner

Image: Maurice Peemen

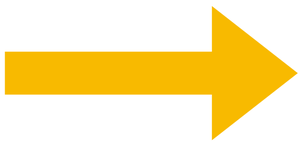
Automatic Kernel Determination

Source layer (image)

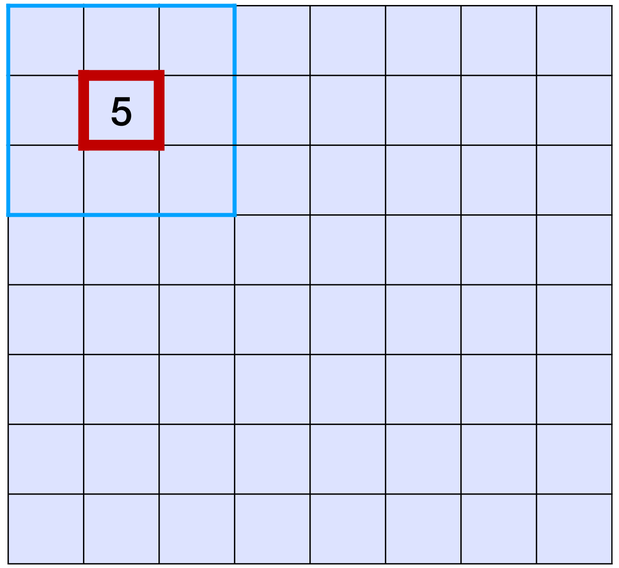
2	2	6	8	2	0	1	2
4	3	4	5	1	9	6	3
3	9	4	4	7	7	6	9
1	3	4	6	8	2	2	1
8	4	6	2	3	1	8	8
5	8	9	0	1	0	2	3
9	2	6	6	3	6	2	1
9	8	8	2	6	3	4	5

w_1	w_2	w_3
w_4	w_5	w_6
w_7	w_8	w_9

Kernel (filter)



Feature map (activation map)

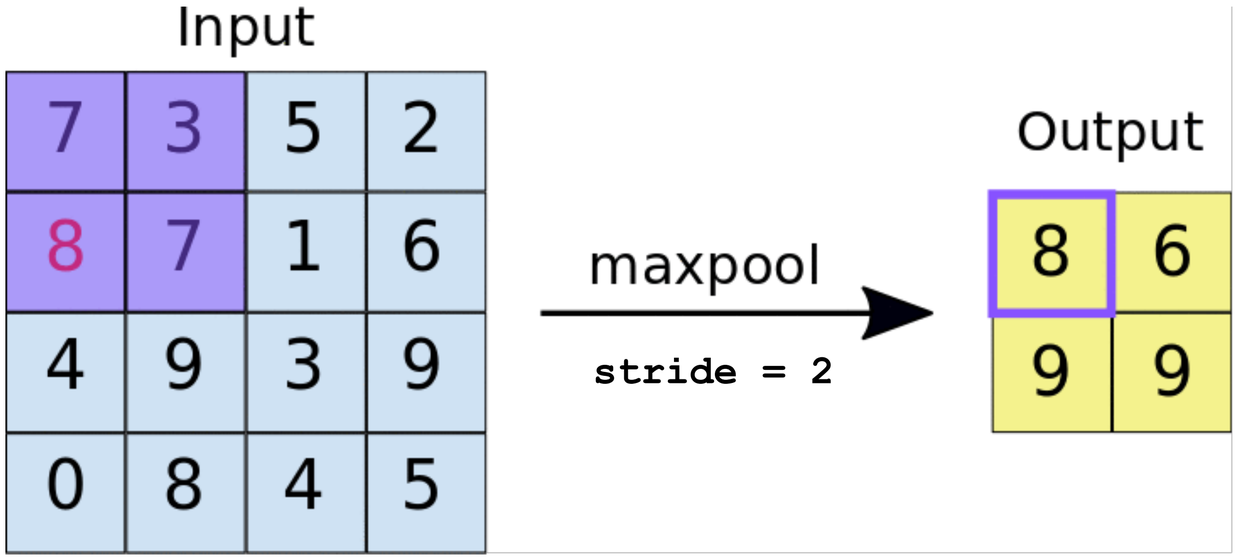


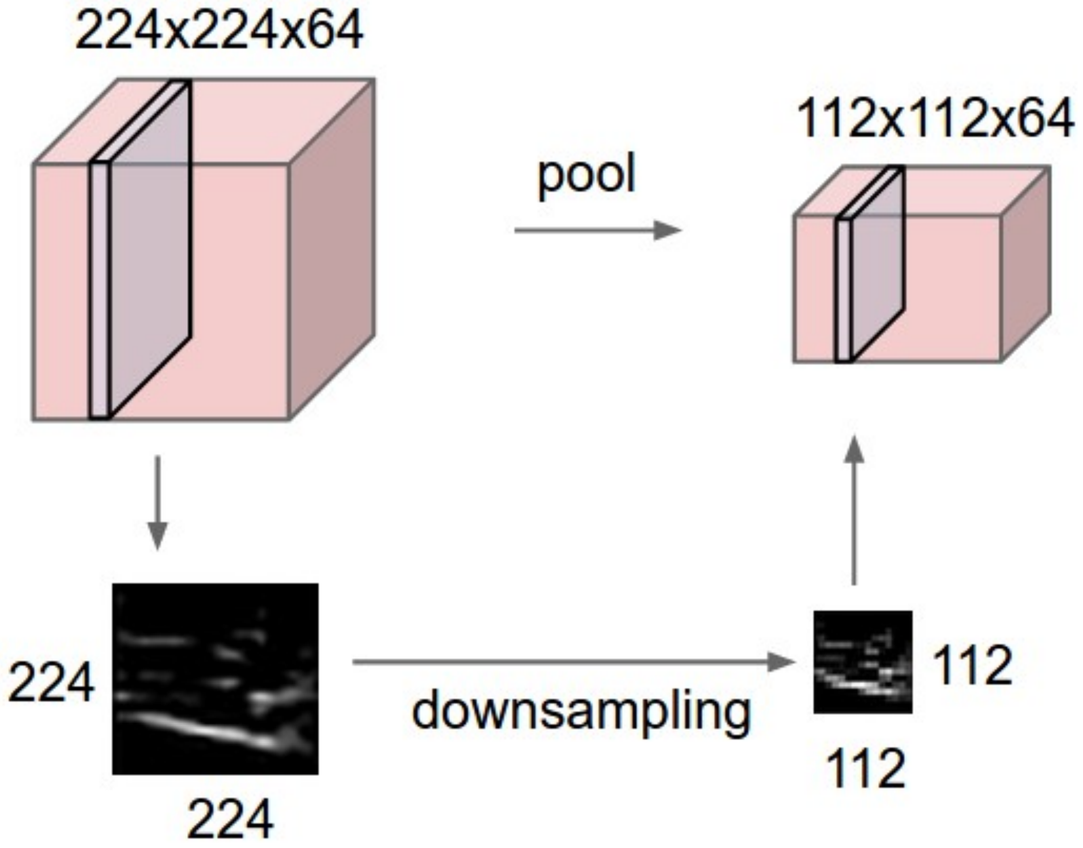
How do we know which kernels to use?

- In **traditional** signal processing, a filter is designed by human experts.
- In **deep learning**, data are too complex and too many different kernels are needed.
- Therefore, kernels are no longer fixed. They are initialized **randomly**.
- Kernels are updated through **backward propagation**, in the way that it **learns** which features to detect.
- **Gradient descent** algorithms are used.

Pooling (downsampling)

We need to **discard** information **gradually**.
Pooling is a way of information **abstraction**.
Pooling is usually applied **after** convolutions.

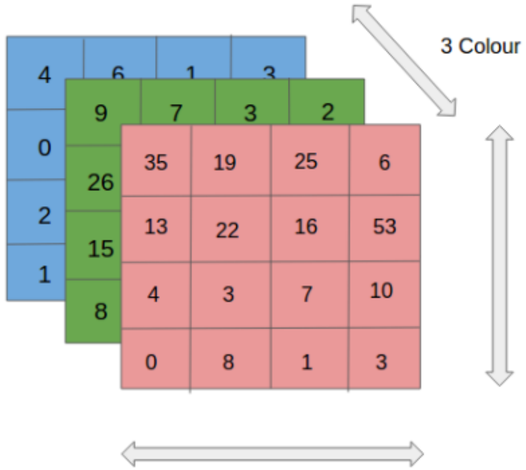


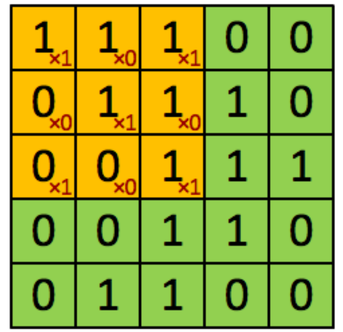


Max pooling: keep the **strongest** signal
Average pooling: use the **local average** as the signal

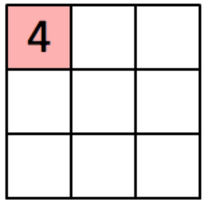
Animation: Google Developers

CNN Architecture

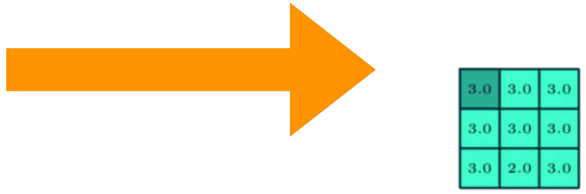


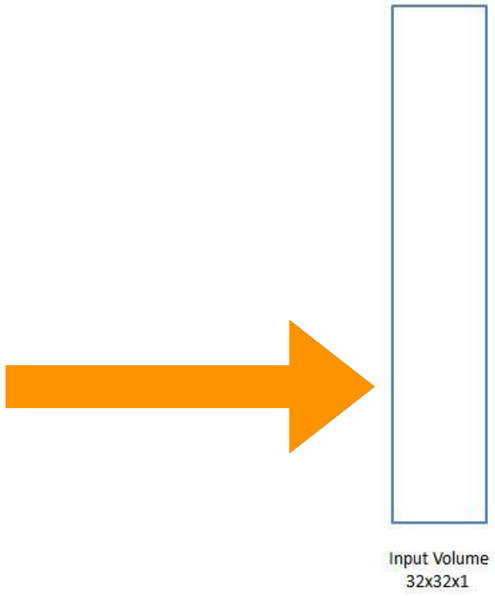


Image

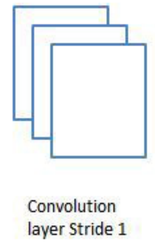


Convolved Feature





Input Volume
32x32x1

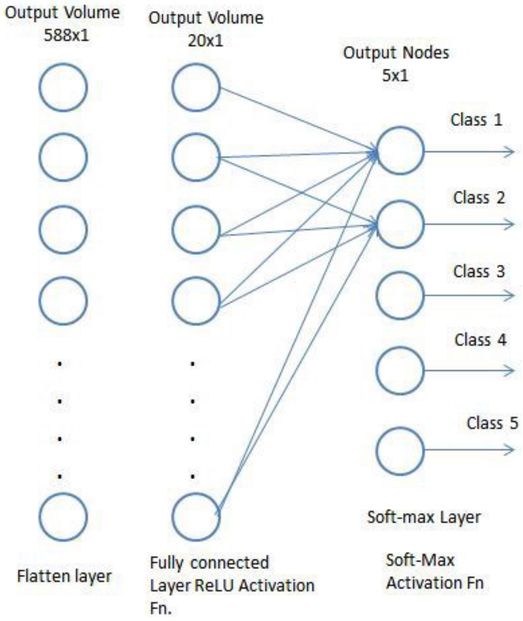


ReLU Activation Fn.
Volume-28x28x3

Convolution
layer Stride 1

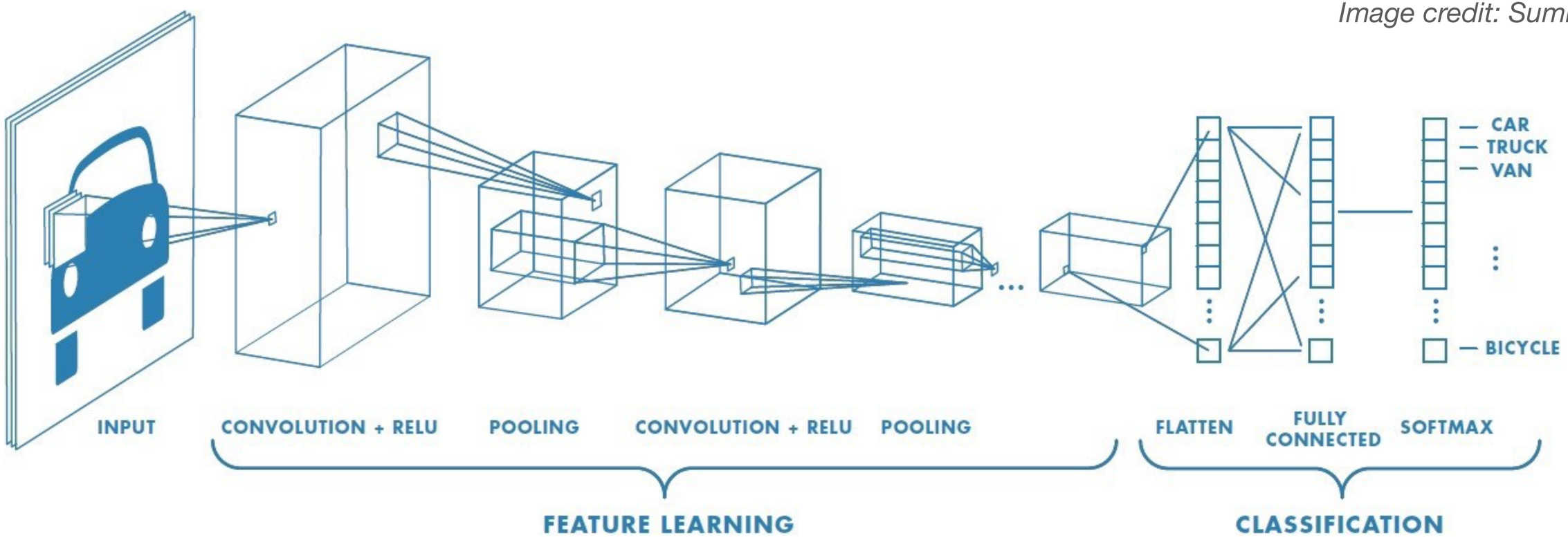
Output Volume
14x14x3

Max Pool
layer Stride 2



Convolution Neural Network (CNN)

Image credit: Sumit Saha



- Typically, **images** become increasingly **smaller** as they go to the **deeper** layers;
- Typically, the number of **filters increases** in the **deeper** layers;
  - Low-level features are limited, thus requires few filters;
  - High-level features are rich, thus requires many filters;
- The **decision making** (i.e., classification) is made in the **last layers**, typically with **dense** layers and the `softmax` activation function.

Transfer Learning

Recall that the convolutional kernels are **learned** during the training process through backward propagation.
The trained kernels contains **knowledge** to detect patterns.
Why not let a new CNN to **inherit these knowledge**?

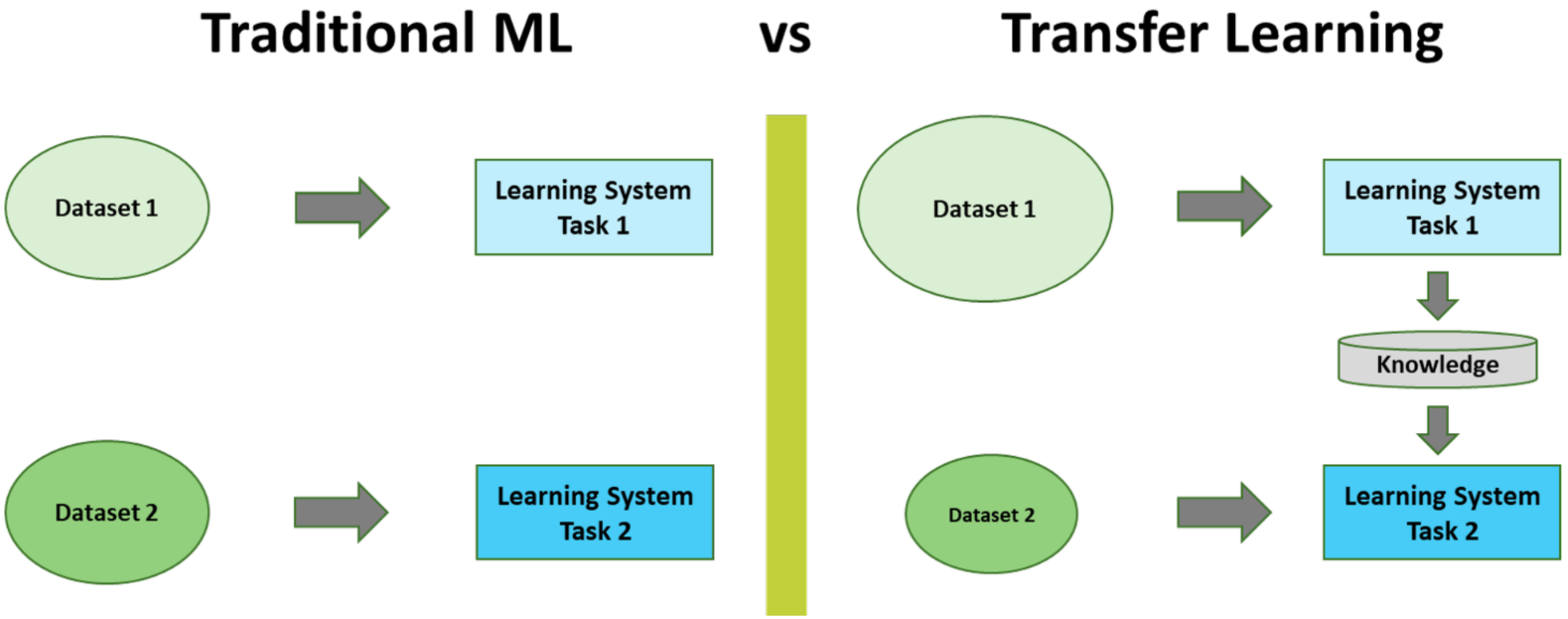


Image source: Dipanjan Sarkar/TowardsDataScience

How to model sequences?

Sequence Modeling

Language translation

Speech recognition

Music generation

Sentiment classification

Video captioning

Chatbot

Text summary

...

“Hoi, hoe gaat het?” ⟷ “Hi, how are you?”

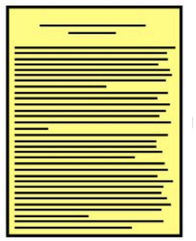
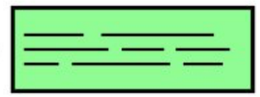
 → “Hi, how are you?”

Style / nothing → 

“Hoi, hoe gaat het?” → ★★★★★

 → A person is running

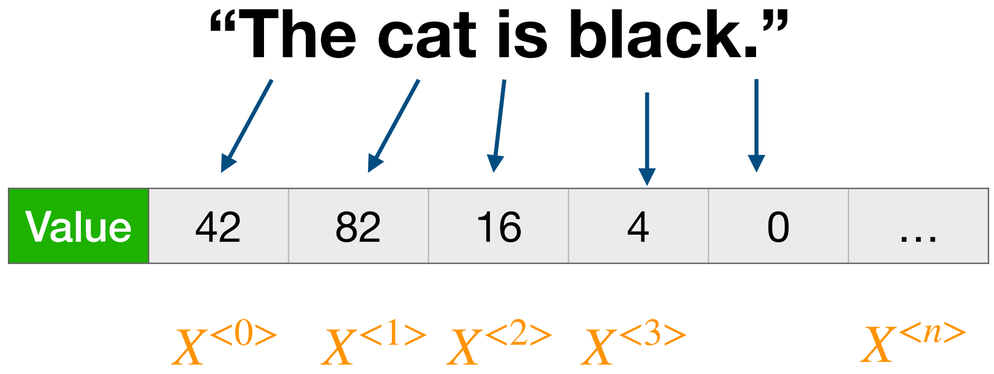
“Tell me my day” → You have two appointments.

 → 

Sequential Data

Sequential data are represented with **1D or 2D arrays**.

Time	24/3	25/3	26/3	27/3	28/3	…
Value	19,722	21,050	21,188	22,532	21,678	…

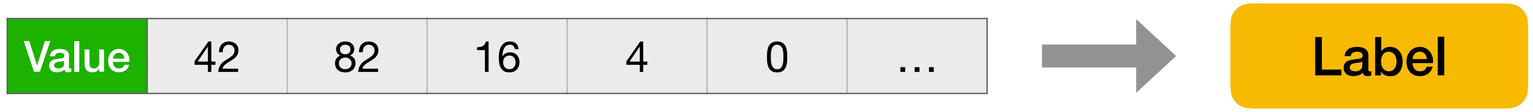


In **natural language processing** (NLP),

- Each **word** is converted into a **token**;
- A token is typically represented as a **numerical** value;
- A **sentence** is a **sequence** of tokens;
- A sequence can have **arbitrary length**;
- Tokens may be **logically related** to each other.

Sequential Data Modeling

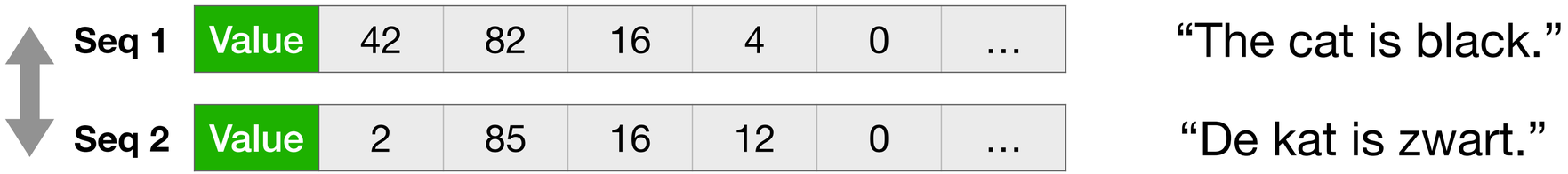
Classification



Generation

Regression

Sequence to Sequence (e.g., Translation)



The fundamental problem in sequence model is to understand the **relations between tokens**/elements.

Sequence modeling with 1D convolution

CNNs works because they can take into account the relation between **nearby** tokens.

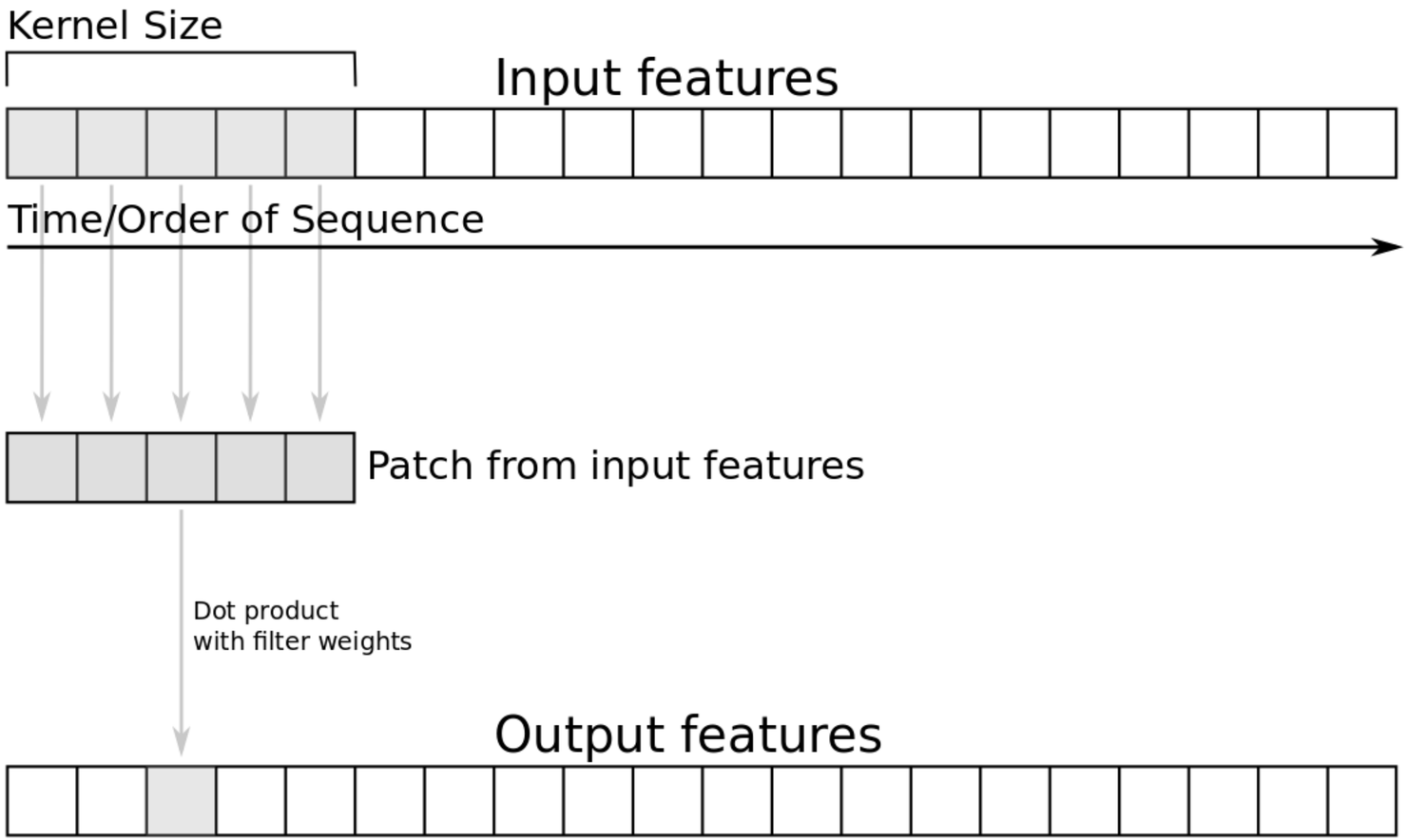
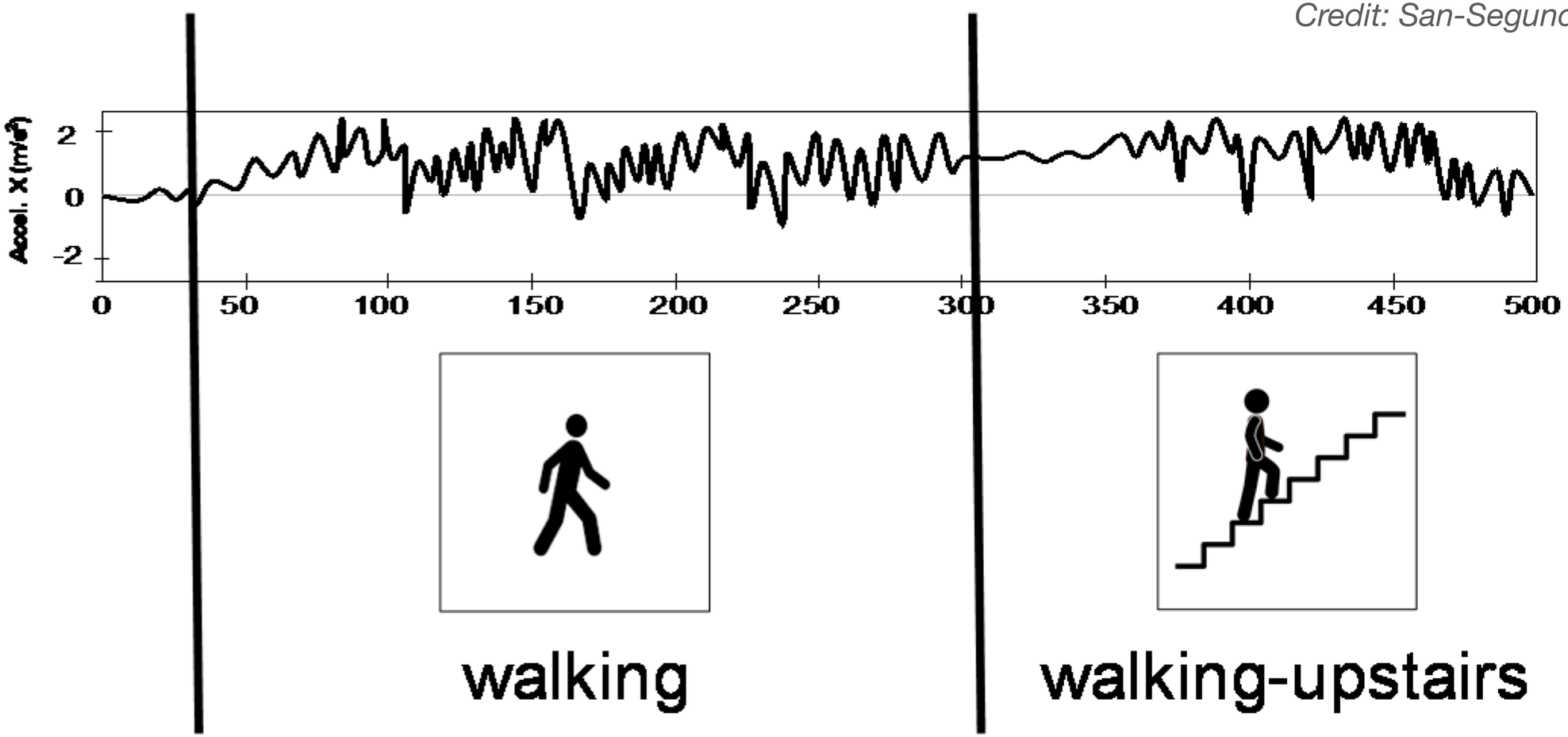


Image source: “Deep Learning With Python” (Francois Chollet)

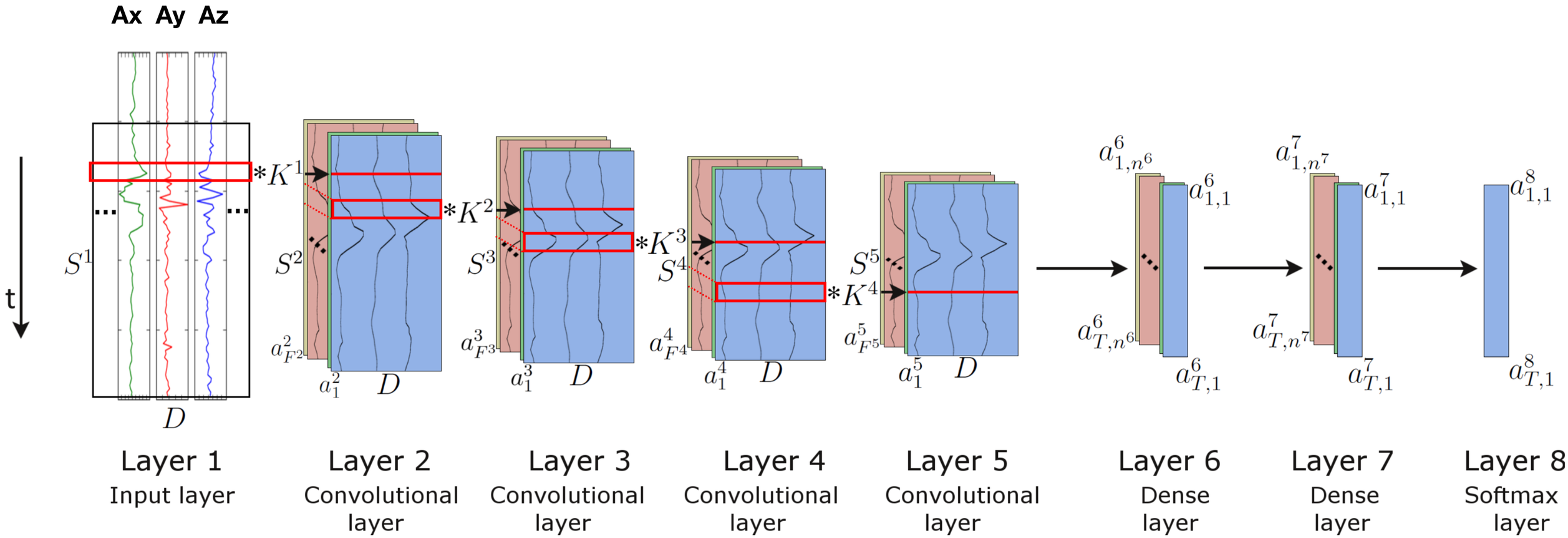
Example: human activity recognition

Credit: San-Segundo et al. (2016)



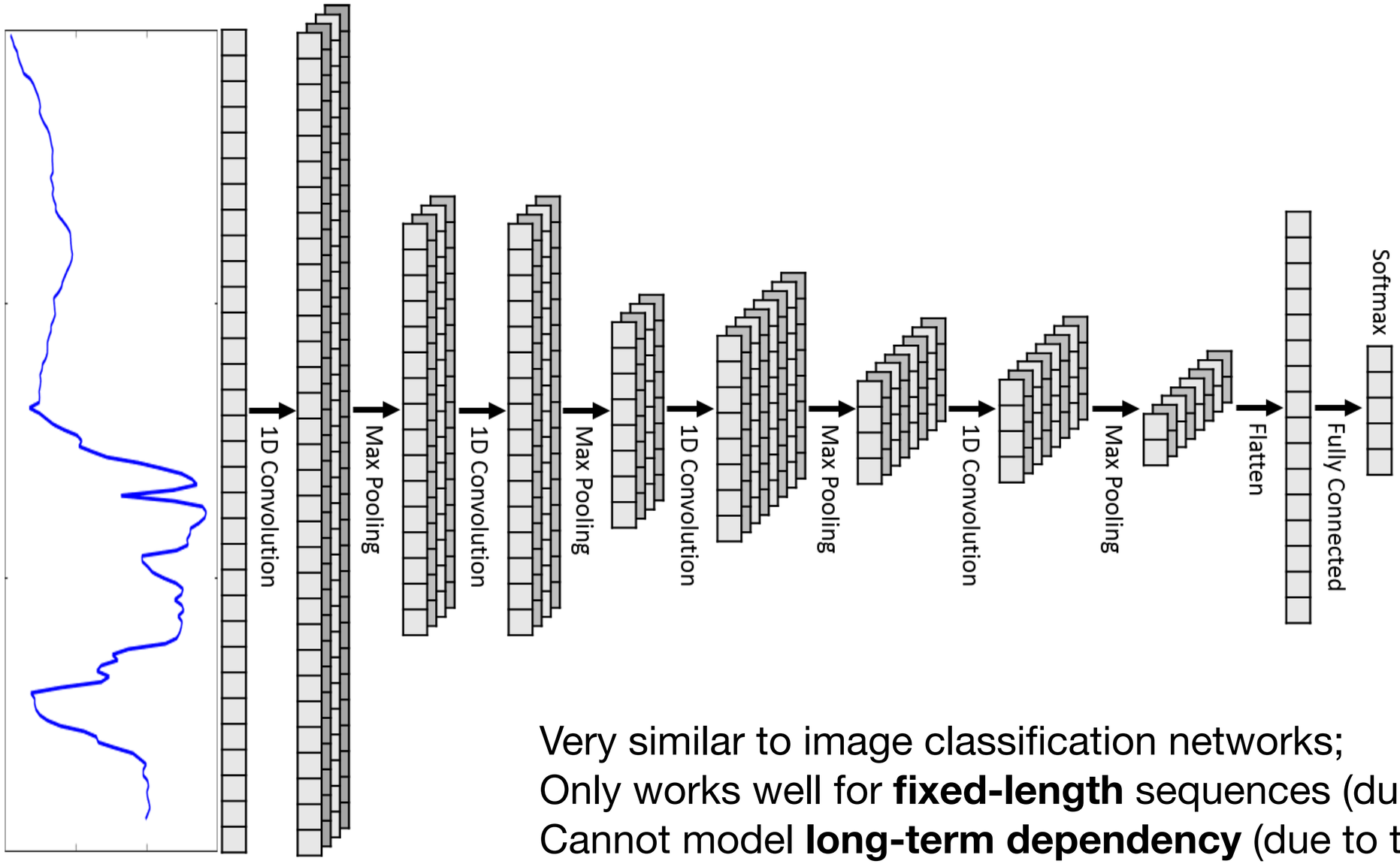
The DNN can be trained with **existing** open datasets!
e.g., https://archive.ics.uci.edu/ml/datasets/human+activity+recognition+using+smartphones

Human activity recognition with 1D Convolution



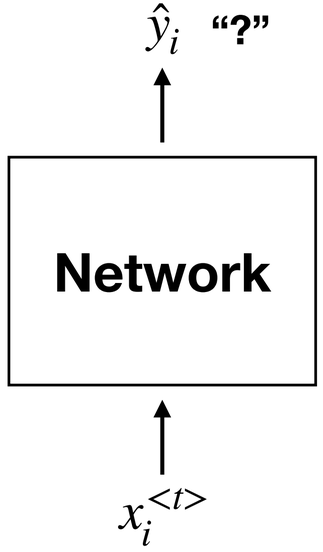
Ordóñez et al. (2016)

Sequence modeling with 1D convolution



Very similar to image classification networks;
Only works well for **fixed-length** sequences (due to the FC layer);
Cannot model **long-term dependency** (due to the limited kernel size).

Naive Approaches v2



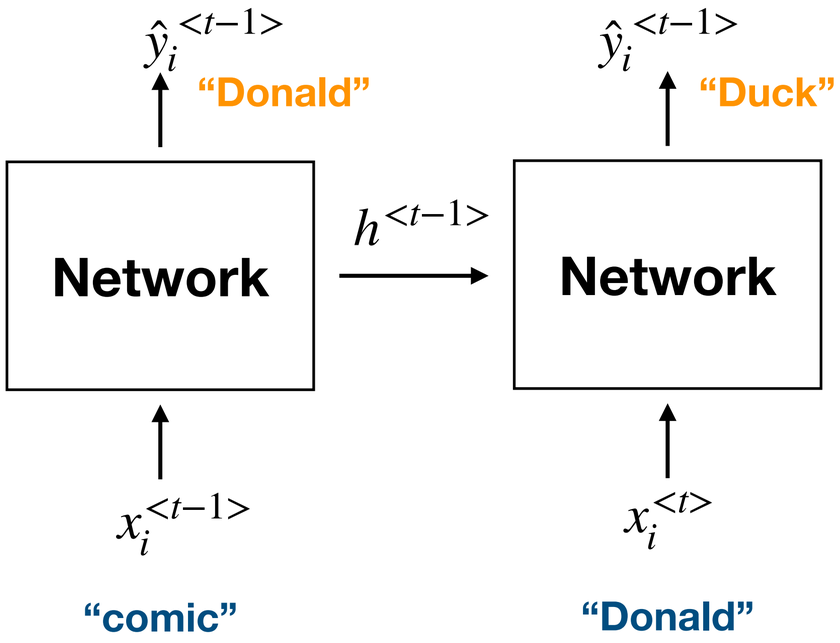
How about modeling just the next word?

The president of the United States is Donald Trump.
Wherever Donald Trump goes, security is tight.

The comic Donald Duck is very famous.

Context matters to the prediction!

Context Propagation



The meaning of the sentence depends on the **context**.

The context at $x_i^{<t-1>}$ is propagated to the next time step via the **hidden state** $h_i^{<t-1>}$.

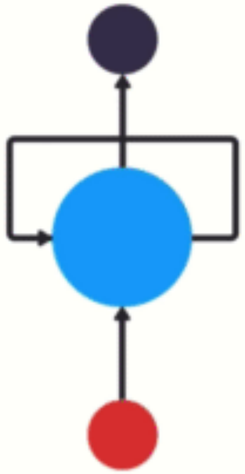
The next prediction is then modeled with both $x_i^{<t>}$ and $h_i^{<t-1>}$.

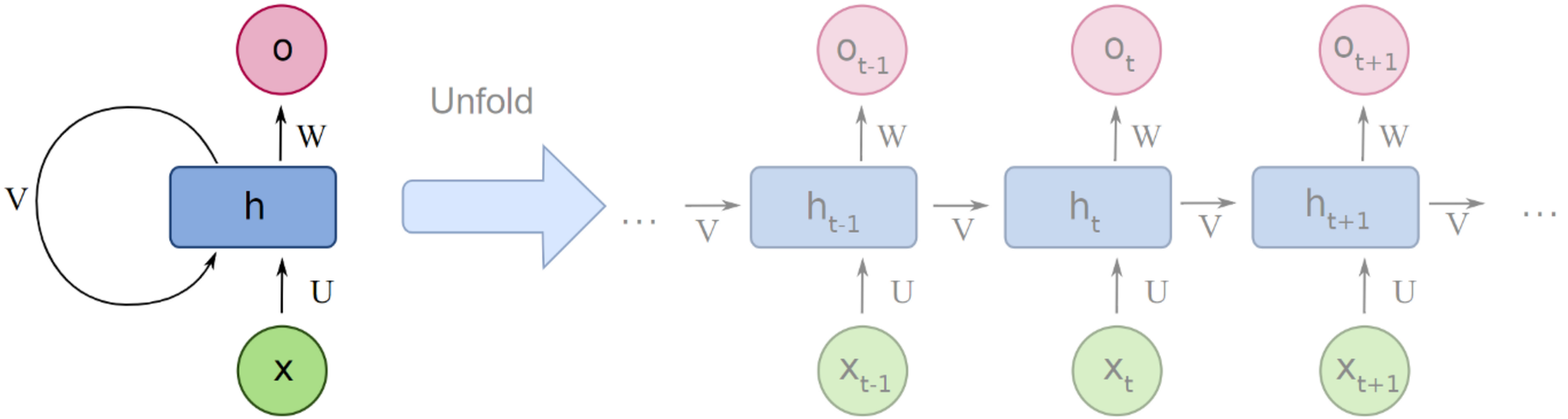
The introduction of the hidden state h_i allows the network to have **memory**.

"The comic Donald Duck is very famous."

Recurrent Neural Networks

In recurrent neural networks (RNNs), weights are **reused** across multiple time steps.





RNN

$$h_t = \sigma(Ux_t + Vh_{t-1} + b_h)$$

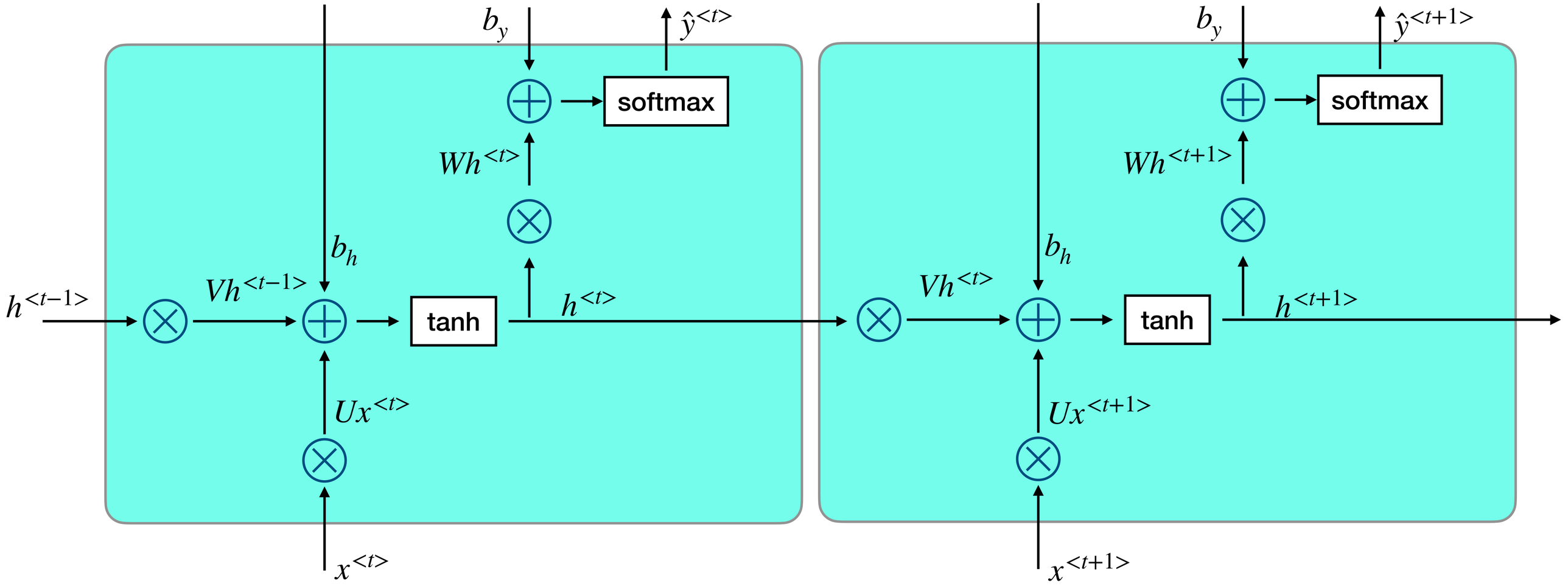
$$O_t = \sigma(Wh_t + b_o)$$

Back propagation through **time**

Non-RNN $O_t = \sigma(Wx_t + b)$

Back propagation through **layers**

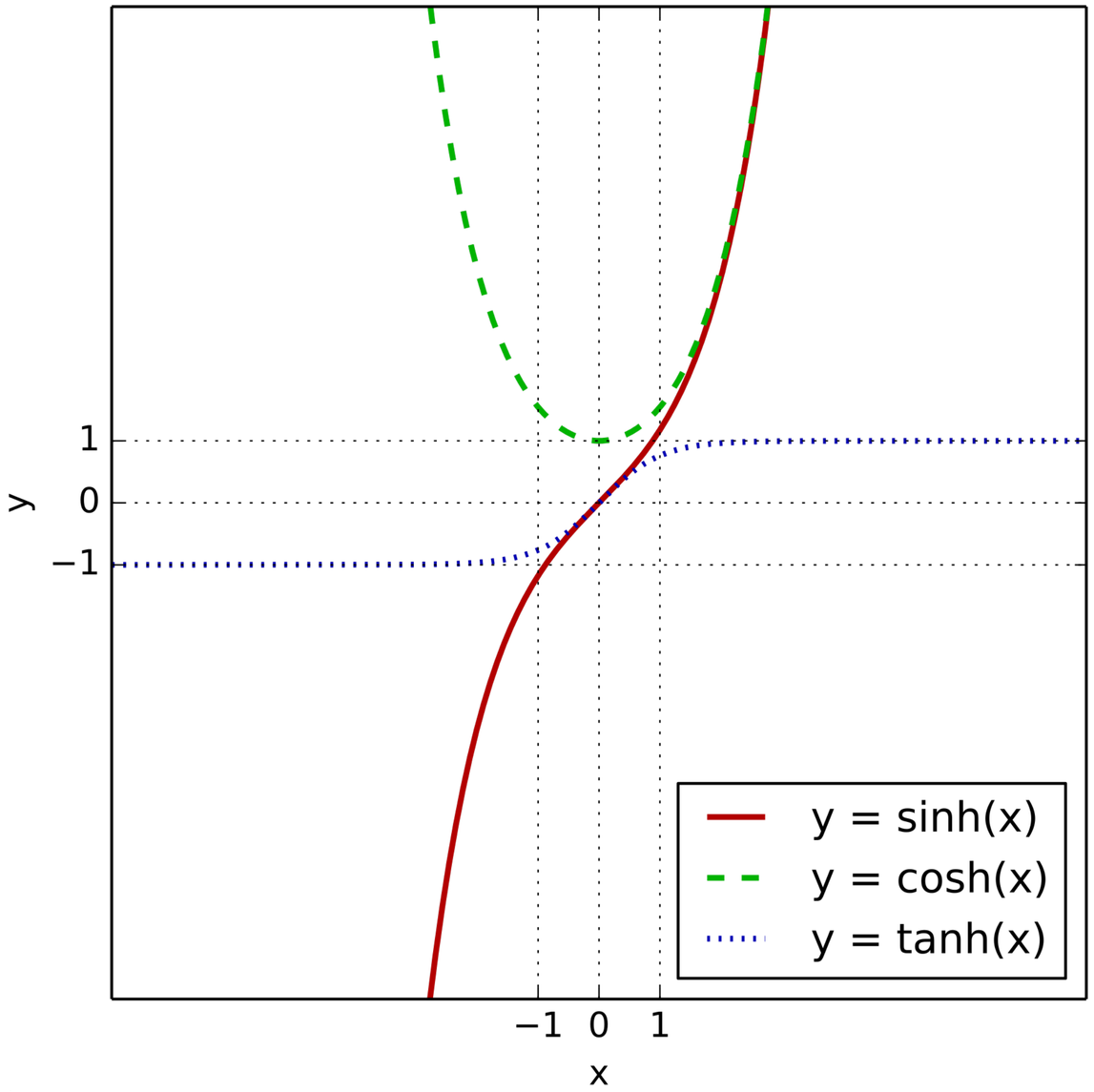
Anatomy of an RNN Cell



$$h^{<t>} = \tanh(Ux^{<t>} + Vh^{<t-1>} + b_h)$$

$$\hat{y}^{<t>} = \text{softmax}(Wh^{<t>} + b_y)$$

Hyperbolic Tangent as an Activation Function



$$\tanh(x) = \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}}$$

Between **[-1, 1]**, the function behaves **linearly** (more or less).

As long as the input range is within [-1,1], the derivative in this range is approximately 1.

The function always scales the input to the well-controlled range of [-1,1].

Limitation of standard RNNs

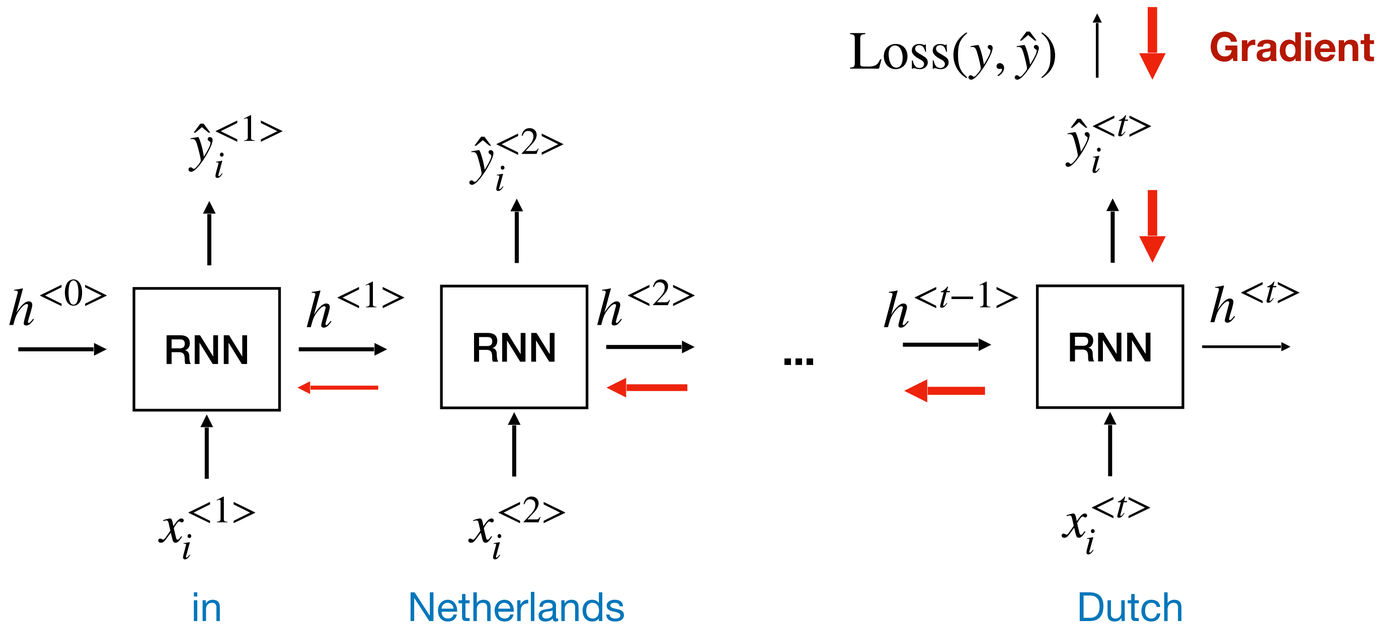
We are not done with the story…

Long-term Dependency

Sometimes, the contexts are far away.

The clouds are in the *sky*.

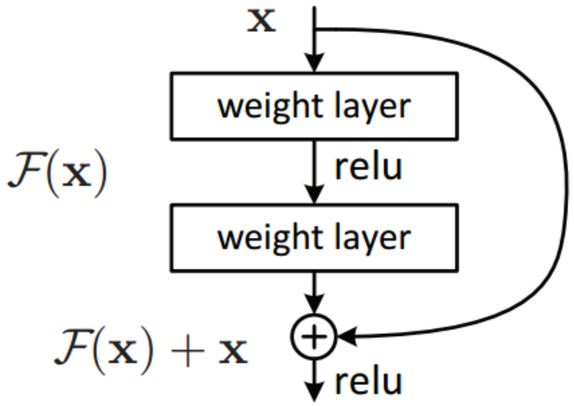
I grew up in the Netherlands… I speak fluent *Dutch*.



Contexts can be **forgotten**; the **gradients** are **vanishing** during back propagation.

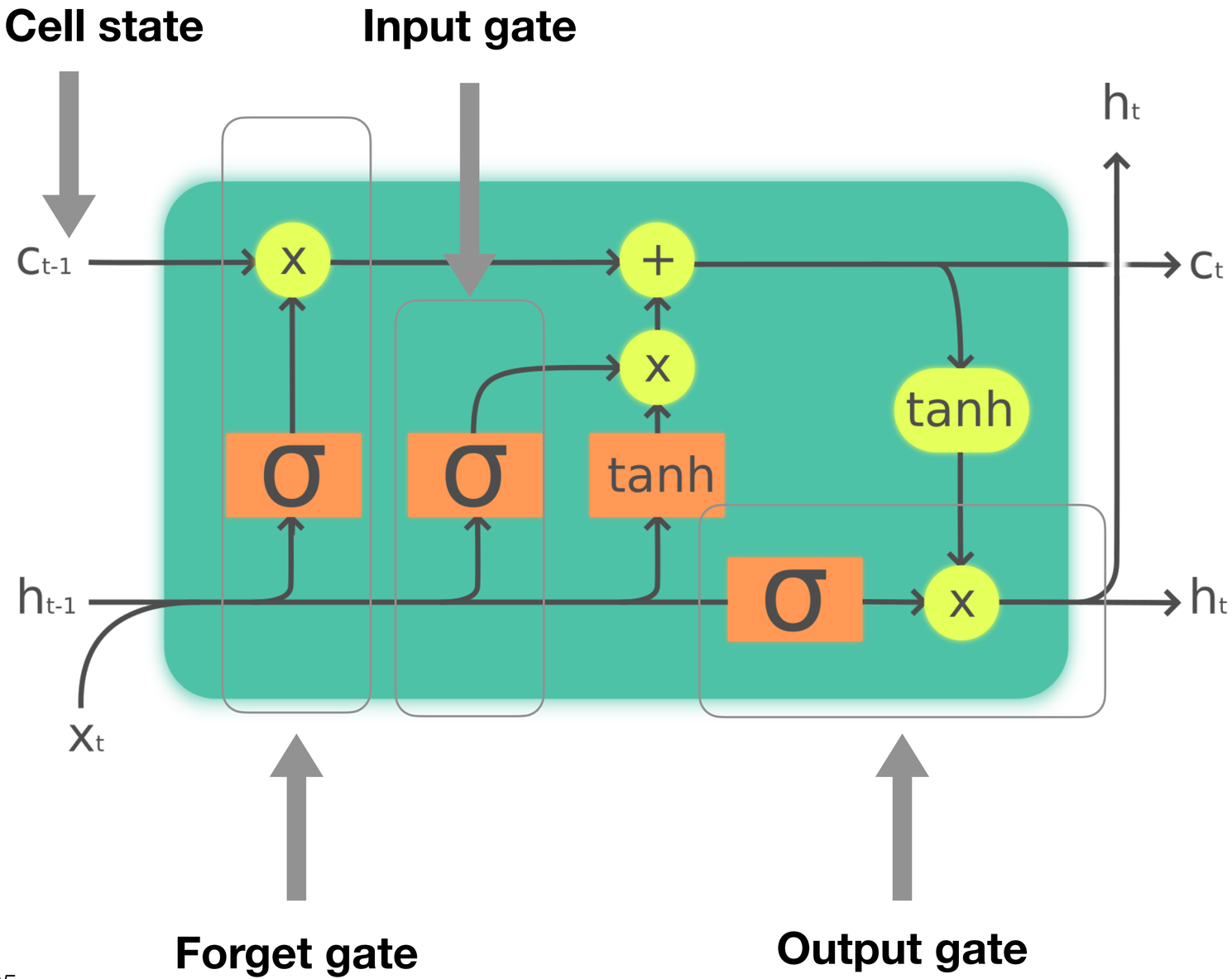
Vanishing Gradient Problem in RNNs

Residual connection is a general solution to the vanishing gradient problem.



However, for very long dependency (which is common in RNNs), this solution is not sufficient.
We should instead regulate which information to **keep** and which to **forget**.

Long Short-term Memory



Hochreiter & Schmidhuber (1997)

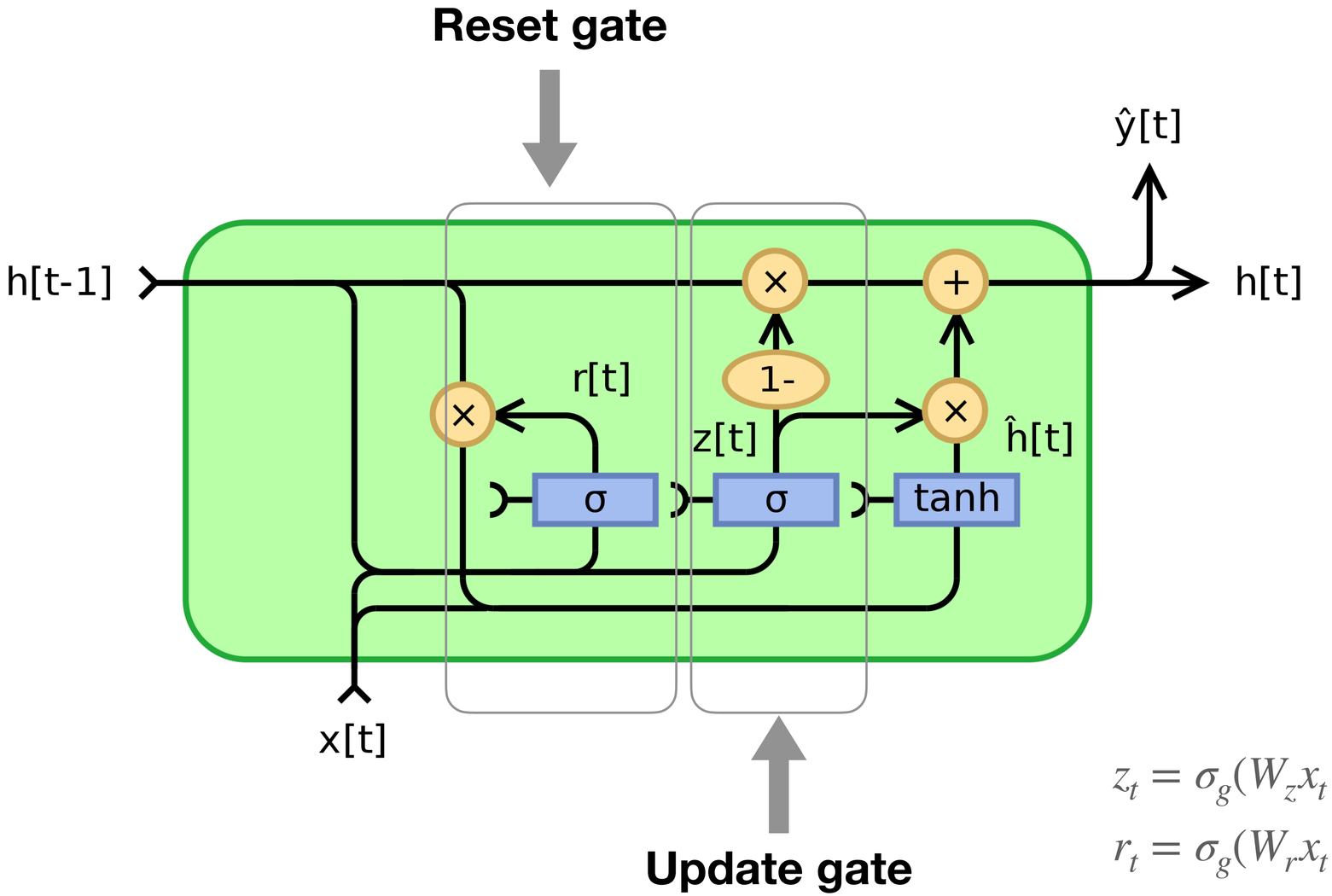
LSTM regulates the flow of information through gates.

- **Input gate**: controls the extent to which a new value flows into the cell;
- **Forget gate**: controls the extent a value remains in the cell;
- **Output gate**: controls the extent to which the value in the cell is used to calculate the output activation.

$$f_t = \sigma_g(W_f x_t + U_f h_{t-1} + b_f)$$
$$i_t = \sigma_g(W_i x_t + U_i h_{t-1} + b_i)$$
$$o_t = \sigma_g(W_o x_t + U_o h_{t-1} + b_o)$$
$$\tilde{c}_t = \sigma_h(W_c x_t + U_c h_{t-1} + b_c)$$
$$c_t = f_t \circ c_{t-1} + i_t \circ \tilde{c}_t$$
$$h_t = o_t \circ \sigma_h(c_t)$$

Image source: Wikipedia

Gated Recurrent Unit



Cho et al. 2014 (arXiv:1406.1078)

GRU regulates the flow of information through gates:

- **Reset gate**: controls how much past information to forget;
- **Update gate**: controls what information to discard and what to keep (similar to the LSTM's input gate and forget gate combined)

$$z_t = \sigma_g(W_z x_t + U_z h_{t-1} + b_z)$$
$$r_t = \sigma_g(W_r x_t + U_r h_{t-1} + b_r)$$
$$h_t = z_t \odot h_{t-1} + (1 - z_t) \odot \phi_h(W_h x_t + U_h(r_t \odot h_{t-1}) + b_h)$$

Generating Input Sequences

To apply a long sequence to a RNN, we need to define the training data x and the labels y:

(1, ...) (2, ...) (3, ...) (4, ...) (5, ...) (6, ...) (7, ...) (8, ...) (9, ...) (10, ...) (11, ...) (12, ...) (13, ...) (14, ...)

We could either **reshape** it:

x (1, ...) (2, ...) (3, ...) (4, ...) (5, ...) (6, ...) (7, ...)

y (8, ...) (9, ...) (10, ...) (11, ...) (12, ...) (13, ...) (14, ...)

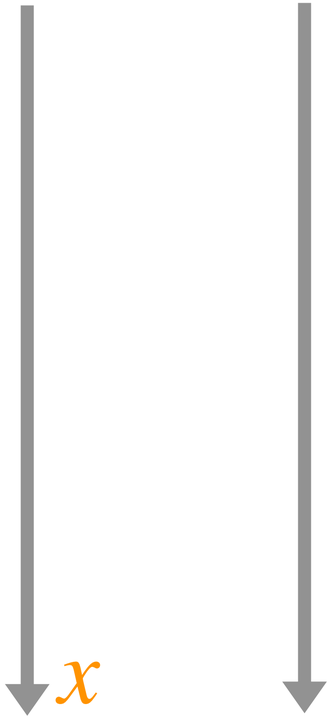
Or truncate it using a **rolling window**:

(1, ...) (2, ...) (3, ...) (4, ...) (5, ...) (6, ...) (7, ...)

(3, ...) (4, ...) (5, ...) (6, ...) (7, ...) (8, ...) (9, ...)

(5, ...) (6, ...) (7, ...) (8, ...) (9, ...) (10, ...) (11, ...)

(7, ...) (8, ...) (9, ...) (10, ...) (11, ...) (12, ...) (13, ...)



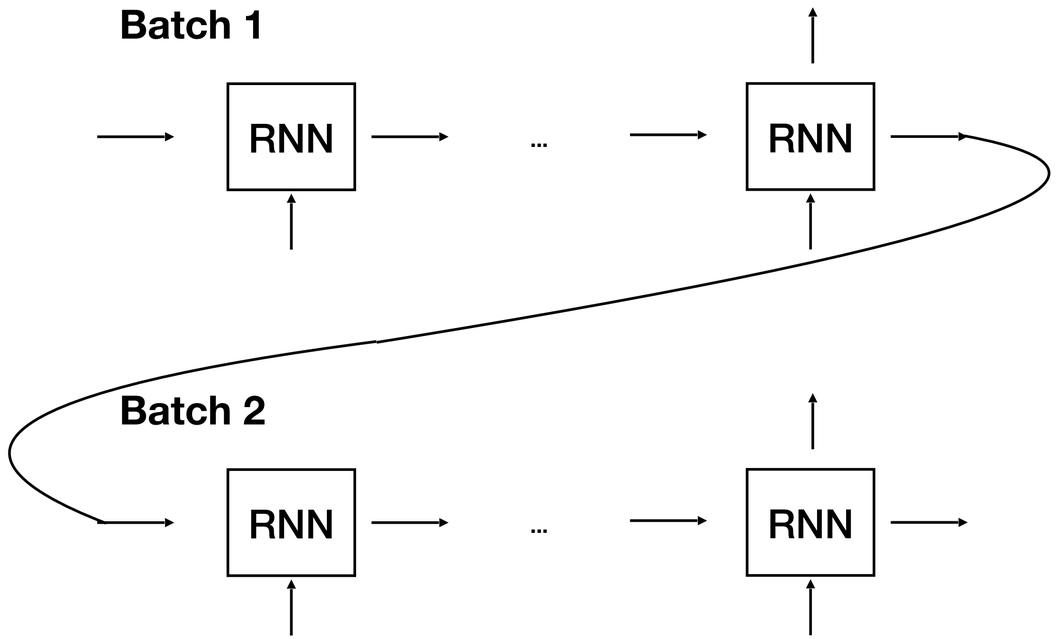
(13, ...)

Stateful RNNs

A stateful RNN passes the **last state** of the **previous batch** as the **initial state** of the **next batch**.

This is useful if there is some connections between batches. This feature essentially allows long sequences to be **folded** into batches.

A non-stateful RNN initialises state of each batch to zero.

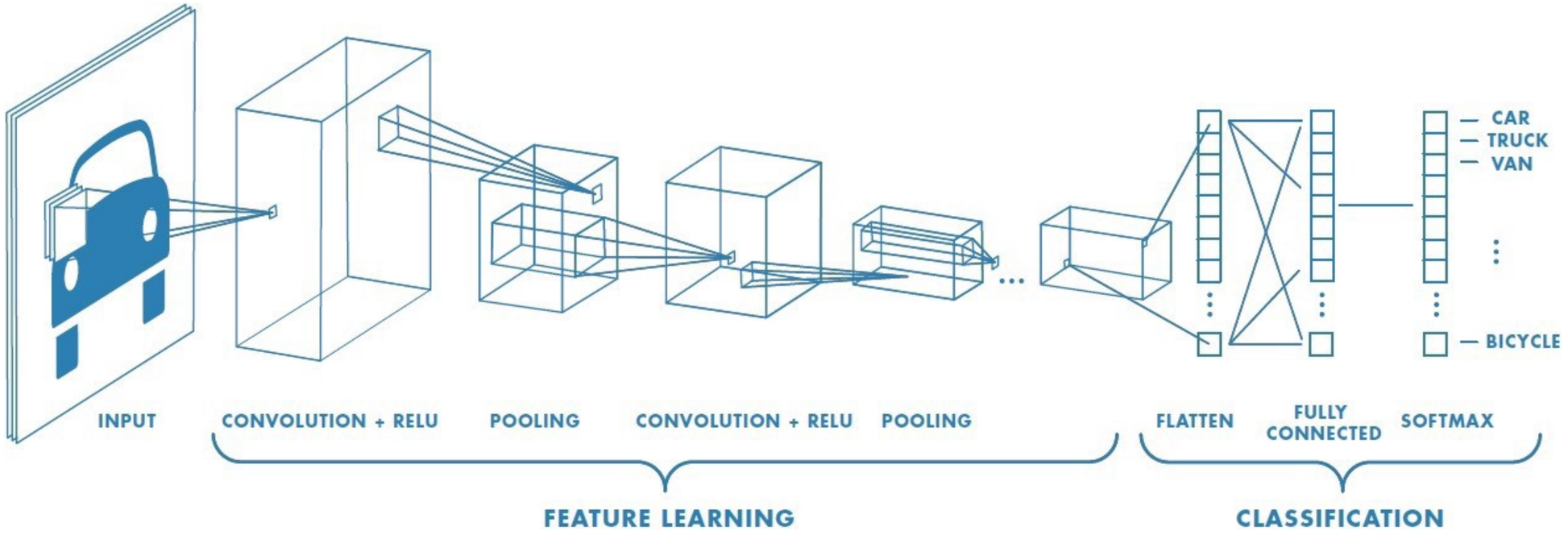


Batch 1	(1, ...) (2, ...) (3, ...) (4, ...) (5, ...) (6, ...) (7, ...)
Batch 2	(8, ...) (9, ...) (10, ...) (11, ...) (12, ...) (13, ...) (14, ...)

Generative Models

Can we invert a CNN classifier?

CNN image classifier



Generative models?

Image credit: Sumit Saha

Can computers have “imaginations”?

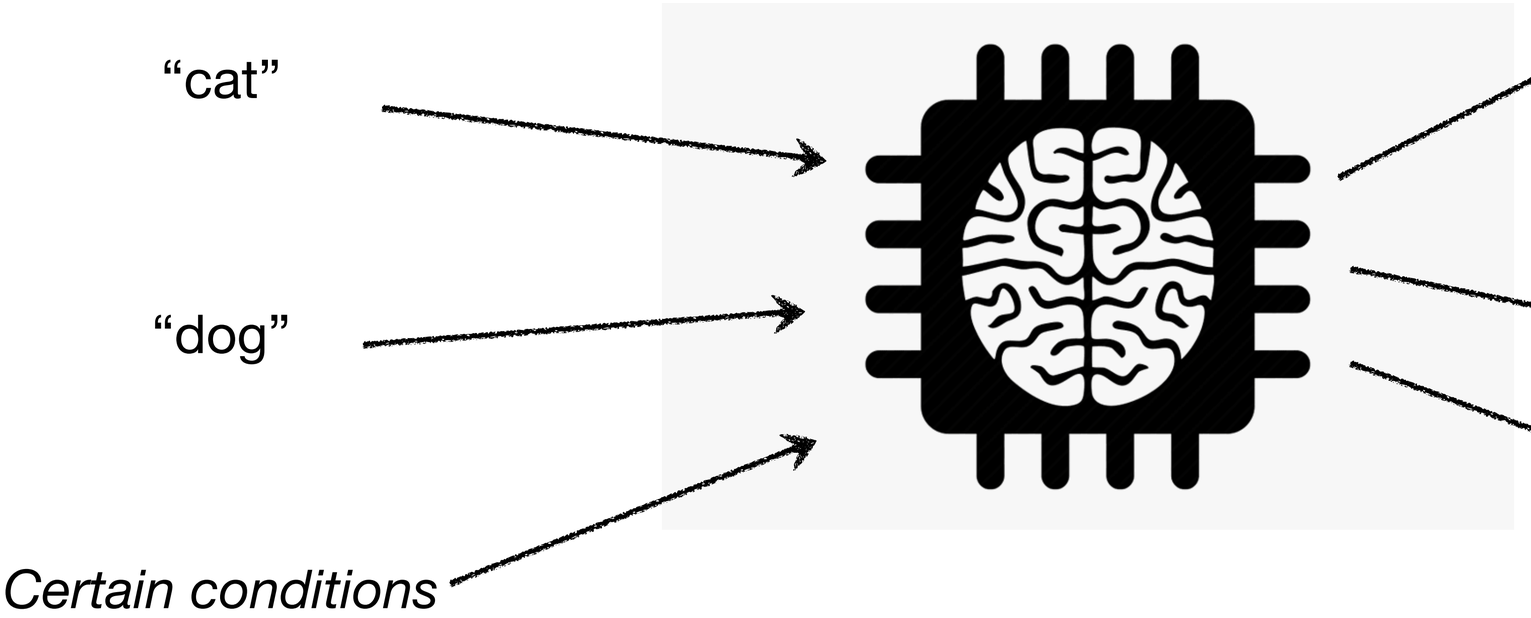
Input

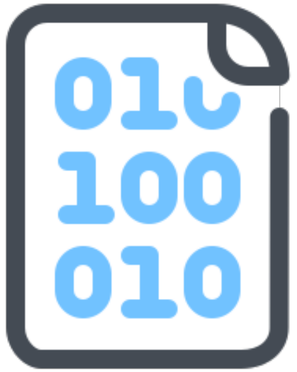
Output

“cat”

“dog”

Certain conditions





If the answer is **yes**, we can **condition** a DNN and make it generate certain outputs!

Move beyond associating inputs and outputs

Classification: mapping a distribution to a **certain** output

Happy cat

Angry cat

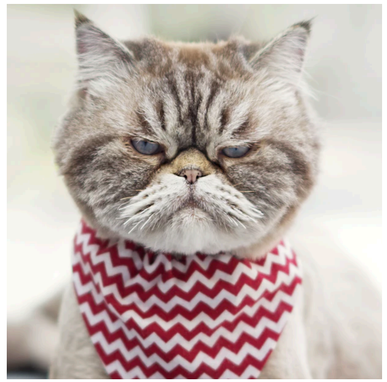
Relaxed cat

“Cats”

Generation: mapping an input to a probability **distribution**

“Cats”

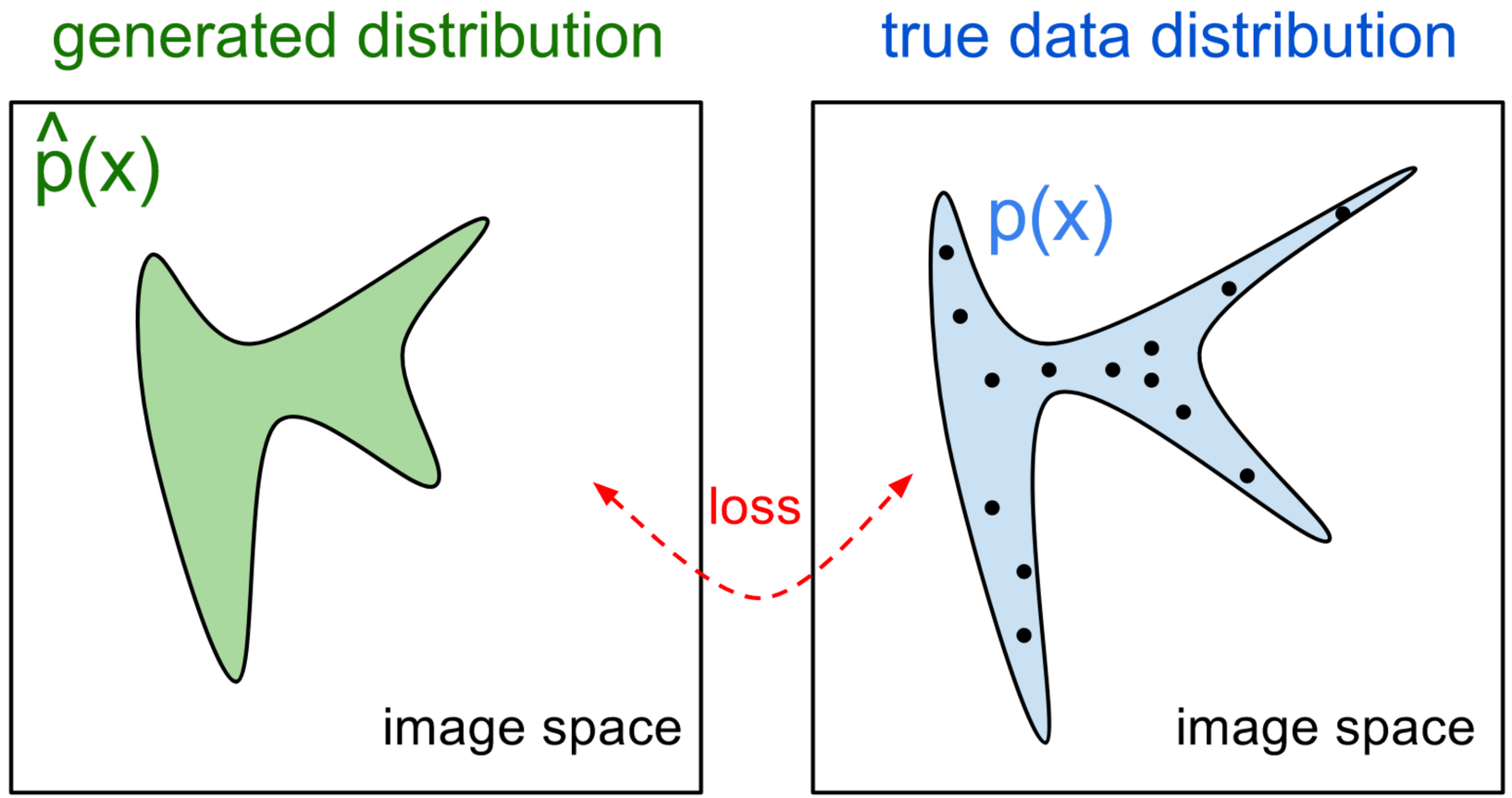
Happy cat



Angry cat

Relaxed cat

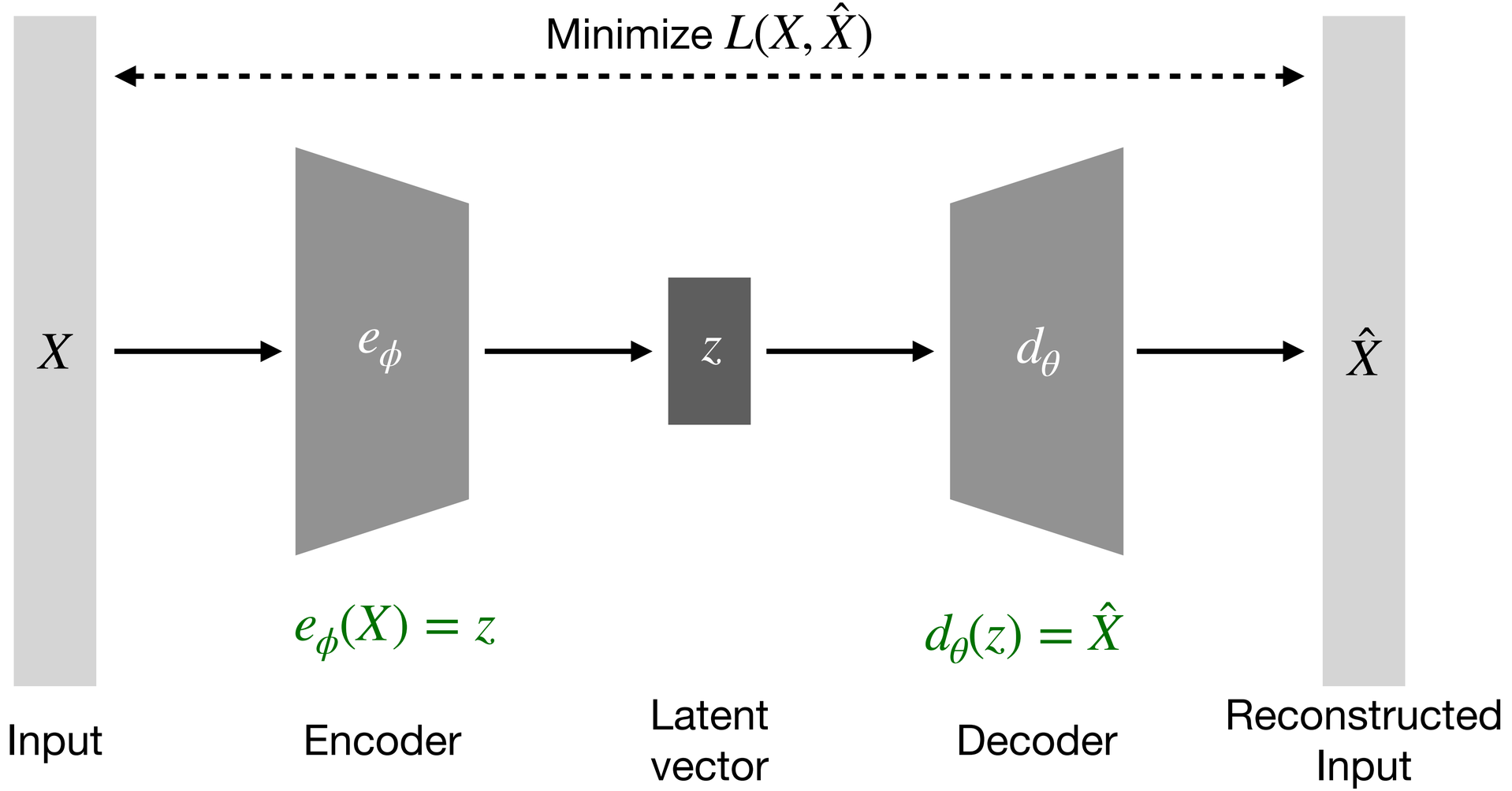
What is a Generative Model?



A (deep) **generative model**
… **learns a distribution** instead of a certain value
… allows **uncertainties** to be **captured**
… allows for (conditional) **density estimation**
… belongs to the category of **unsupervised learning**

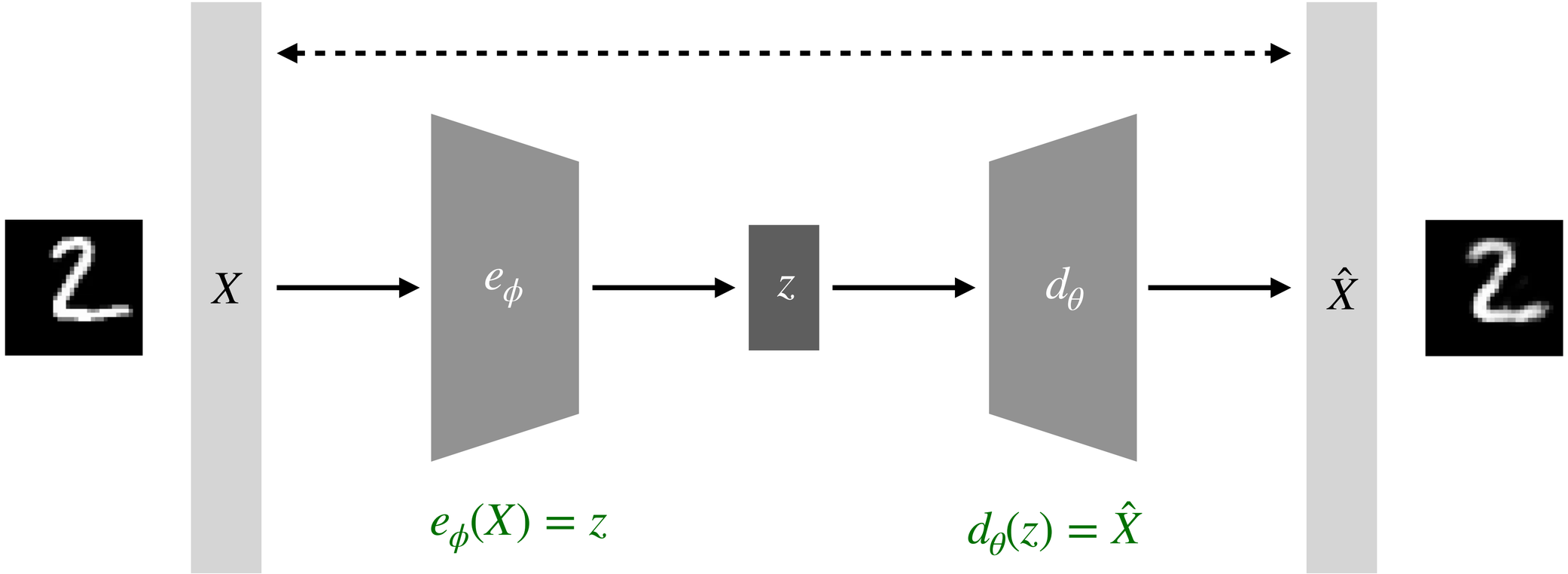
Image: OpenAI

Autoencoder



Hinton & Salakhutdinov (2006, Science)

Autoencoder



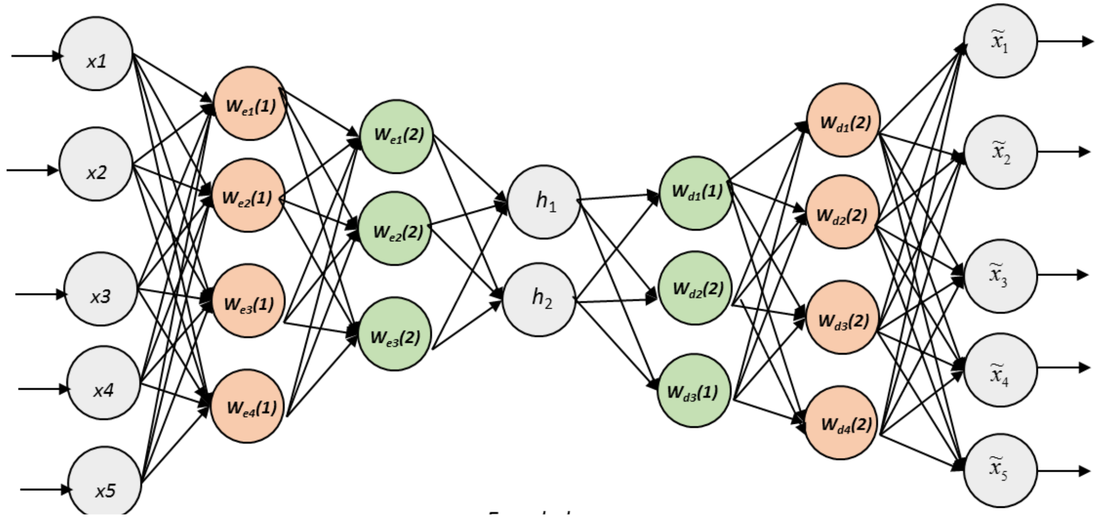
It looks like an autoencoder trivially copies X to $\hat{X}$, **but**:

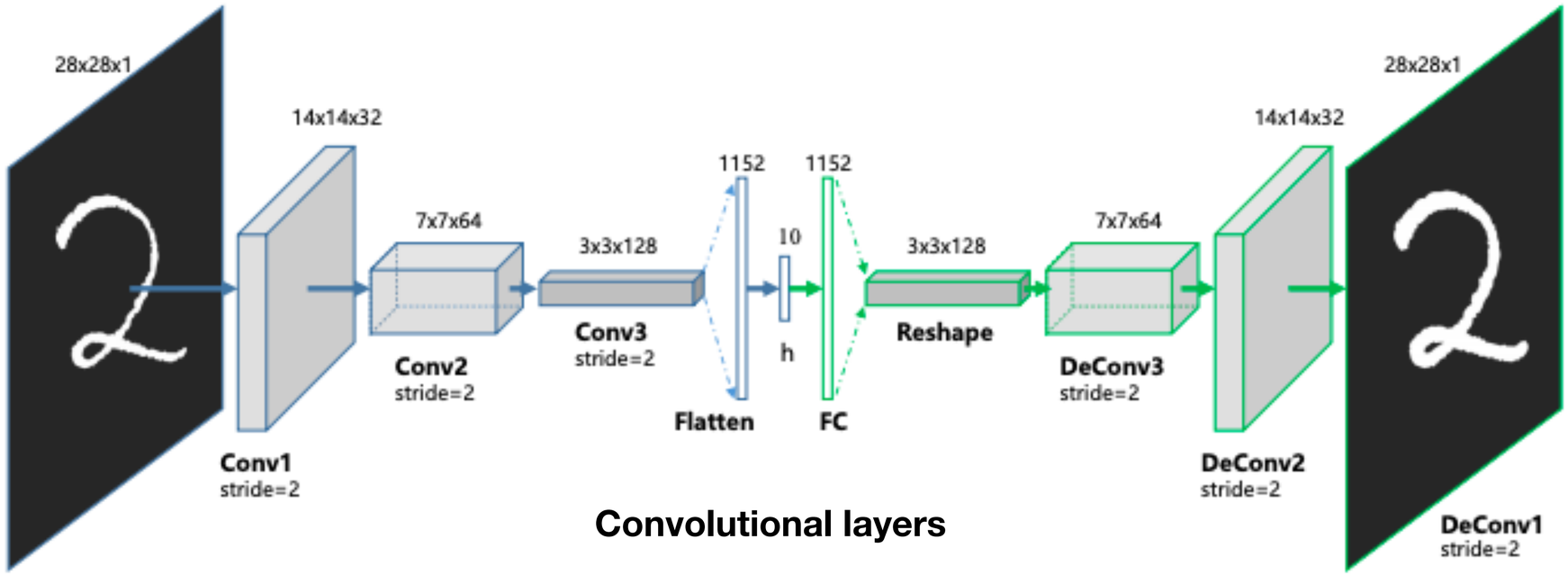
- The **latent vector** z has lower dimension than the input X, and therefore information are **compressed**.
- A good autoencoder selects relevant information and **discards irrelevant information**.

Hinton & Salakhutdinov (2006, Science)

Autoencoder: Basic Implementations

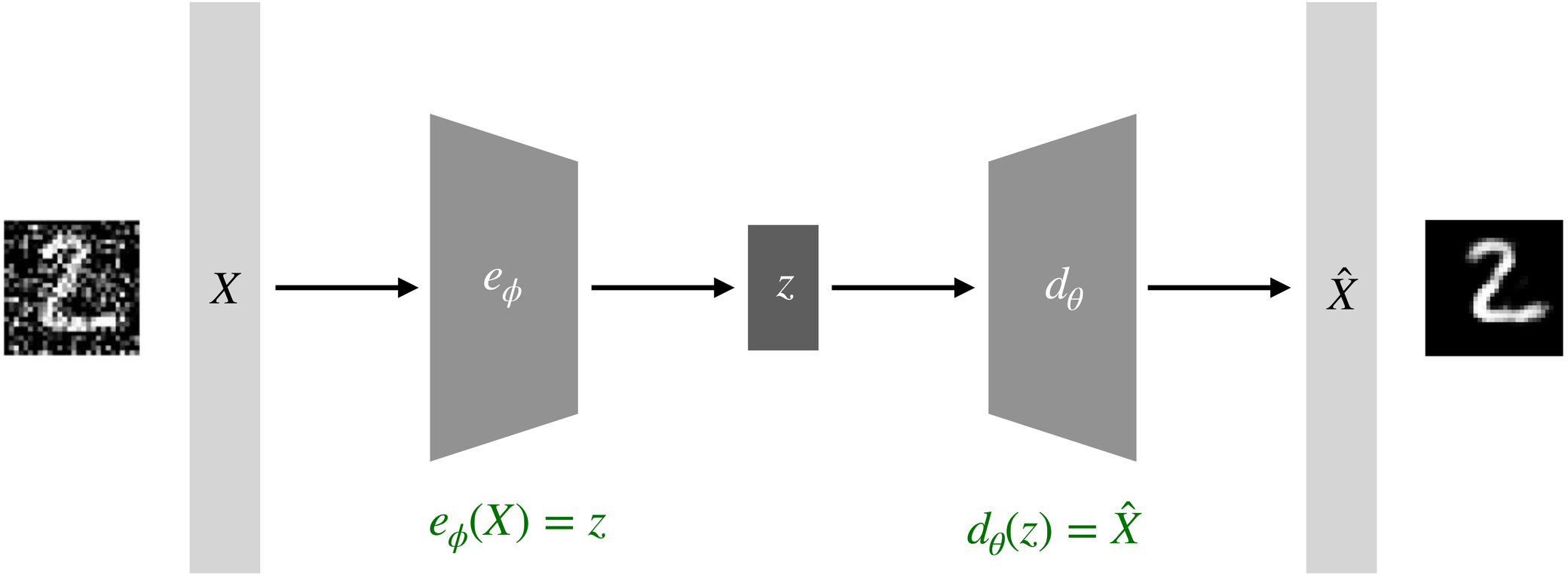
Fully connected layers





Convolutional layers

Autoencoder

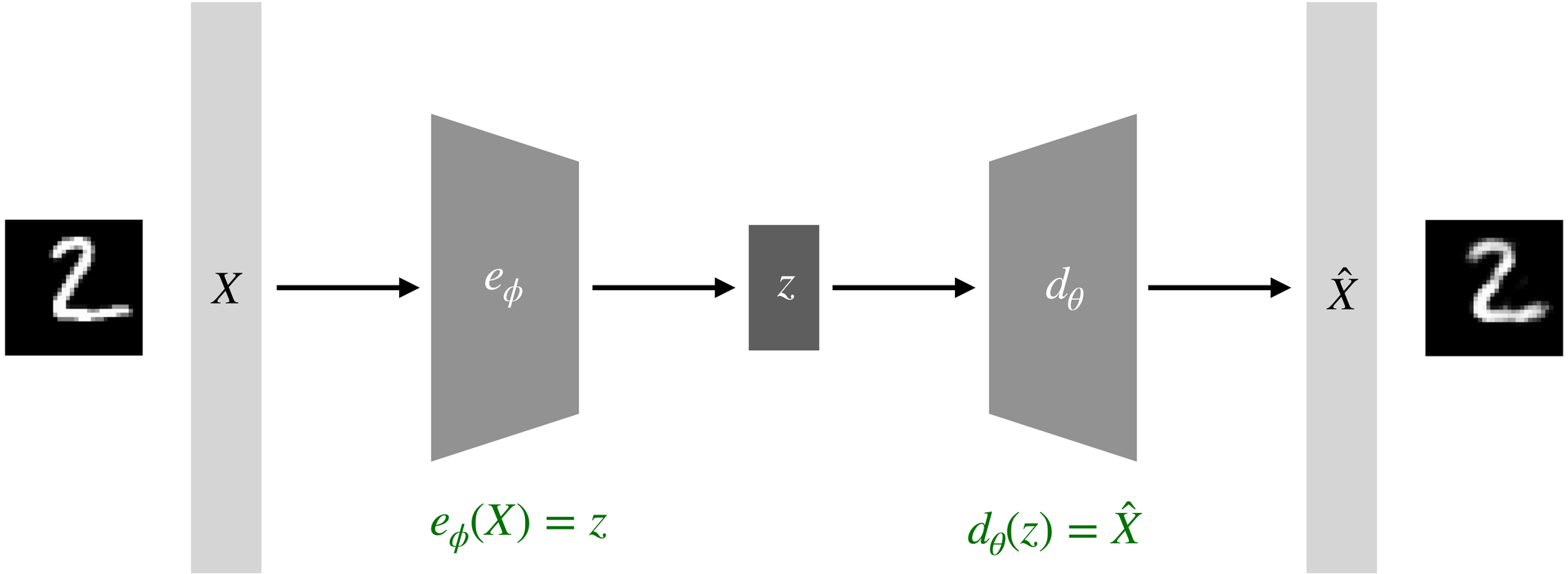


Denoising autoencoder:

- Trained with noisy (perturbed) input data;
- The bottleneck z has limited capacity, and therefore **prevents overfitting**;
- The reconstruction data is clean of noise, because z doesn't have enough capacity to learn noise.

Hinton & Salakhutdinov (2006, Science)

Autoencoder



Autoencoder for anomaly detection:

- Trained with regular input data (i.e., no anomaly);
- The bottleneck z encodes the statistical properties of the input data;
- Anomalies have different statistical properties; the autoencoder can't properly reconstruct them;
- Large reconstruction error → Anomaly.

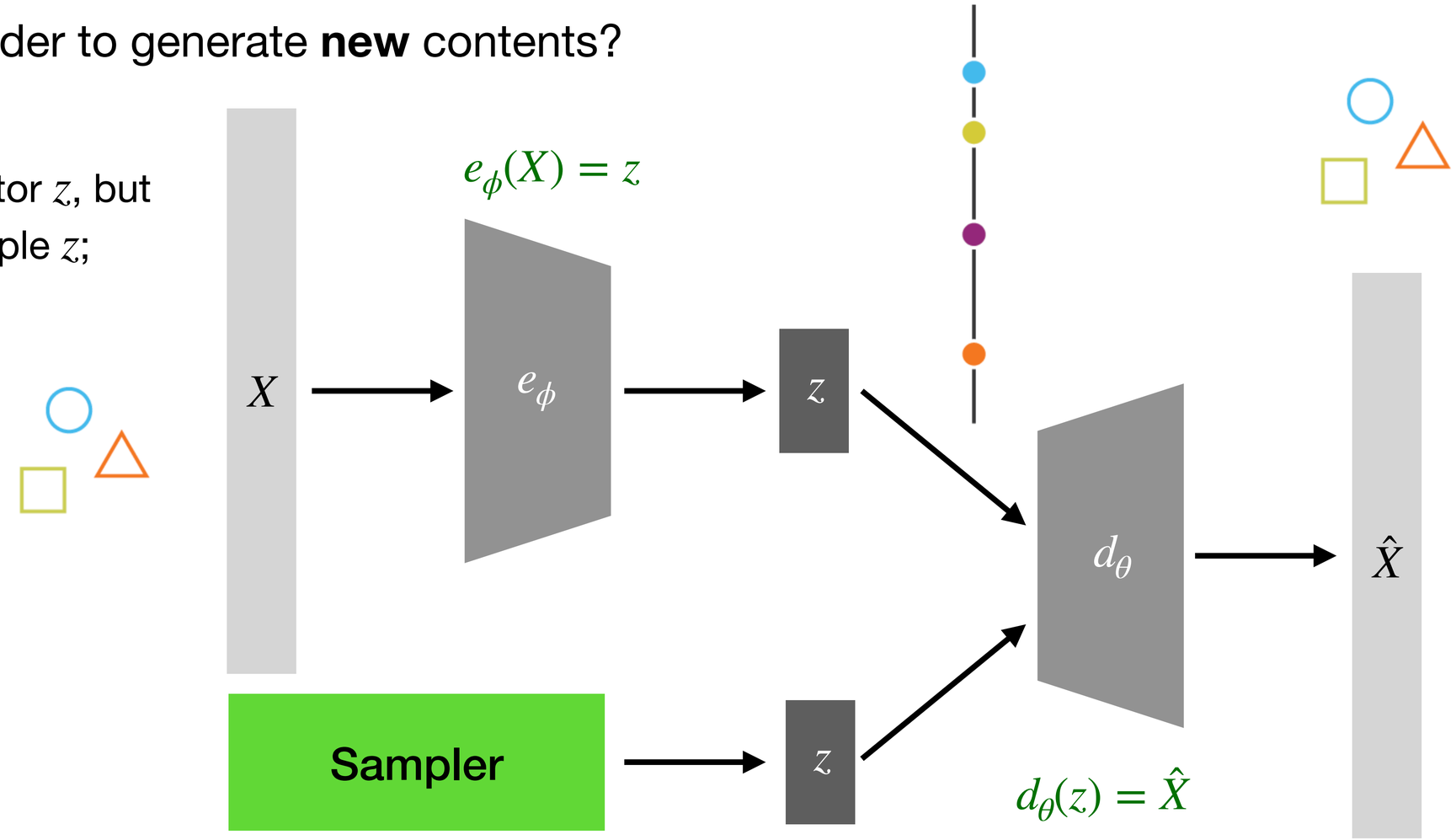
Hinton & Salakhutdinov (2006, Science)

Autoencoder

How can we let an autoencoder to generate **new** contents?

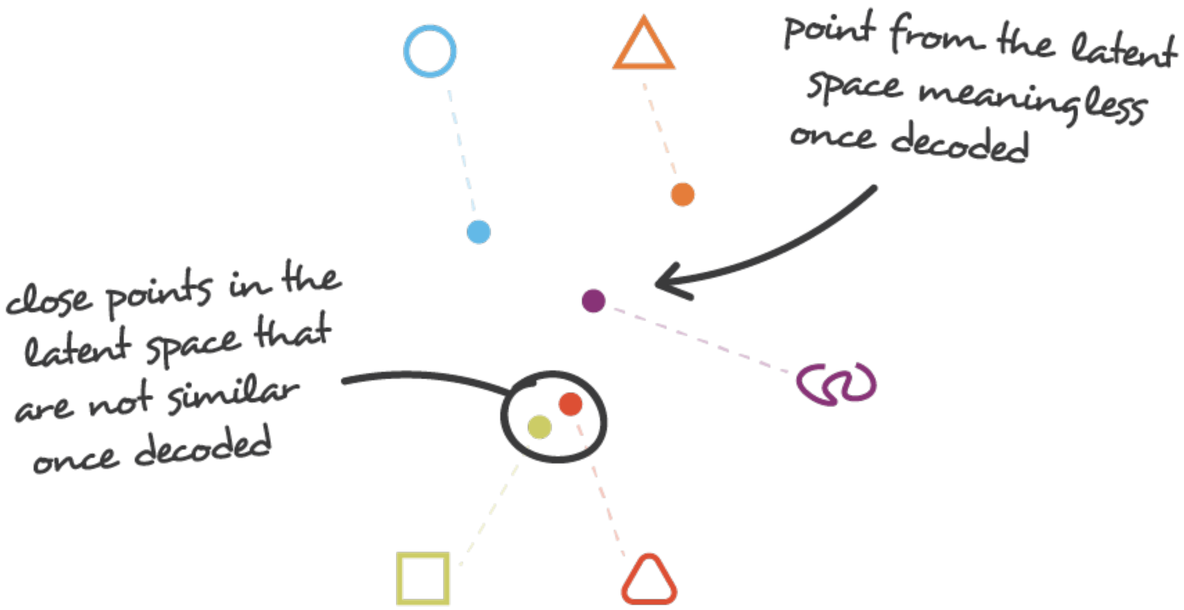
We can sample the latent vector z, but

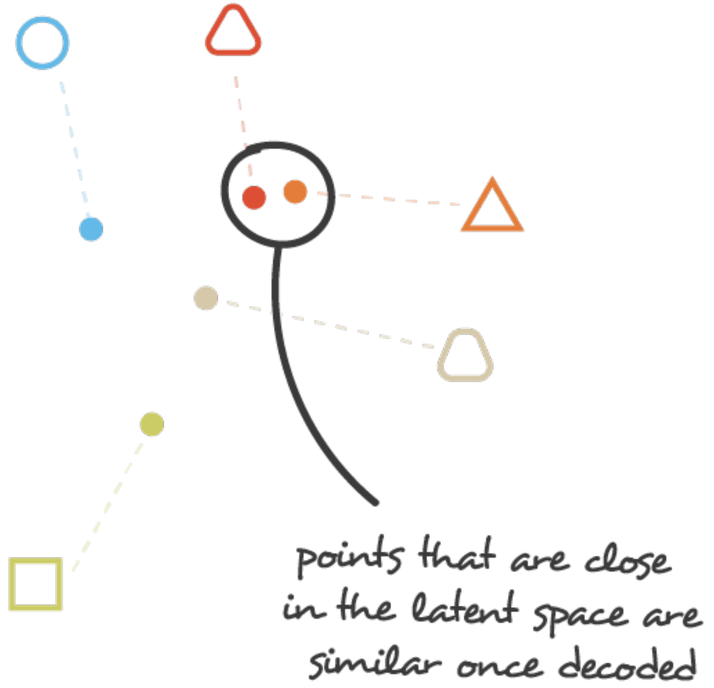
- We don't know how to sample z;
- z can be very irregular.



We need to **regularize** the distribution (i.e., arrangement) of the latent space!

Latent Space Distribution





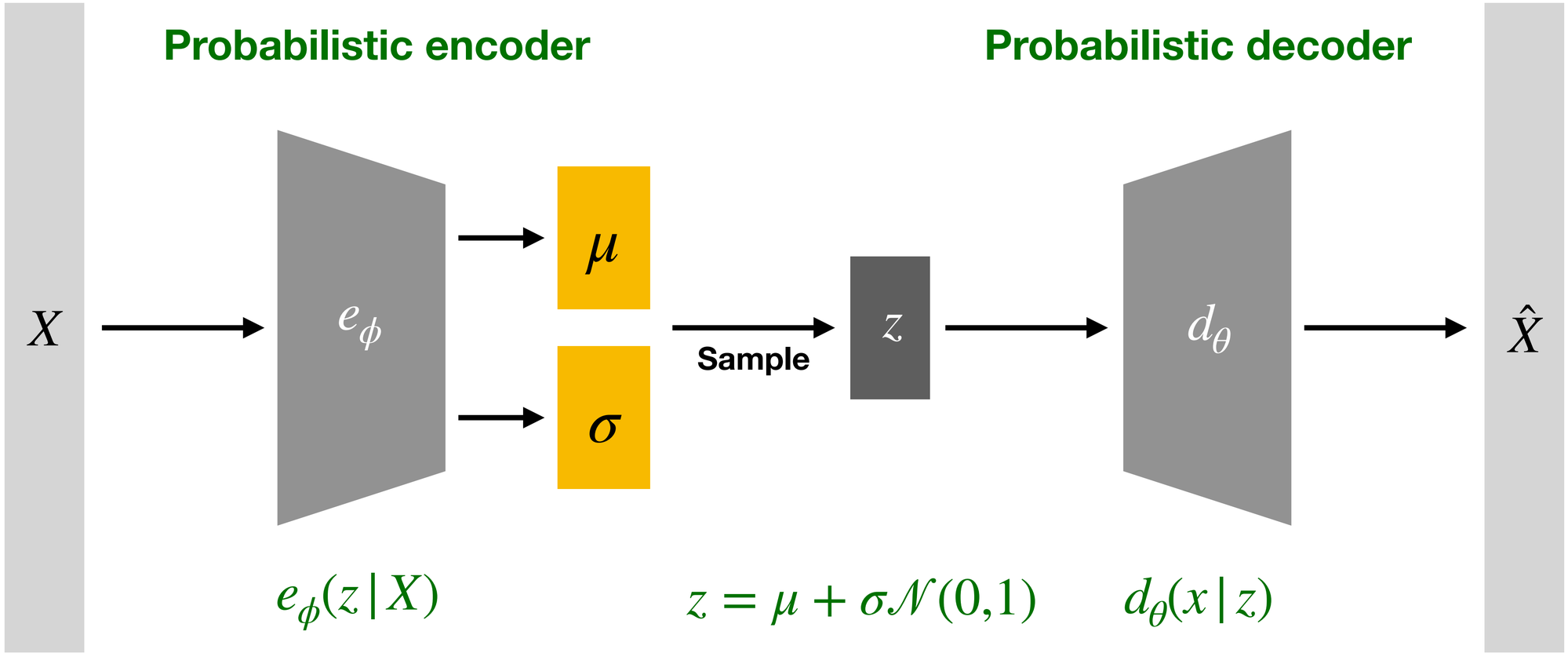
irregular latent space

regular latent space

A regular latent space allows us to do **interpolation**.
New contents are generated **by interpolating** the latent space.

Image: Joseph Rocca (TowardDataScience)

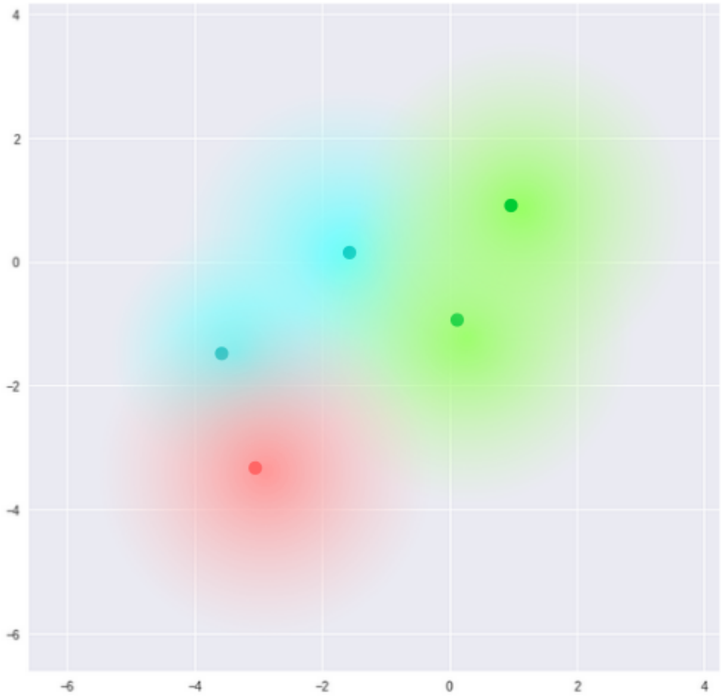
Variational Autoencoder



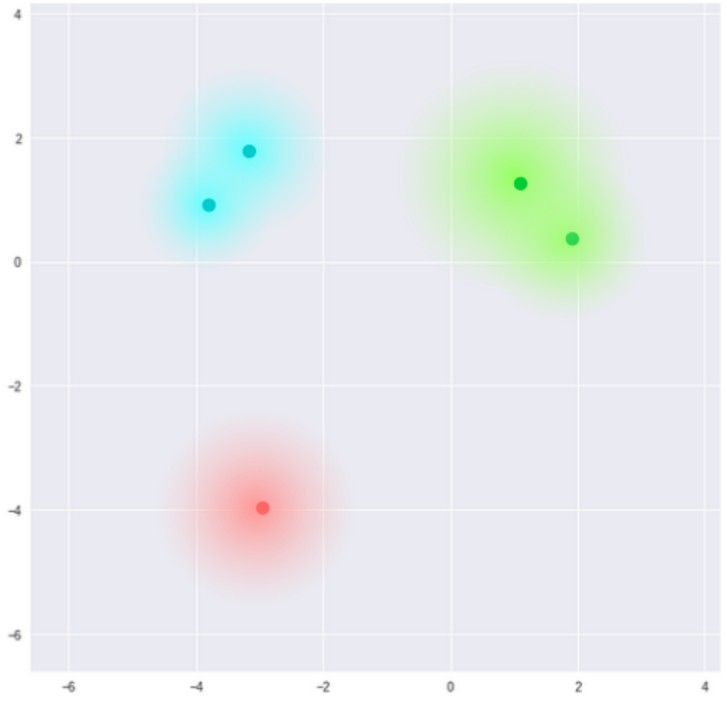
Kingma & Welling (2013, arXiv:1312.6114)

Latent space: tight, smooth, and complete

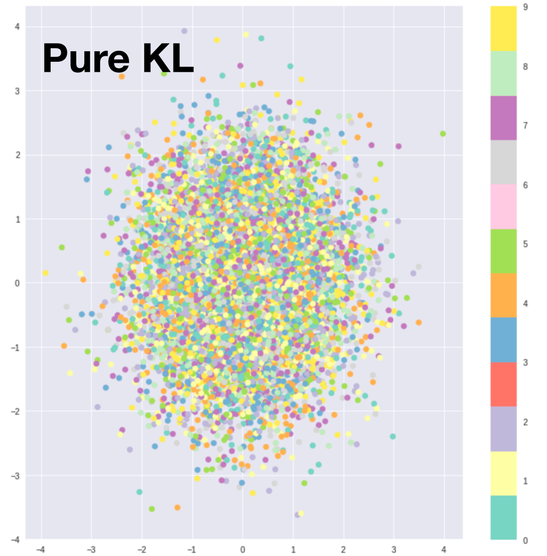
Without constraining μ and σ:

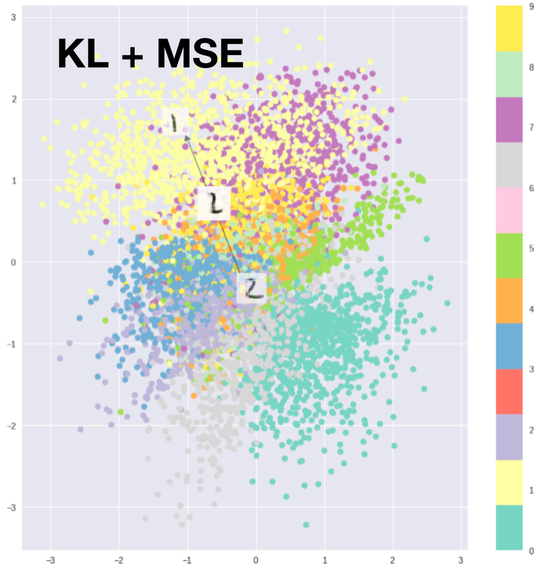


What we require



What we may inadvertently end up with

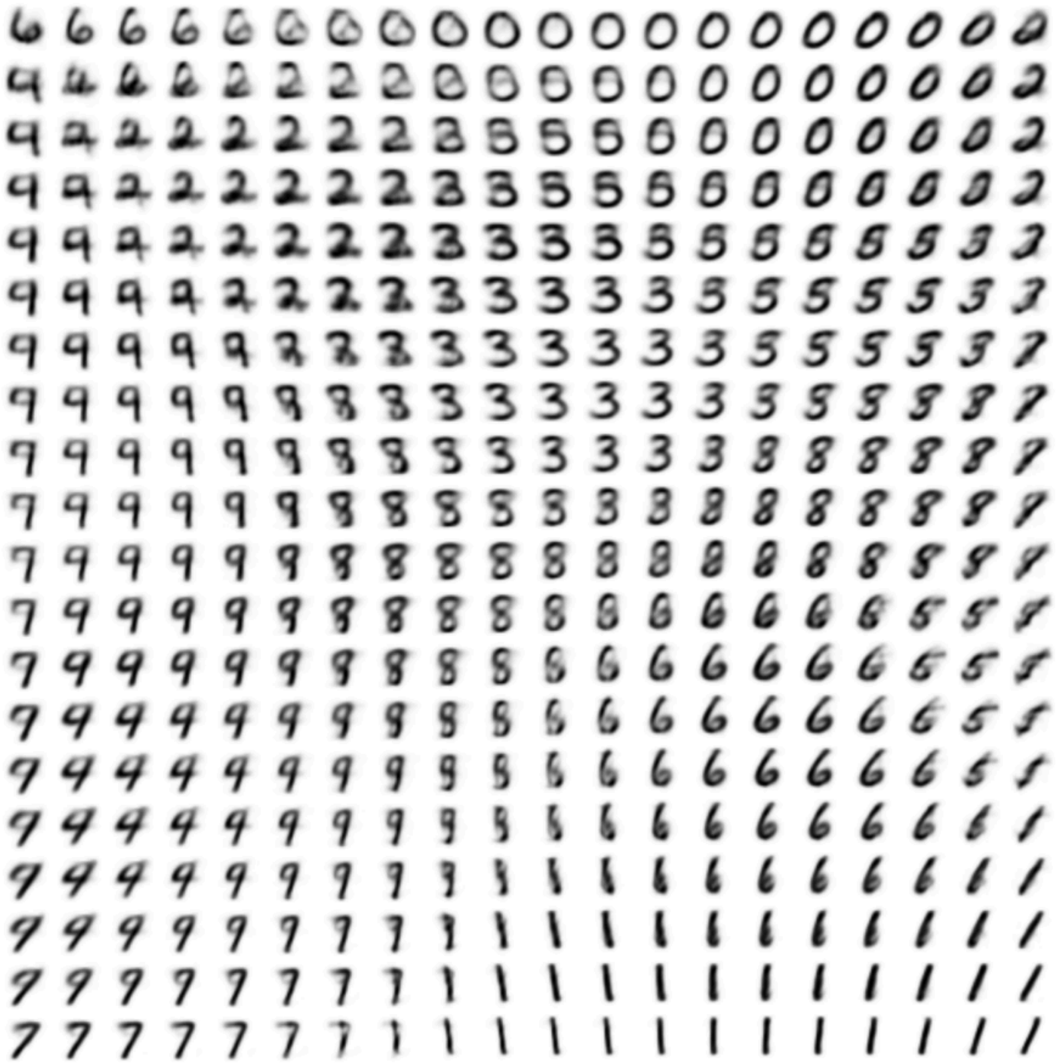


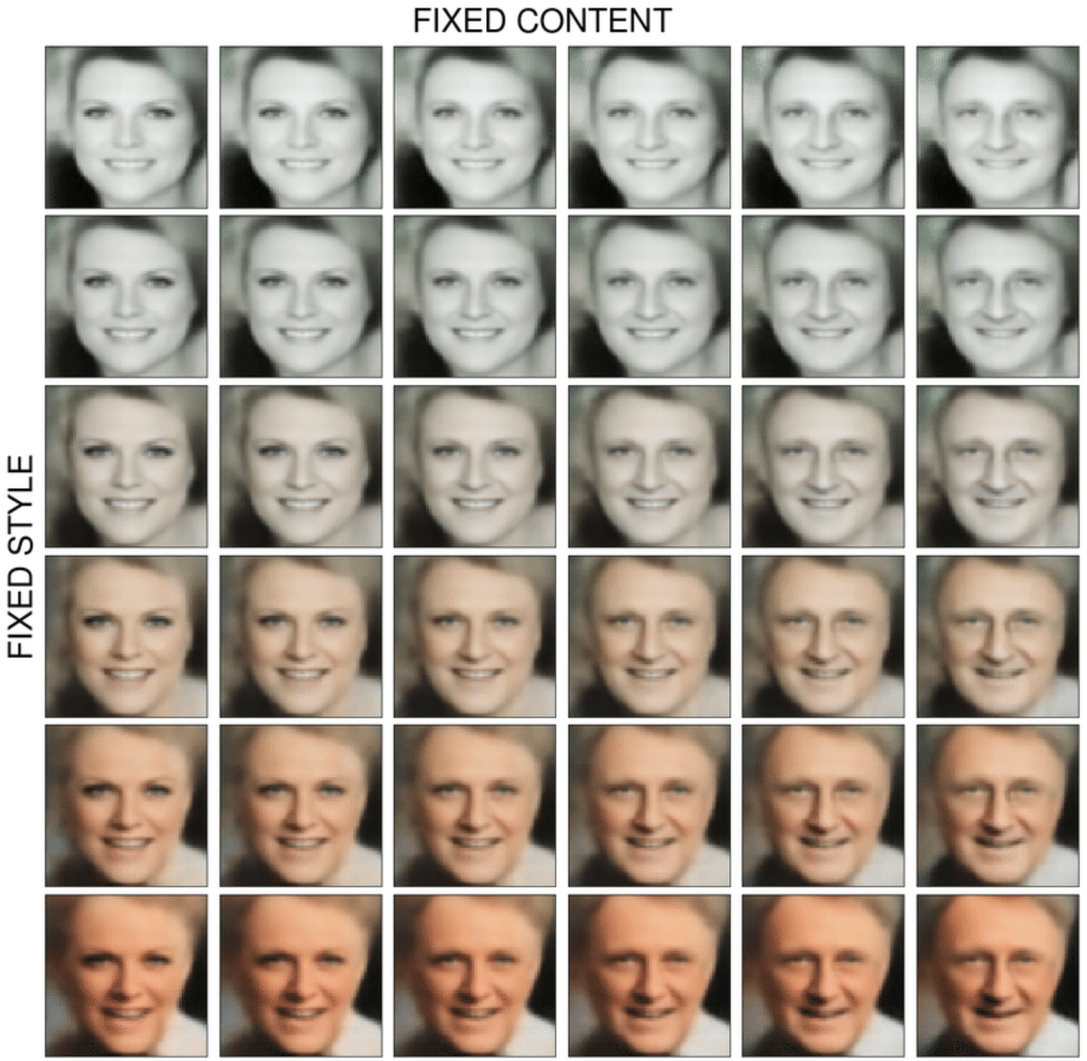


Solution:

- Use **KL divergence** to force clusters to get **close to each other**;
- Use **reconstruction losses** (e.g., MSE) to **avoid** clusters from **overlapping**.

Latent vector interpolation

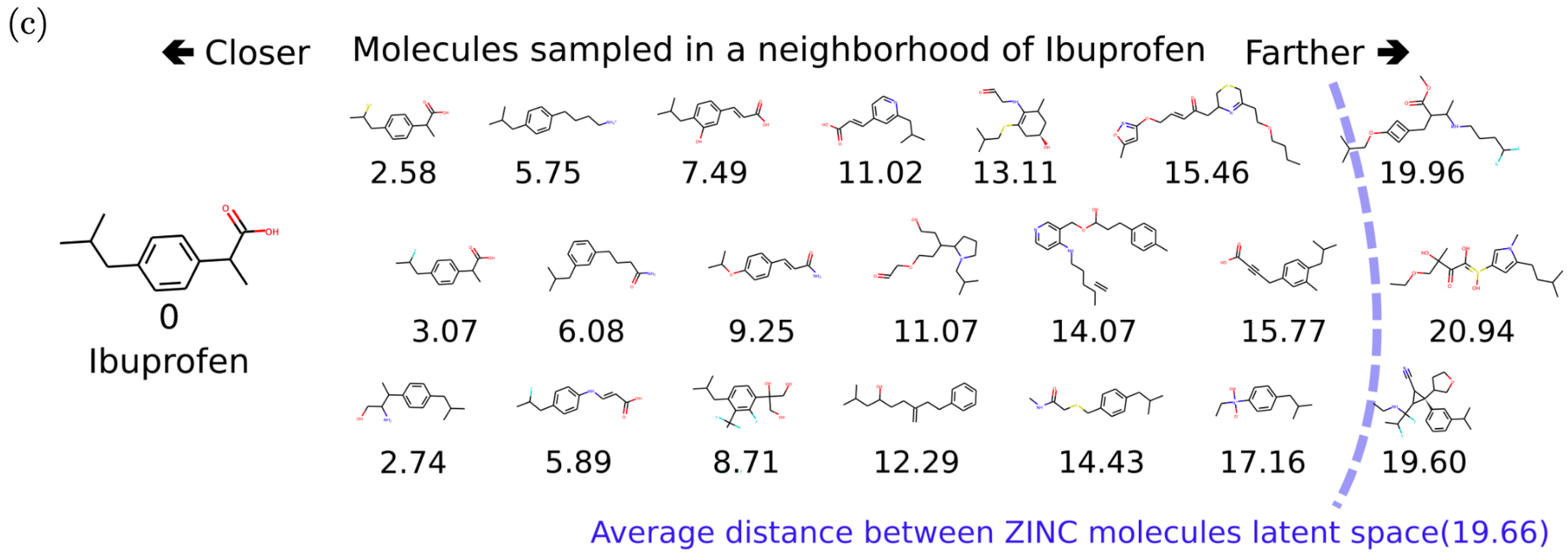




Bouchacourt, Tomioka & Nowozin (2017).

Application: VAE for Drug Discovery

Proposing candidate molecules by interpolating the latent space.



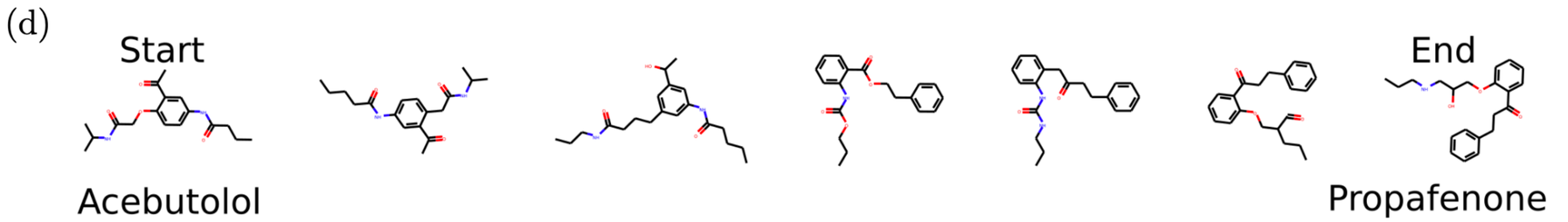


Fig.2 of Gómez-Bombarelli et al. (2016, arXiv:1610.02415)

Alternative Approaches?

Variational autoencoders is elegant and theoretically pleasing.
However, the generated images (data) are **blurry** (causes unknown).

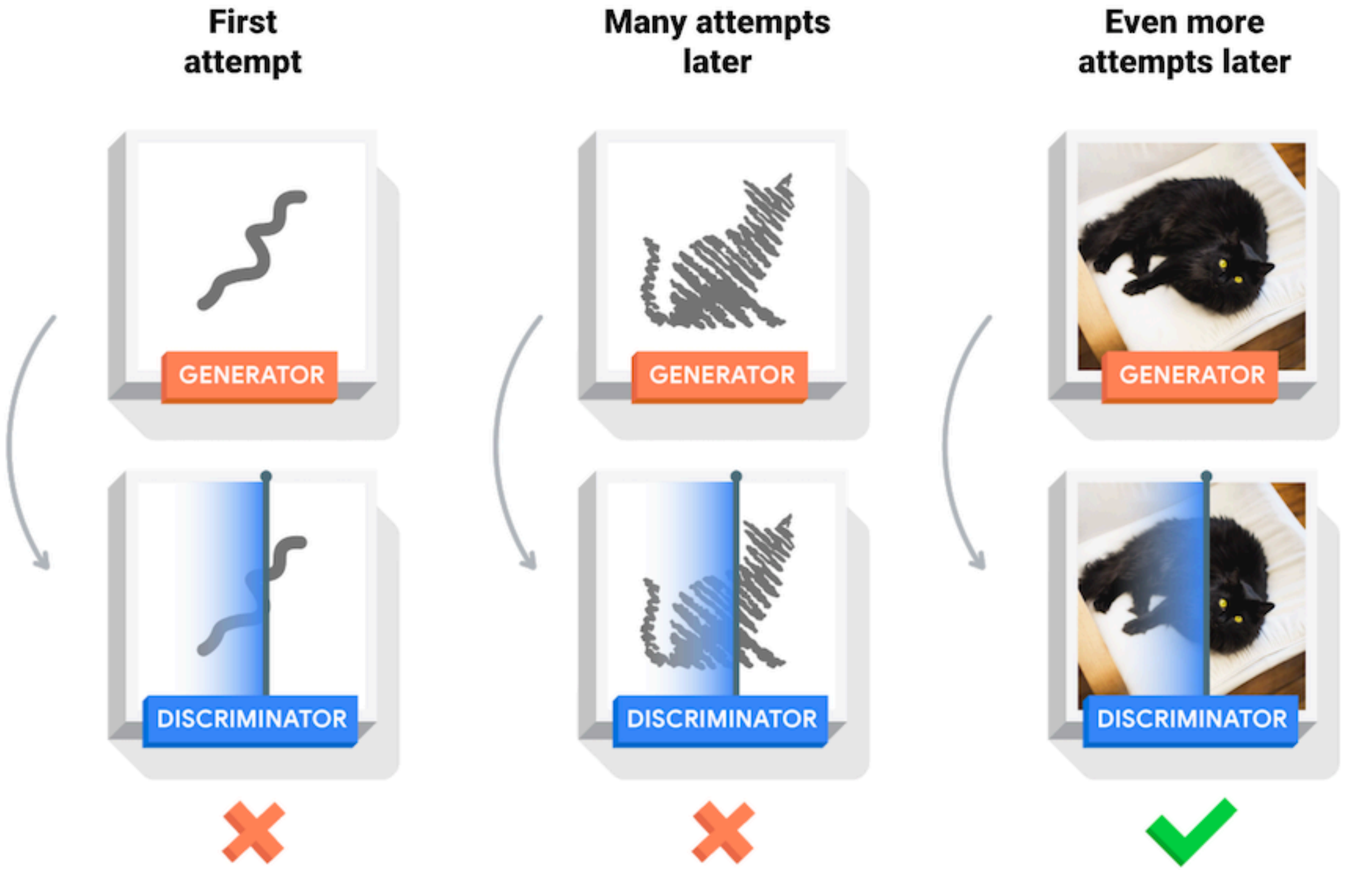
How to generate high resolution images (data)?

Image: https://www.secretservice.gov/data/KnowYourMoney.pdf

Adversarial Training

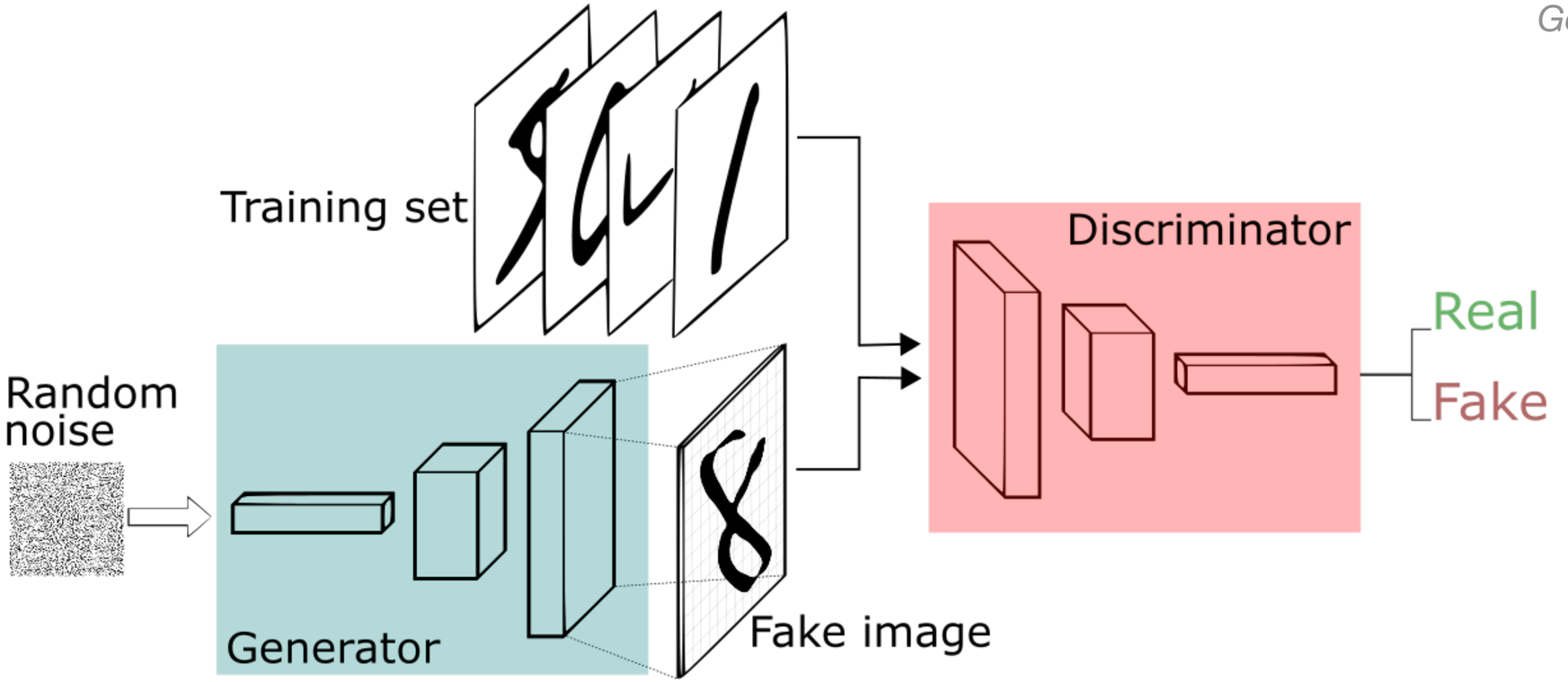
During the training:

- The **generator** progressively **becomes better** in creating images that looks real;
- The **discriminator** progressively **becomes better** in telling them apart.
- The process reaches an **equilibrium** when the discriminator can no longer distinguish real images from fakes.



Adversarial Training

Goodfellow et al. (2014, arXiv:1406.2661)



Log proba of D predicting that the **real** images are **genuine**

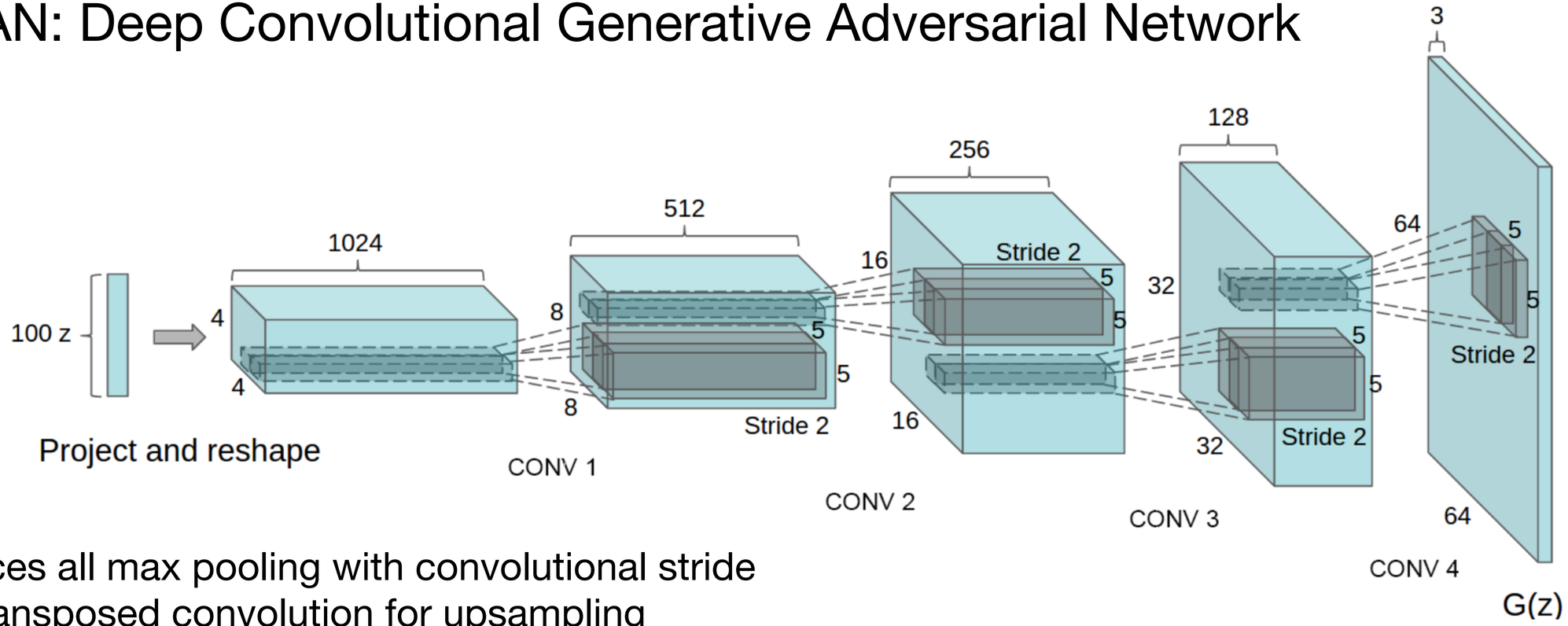
Log proba of G predicting that the **generated** images are **fake**

Nash equilibrium: $$\min_G \max_D V(D,G) = \mathbb{E}_{x\sim p_{\text{data}}(x)}[\log D(x)] + \mathbb{E}_{z\sim p_{\text{model}}(z)}[\log(1 - D(G(z)))]$$

"Nash equilibrium is a proposed solution of a **non-cooperative game** involving two or more players in which each player is assumed to know the equilibrium strategies of the other players, and no player has anything to gain by changing only their own strategy." — Wikipedia

Implementation: DCGAN

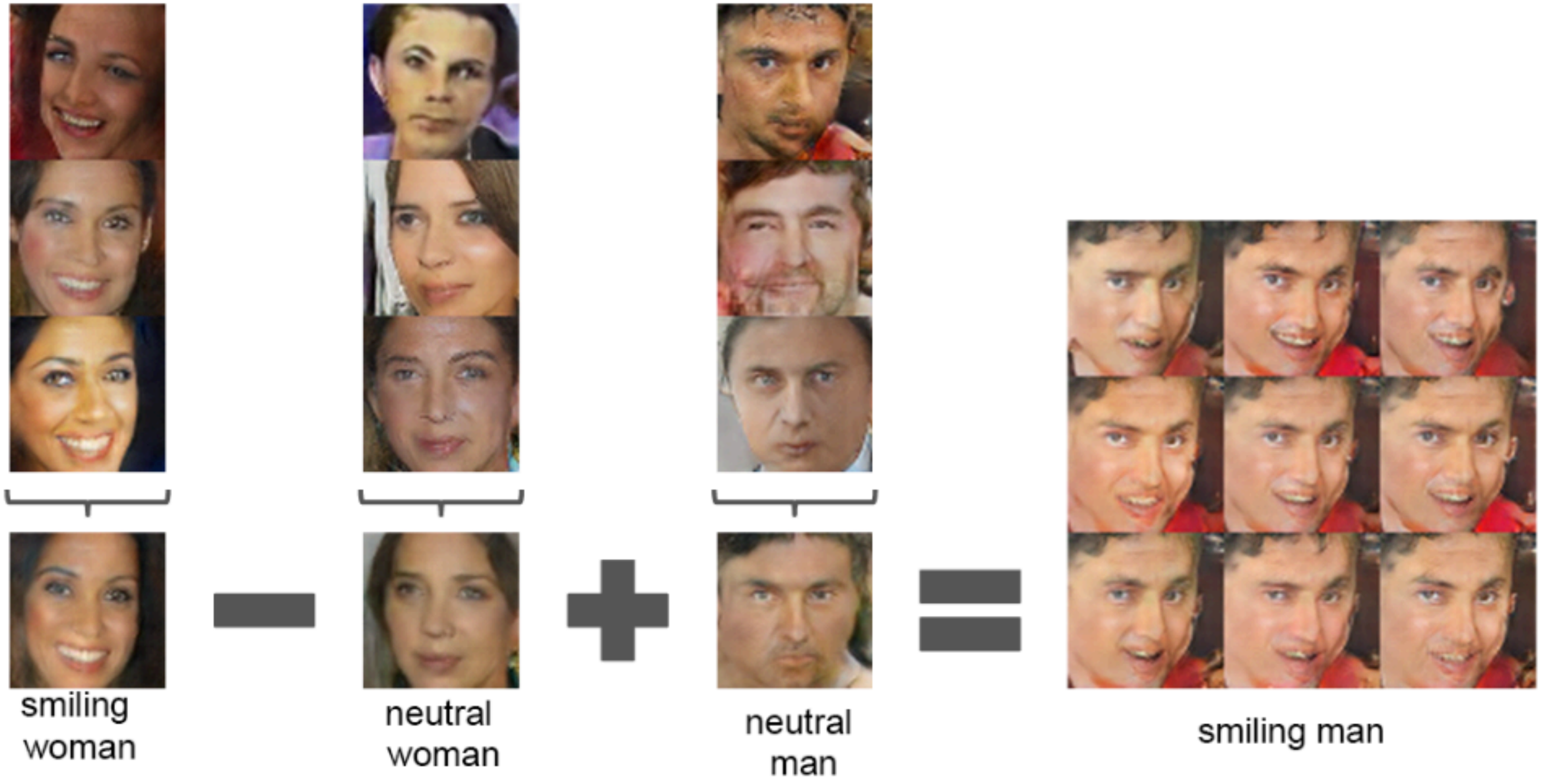
DCGAN: Deep Convolutional Generative Adversarial Network



- Replaces all max pooling with convolutional stride
- Use transposed convolution for upsampling
- Eliminate fully connected layers
- Use batch normalization except the output layer for the generator
- Use batch normalization for the input layer of the discriminator
- Use ReLU in the generator except for the output (which uses tanh)
- Use LeakyReLU in the discriminator.

Radford, Metz & Chintala (2015, arXiv:1511.06434)

Implementation: DCGAN



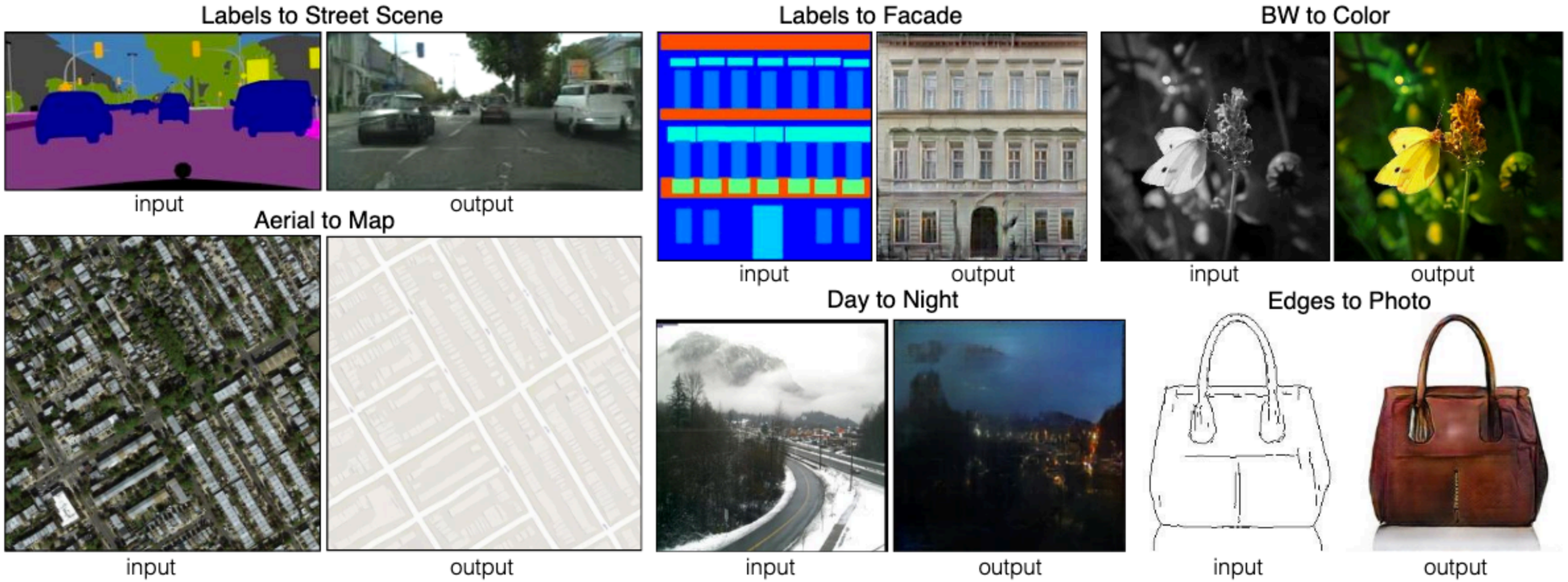
Radford, Metz & Chintala (2015, arXiv:1511.06434)

Implementation: CGAN

CGAN: Conditional Generative Adversarial Network

Normal GAN: $$\min_G \max_D V(D,G) = \mathbb{E}_{x\sim p_{\text{data}}(x)}[\log D(x)] + \mathbb{E}_{z\sim p_{\text{model}}(z)}[\log(1 - D(G(z)))]$$

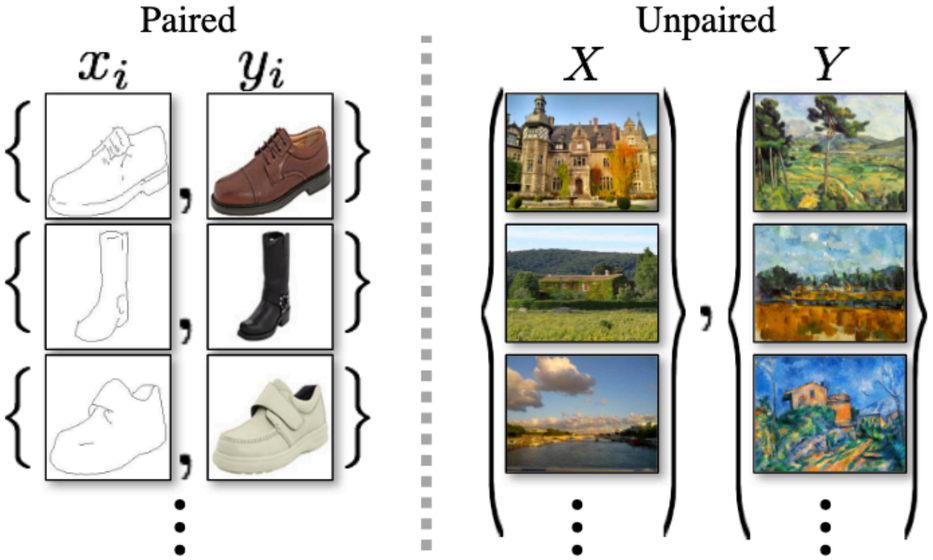
Conditional GAN: $$\min_G \max_D V(D,G) = \mathbb{E}_{x\sim p_{\text{data}}(x)}[\log D(x\,|\,y)] + \mathbb{E}_{z\sim p_{\text{model}}(z)}[\log(1 - D(G(z\,|\,y)))]$$

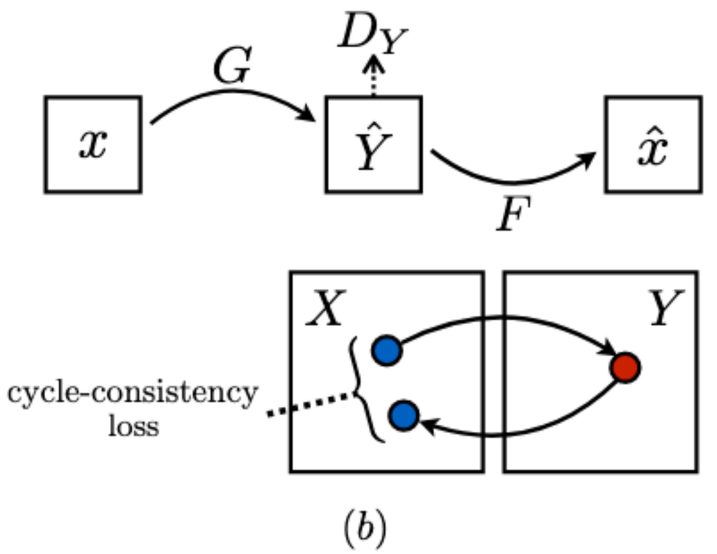


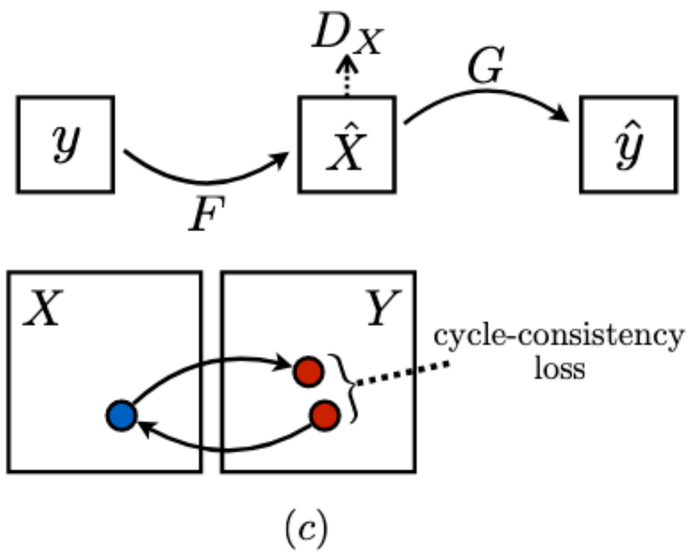
Mirza & Osindero (2014, arXiv:1411.1784); Isola et al. (2016, arXiv:1611.07004)

Implementation: CycleGAN

Image translation typically requires **paired** datasets. What if we don't have paired datasets?





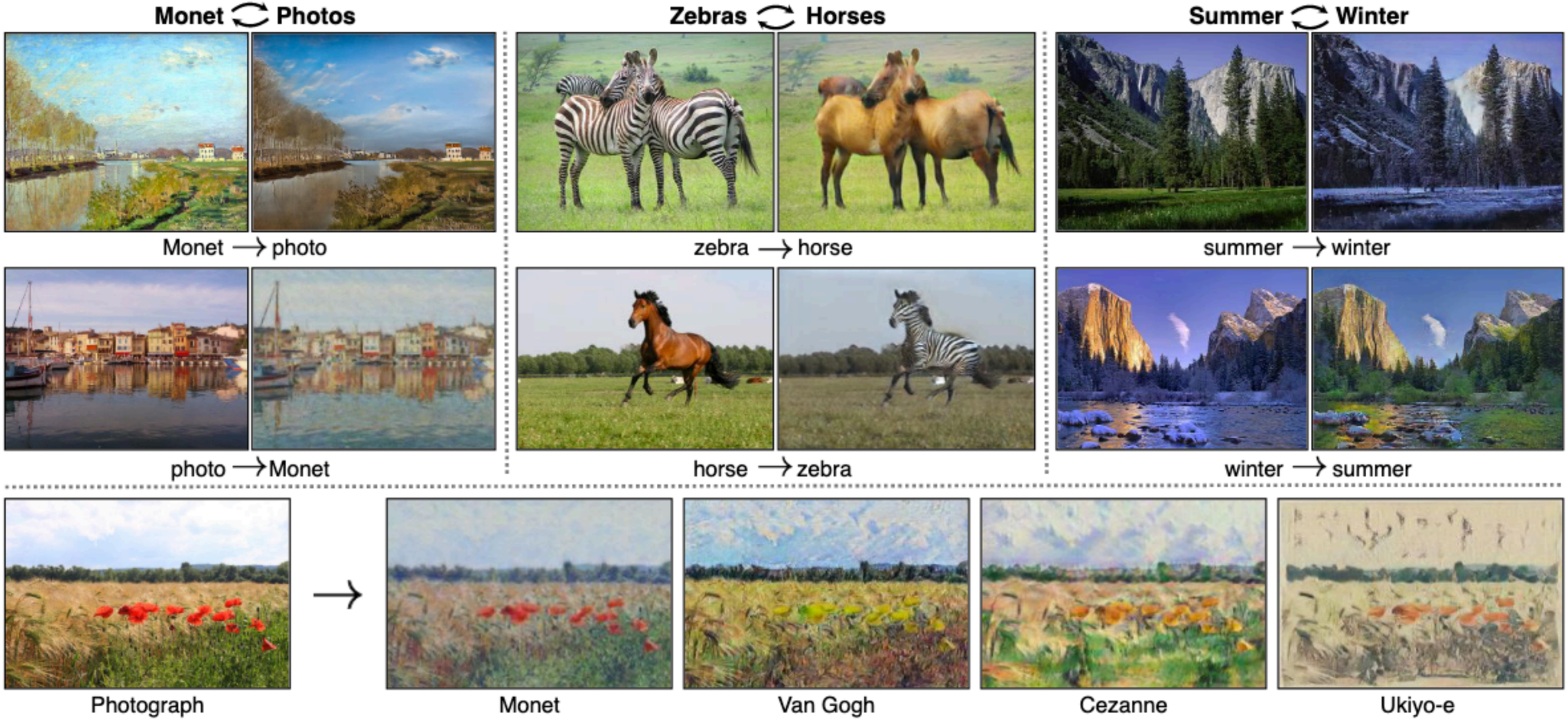


$x \rightarrow G(x) \rightarrow F(G(x)) \approx x$

$y \rightarrow F(y) \rightarrow G(F(y)) \approx y$

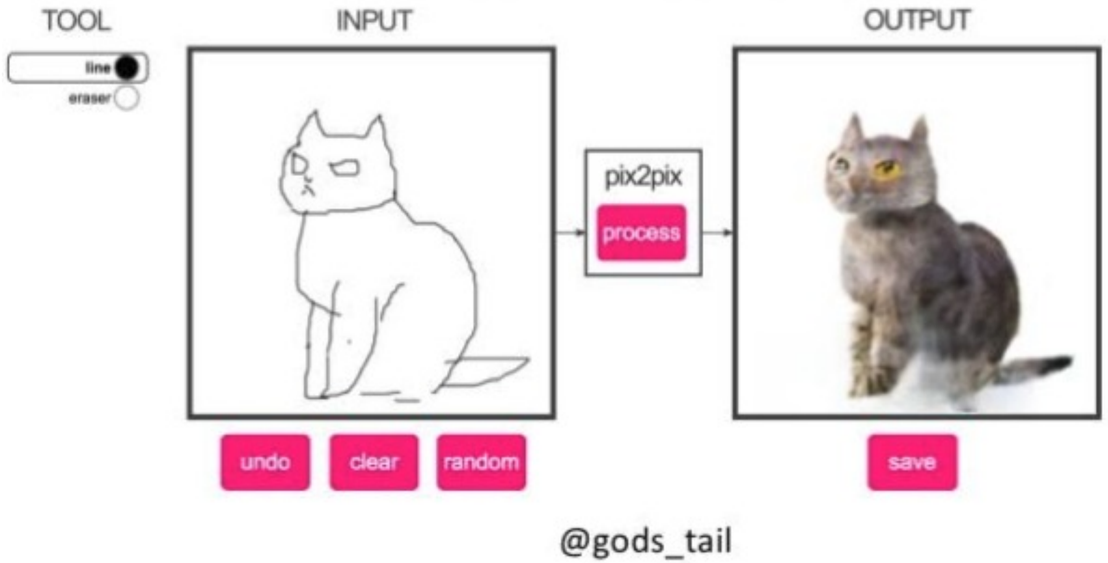
Zhu et al. (2017, arXiv:1703.10593)

Implementation: CycleGAN



Zhu et al. (2017, arXiv:1703.10593)

Implementation: CycleGAN



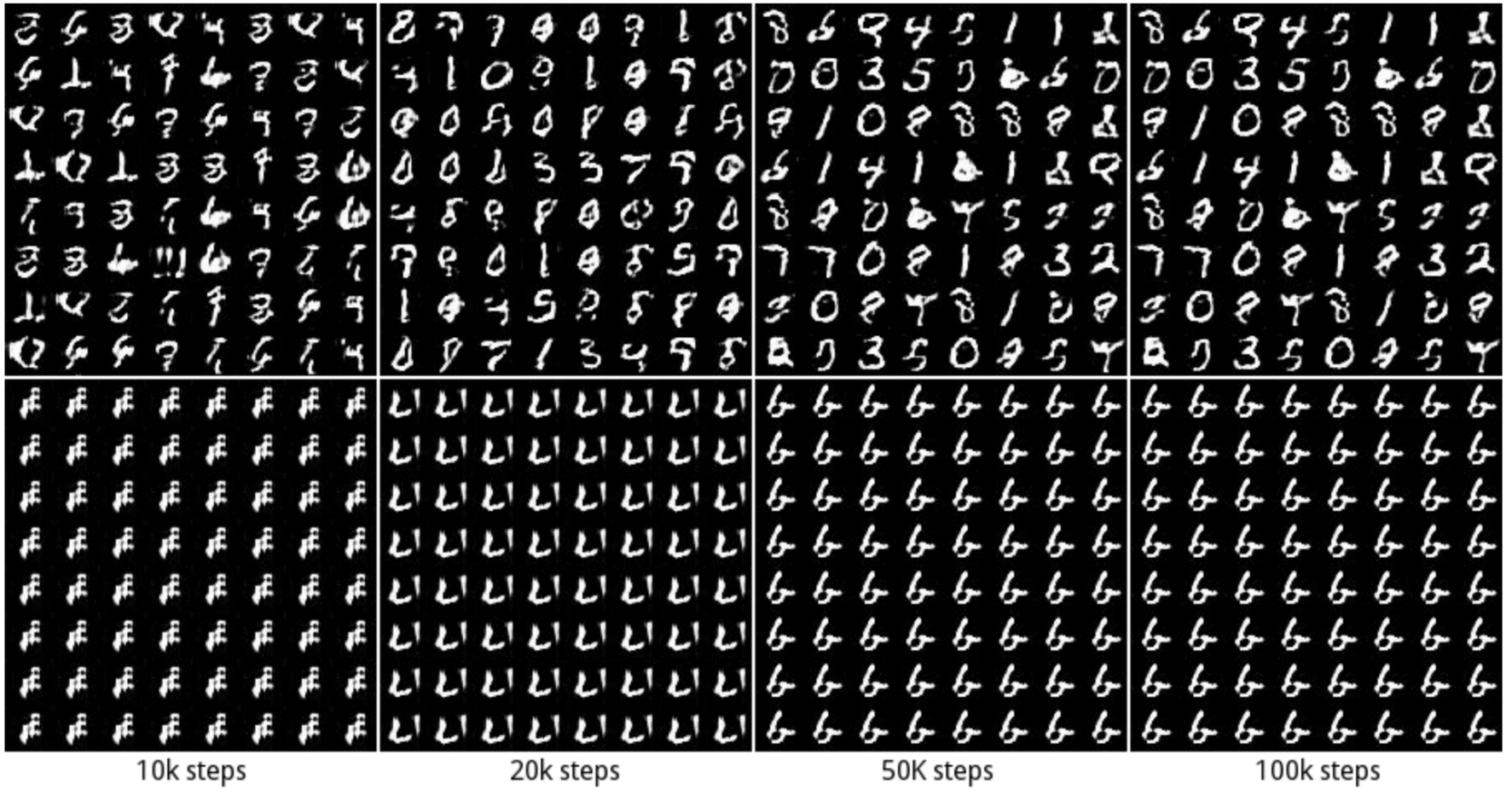
Works!

Hmmm…

The quality of GAN-generated images

Problems with GANs

Convergence not guaranteed: the two models may oscillate and never converge.
Mode collapse: the generator only produces limited variation.
Diminished gradient: the discriminator gets too successful and the generator learns nothing.

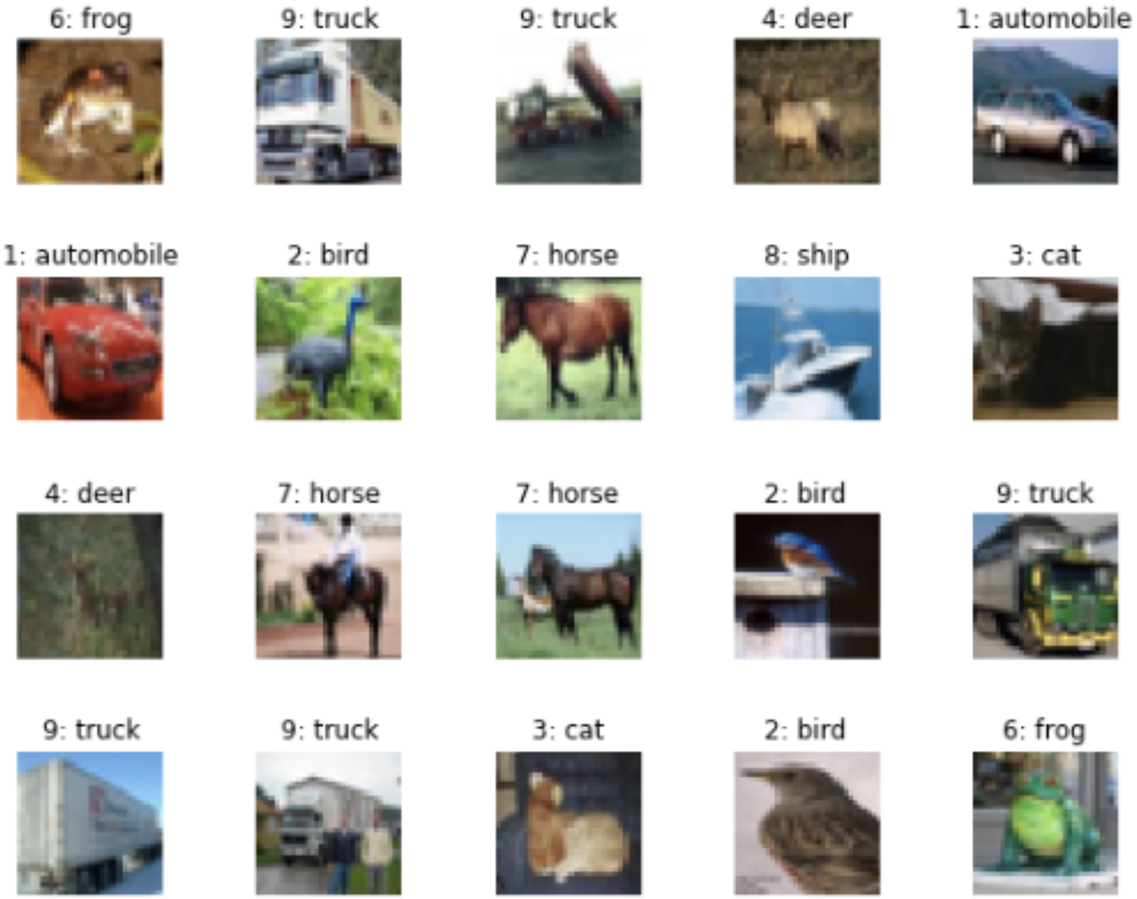


Mode collapse of GANs

Metz et al. 2016 (arXiv:1611.02163)

jupyter

https://jupyter.lisa.surfsara.nl/jhlptc001/



CNN Classification on the CIFAR-10 Dataset

CIFAR = Canadian Institute for Advanced Research