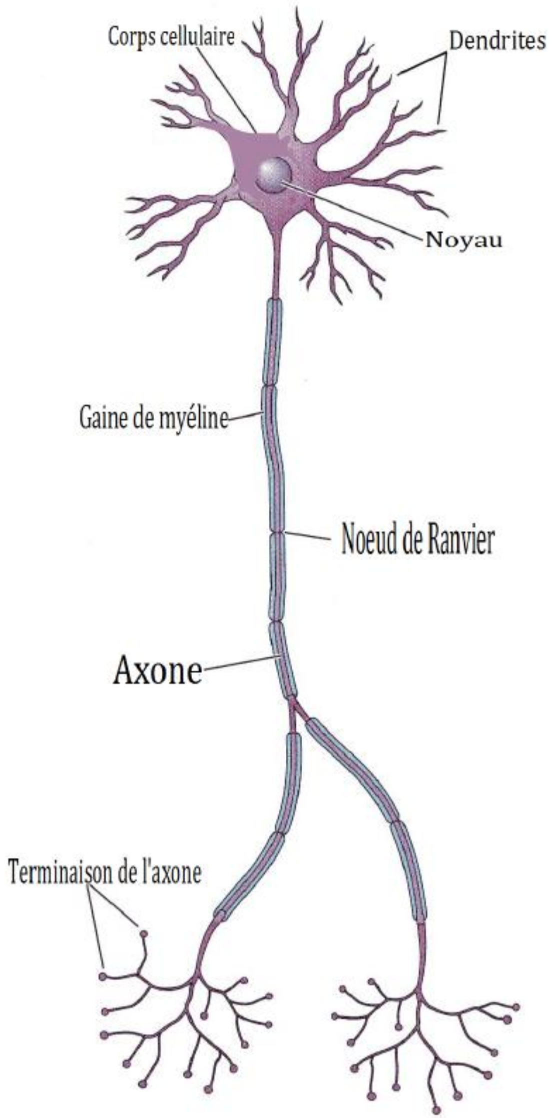
Initiation à l’apprentissage automatique en science des matériaux

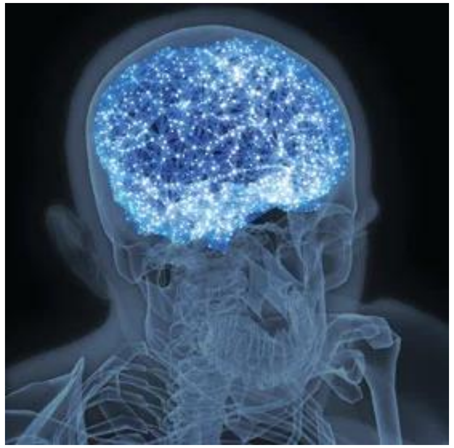
5. Neural Network

J.-C. Crivello, LINK : jean-claude.crivello@cnrs.fr
C. Barreteau, ICMPE : celine.barreteau@cnrs.fr
S. Junier, ICMPE : sebastien.junier@cnrs.fr

https://link.cnrs.fr/ML/

Inspired by nature



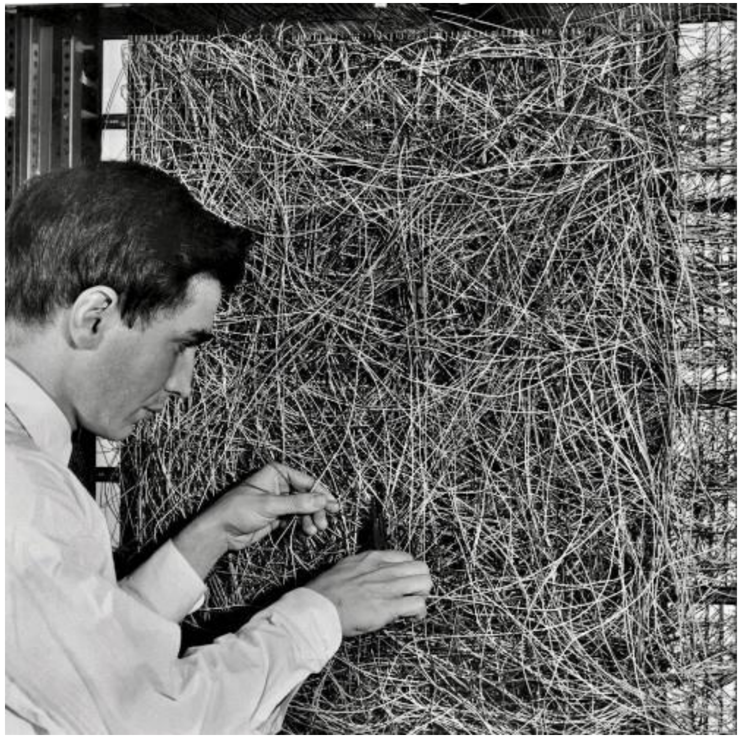


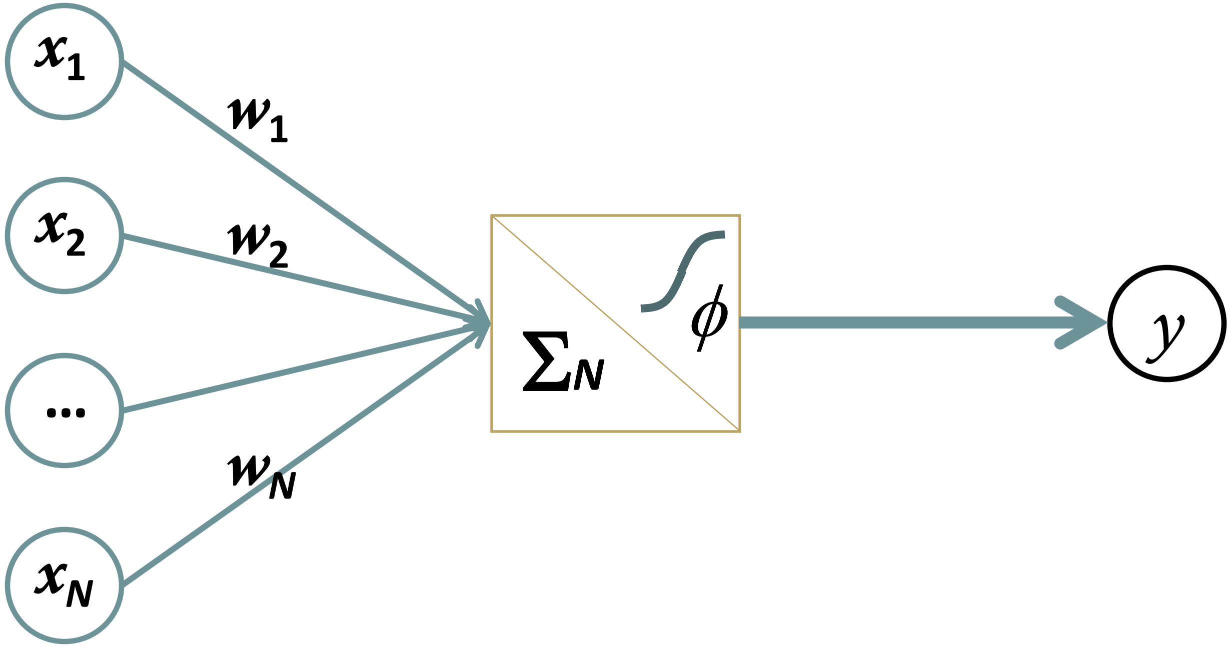
Human:

$100\ .10^9$ neurons
10^3 synapses/neurons
200.10^3 electric bonds

Artificial neuron

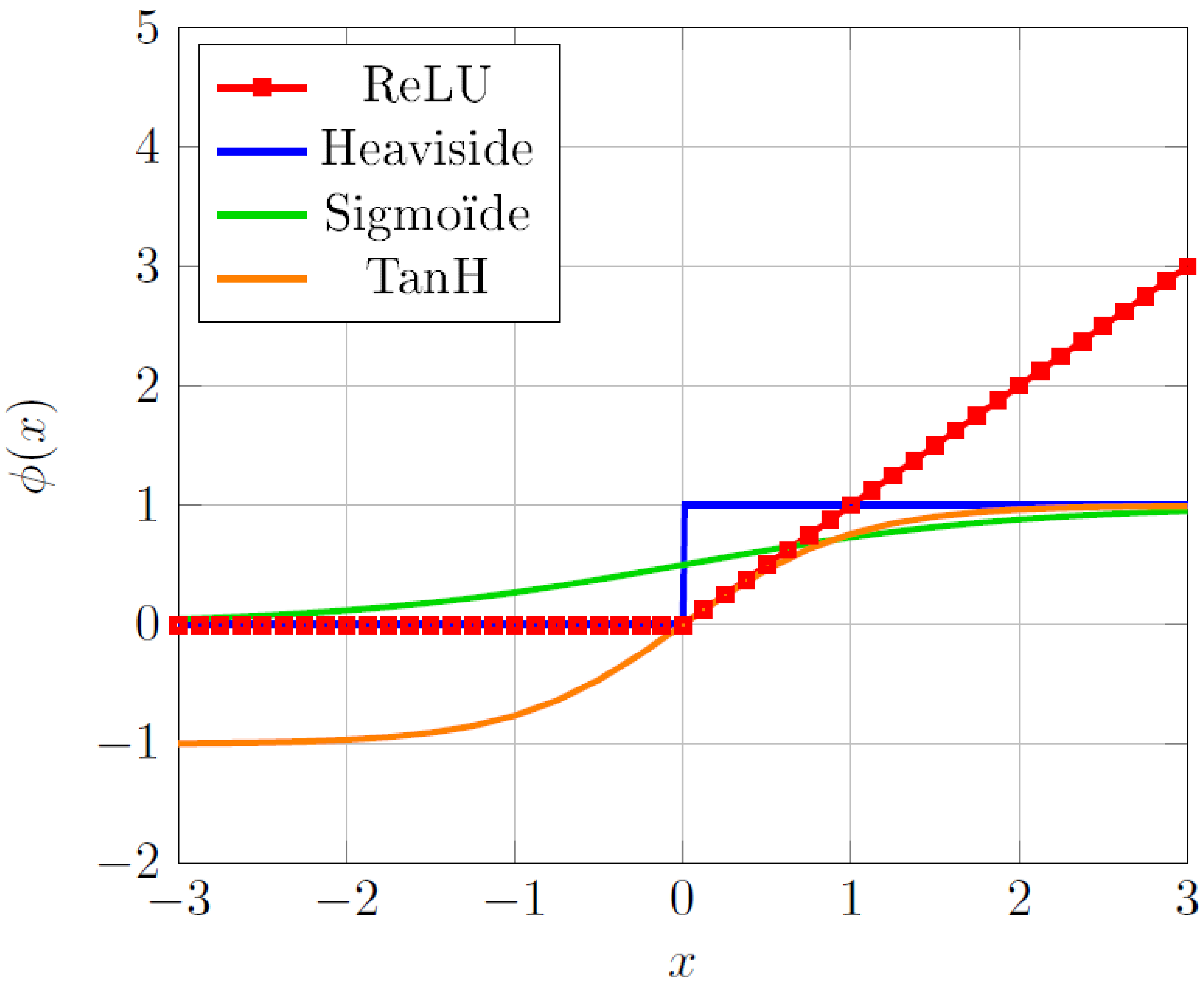
Perceptron, 1957





$$y = \phi\left(\sum_{n=1}^{N} \omega_n x_n - \omega_0\right)$$

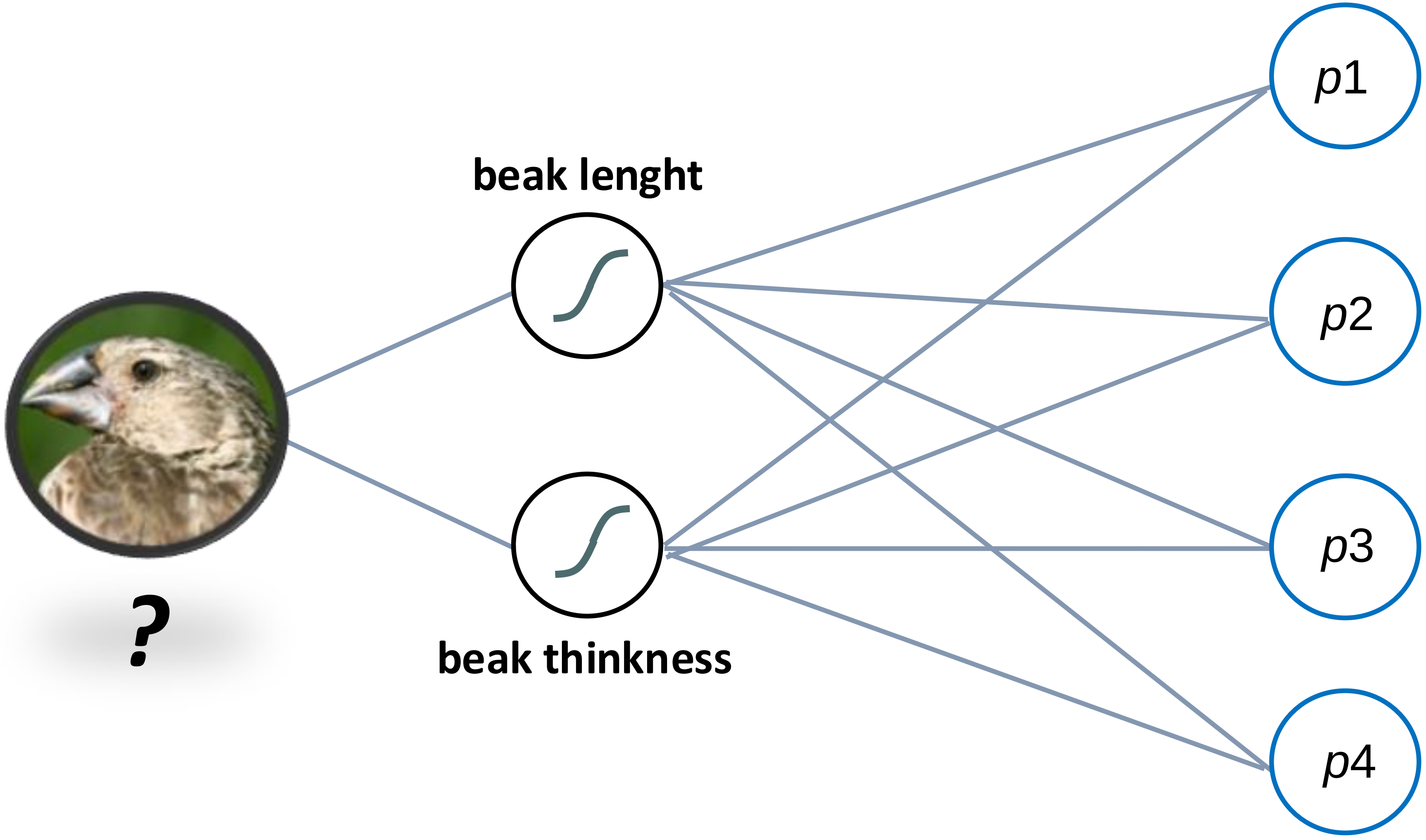
Activation function

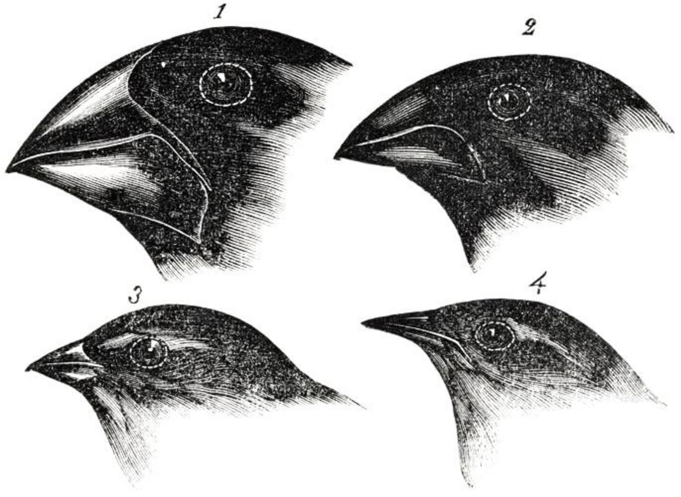


$$y = \phi\left(\sum_{n=1}^{N} \omega_n x_n - \omega_0\right)$$

The artifical neural network

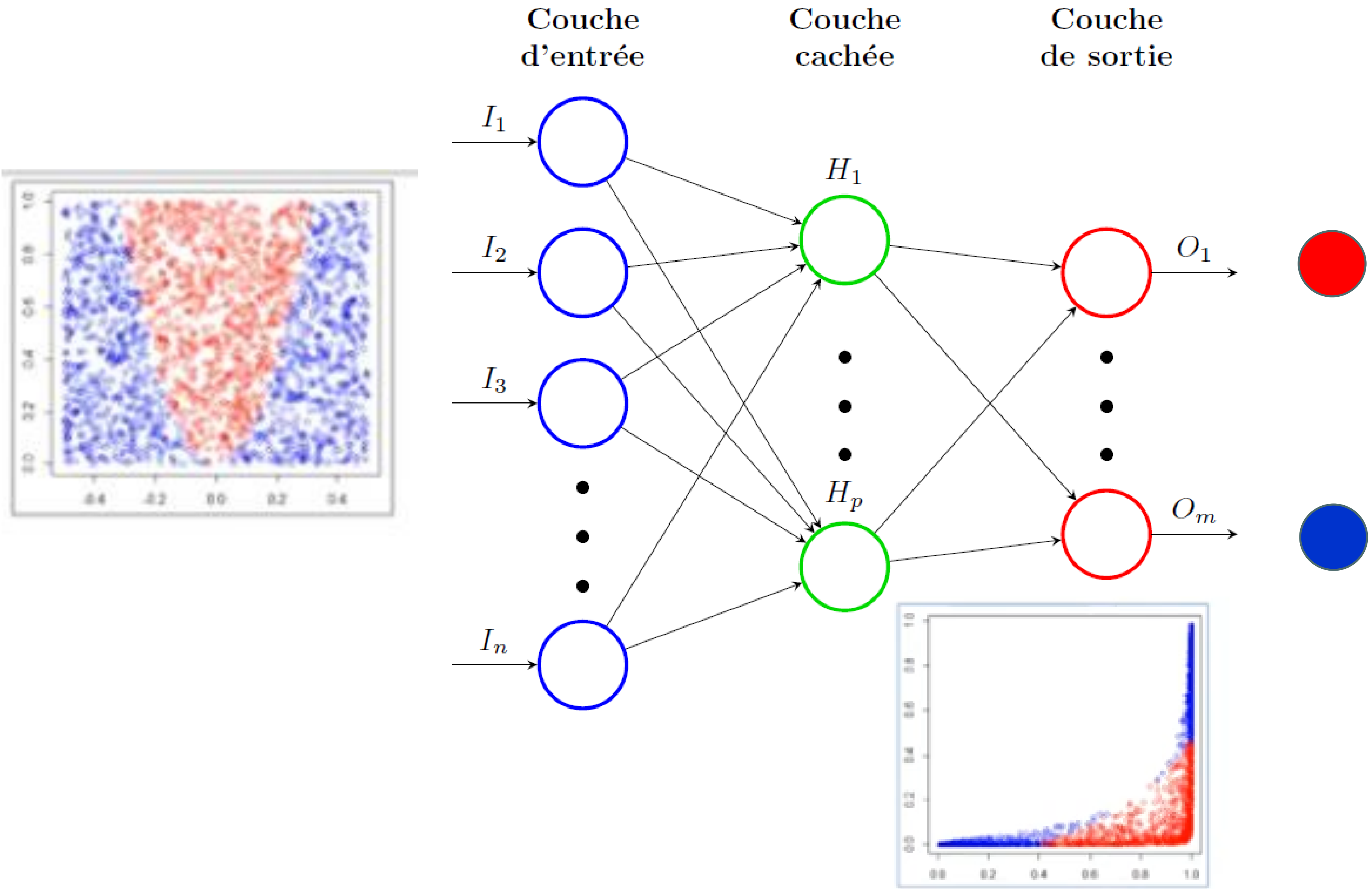
Classification of Darwin's finches



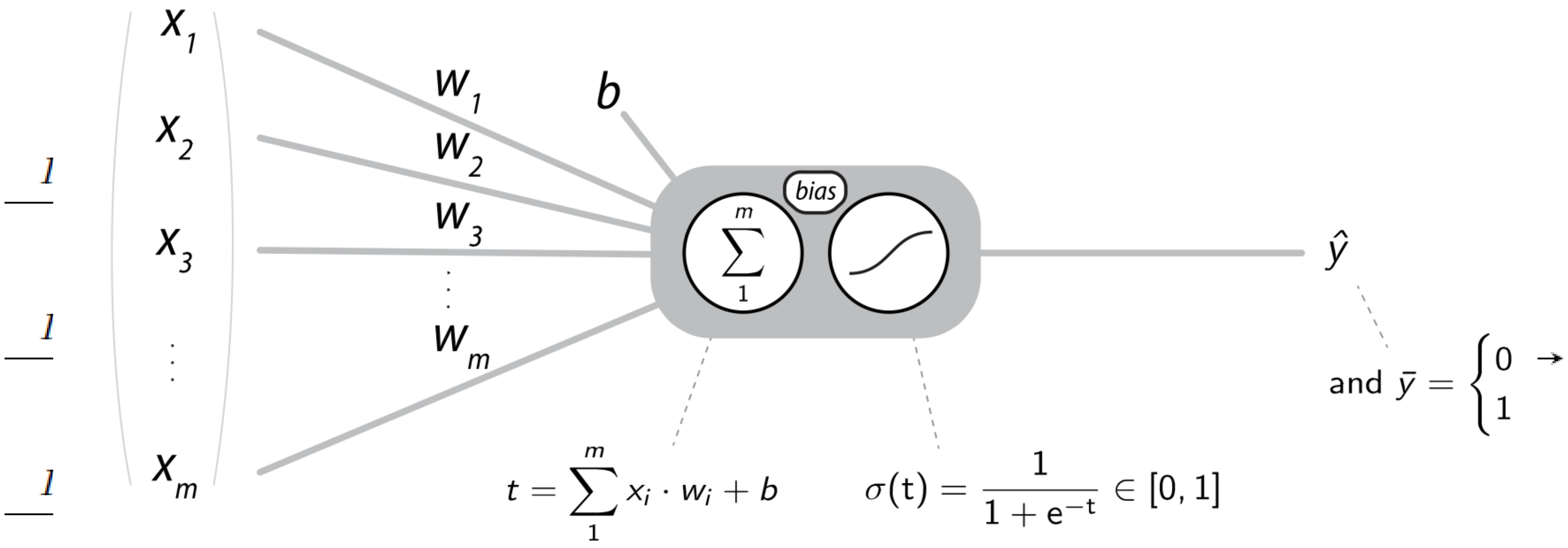


1.Geospiza magnirostris
2.Geospiza fortis
3.Geospiza parvula
4.Certhidea olivacea

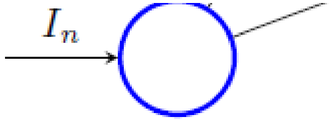
Neural network / Perceptron multicouche MLP



multilayer perceptron MLP

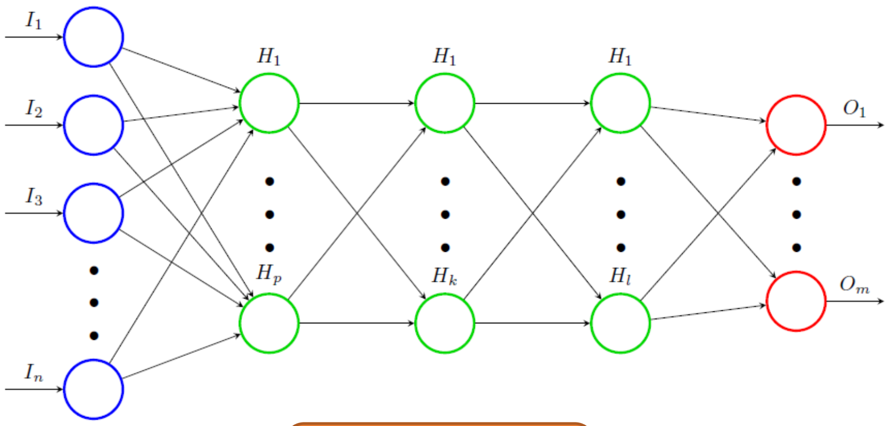


Input	Bias / Weight	Activation function	Output
X	Θ	$\sigma(t)$	$\hat{y}$



Back-propagation

X,
w



feed forward

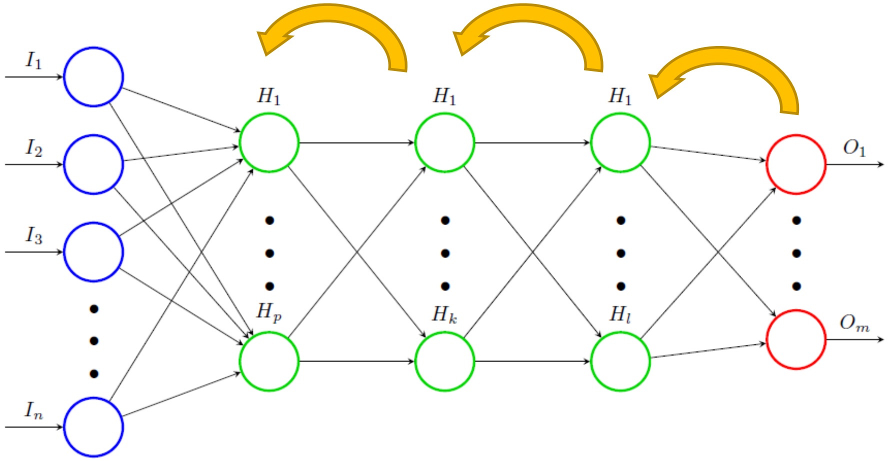
y

ŷ

loss function

$E_w(y, \hat{y})$

back propagation



$$w_{ij} = w_{ij} - \alpha \frac{dE}{dw}$$

How to adjust w_{ij} ?

$$w_{ij} = w_{ij} - \alpha \frac{dE}{dw}$$

α: learning rate

if $E_w(y, \hat{y}) = ½ (\hat{y} - y)^2$

$$\rightarrow \frac{dE}{dy} = \hat{y} - y$$

$$\frac{dE}{dX} = \frac{dE}{dy}\frac{dy}{dX}$$

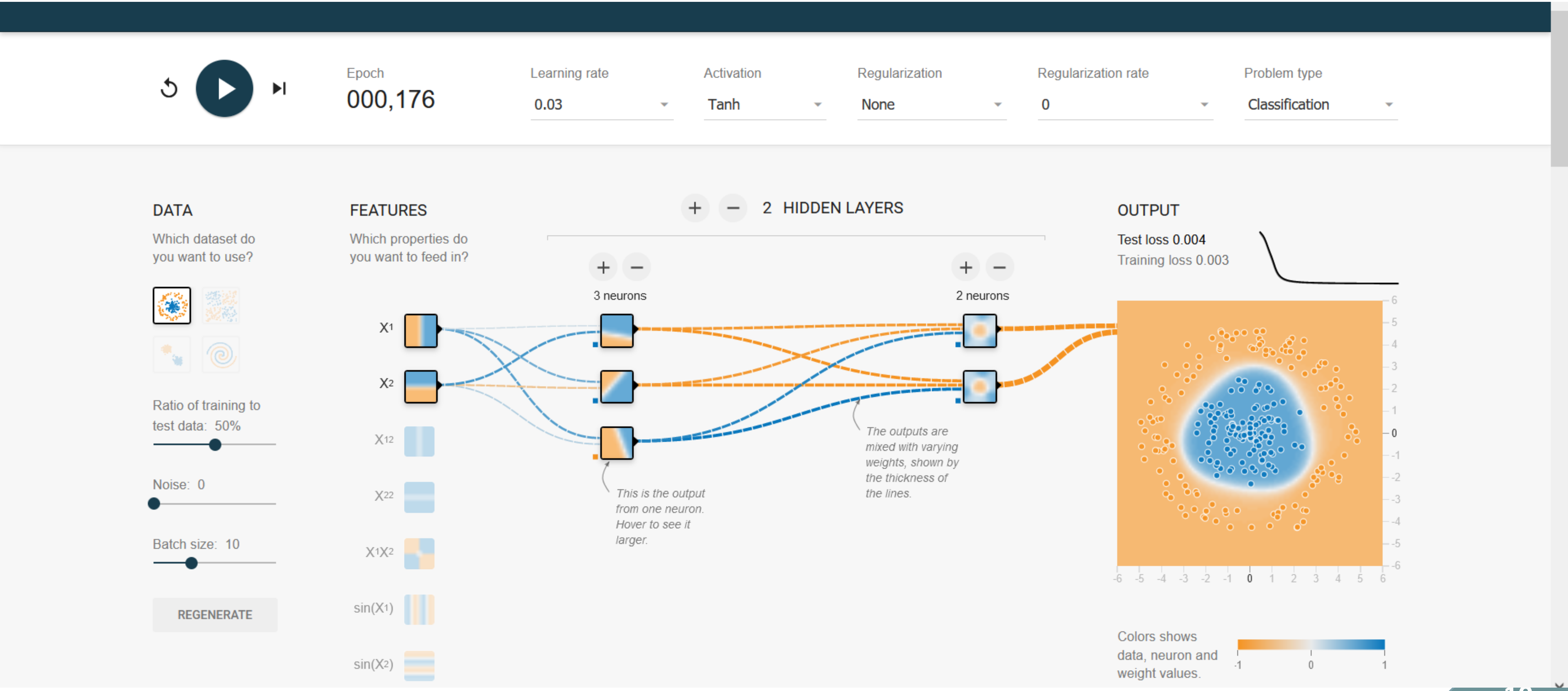
$$= \frac{dE}{dy}\frac{d}{dX}\phi(X)$$

$$= (\hat{y} - y)\frac{d}{dX}\phi(X)$$

$$\frac{dE}{dw} = \frac{dE}{dX}\frac{dX}{dw}$$

$$= \frac{dE}{dX}y$$

https://playground.tensorflow.org/



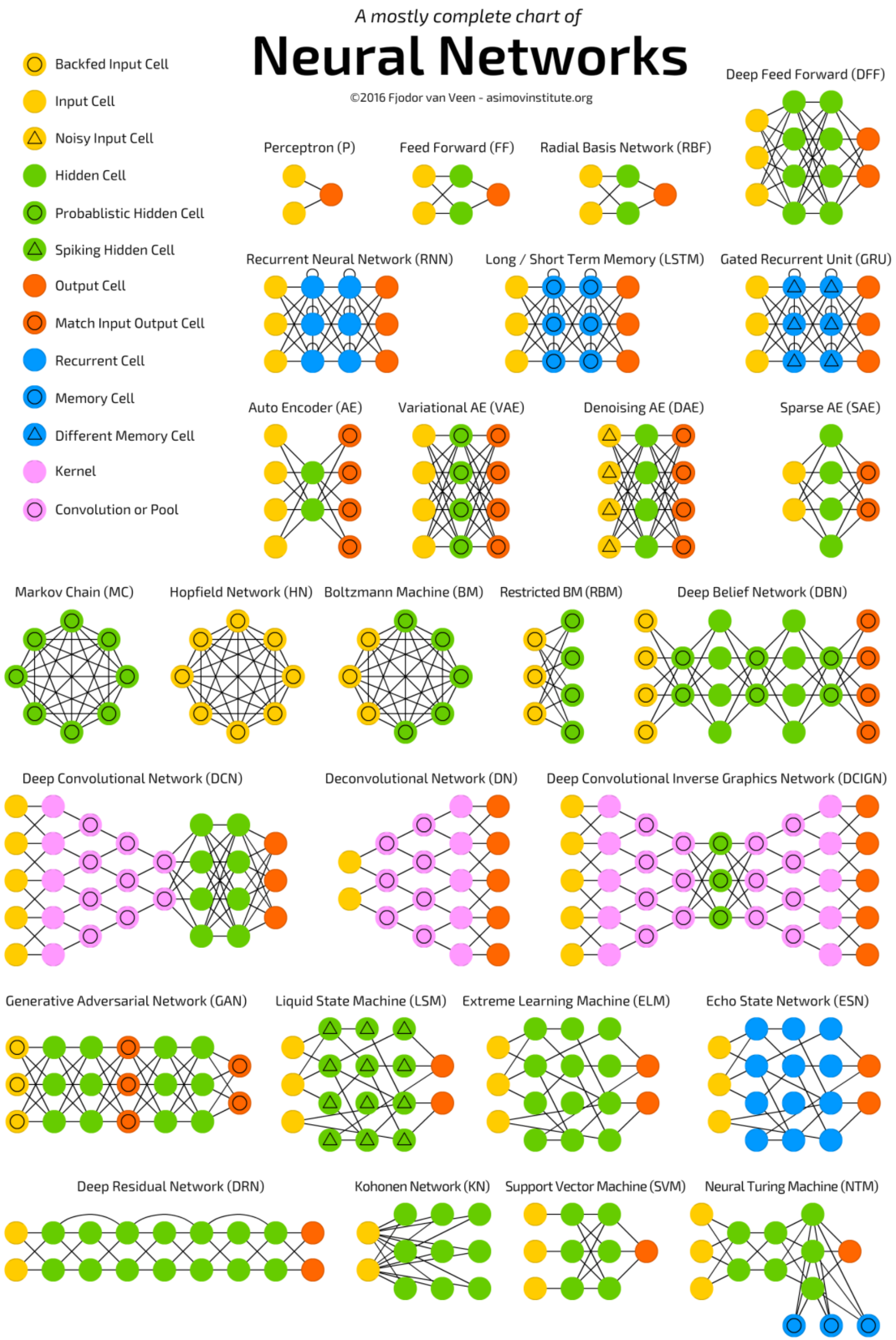
Neural network

Strengths:

- Model can read any data without any knowledge
- Consideration of complex correlations
- Really efficient

Weaknesses:

- Black box
- Too many connections
- Slow to learn



About images

0.0008 Mpixels
28x28 px
8 bits

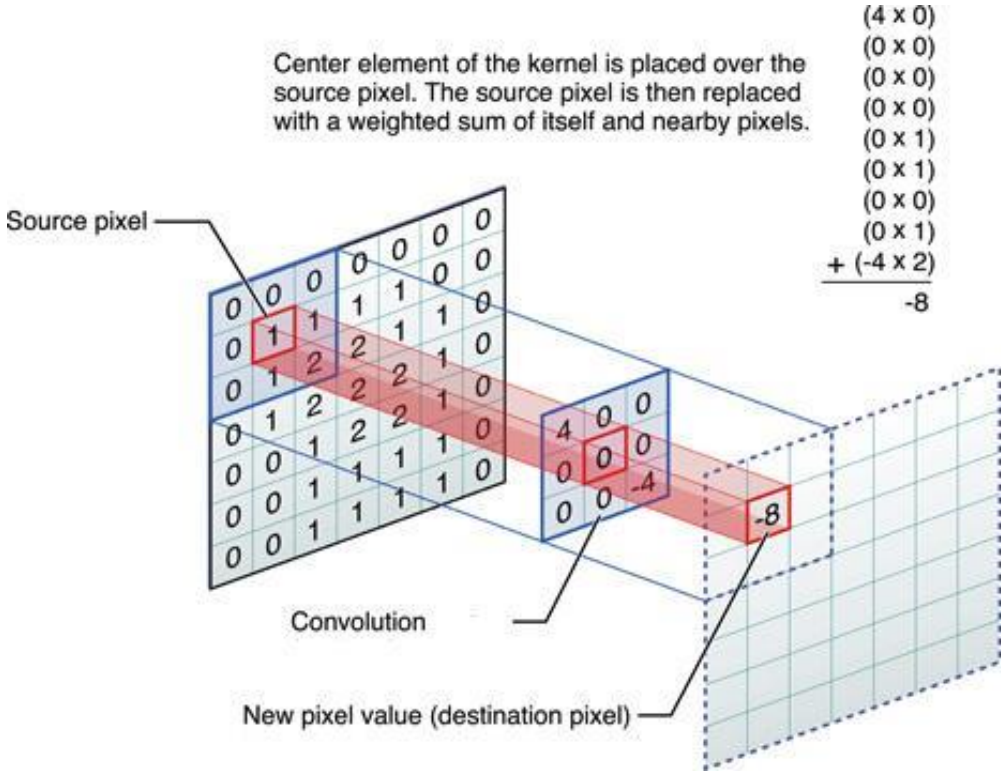
24 Mpixels
3*8bits

With a fully connected NN of 1000 neurones:

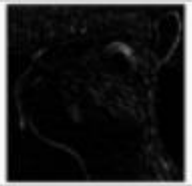
→ 785 000 parameters

→ 72.10^9 parameters

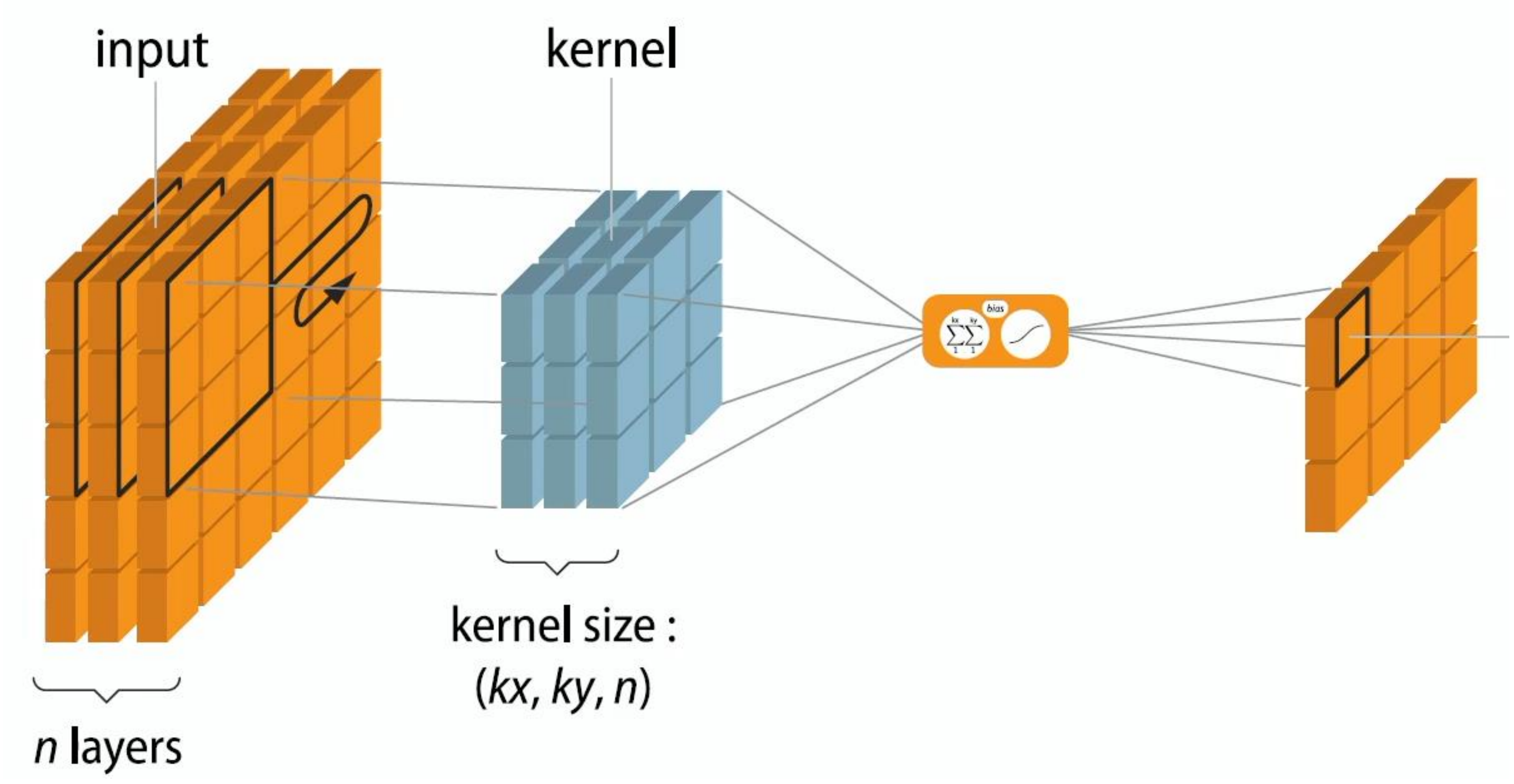
Image convolution



Hanamard product by a kernel

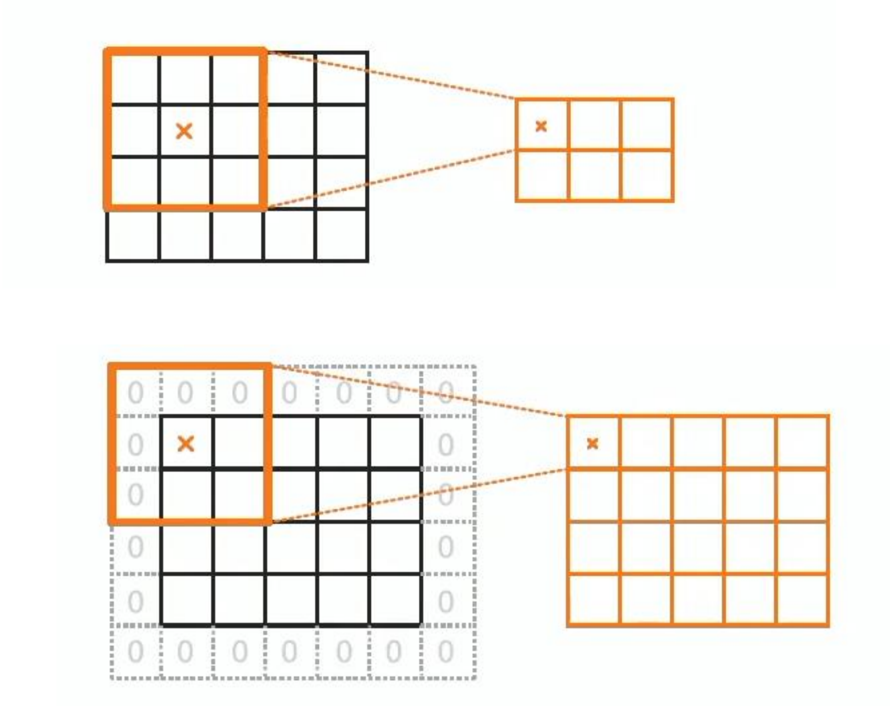
Operation	Filter	Convolved Image
Identity	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	
Edge detection	$\begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix}$	
	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{bmatrix}$	
	$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$	
Sharpen	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 5 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	
Box blur (normalized)	$\frac{1}{9}\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$	
Gaussian blur (approximation)	$\frac{1}{16}\begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$	

Convolution

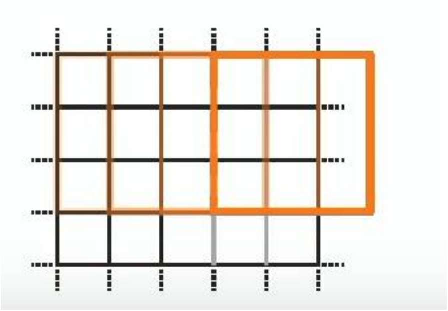


Several operations

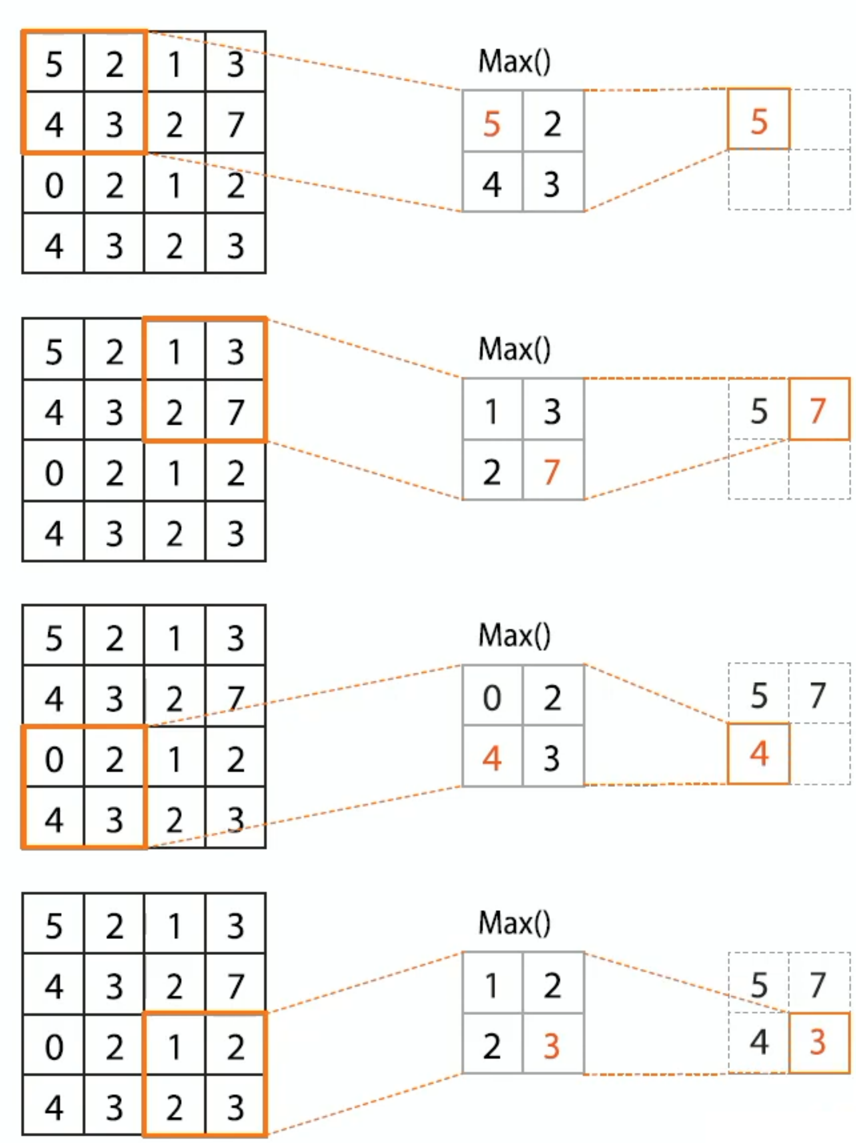
padding



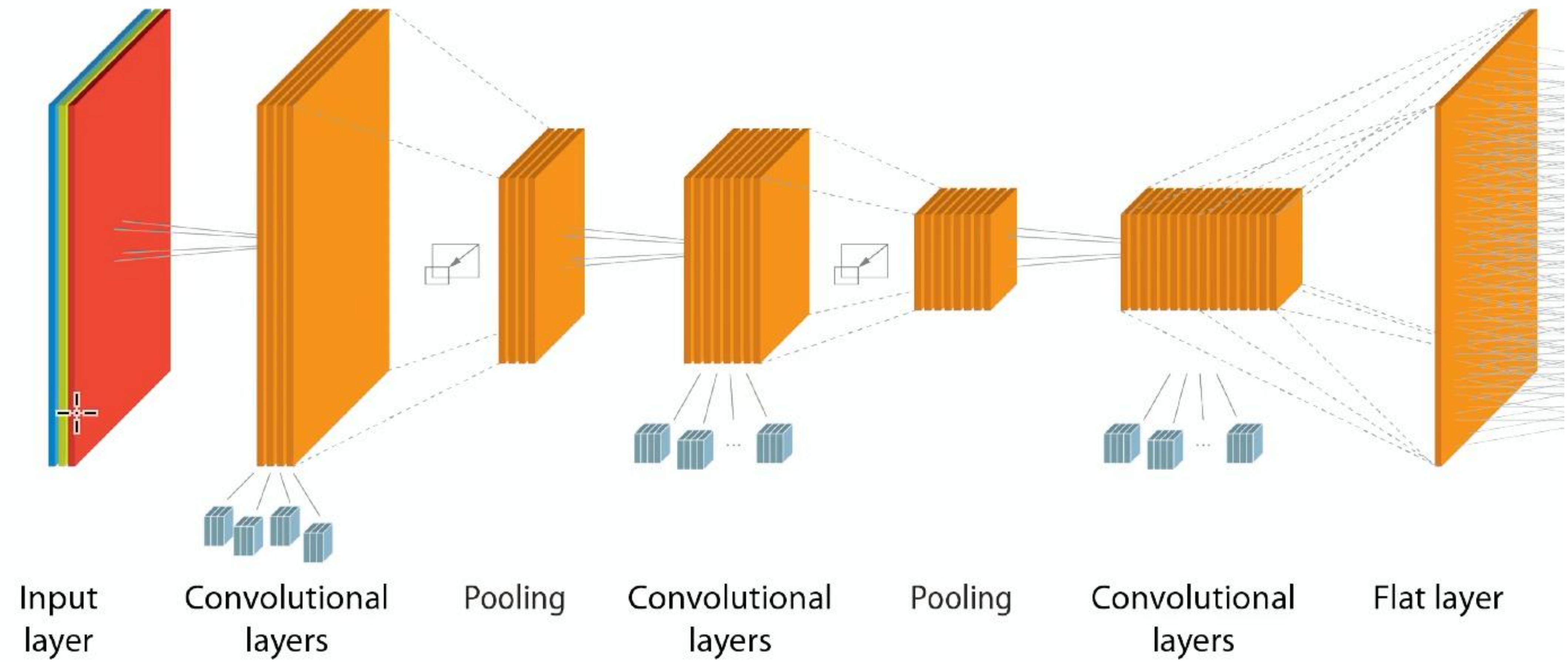
strides



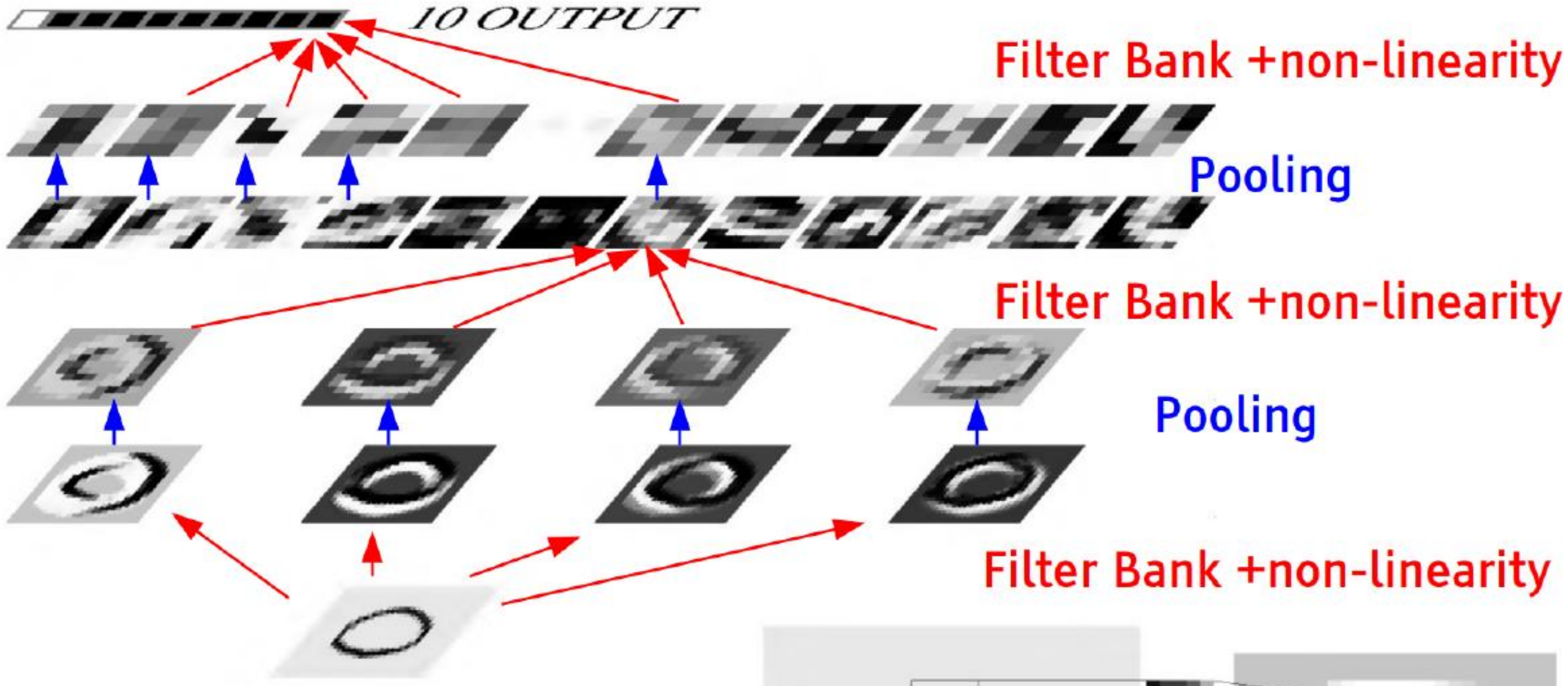
pooling

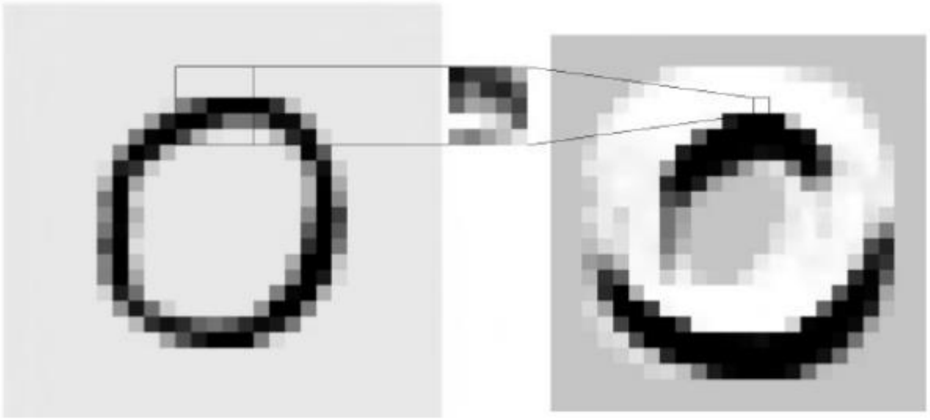


Convolution



Convolution for classification



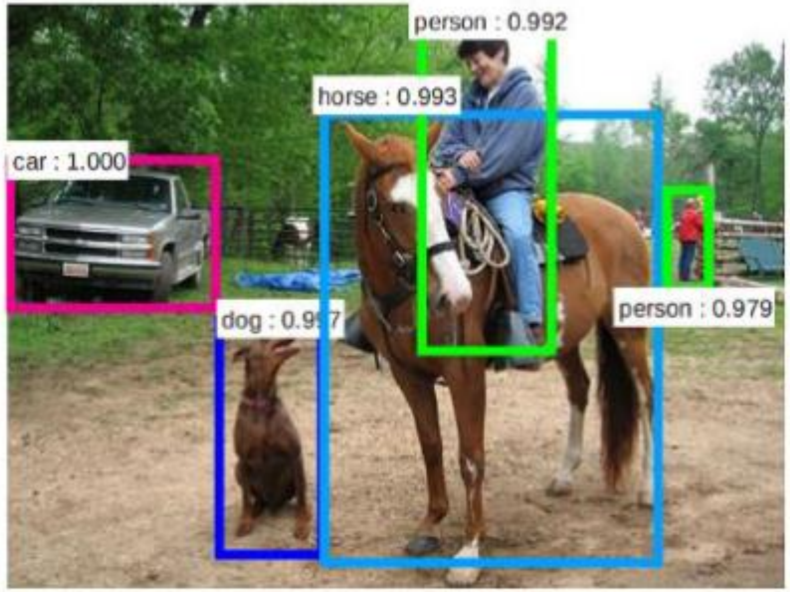


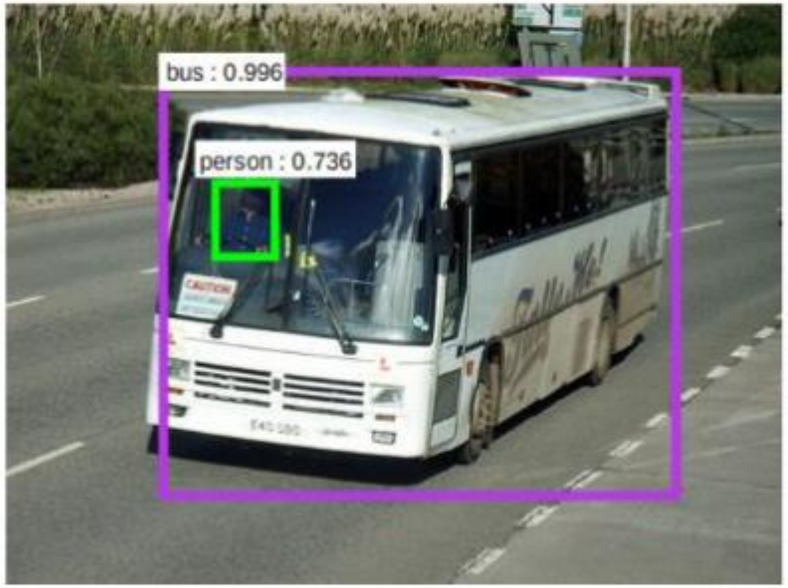
LeCun et al., NIPS (1989)

Convolution network

Strengths:
- Can treat complex images
- More simple than MPL (same weight)
- Reduce size by pooling
- Learn from deep information hidden by data
- Adapted for GPU (60 times faster)

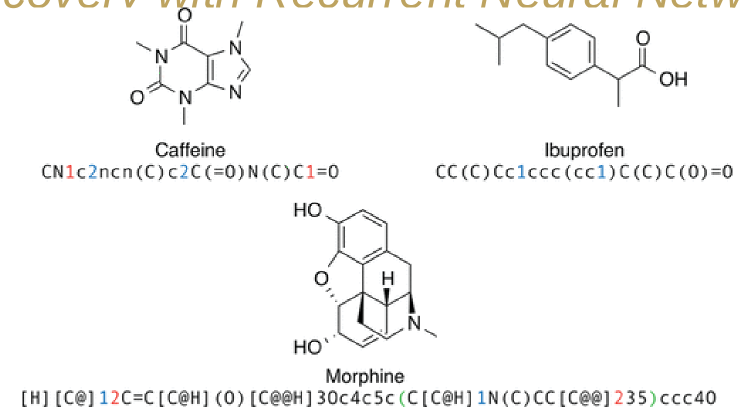
Weaknesses:
- Black box
- Slow to learn
- Need a large DB



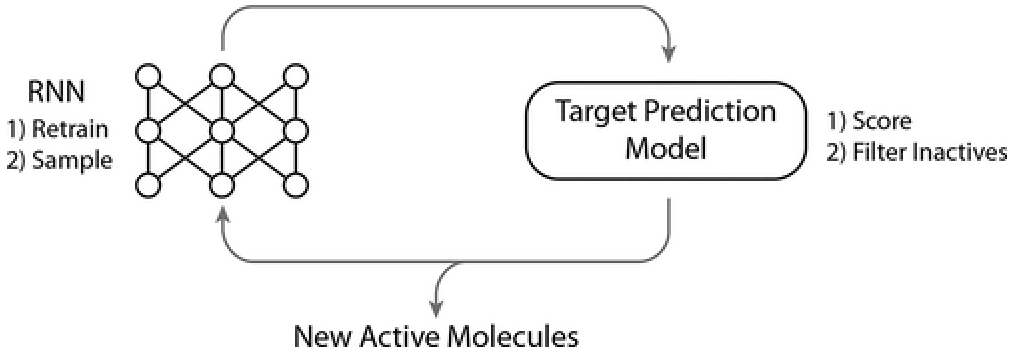


Generative methods

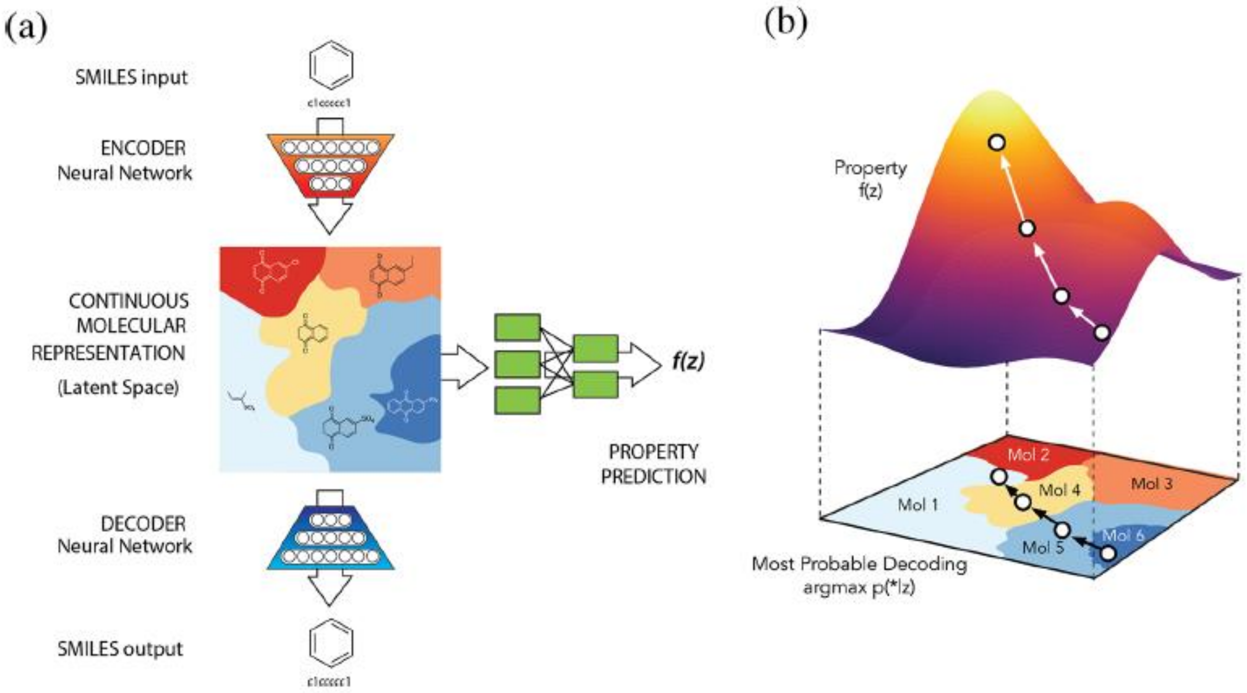
Segler *et al*. ACS central science (2018)
Generating Focused Molecule Libraries for Drug Discovery with Recurrent Neural Networks



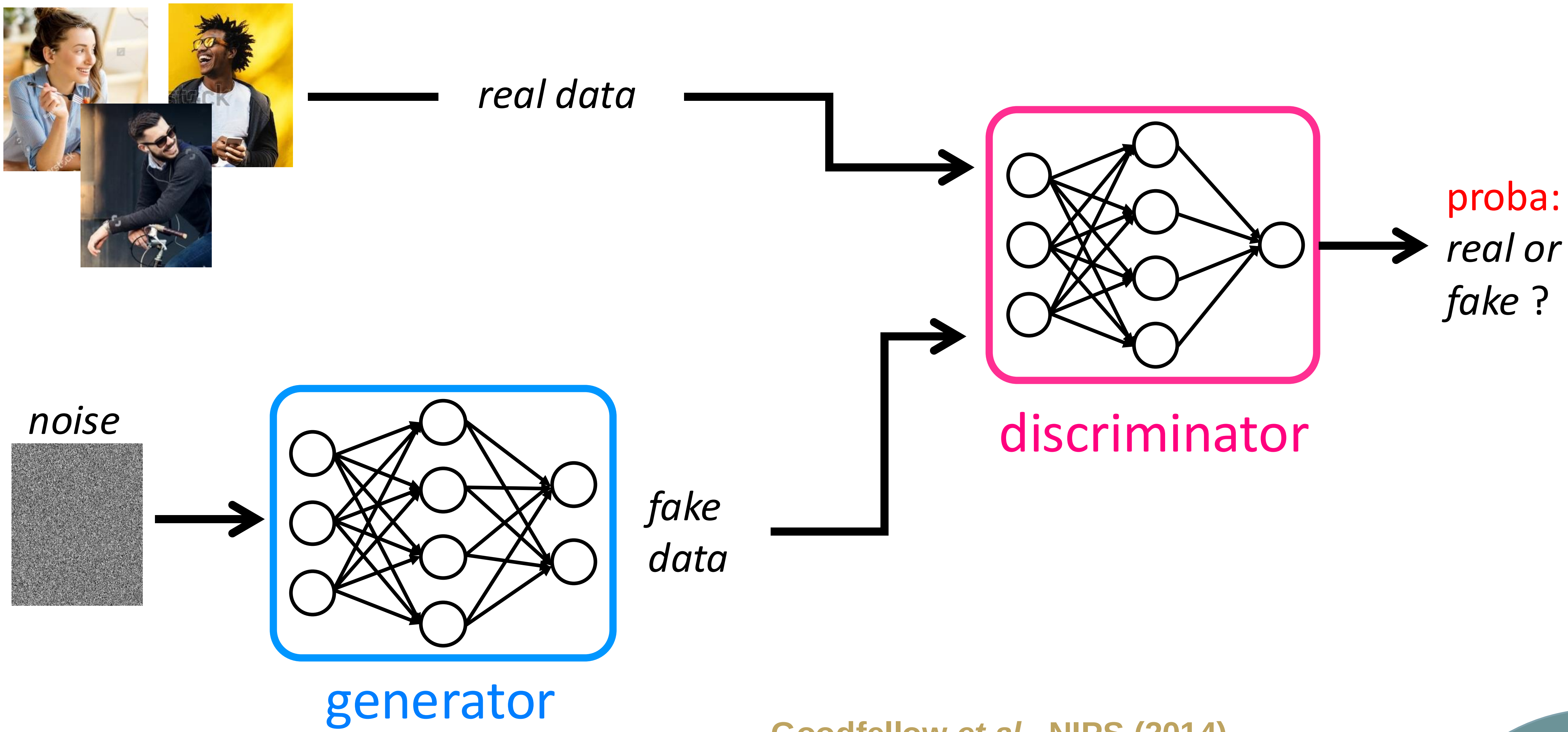
Batch	Generated Example	valid
0	Oc.BK5i%ur+7oAFc7L3T=F8B5e=n)CS6RCTAR((OVCp1CApb)	no
1000	OF=CCC2OCCCC)C2)C1CNC2CCCCCCCCCCCCCCCCCCCCCCCC	no
2000	O=C(N)C(=O)N(c1occc1OC)c2ccccc2OC	yes
3000	O=C1C=2N(c3cc(ccc3OC2CCC1)CCCc4cn(c5c(Cl)cccc54)C)C	yes



Gomez-Bombarelli *et al*. ACS central science (2018)
Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules

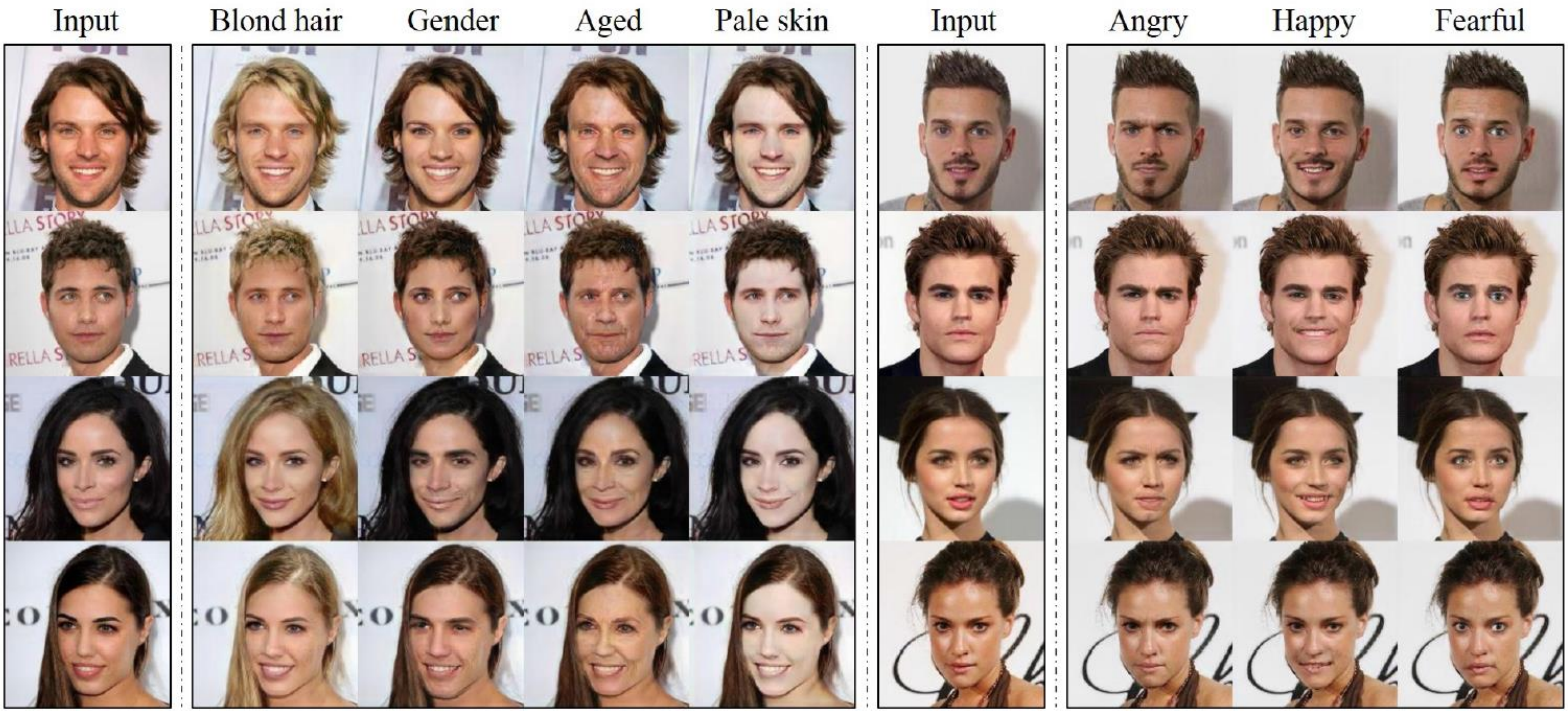


Generative adversarial networks (GAN)

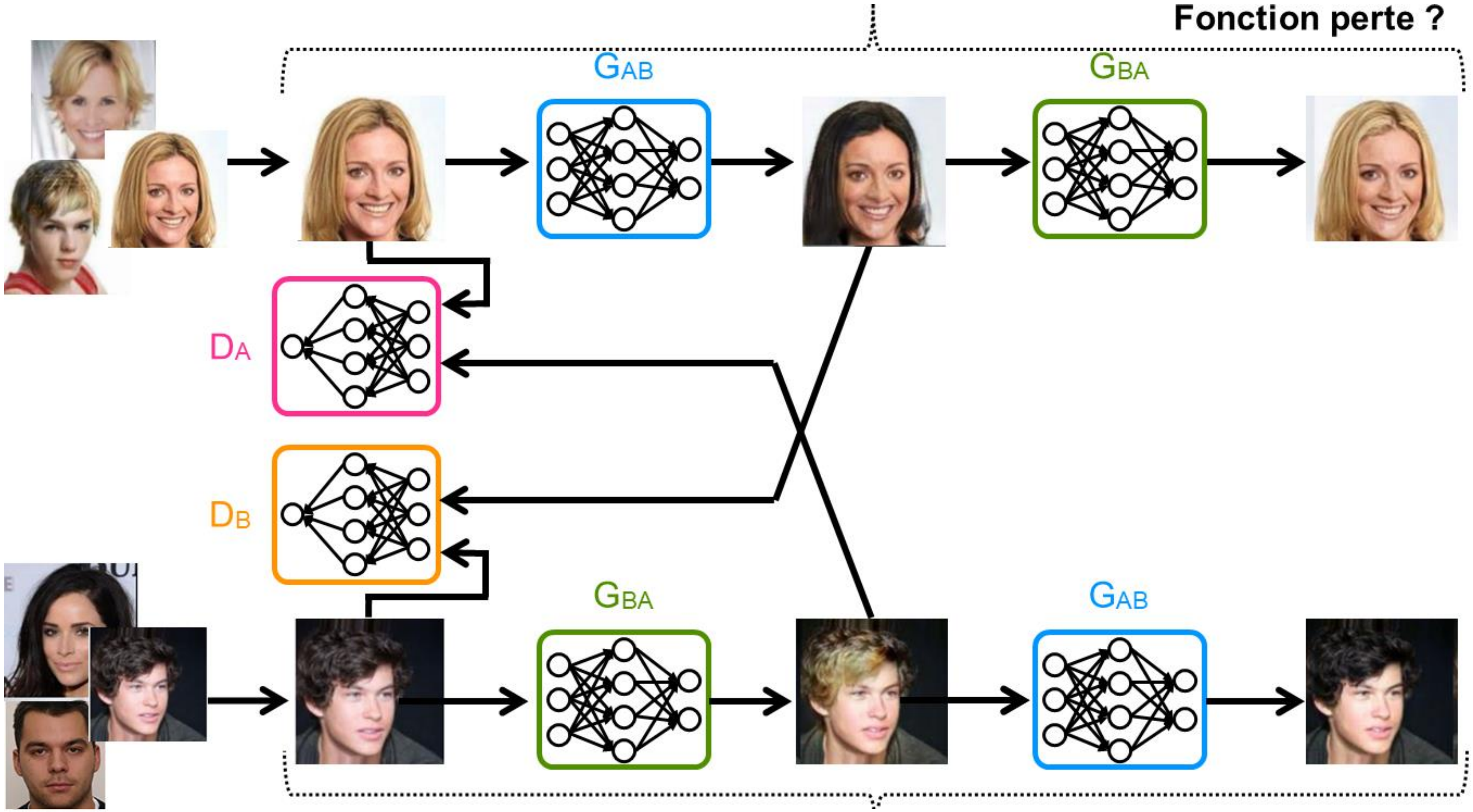


Goodfellow *et al*., NIPS (2014)

Generative adversarial networks (GAN)

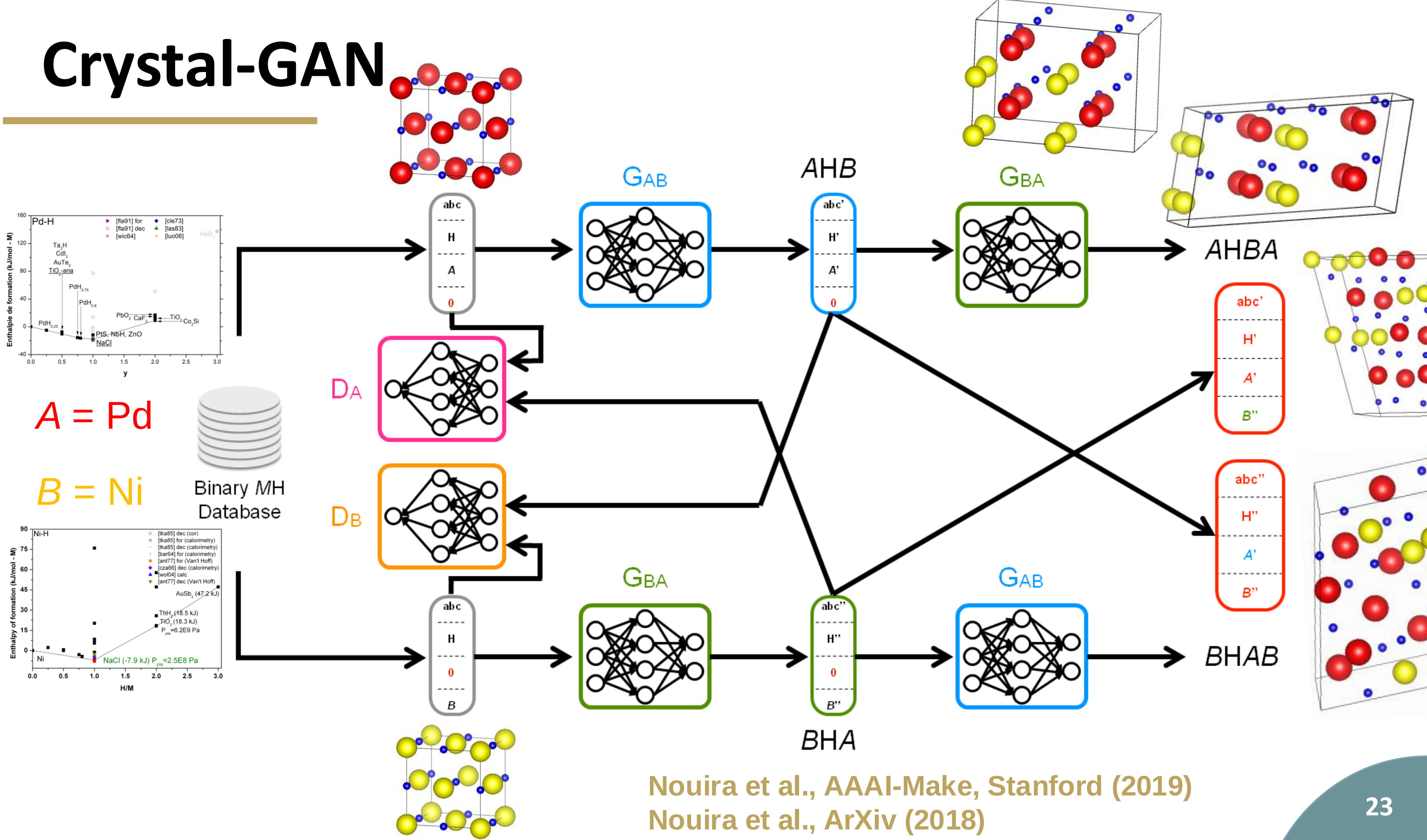


Cross-domain GAN (DiscoGAN)



Kim et al., ICML (2017)

Crystal-GAN



Nouira et al., AAAI-Make, Stanford (2019)
Nouira et al., ArXiv (2018)

Generative methods: many applications

Generate a picture

"a cabin in the mountains"

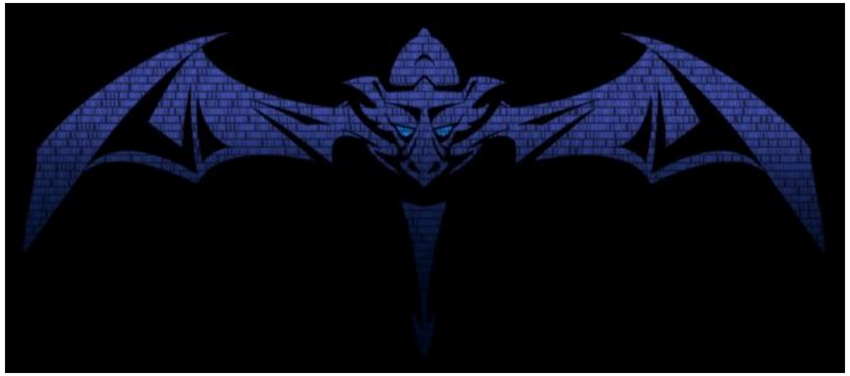
https://huggingface.co/spaces/akhaliq/VQGAN_CLIP

2020: DALLE3

Generate a narration (GPT3)

https://play.aidungeon.io

2023: GPT4 (1000 G parameters)



Generate a sound track

https://openai.com/blog/jukebox/