Deep learning with PyTorch

Luca Antiga, Orobix

Deep learning with PyTorch

- **Neural networks and back-propagation**
- PyTorch basics
- Deep learning with PyTorch
- Deep learning for g2net data

Neural networks and back propagation

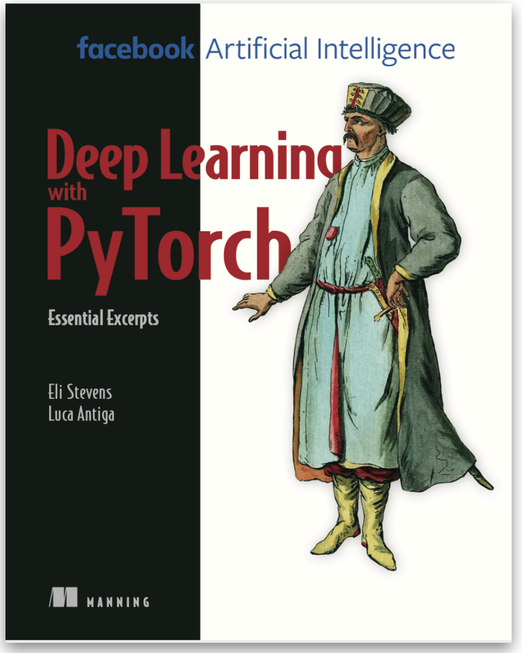
Luca Antiga, Orobix

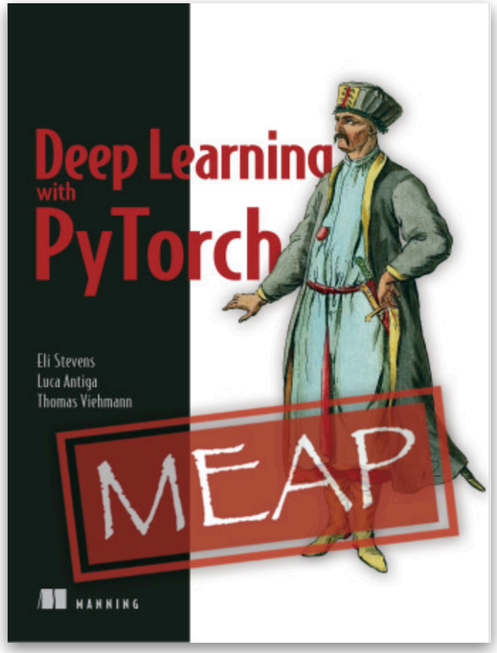
Who am I

- Co-founder at Orobix Srl, and Tensorwerk Inc
- Former PyTorch contributor
- Co-author of “Deep learning with PyTorch”
- ESCAPE project partner

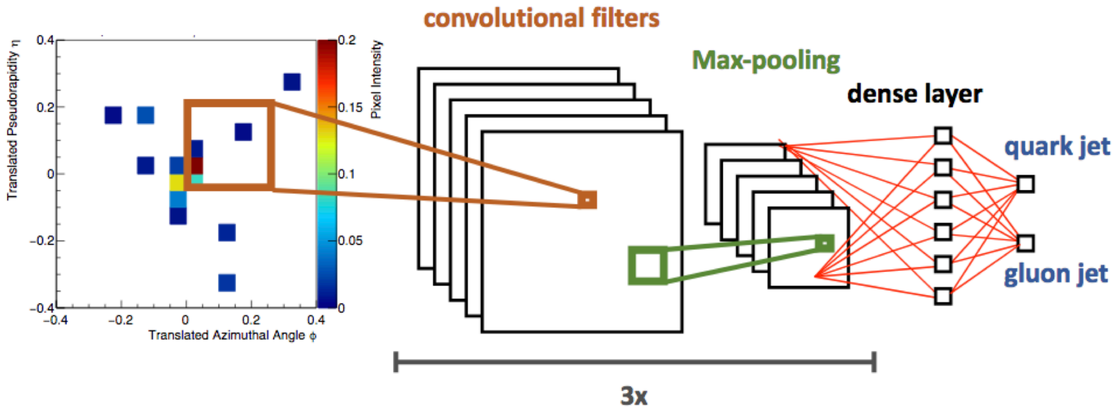
This slide deck contains:

- Figures from Deep learning with PyTorch, FB AI ed
  `https://pytorch.org/deep-learning-with-pytorch`
- Slides from Gilles Louppe’s course
  `https://github.com/glouppe/info8010-deep-learning`

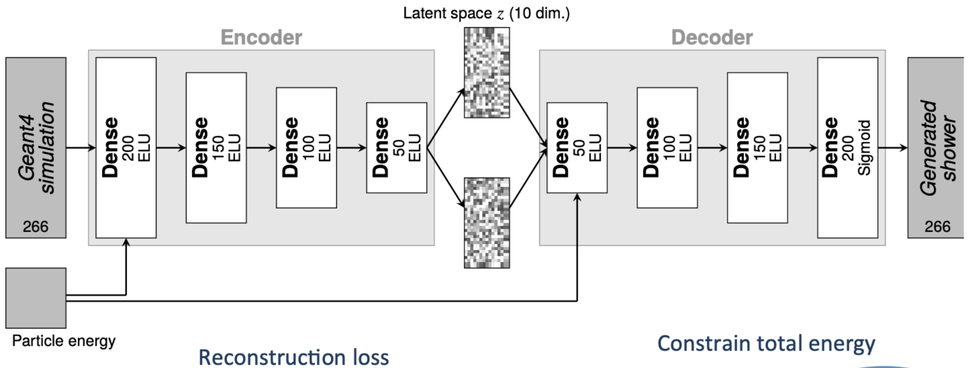




Deep learning in physics



Variational Auto-Encoder (VAE) architecture: [ATL-SOFT-PUB-2018-001]



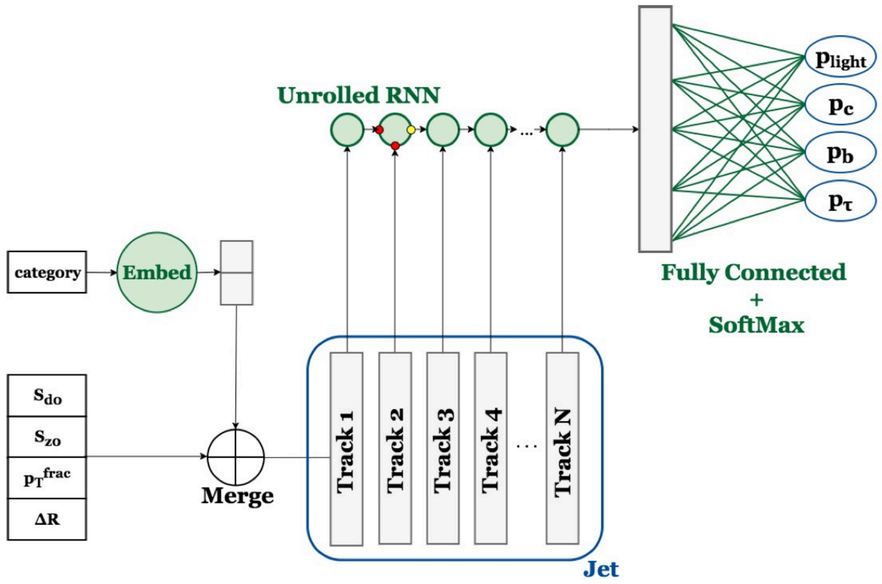
Reconstruction loss

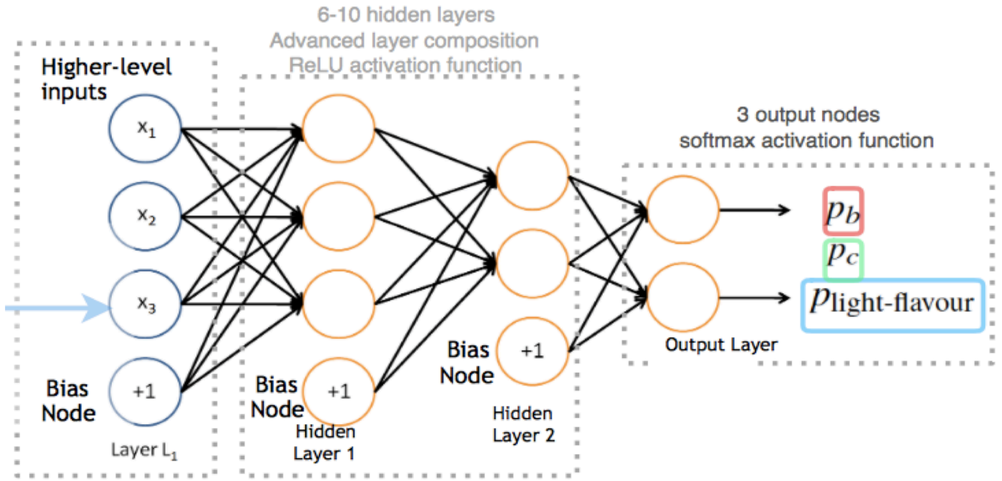
Constrain total energy

$$L_{\mathrm{VAE}}(x,\tilde{x}) = w_{\mathrm{reco}} E_{z\sim q_\theta(z|x)}[\log p_\phi(x|z)] + w_{\mathrm{KL}} \mathrm{KL}(q_\theta(z|x)||p(z)) + w_{E_{\mathrm{tot}}} L_{E_{\mathrm{tot}}}(x,\tilde{x}) + \sum_i^M w_i L_{E_i}(x,\tilde{x})$$

Kullback-Leibler divergence

Constrain energy fractions in layers



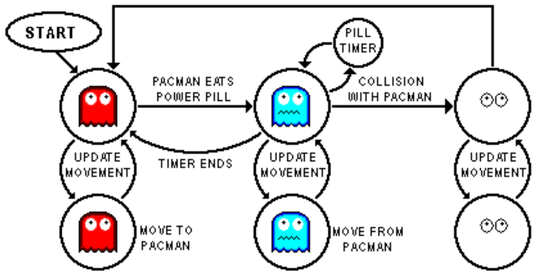


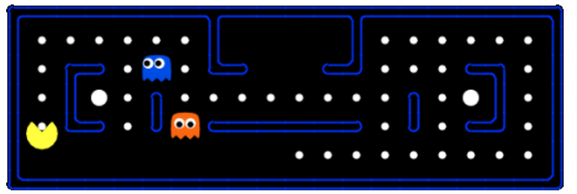
[ATL-PHYS-PUB-2017-013]

From rules to end-to-end learning

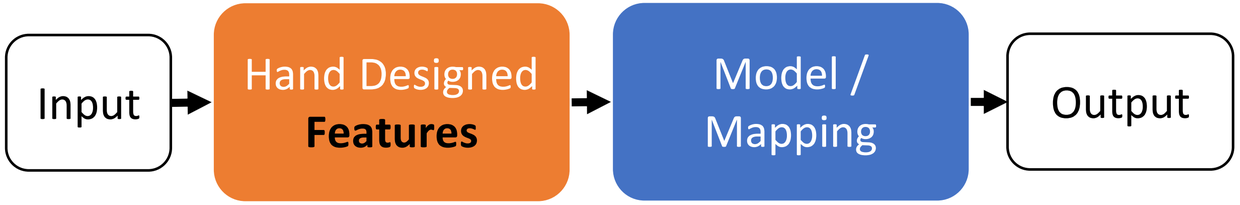
Rule Based Systems [1950 : now]

Example [Pac-Man Game Logic]

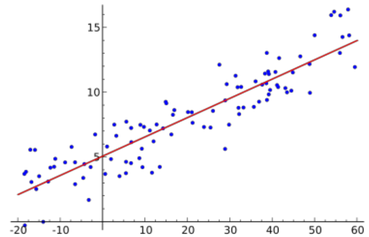


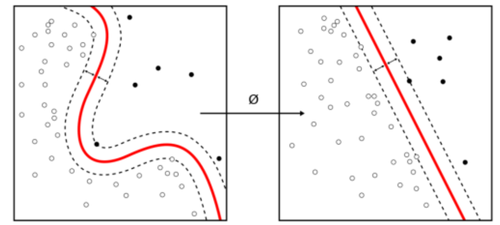


Classic Machine Learning [1990 : now]



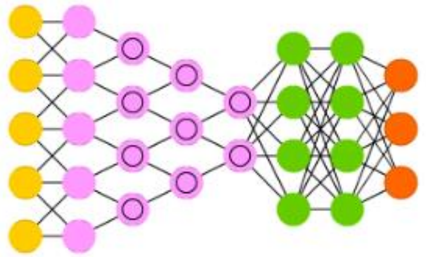
Examples [Regression and SVMs]



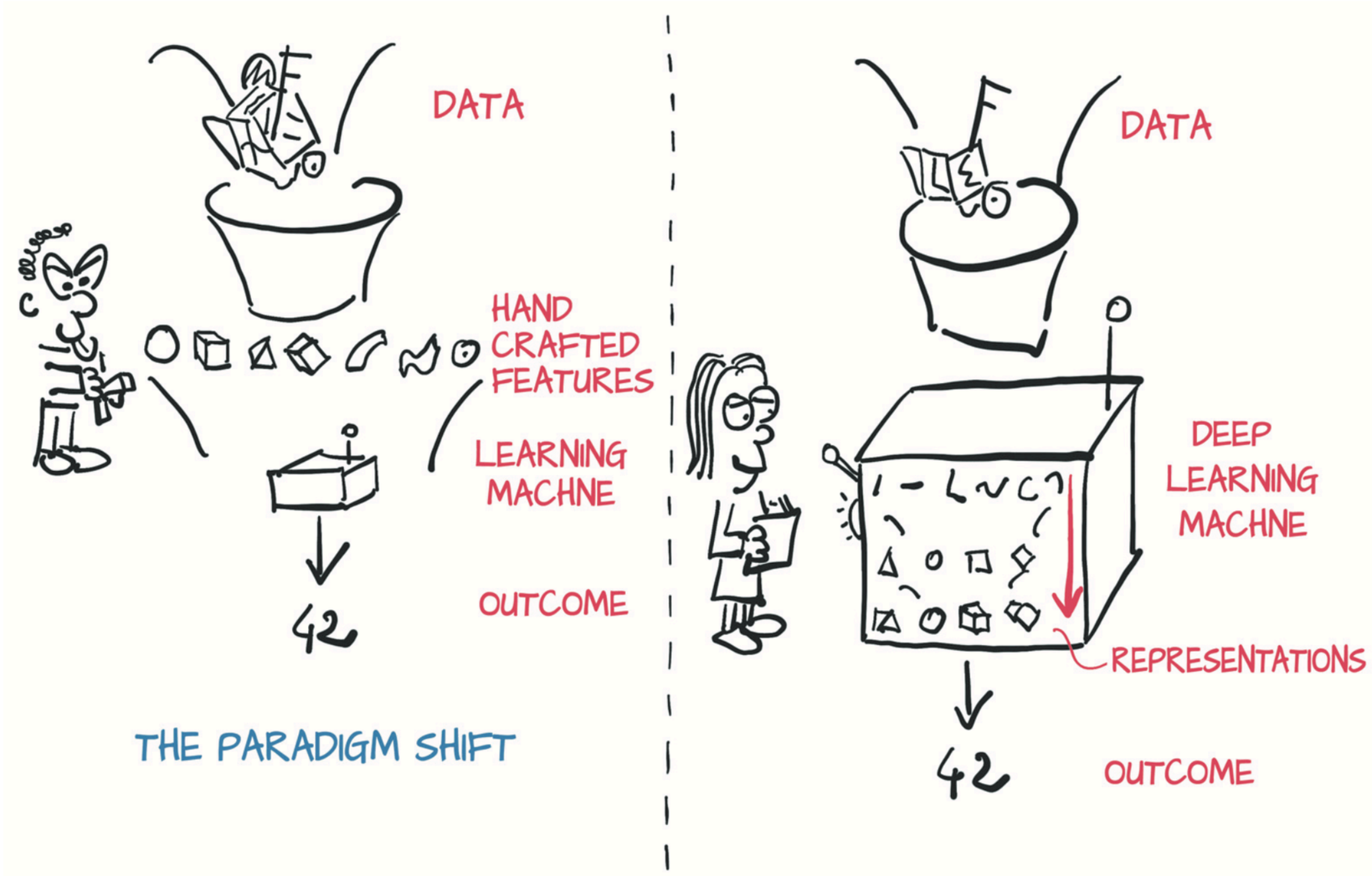


Deep/End-to-End Learning [2012 : now]

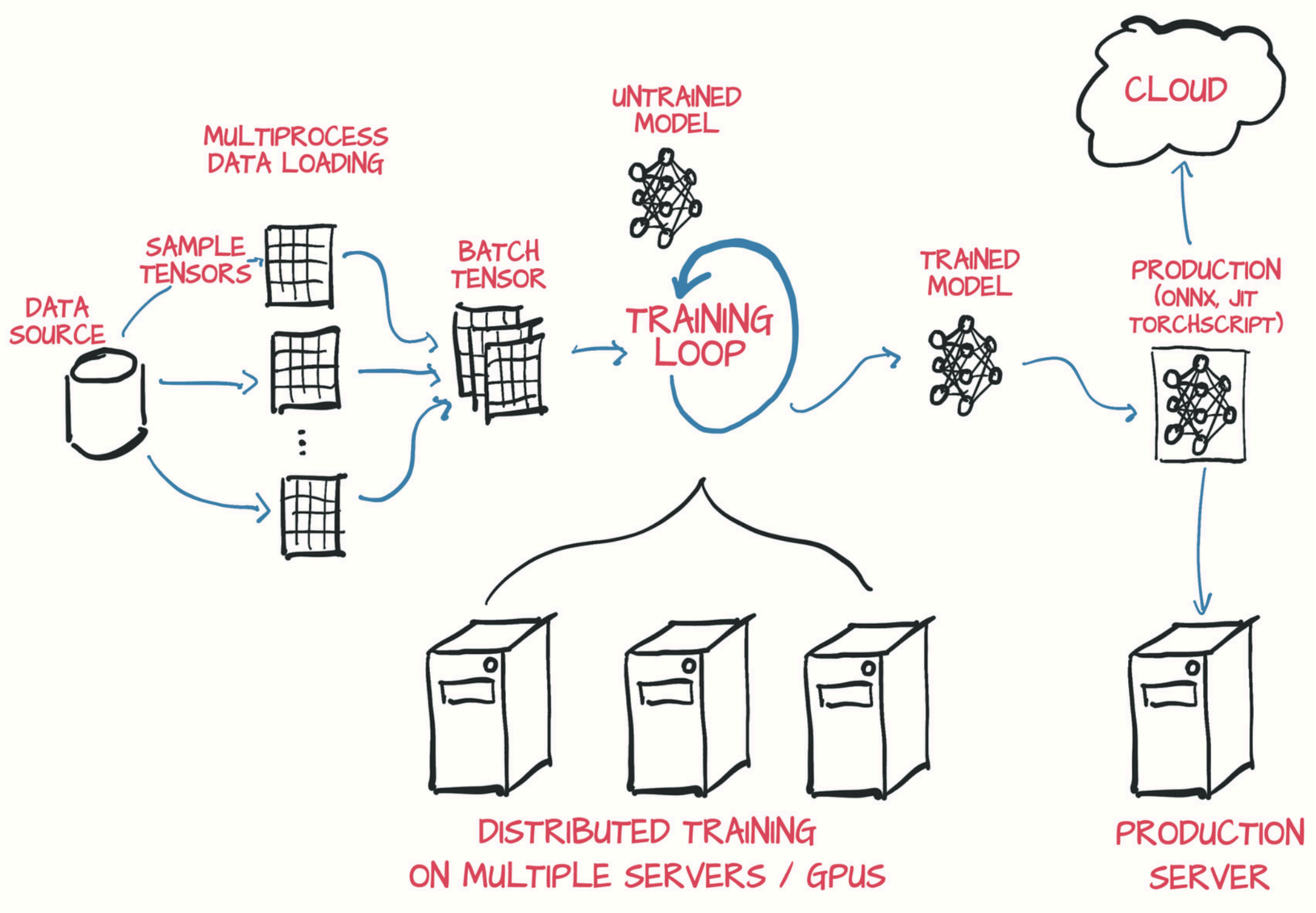
Example [Conv Net]



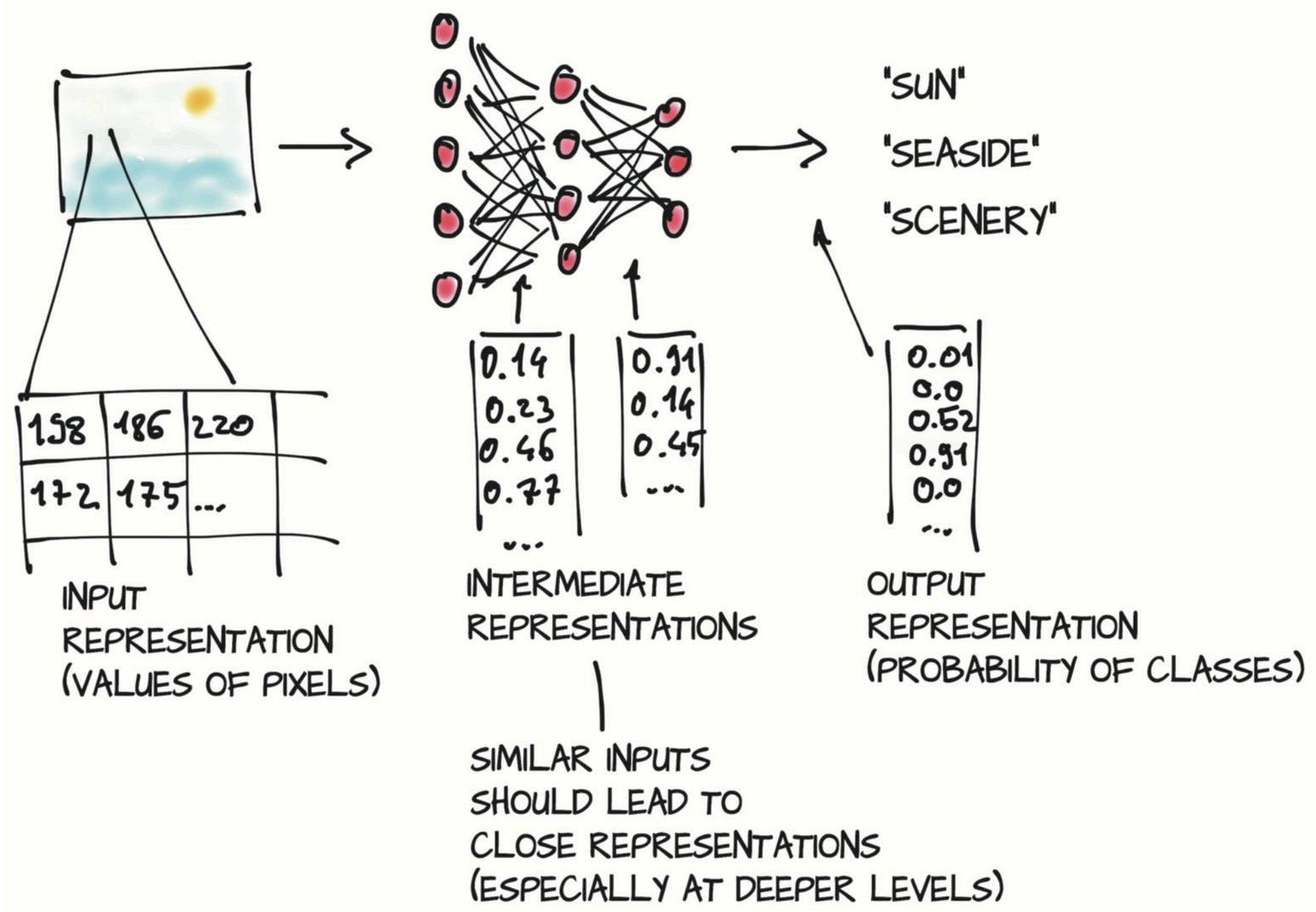
The paradigm shift



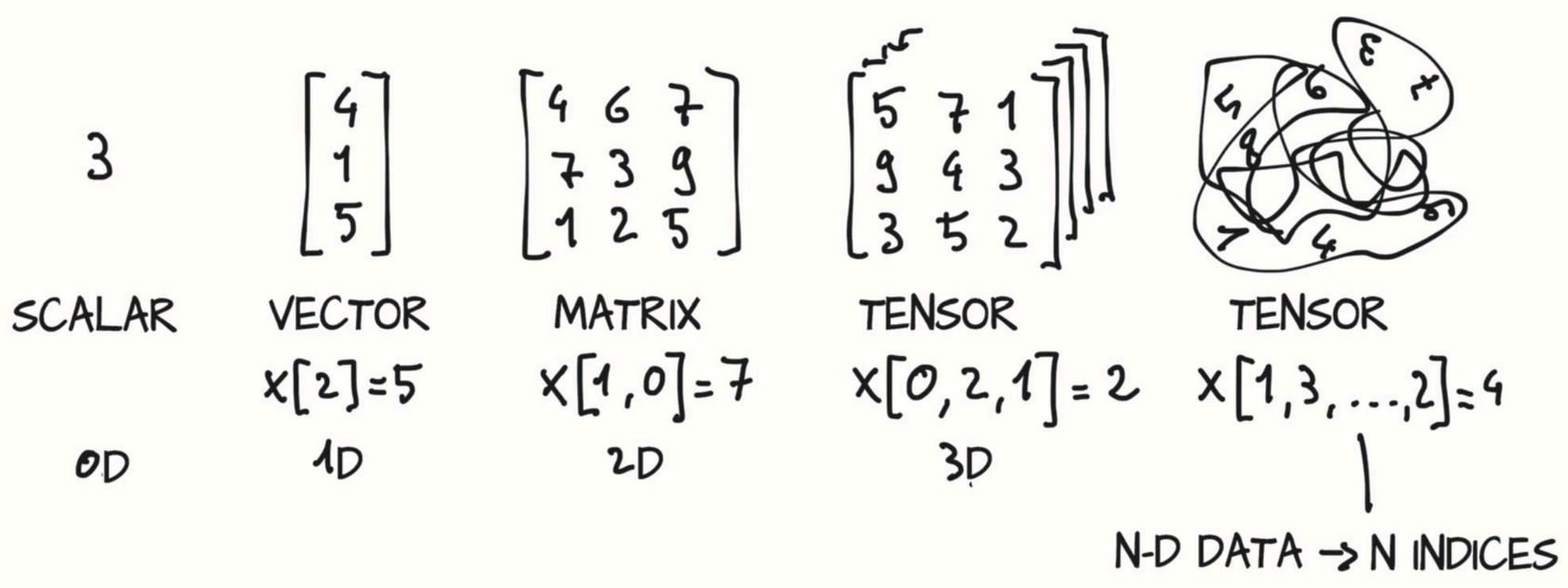
The mental model



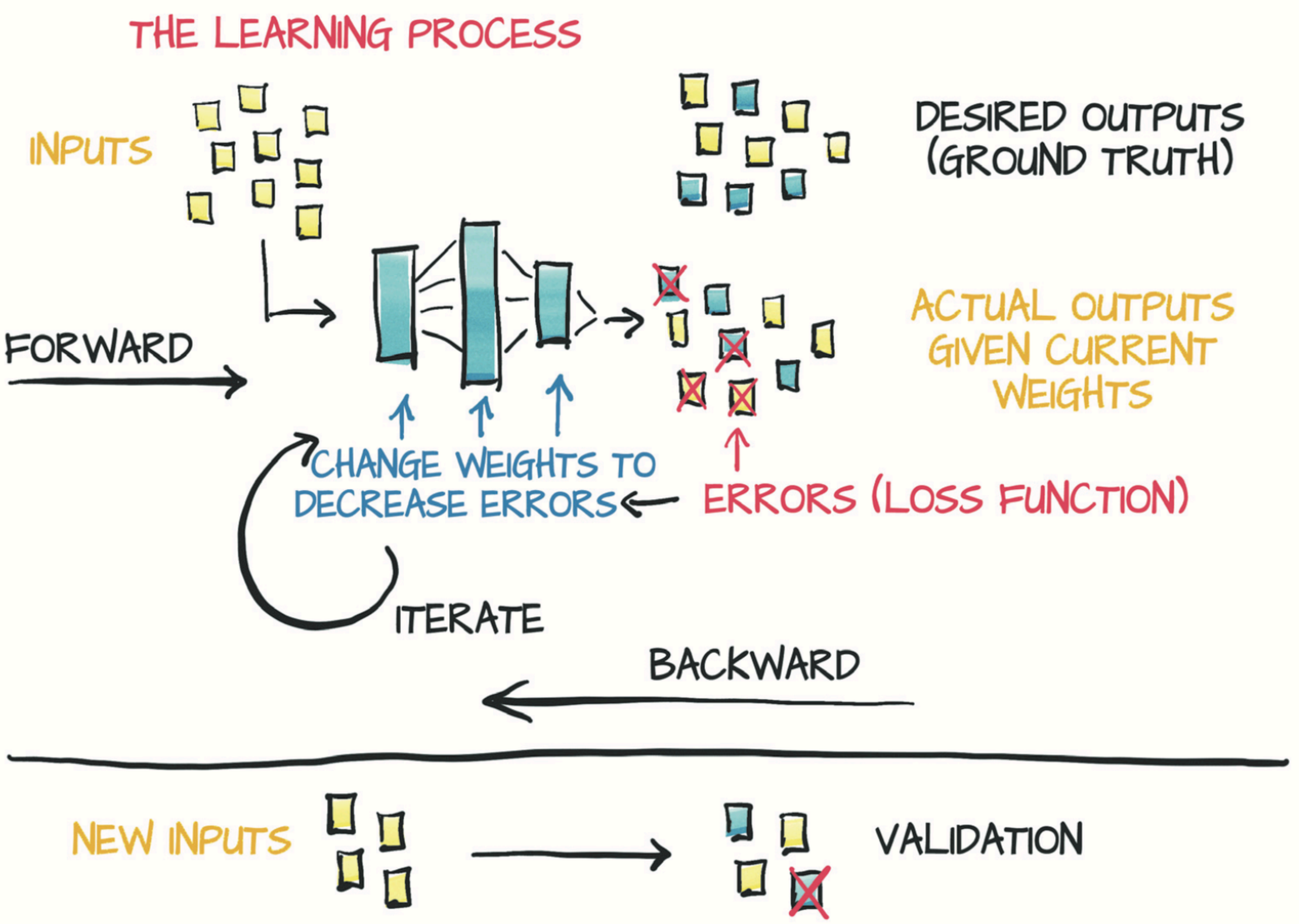
Neural network



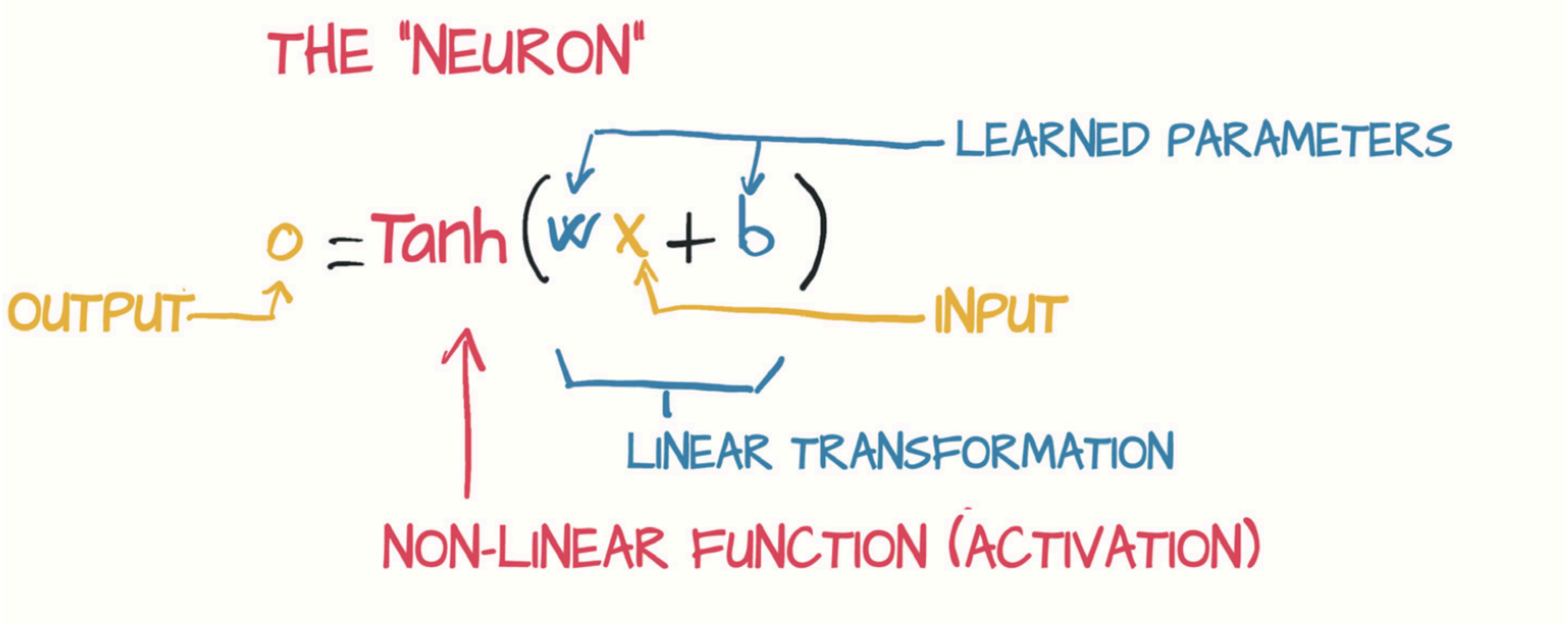
Tensors


3
SCALAR
0D
VECTOR
x[2]=5
1D
MATRIX
x[1,0]=7
2D
TENSOR
x[0,2,1]=2
3D
TENSOR
x[1,3,...,2]=4
N-D DATA → N INDICES

The learning process



The neuron

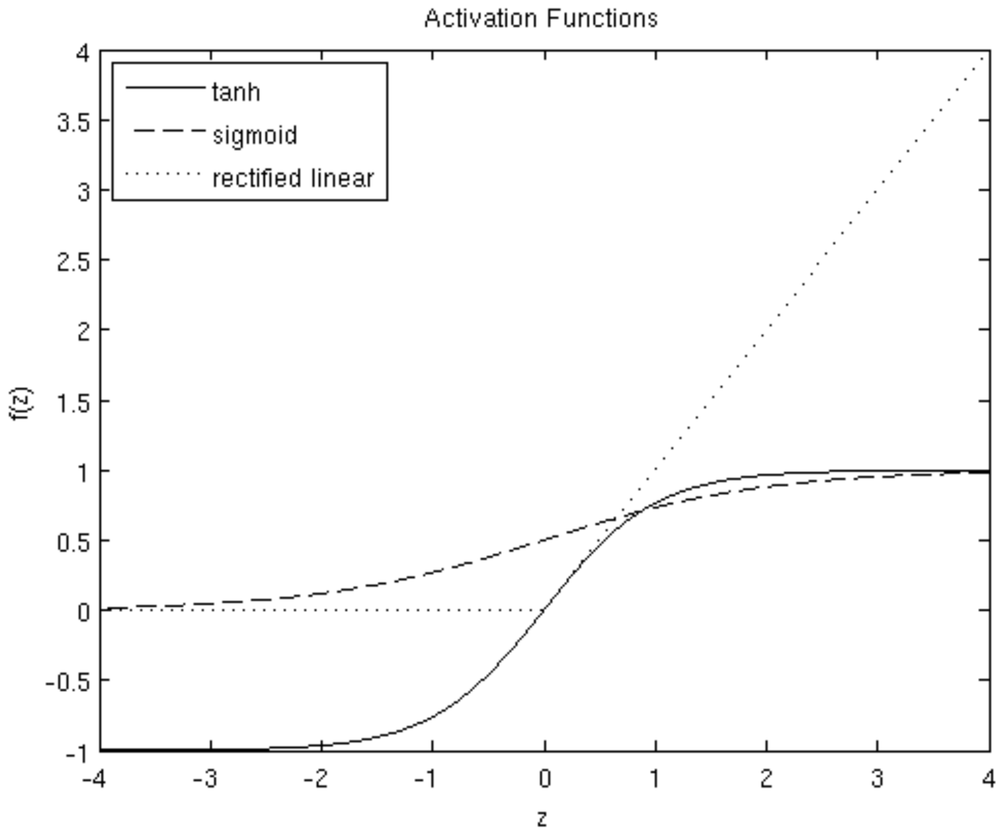

THE "NEURON"
LEARNED PARAMETERS
o = Tanh (w x + b)
OUTPUT
INPUT
LINEAR TRANSFORMATION
NON-LINEAR FUNCTION (ACTIVATION)

Non-linear activations

$$f(z) = \tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}.$$

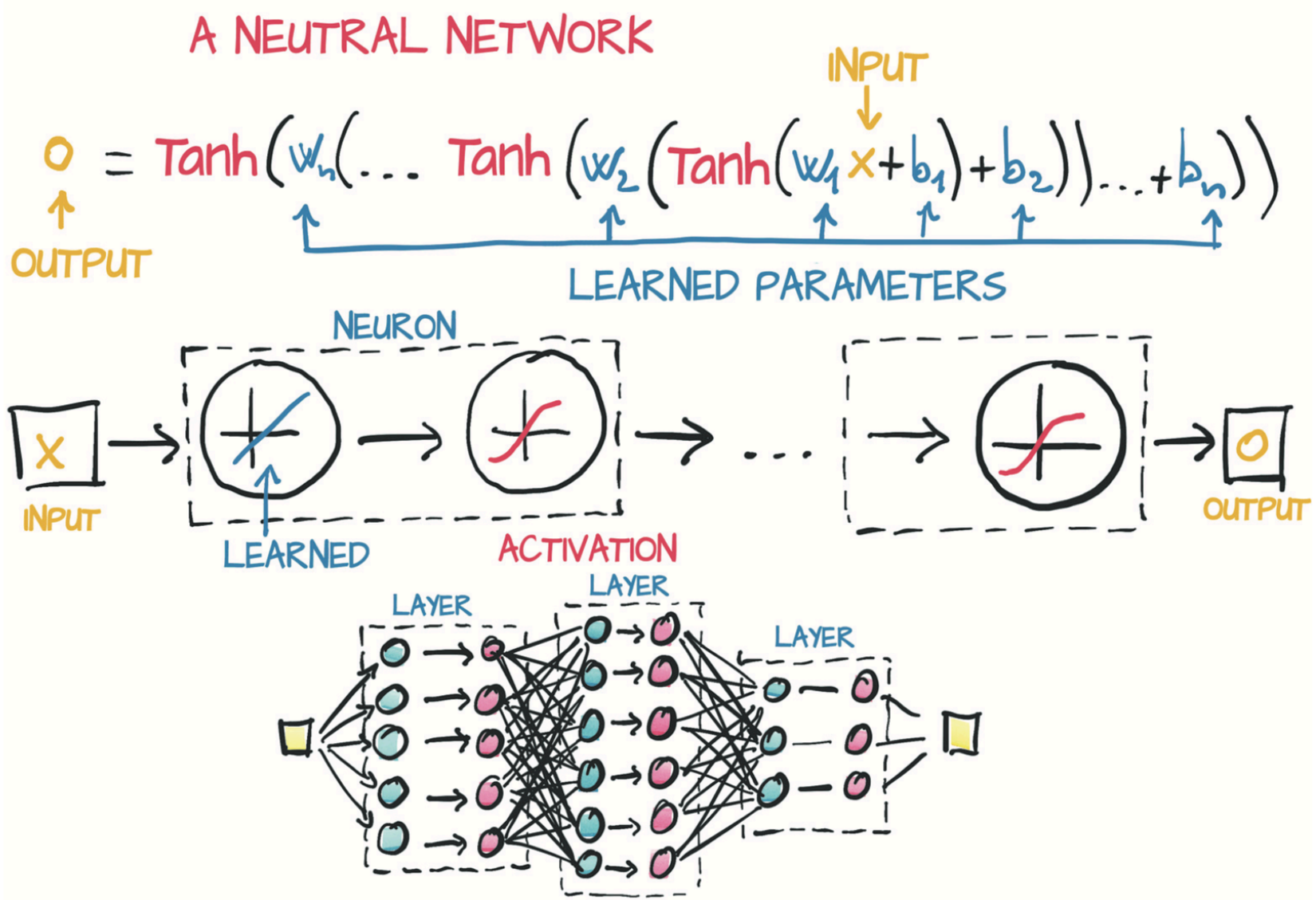
$$f(z) = \frac{1}{1 + \exp(-z)}.$$

$$f(z) = \max(0, x).$$



http://ufldl.stanford.edu/tutorial/supervised/MultiLayerNeuralNetworks/

A neural network



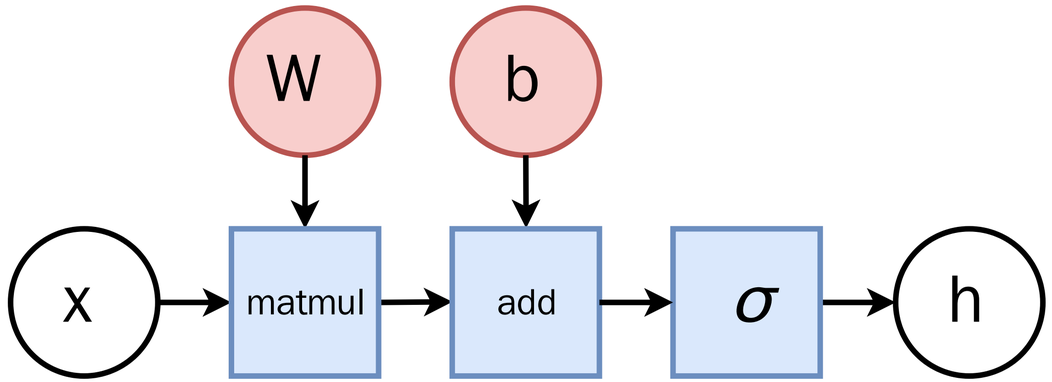
Layers

So far we considered the logistic unit $h = \sigma\left(\mathbf{w}^T\mathbf{x} + b\right)$, where $h \in \mathbb{R}, \mathbf{x} \in \mathbb{R}^p$, $\mathbf{w} \in \mathbb{R}^p$ and $b \in \mathbb{R}$.

These units can be composed in parallel to form a layer with q outputs:

$$\mathbf{h} = \sigma(\mathbf{W}^T\mathbf{x} + \mathbf{b})$$

where $\mathbf{h} \in \mathbb{R}^q, \mathbf{x} \in \mathbb{R}^p, \mathbf{W} \in \mathbb{R}^{p \times q}, b \in \mathbb{R}^q$ and where $\sigma(\cdot)$ is upgraded to the element-wise sigmoid function.



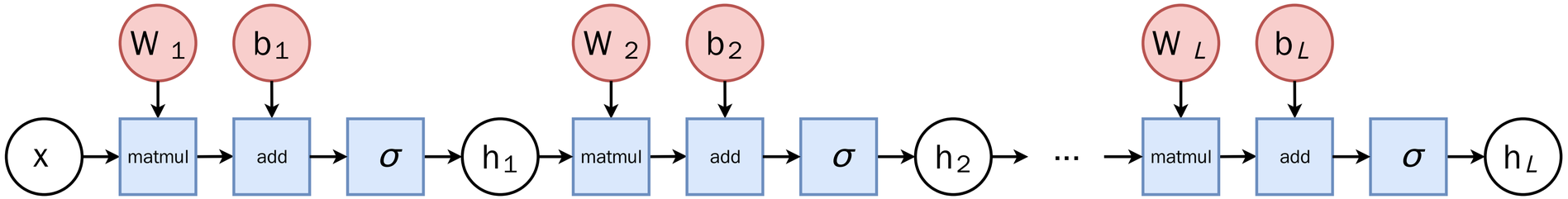
Feed forward example

Similarly, layers can be composed in series, such that:

$$
\begin{aligned}
\mathbf{h}_0 &= \mathbf{x} \\
\mathbf{h}_1 &= \sigma(\mathbf{W}_1^T \mathbf{h}_0 + \mathbf{b}_1) \\
&\dots \\
\mathbf{h}_L &= \sigma(\mathbf{W}_L^T \mathbf{h}_{L-1} + \mathbf{b}_L) \\
f(\mathbf{x}; \theta) = \hat{y} &= \mathbf{h}_L
\end{aligned}
$$

where θ denotes the model parameters $\{\mathbf{W}_k, \mathbf{b}_k, ... | k = 1, ..., L\}$.

This model is the multi-layer perceptron, also known as the fully connected feedforward network.

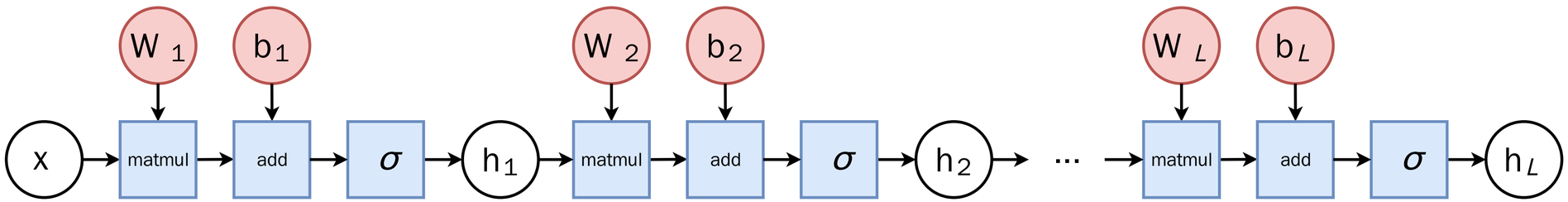


Classification

- For binary classification, the width q of the last layer L is set to 1, which results in a single output $h_L \in [0, 1]$ that models the probability $P(Y = 1|\mathbf{x})$.
- For multi-class classification, the sigmoid action σ in the last layer can be generalized to produce a (normalized) vector $\mathbf{h}_L \in [0, 1]^C$ of probability estimates $P(Y = i|\mathbf{x})$.

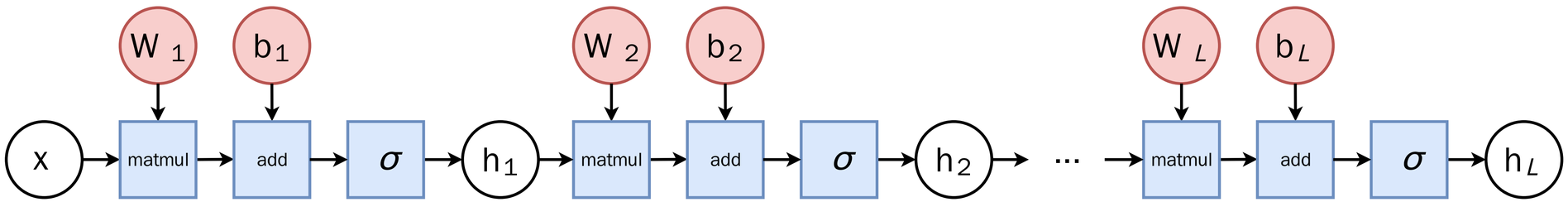
  This activation is the $\mathrm{Softmax}$ function, where its i-th output is defined as

$$\mathrm{Softmax}(\mathbf{z})_i = \frac{\exp(z_i)}{\sum_{j=1}^{C} \exp(z_j)},$$



Regression

The last activation σ can be skipped to produce unbounded output values $h_L \in \mathbb{R}$.



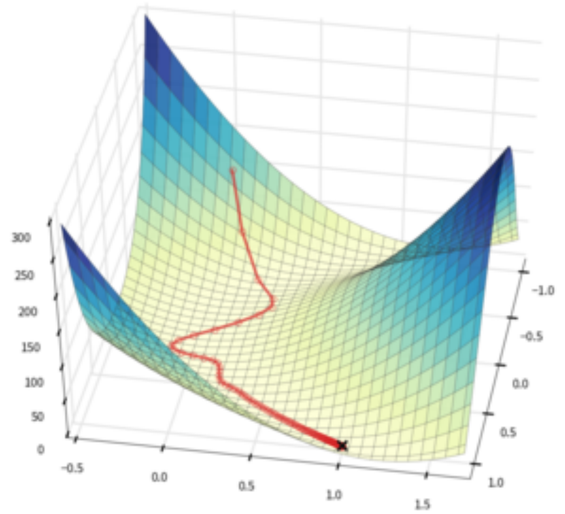
The learning process

Define J (loss); optimize J by changing W, b.
Stochastic gradient descent: compute descent on one sample or mini-batch.

$$J(W,b) = \left[\frac{1}{m}\sum_{i=1}^{m} J(W,b;x^{(i)},y^{(i)})\right] + \frac{\lambda}{2}\sum_{l=1}^{n_l-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}}\left(W_{ji}^{(l)}\right)^2$$

$$W_{ij}^{(l)} = W_{ij}^{(l)} - \alpha\frac{\partial}{\partial W_{ij}^{(l)}}J(W,b)$$

$$b_i^{(l)} = b_i^{(l)} - \alpha\frac{\partial}{\partial b_i^{(l)}}J(W,b)$$



http://ufldl.stanford.edu/tutorial/supervised/MultiLayerNeuralNetworks/

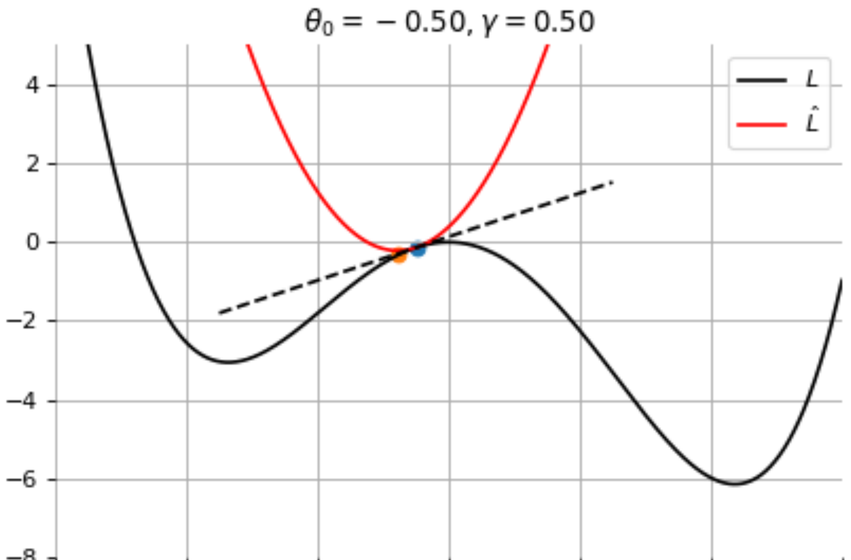
Gradient descent

Let $\mathcal{L}(\theta)$ denote a loss function defined over model parameters θ (e.g., $\mathbf{w}$ and b).

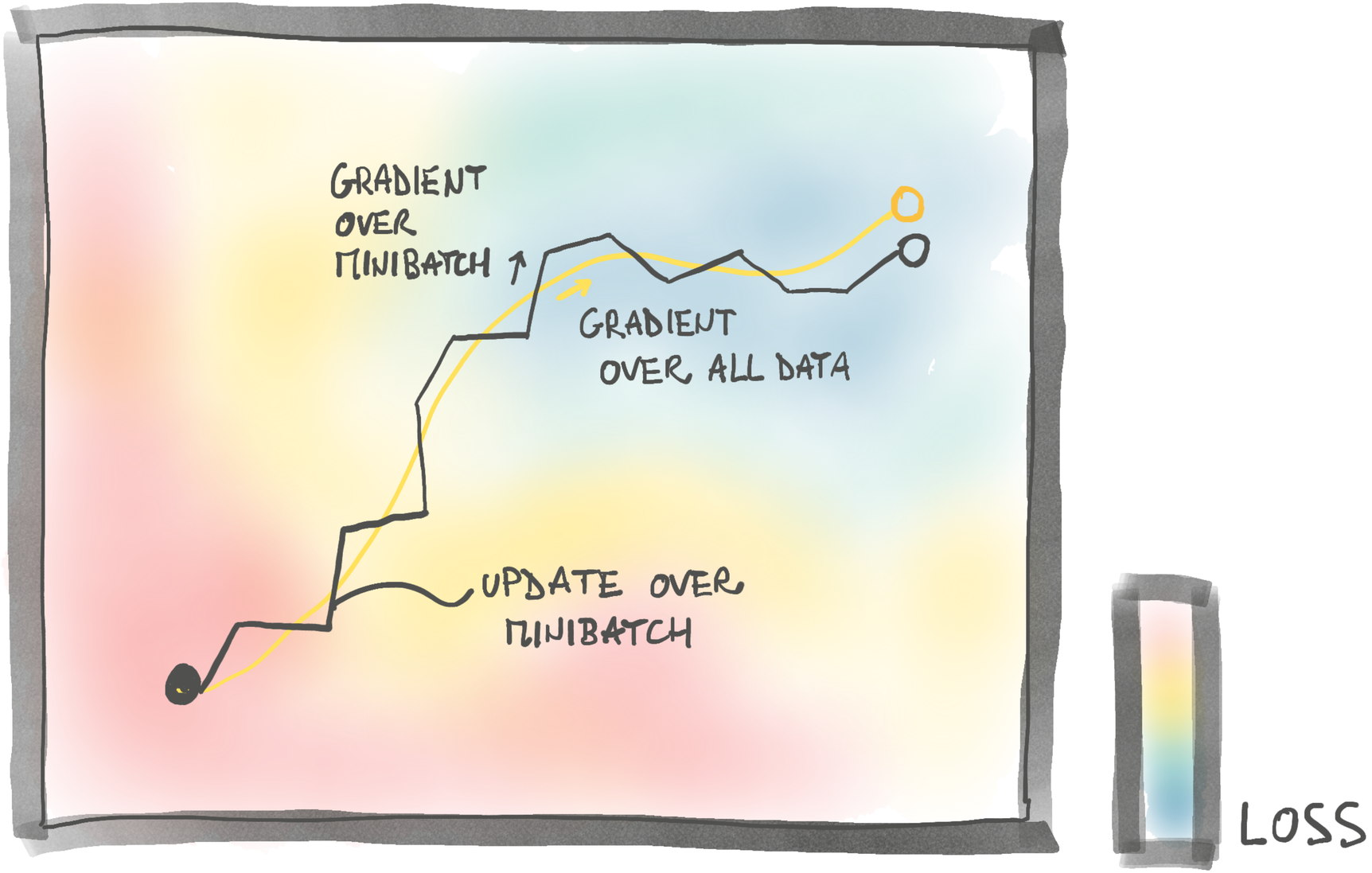
To minimize $\mathcal{L}(\theta)$, gradient descent uses local linear information to iteratively move towards a (local) minimum.

For $\theta_0 \in \mathbb{R}^d$, a first-order approximation around θ_0 can be defined as

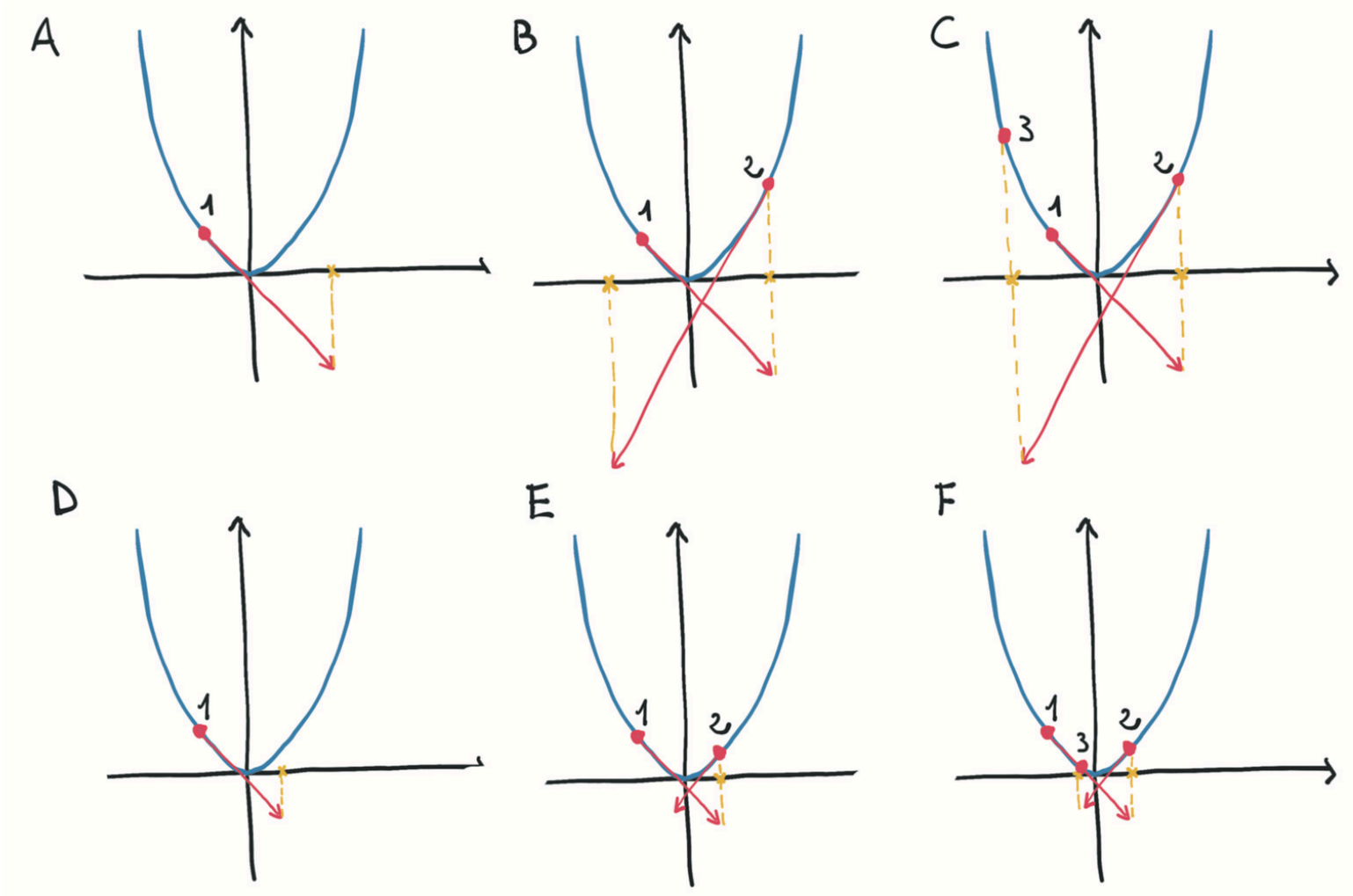
$$\hat{\mathcal{L}}(\theta_0 + \epsilon) = \mathcal{L}(\theta_0) + \epsilon^T \nabla_\theta \mathcal{L}(\theta_0) + \frac{1}{2\gamma} ||\epsilon||^2.$$



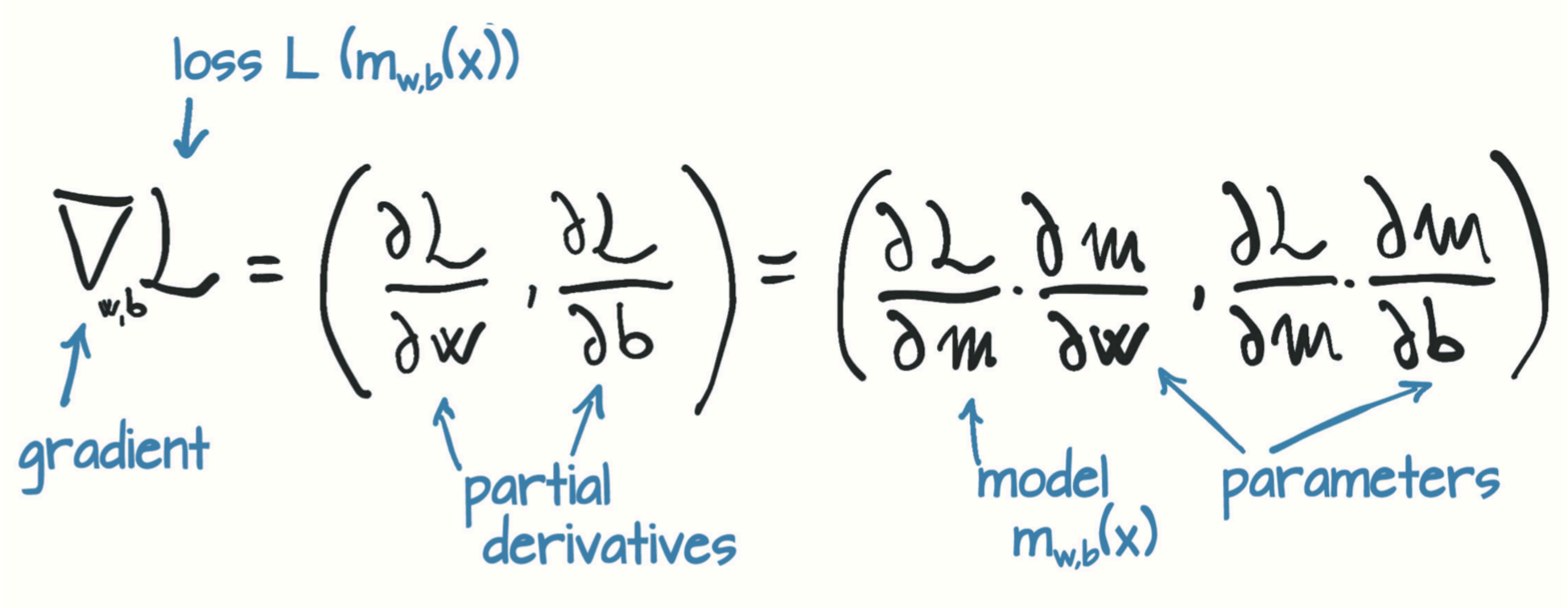
Stochastic gradient descent



Learning rate

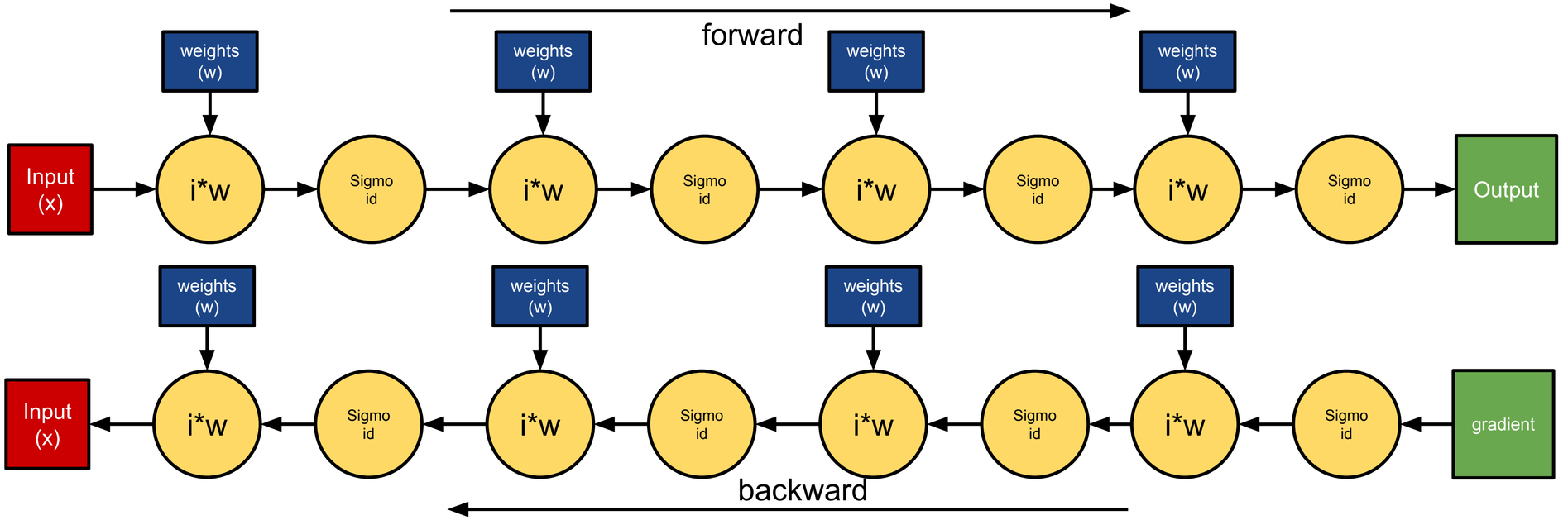


Gradient and chain rule



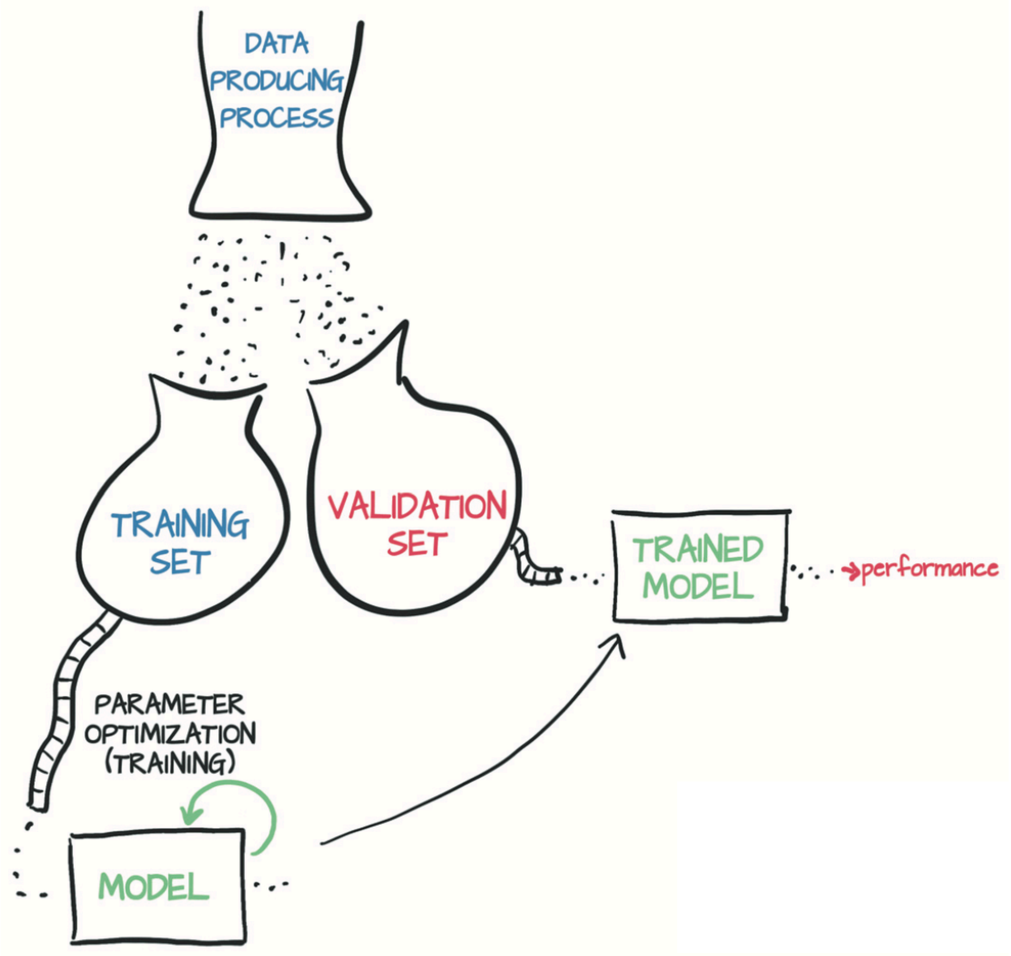
Back propagation

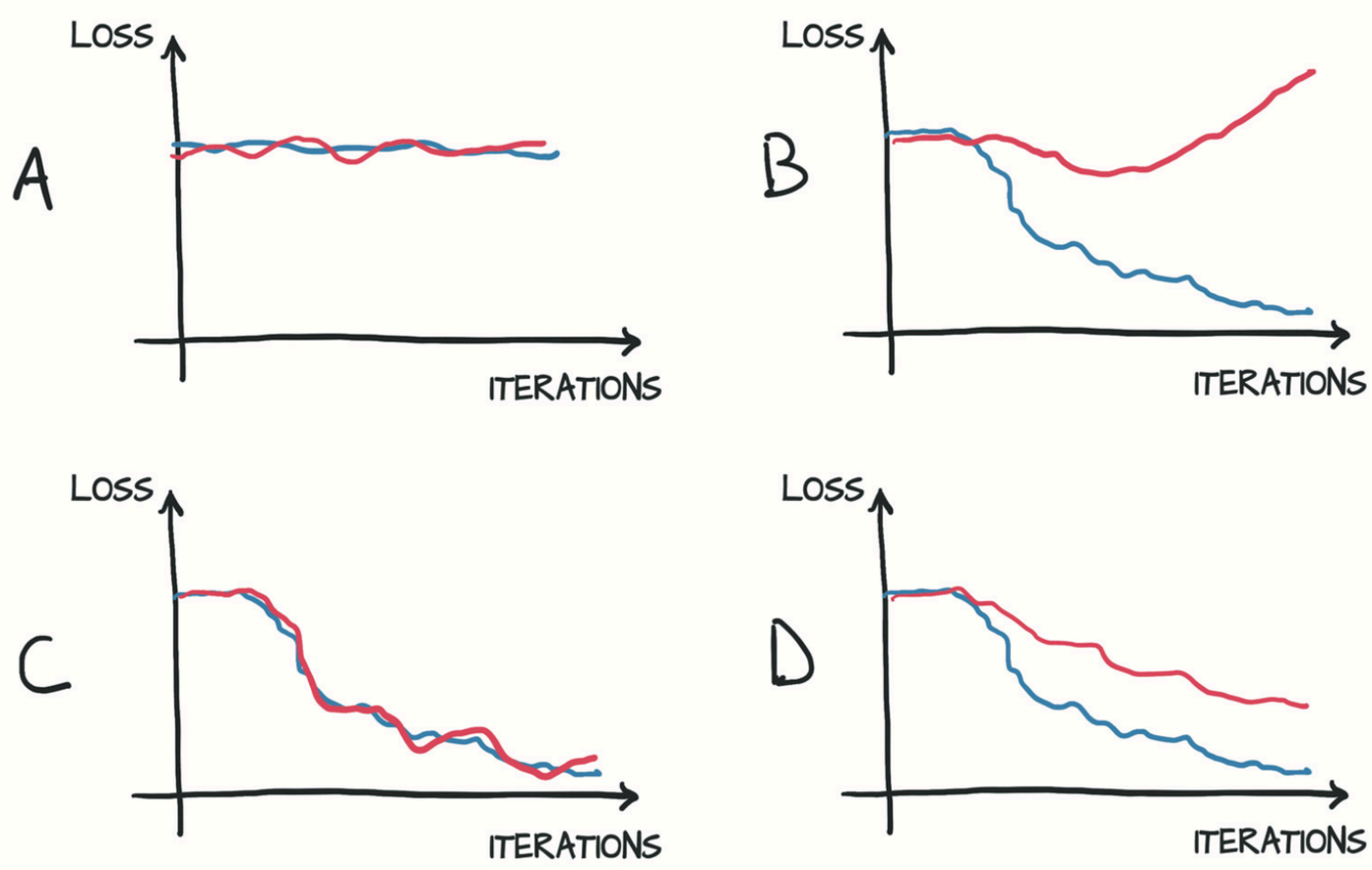
$$W_{ij}^{(l)} = W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W, b)$$



The Deep Learning Revolution: Rethinking Machine Learning Pipelines. Soumith Chintala

Loss behaviors





What makes things work

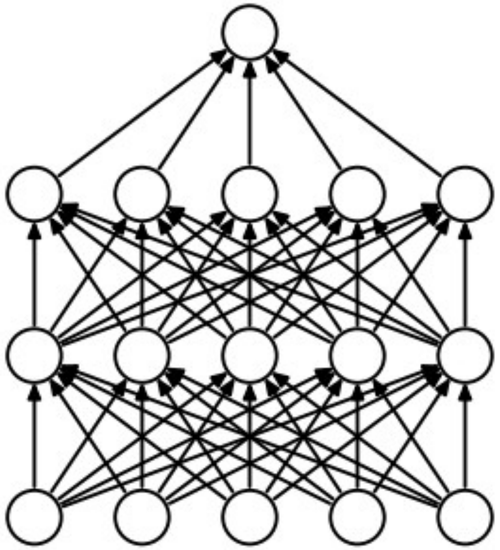
Dropout

Batch normalization

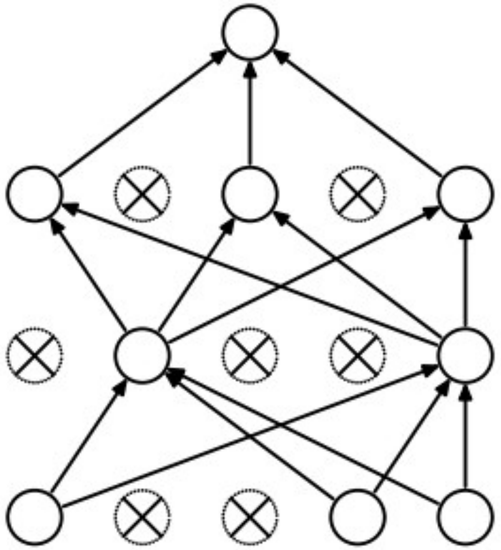
Stochastic depth

Noise injection

Data augmentation



(a) Standard Neural Net



(b) After applying dropout.

Playground

http://playground.tensorflow.org

Universal approximation

Hornik et al (1989): A one hidden layer feedforward neural network is capable of approximating uniformly any continuous multivariate function, to any desired degree of accuracy.

Kolmogorov, A. N. (1957). On the representation of continuous functions of many variables by superposition of continuous functions of one variable and addition.

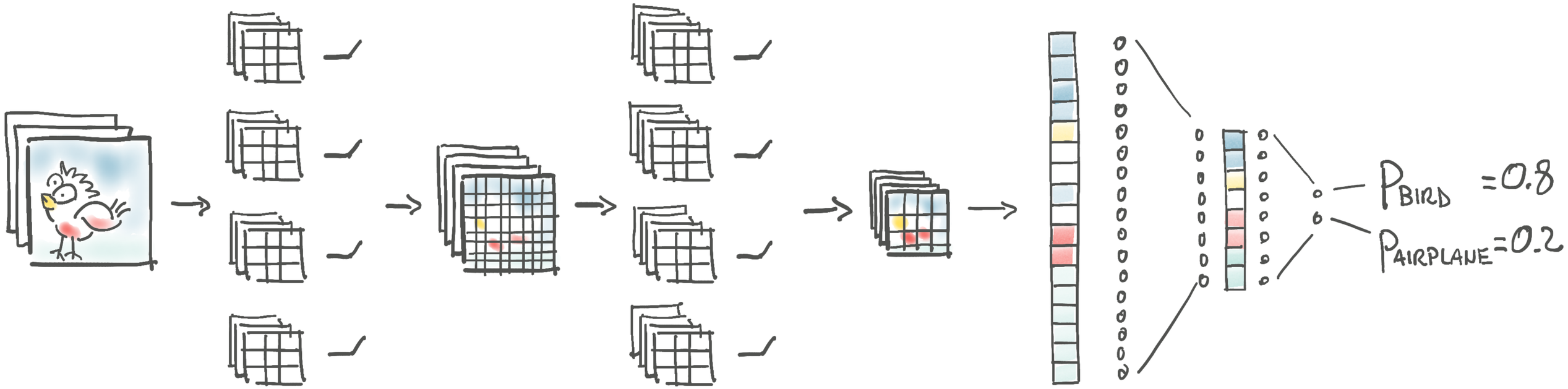
Theorem 1.1. (Kolmogorov 1957). *There exist fixed increasing continuous functions $h_{pq}(x)$, on $I = [0,1]$ so that each continuous function f on I^n can be written in the form*

$$f(x_1, \ldots, x_n) = \sum_{q=1}^{2n+1} g_q\left(\sum_{p=1}^{n} h_{pq}(x_p)\right),$$

where g_q are properly chosen continuous functions of one variable.

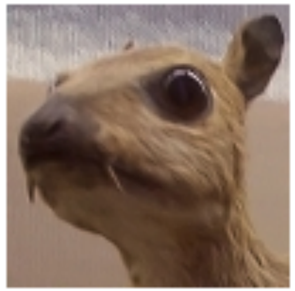
https://theneural.wordpress.com/2013/01/07/universal-approximation-and-depth/

Convolutional neural networks



Convolutions

Input image



Convolution Kernel

$$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$$

Feature map

$1_{\times 1}$	$1_{\times 0}$	$1_{\times 1}$	0	0
$0_{\times 0}$	$1_{\times 1}$	$1_{\times 0}$	1	0
$0_{\times 1}$	$0_{\times 0}$	$1_{\times 1}$	1	1
0	0	1	1	0
0	1	1	0	0

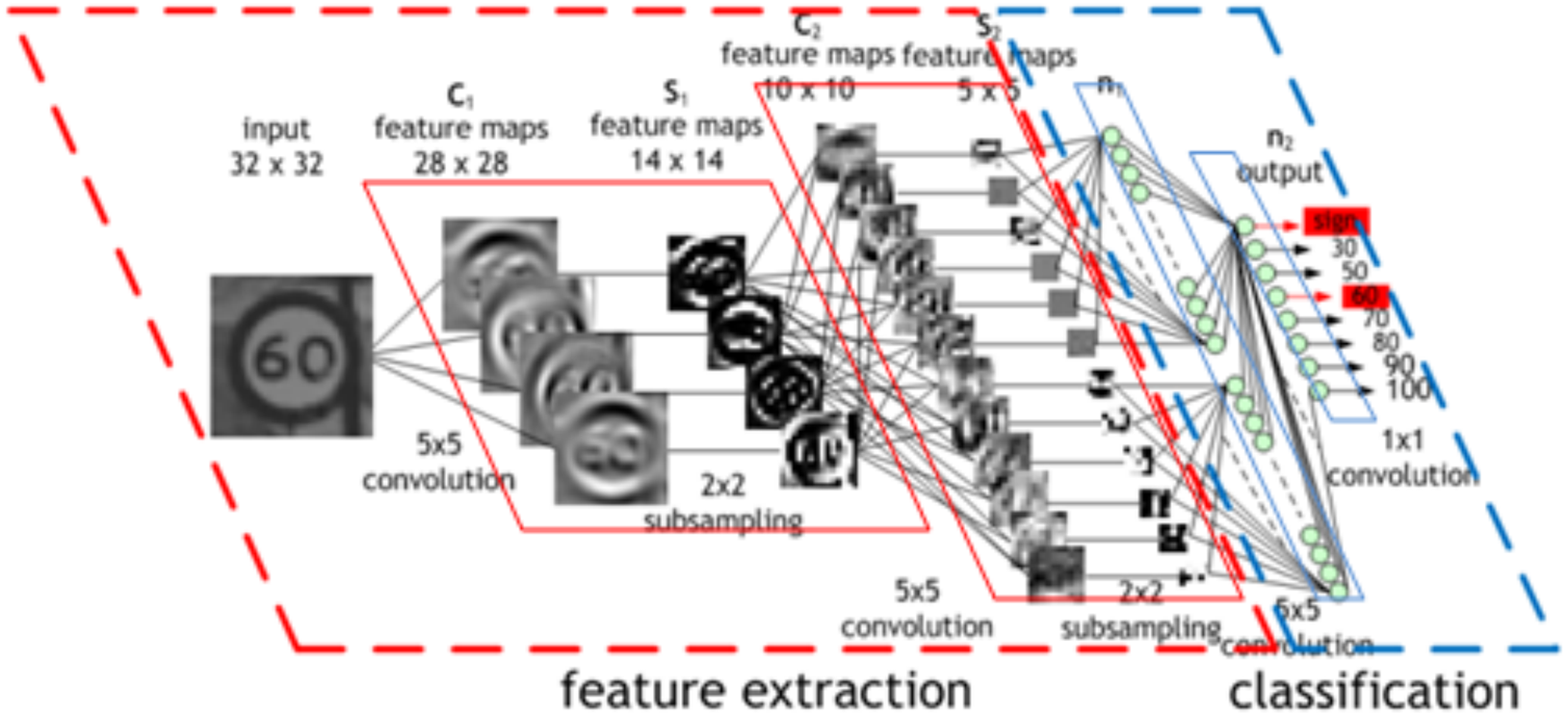
Image

4		

Convolved Feature

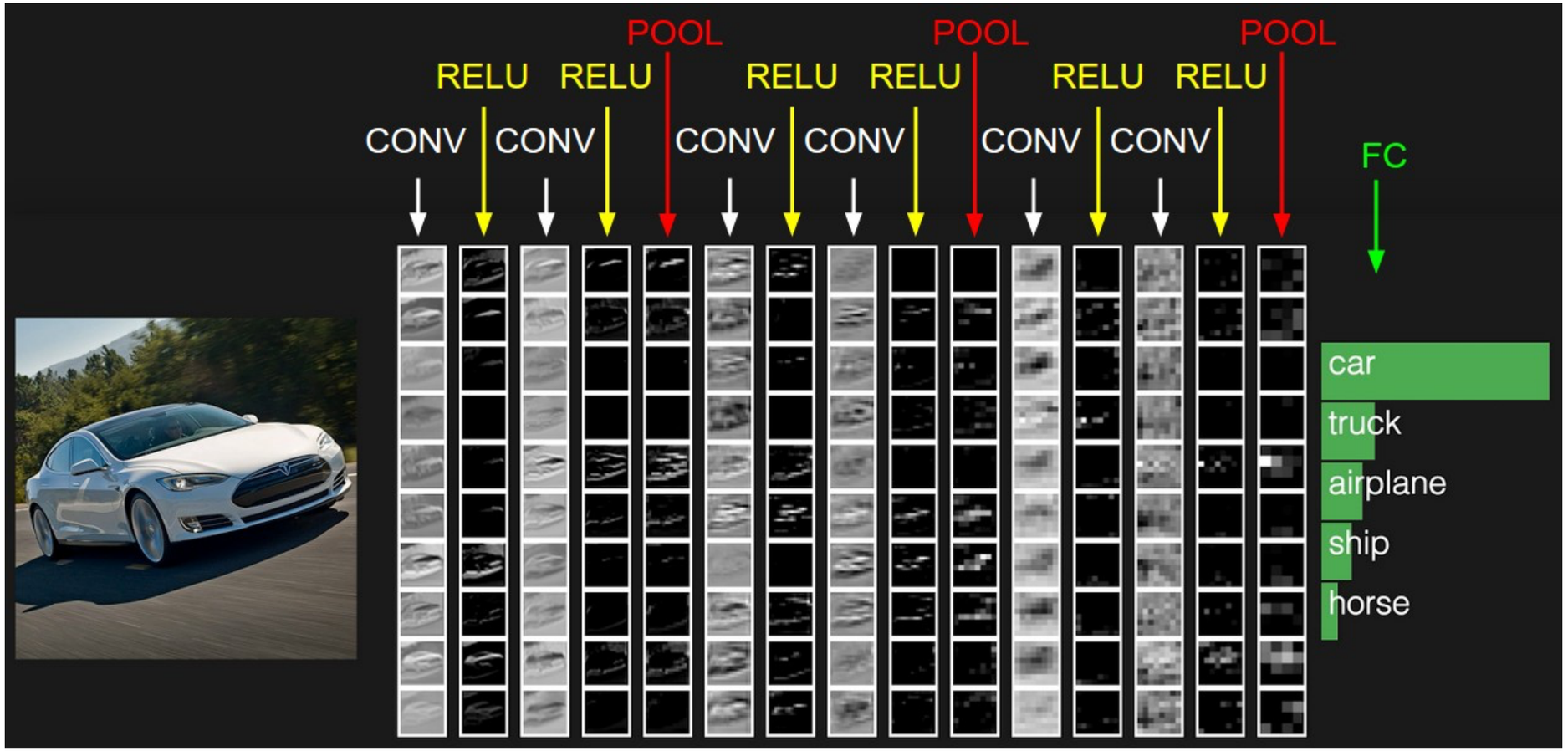
https://devblogs.nvidia.com/parallelforall/deep-learning-nutshell-core-concepts/

Convolutional networks



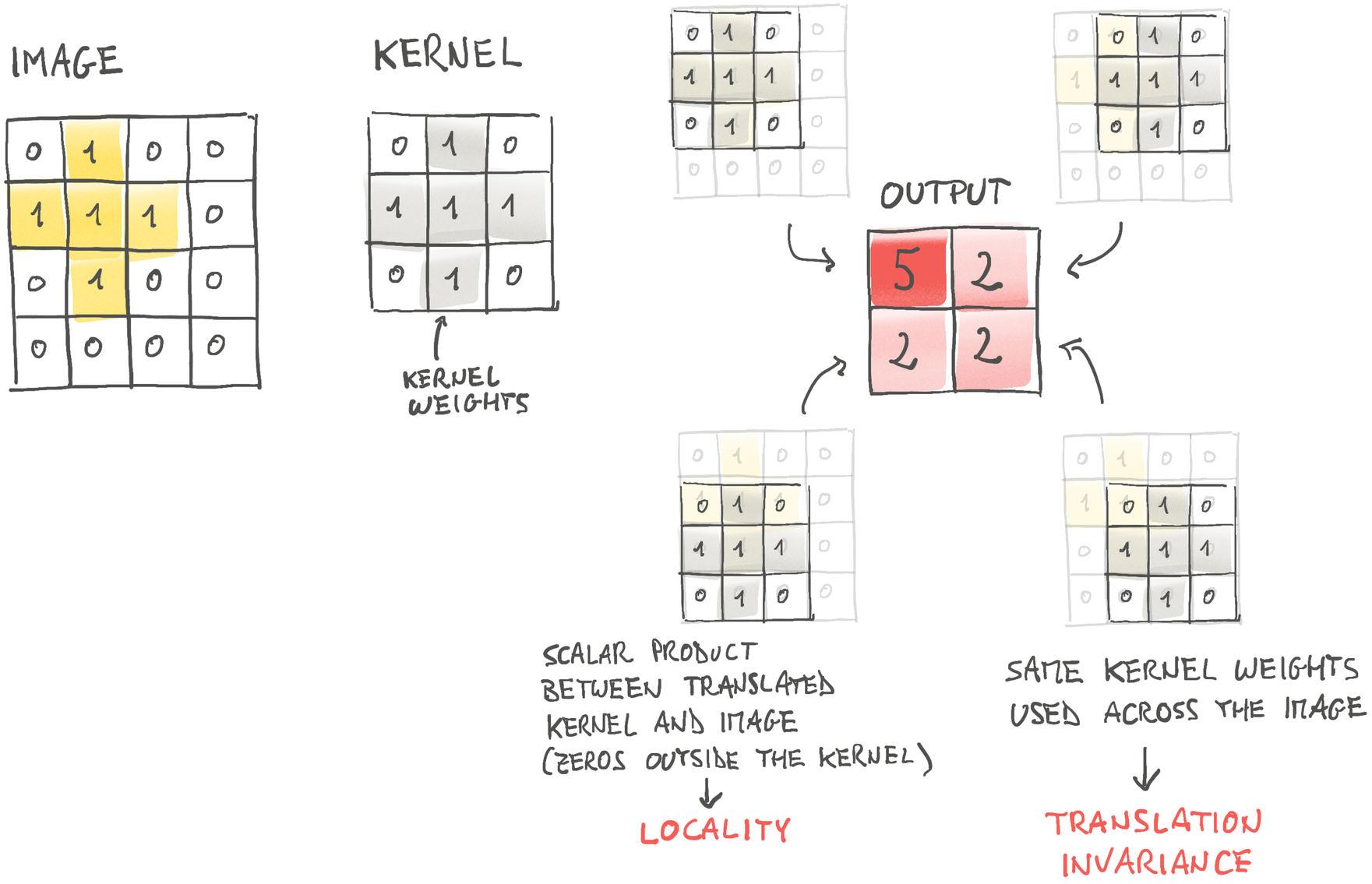
https://devblogs.nvidia.com/parallelforall/deep-learning-nutshell-core-concepts/

Convolutional networks

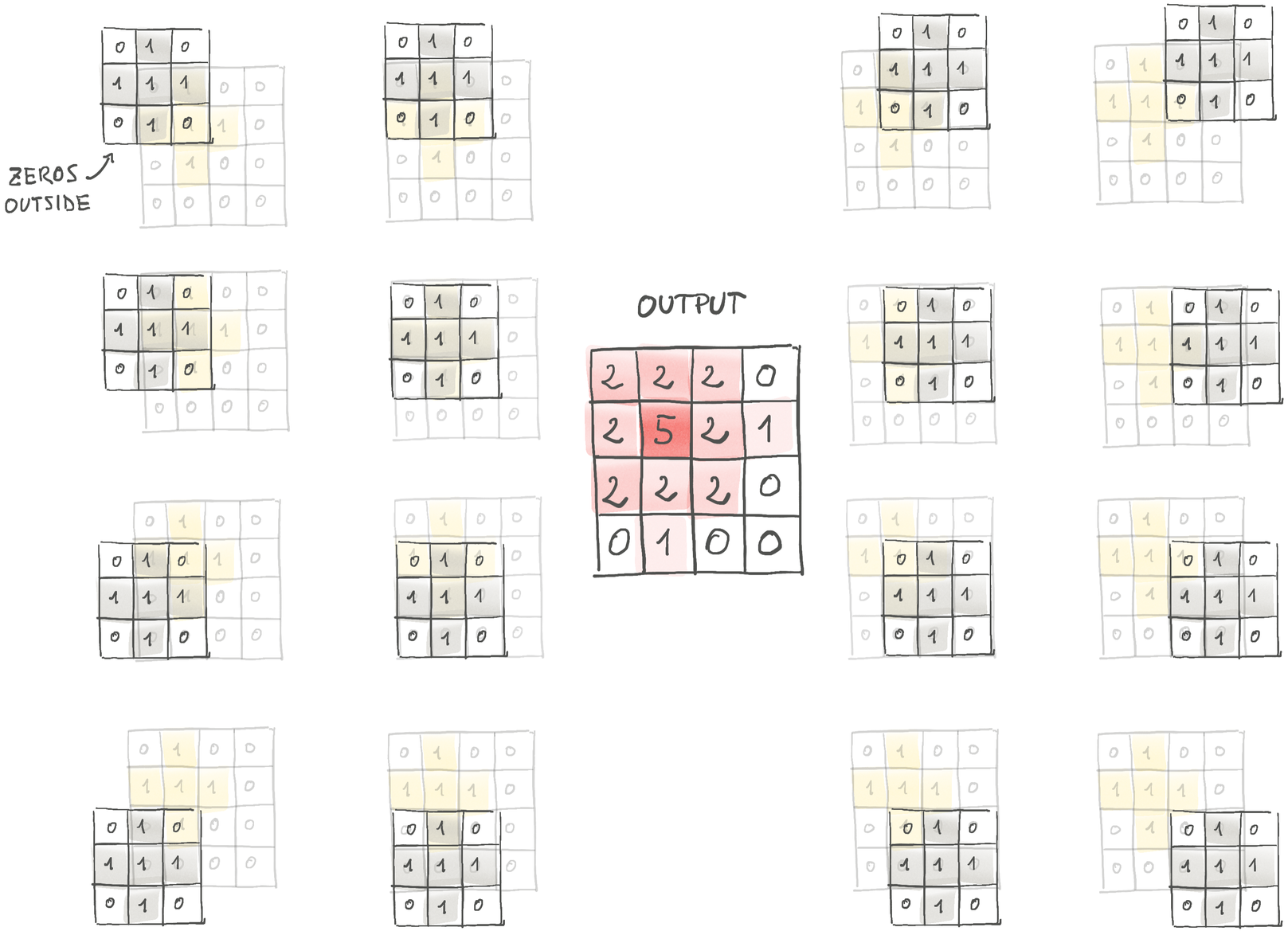


http://cs231n.github.io/convolutional-networks/

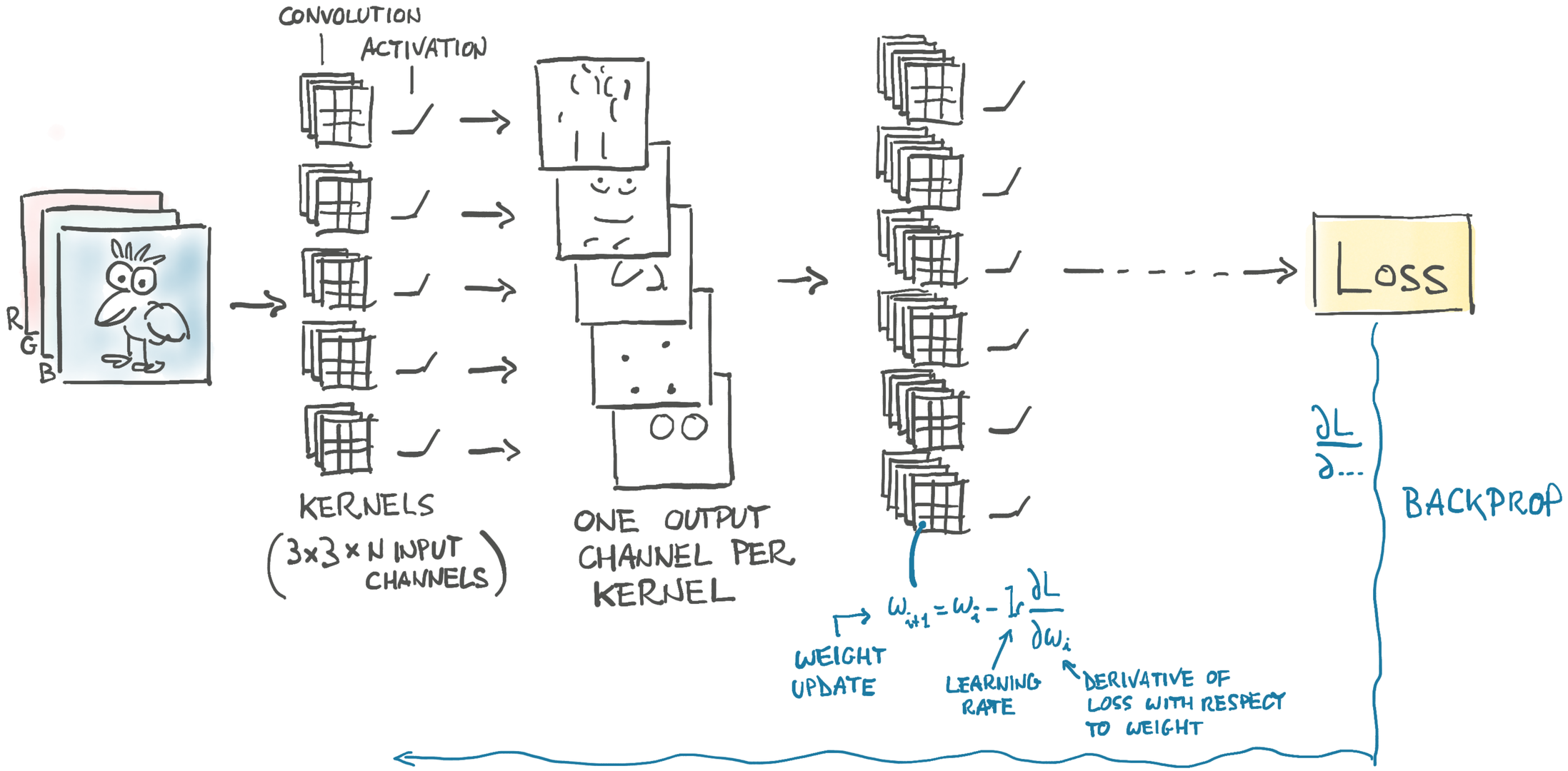
Convolution



Zero padding



Convolutional neural network



Playground

https://cs.stanford.edu/people/karpathy/convnetjs/