Deep Learning: Introduction

MLP, backpropagation, CNN

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Outline

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Perceptron : Basic principle

Motivation : Build a Bio-inspired parametric model, with possibly "high" complexity.

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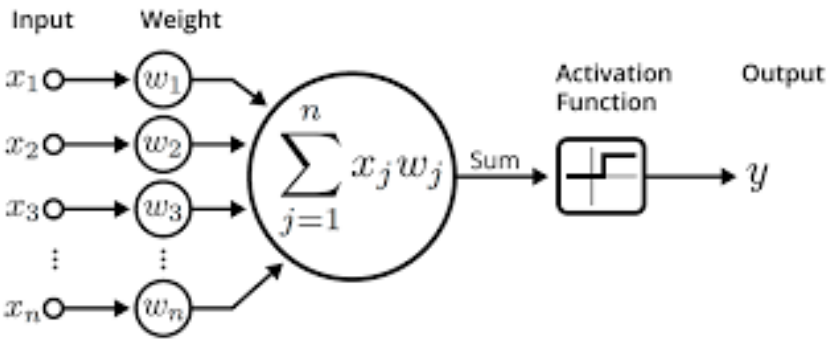

An illustration of an artificial neuron. Source: Becoming Human.

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- Hugely influential, esp. since the coming back of neural networks.
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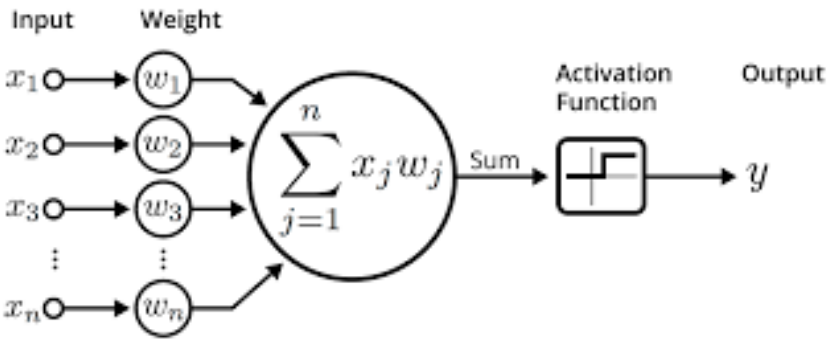

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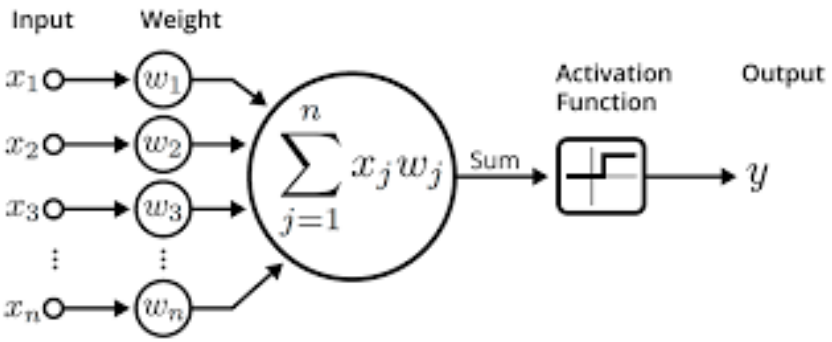

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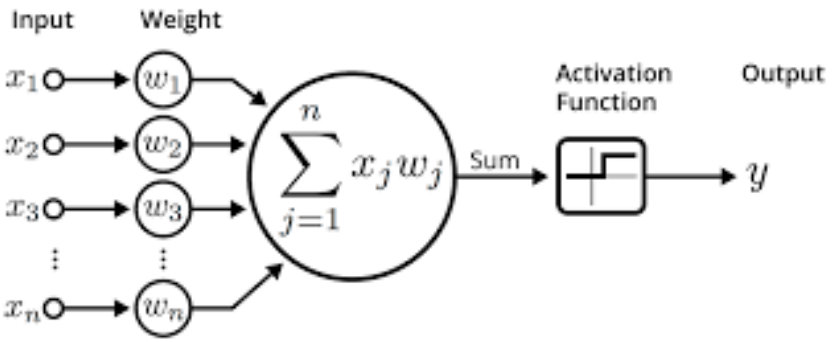

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$$a(x_i) = \sum_{j=1}^{d} w_j x_{ij} = w^\top x_i, \quad \hat{y}_i = f(x_i) = g(a(x_i))$$

This is just a linear model with an additional "activation" !

Remarks

- It is often convenient to introduce a bias to account for possible affine separating hyperplane : x is replaced by $[1, x_1, \ldots, x_p]$ and w by $[w_0, w_1, \ldots, w_d] \in \mathbb{R}^{d+1}$

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  - In order to predict the probability of x to be in a given class :

$$g(a(x)) = \frac{1}{1 + e^{a(x)}}$$

Sigmoidal, same expression than logistic function, but don't confuse loss function and activation function ! *We used max-likelihood for logistic regression. None of this here.*

Training the perceptron

As for other ML approaches, minimize the empirical risk, i.e. an averaged cost function : $\min_f \frac{1}{n} \sum_i L(f(x_i), y_i)$. This is done by using gradient descent.

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Originally, the perceptron is optimized by taking the examples one by one, which is similar to online learning (samples arrive in a stream) or Stochastic Gradient Descent (samples are taken randomly to decrease the computational cost). This is opposed to full-batch learning.

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  - if ν is too large : possible instability
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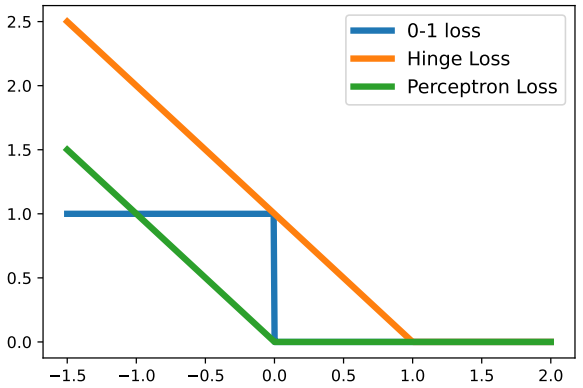
- ν is the learning rate. In practice, ν is often decreased when the risk is close to the minimum.
  - if ν is too large : possible instability
  - if ν is too small : slow convergence
- A full cycle on the training set is an epoch. Many epochs may be performed on the whole training set.

Historical example : binary classifier

- $g(a) = a$ and (almost) hinge loss
  $L(y, \hat{y}) = \max(0, -y\hat{y})$

$$\Rightarrow w_j \leftarrow \begin{cases} w_j & \text{if } y_i w^T x_i > 0 \\ w_j + \nu y_i x_{ij} & \text{if } y_i w^T x_i \leq 0 \end{cases}$$



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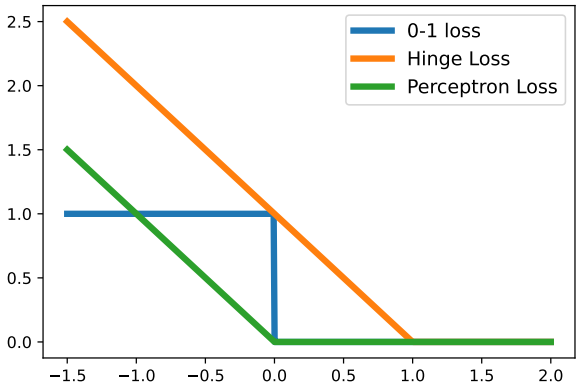

Albert Novikov theorem, 1962

Let $\mathcal{T} = \{(x^i, y^i), i = 1 \ldots, N\}$ be the training set. Let $D, \gamma \in \mathbb{R}^{+*}$, then

IF

- $\forall x_i \in \mathcal{T}, \|x_i\|^2 < D$ (← bounded support)
- $\exists u \in \mathbb{R}^{n+1}, \|u\|^2 = 1$ s.t. $\forall (x_i, y_i) \in \mathcal{T}, y^i u^T x^i \geq \gamma$ (← margin condition)

THEN the perceptron algorithm converges in less than $\left(\frac{D}{\gamma}\right)^2$ iterations.

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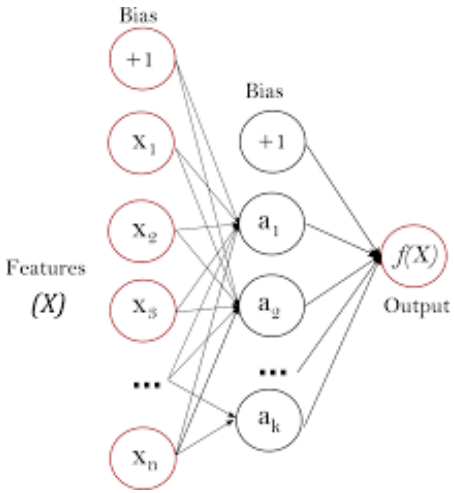
Single Hidden Layer Perceptron



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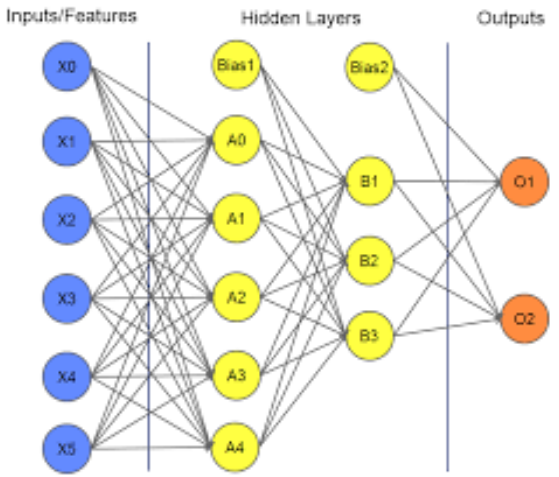

It can be represented graphically : each edge is a scalar product associated to a coefficient that must be estimated. A "fully connected" layer is just a matrix-vector multiplication.

Notations

w_{ij}^k : weight for node j in layer l_k for incoming node i
b_i^k : bias for node i in layer l_k
a_i^k : activation for node i in layer l_k
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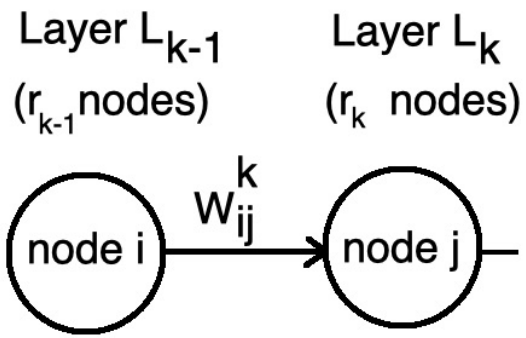

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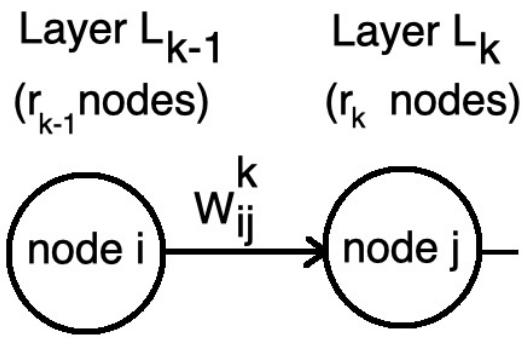

Then

- Input : $r_0 = p$ and $o_j^0 = x_{ij}$
- At layer $k = 1, \ldots, L$: $a_j^k = b_j^k + \sum_{i=1}^{r_{k-1}} w_{ij}^k o_i^{k-1}$ and $o_j^k = g(a_j^k)$
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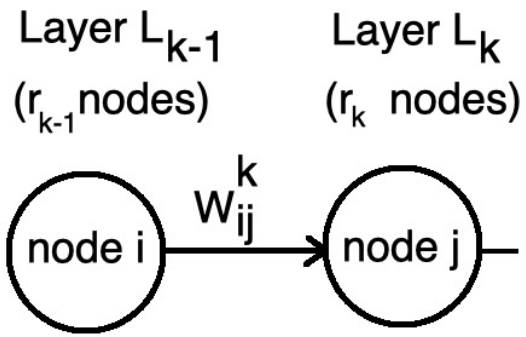

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- Output : $f(x_i)_j = g_o(a_j^L)$

In vectorial form, this is just $o^k = g(W^k o^{k-1} + b^k)$ where g is applied pointwise and $o^k, b^k \in \mathbb{R}^{r_k}$, $W^k \in \mathbb{R}^{r_{k-1} \times r_k}$.

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Gradient backpropagation algorithm

Recall that our goal is to minimize the empirical risk (or loss)

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We have :

$$\frac{\partial F(\theta)}{\partial \theta} = \frac{1}{n} \sum_\ell \frac{\partial}{\partial \theta} L(f_\theta(x_\ell), y_\ell), \quad \text{and} \quad \frac{\partial}{\partial \theta} = \left[\frac{\partial}{\partial w_{ij}^k} \right]_{ijk}$$

For each weight/parameter w_{ij}^k and sample x_ℓ, we need to evaluate $\frac{\partial E}{\partial w_{ij}^k}$ for $E = E_\ell = L(f_\theta(x_\ell), y_\ell)$. Rk : w include the bias here

Backprop

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For $k \geq 1$ we write

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We have easily $\frac{\partial o_j^k}{\partial a_j^k} = g'(a_j^k)$ (or g_o if $k = L$) and $\frac{\partial a_j^k}{\partial w_{ij}^k} = o_i^{k-1}$ ($= x_{\ell i}$ if $k = 1$), it remains the first term.

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If $k = L$

Taking $r_L = 1$ for simplicity, $E = L(\hat{y}_\ell, y_\ell) = L(o_1^L, y_\ell)$, so

$$\frac{\partial E}{\partial o_1^L} = L'(\hat{y}_\ell, y_\ell) \Rightarrow \delta_1^L = L'(\hat{y}_\ell, y_\ell) g_o'(a_1^L)$$

Only requires to know the prediction $\hat{y}_\ell$: a forward pass is required before a backward pass (that is, just applying the network on x_ℓ).

Backprop - cont'd

If $k < L$

We use the "total derivative rule" : given a multivariate function $F(f_1, \ldots, f_r)$ and r functions $f_1, \ldots, f_r$,

$$f(x) = F(f_1(x), \ldots, f_r(x)) \Rightarrow \frac{\partial f(x)}{\partial x} = \sum_i \frac{\partial F}{\partial f_i} \cdot f_i'(x)$$

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- δ_j^k can be computed if all the δ_i^{k+1} are known.
- Backpropagation : evaluate the gradients by decreasing order of layers $k = L, L-1, \ldots$ ("backward" propagation)

BACKPROPAGATION ALGO, Main equations

The gradients are given by

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  - $\delta_1^L = g_o'(a_1^L) L'(\hat{y}_\ell, y_\ell)$
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Note that if $L(\hat{y}_\ell, y_\ell)$ reach its minimum in $\hat{y}_\ell$ and $L'(\hat{y}_\ell, y_\ell) = 0$, then all the gradients are zero !

Then the gradient corresponding to b samples x_ℓ, y_ℓ are averaged (full batch $b = n$, online $b = 1$, SGD...), and a gradient step is performed

$$w_{ij}^k \leftarrow w_{ij}^k - \nu \left(\frac{1}{b} \sum_{\ell=1}^{b} \frac{\partial L(f_\theta(x_\ell), y_\ell)}{\partial w_{ij}^k} \right)$$

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Backprop today...

- is automatic in Pytorch and Tensorflow ! Just implement the forward pass using only Pytorch/Tensorflow operations and elements, then call `.backward()` (or equivalent)
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- The use of GPU is completely transparent. The practical sessions will be done on CPU, the code almost does not change for GPU.
- Can be applied to any functions ! (... that are composition of elementary operations). Consequences far beyond deep learning...

Pros and cons

- Empirical risk minimization for multilayer perceptron (or any deep net) is an ill-posed and ill-conditioned NON CONVEX problem.
- Hyperparameters (weights initialization values, learning rate, choice of $g()$, L, r_k...) all influence the result !
- To avoid saturation effects of node outputs (either to 0 or to 1), l_2 regularization (or other regularization) of $L(f(x), y)$ may be applied on θ.

Vanishing/exploding gradient problem

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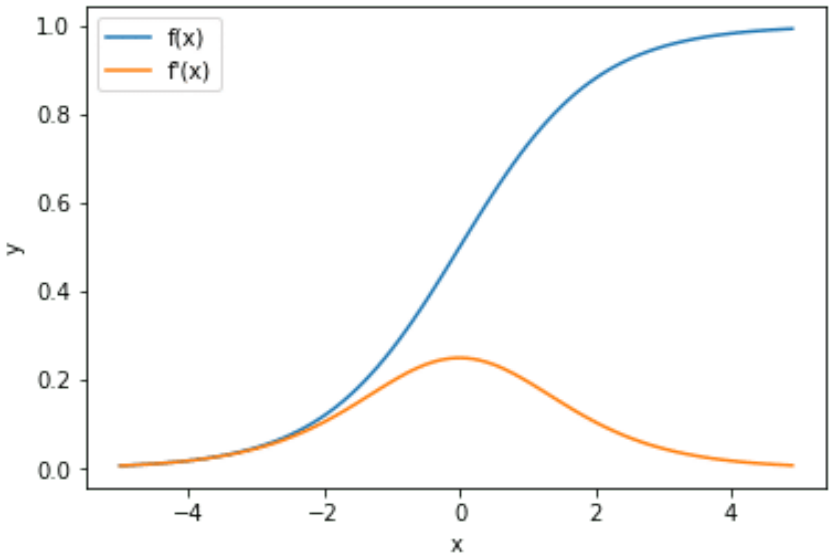
- Consider a 3-layers DNN with sigmoid activation. The chain rule leads to equation that look (roughly) like

$$\frac{\partial L}{\partial U} = \frac{\partial L_3}{\partial out_3}\frac{\partial out_3}{\partial h_3}\frac{\partial h_3}{\partial h_2}\frac{\partial h_2}{\partial h_1}\frac{\partial h_1}{\partial h_0}\frac{\partial h_0}{\partial U}$$

In this product of gradients, each involves to evaluate the gradient of a sigmoid function : may be very small (which occurs if the output is close to either 0 or 1), the product becomes exponentially small. Other activation function may lead to exploding gradients instead.



ResNets

- Important solution : **Residual Networks** (ResNet, He et al. 2015), which includes *skip connections* and fit the residual signal :

$$x^{\ell} = x^{\ell-1} + \mathcal{F}(x^{\ell-1})$$

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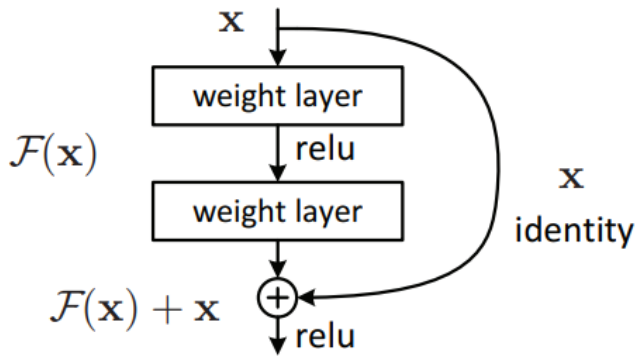
- All modern DNNs include skip connections. ResNets are still (!) state-of-the-art in several tasks



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Stochastic Gradient method

At each iteration, rather than computing

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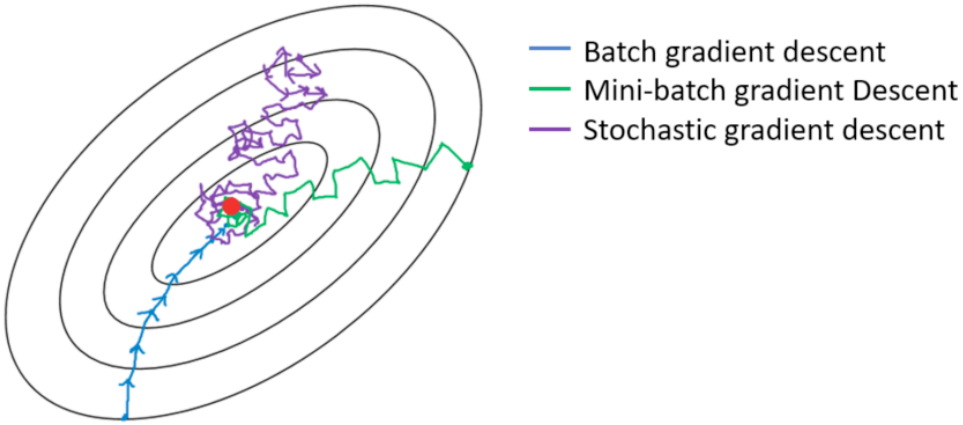
In a generalized case, at each iteration a mini-batch $\mathcal{B}$ that consists of indices for training data instances may be sampled at uniform with replacement.

$$\nabla E_\mathcal{B} = \frac{1}{|\mathcal{B}|} \sum_{\ell \in \mathcal{B}} \nabla E_\ell$$

update θ as

$$\theta := \theta - \nu \nabla E_\mathcal{B}$$



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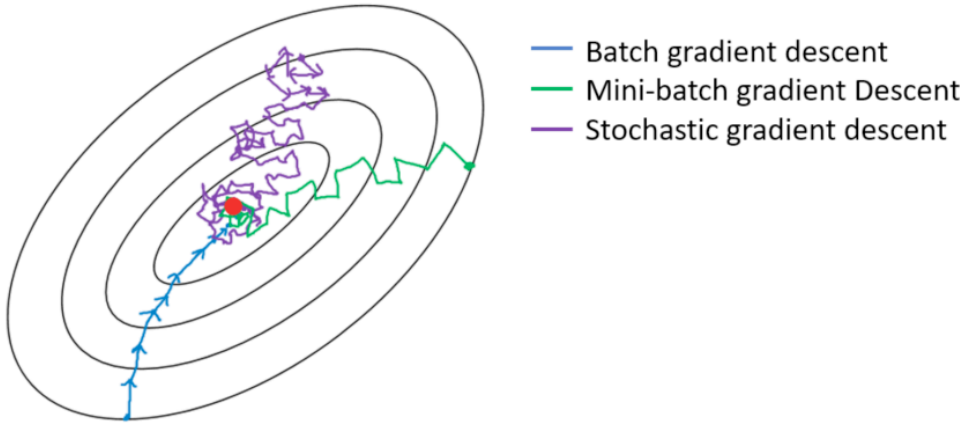

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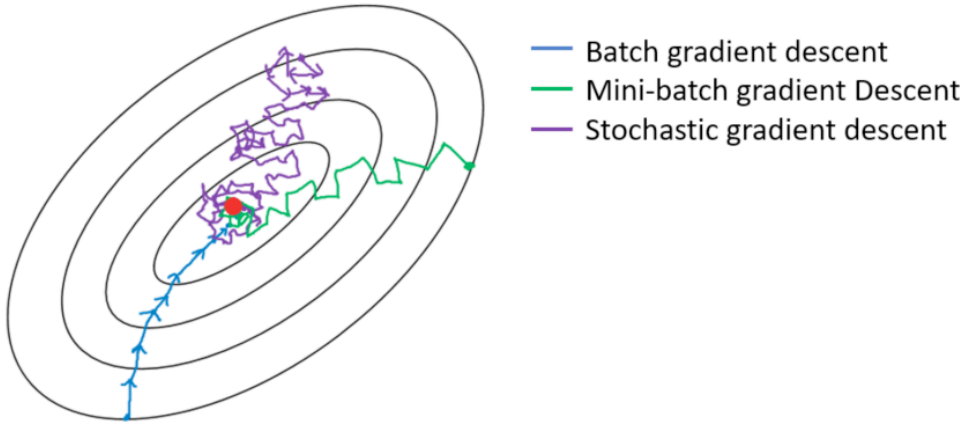

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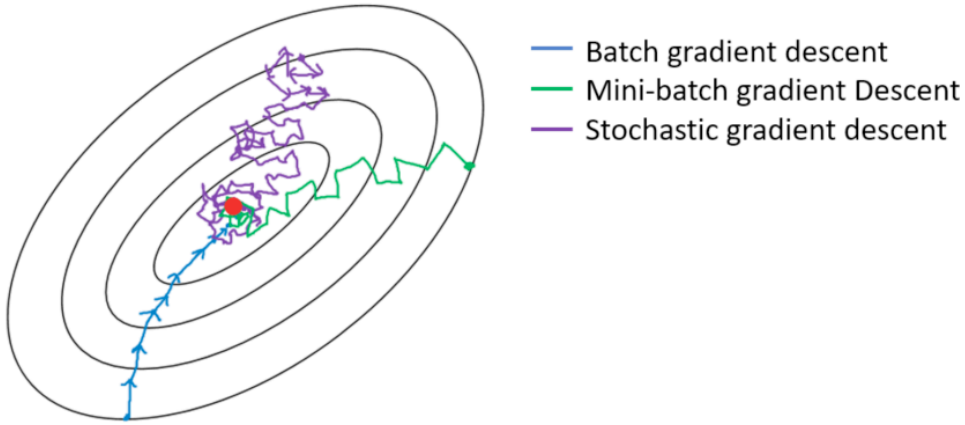

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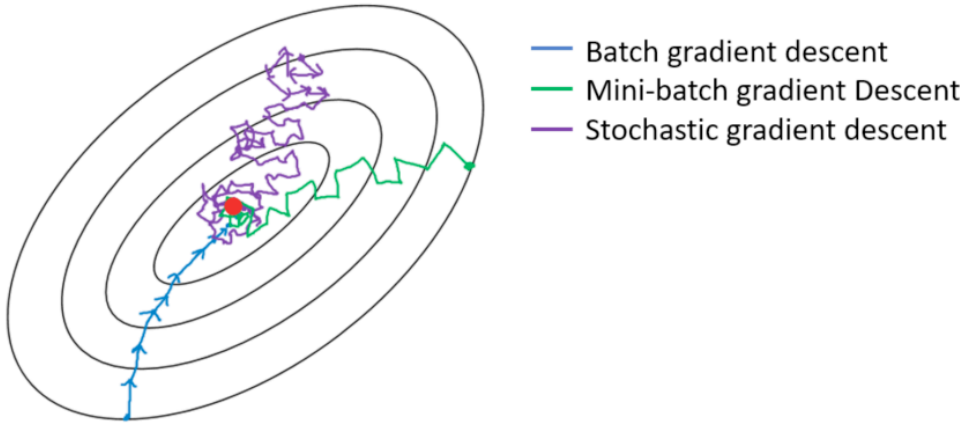

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- Globally, the batch size in an important hyperparameter, whose effects are not often predictable, and still only partially understood in theory.
- Many variants of SGD : with momentum, etc. Popular ones include Adam ("just use Adam"), RMSProp,...

Backprop in Practice

Y LeCun

- Use ReLU non-linearities
- Use cross-entropy loss for classification
- Use Stochastic Gradient Descent on minibatches
- Shuffle the training samples (← very important)
- Normalize the input variables (zero mean, unit variance)
- Schedule to decrease the learning rate
- Use a bit of L1 or L2 regularization on the weights (or a combination)
  - But it's best to turn it on after a couple of epochs
- Use "dropout" for regularization
- Lots more in [LeCun et al. "Efficient Backprop" 1998]
- Lots, lots more in "Neural Networks, Tricks of the Trade" (2012 edition) edited by G. Montavon, G. B. Orr, and K-R Müller (Springer)
- More recent: Deep Learning (MIT Press book in preparation)

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Brief insights into Convolutional Neural networks (CNN)

"Universal approximation theorem" (Cybenko 89, Hornik 89, Pinkus 99)

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- MLP totally ignore potentially existing structure in the data. This is essential : **deep learning is not automatic !**

CNN : historic origin

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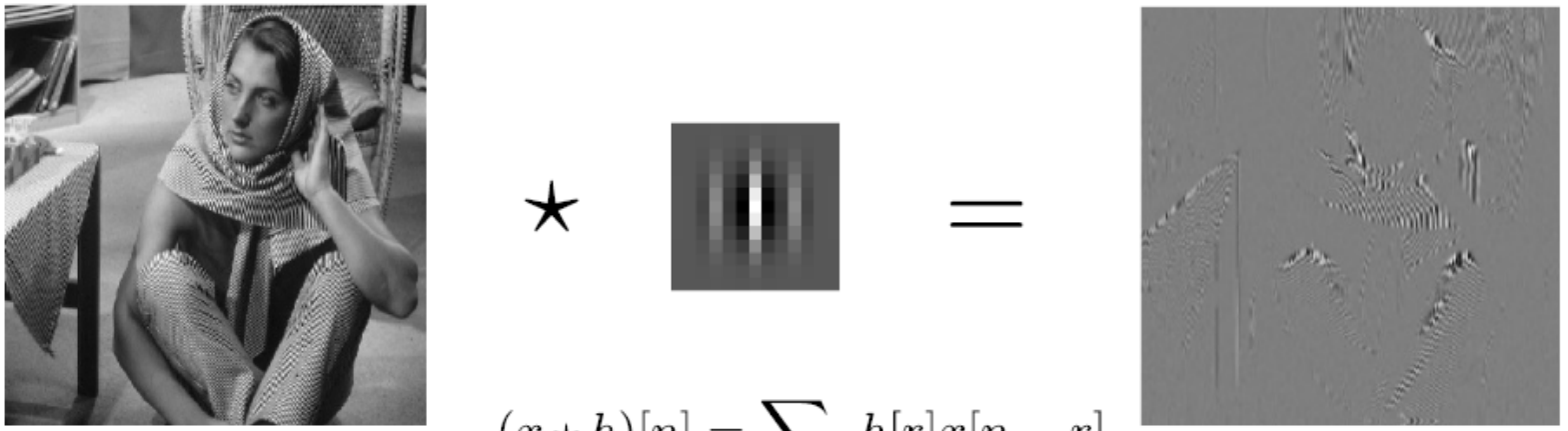

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$\star$

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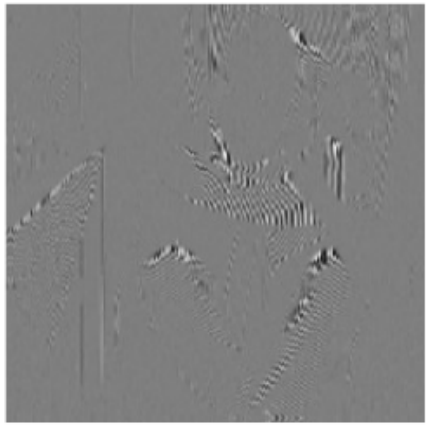

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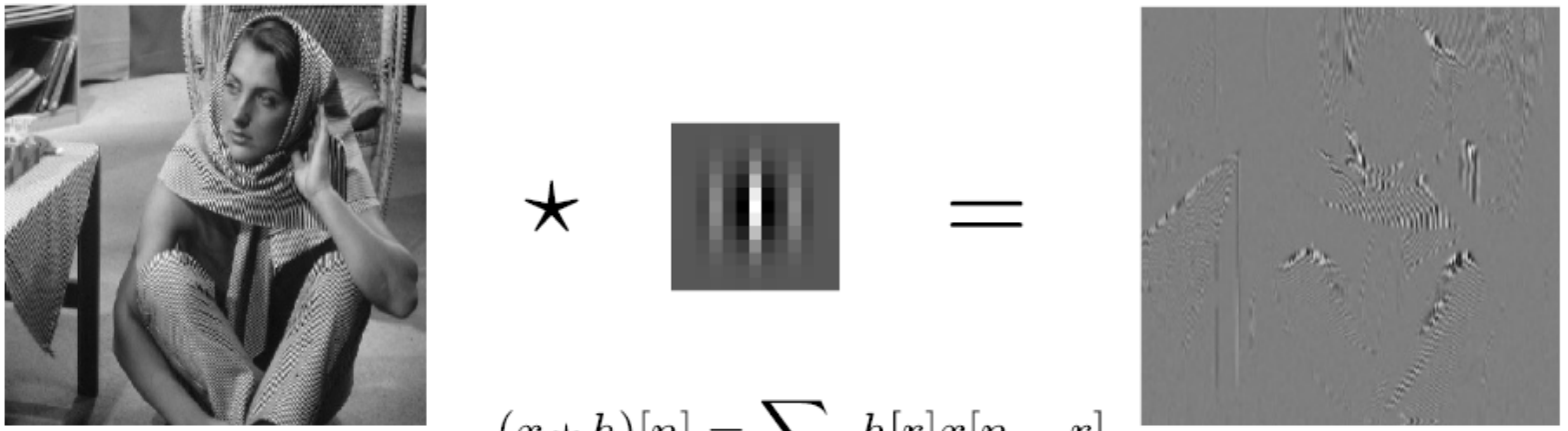

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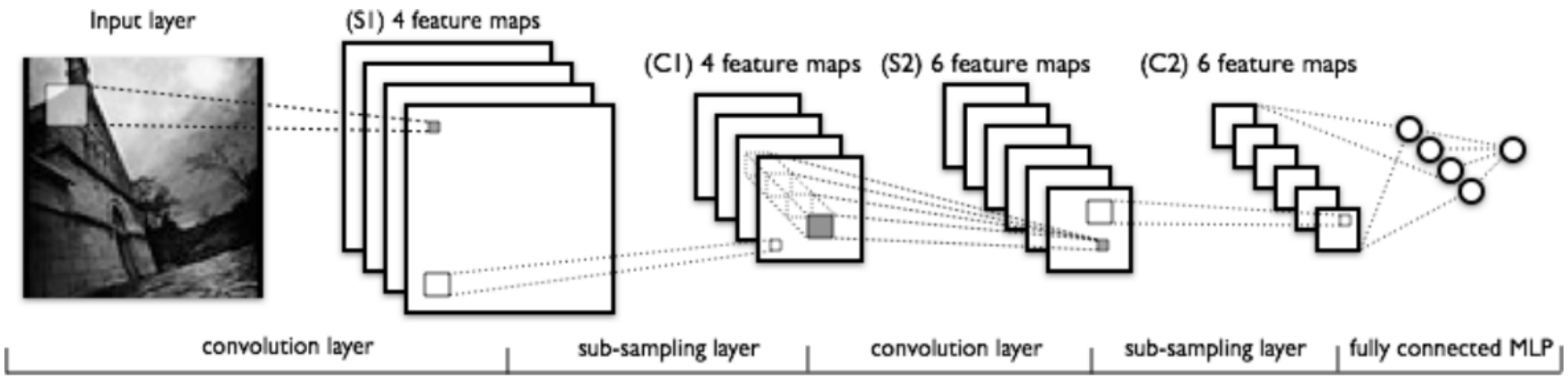
But :

- Impossible to try every pattern !
- Patterns have a hierarchical structure : small patterns are "combined" to make bigger objects, etc.

Ingredients of a CNN

- Convolution filters : the convolution kernels are learned (unlike wavelets)



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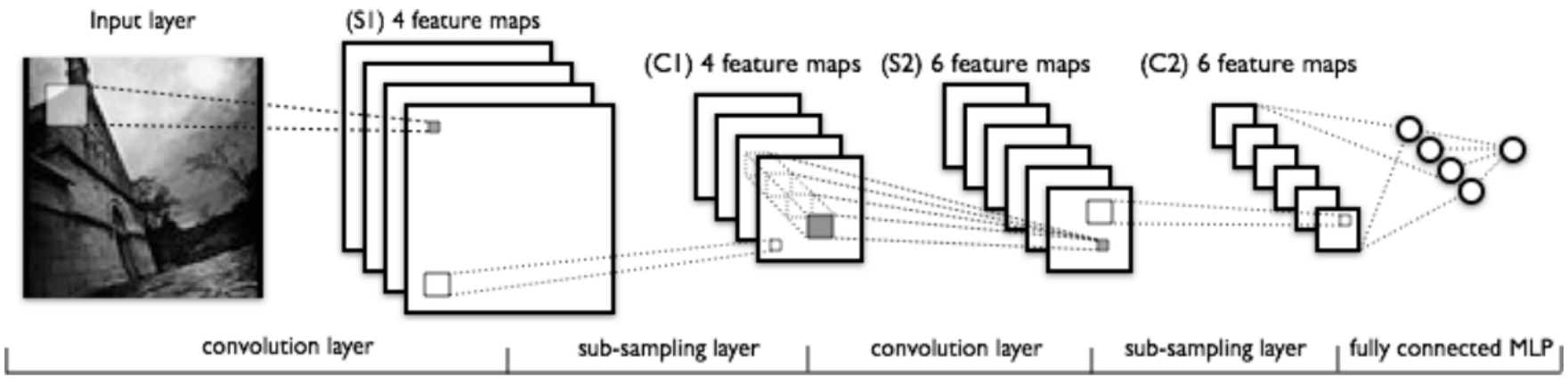

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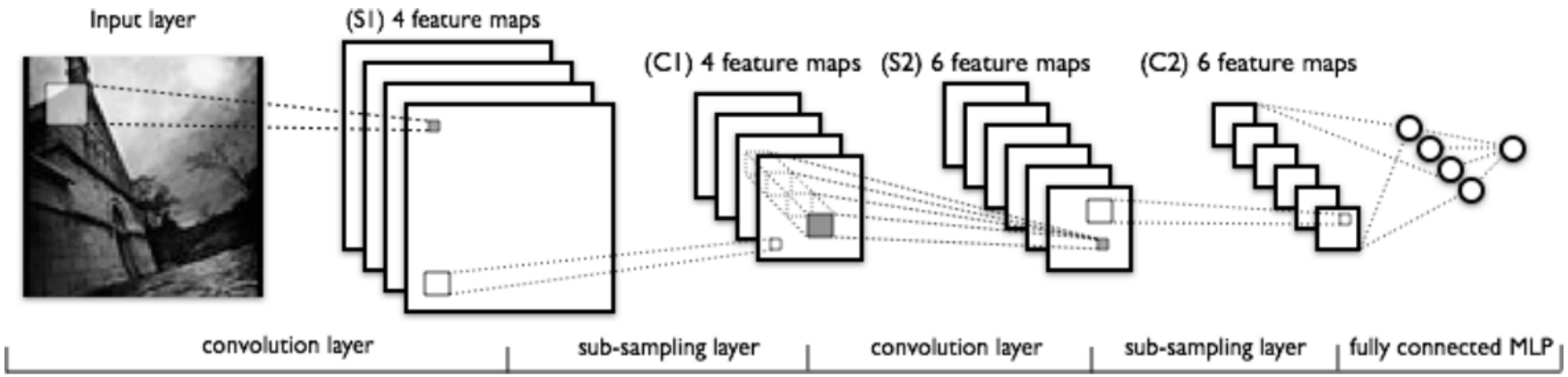

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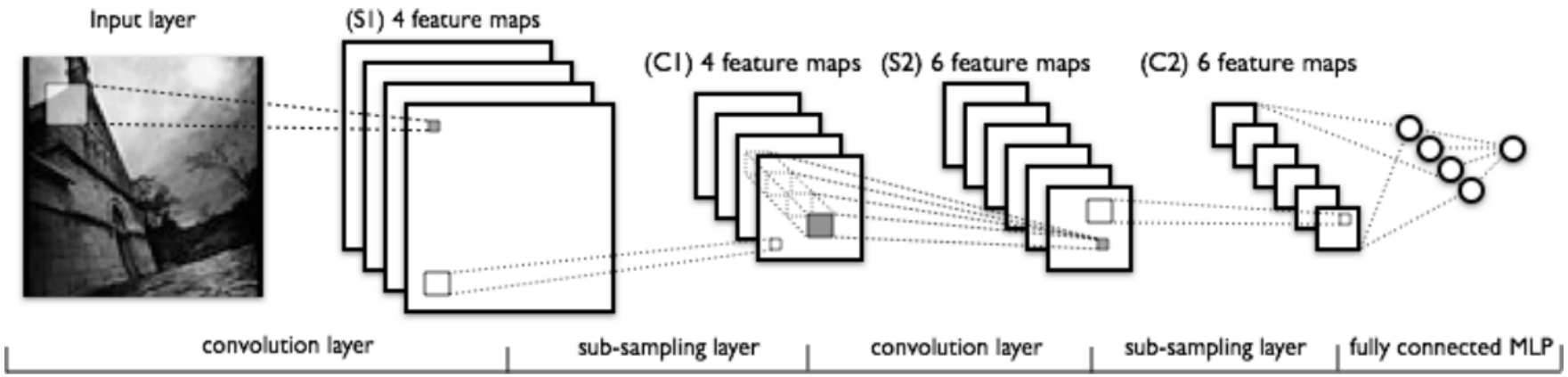
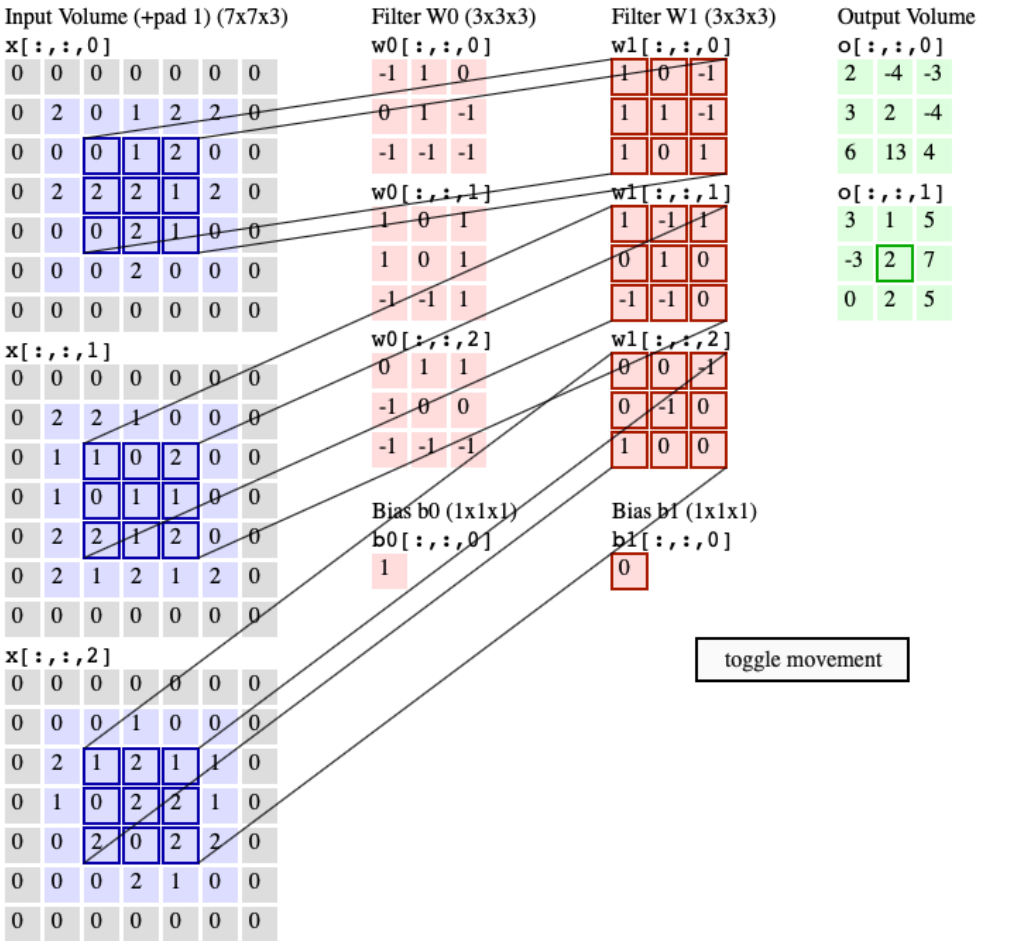


- Similar to an MLP, but with significant zeroed weights and weight-sharing (instead of dense parameter matrices, use block matrices with same, structured blocks)

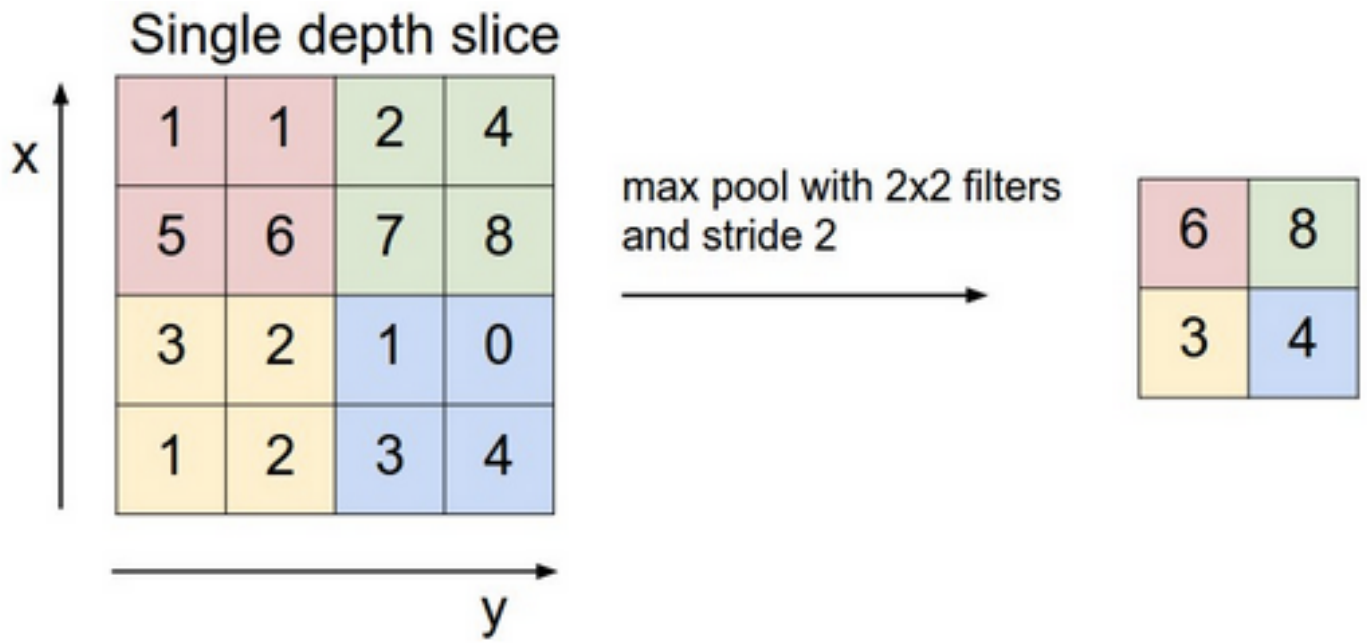
CNN Convolutive Layer example

RGB Channels Filter 1 Filter 2 Output Stack



Pooling / Downsampling within CNNs

Example : Max Pooling



- Only the locations on the image that shows the strongest correlation to each feature (the max value) are preserved, and those max values combine to form a lower-dimensional space
- Other examples : mean pooling, softmax...

CNNs : remark

- Depth is important to make the model hierarchical : it is impossible to enumerate all objects, but small patterns are combined to learn bigger objects

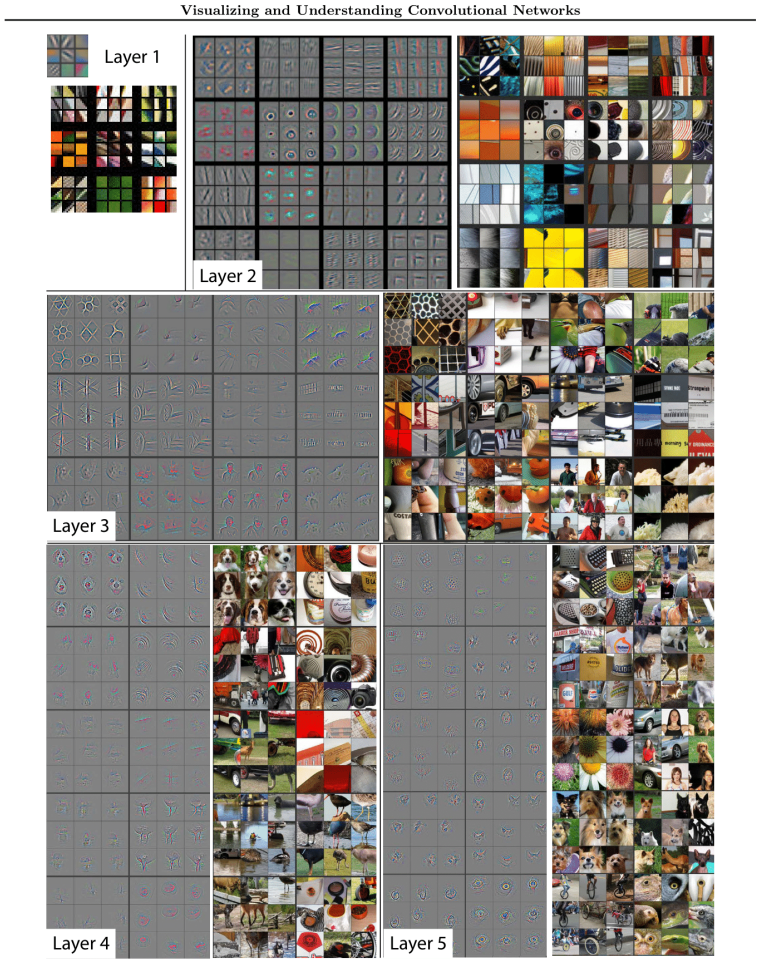
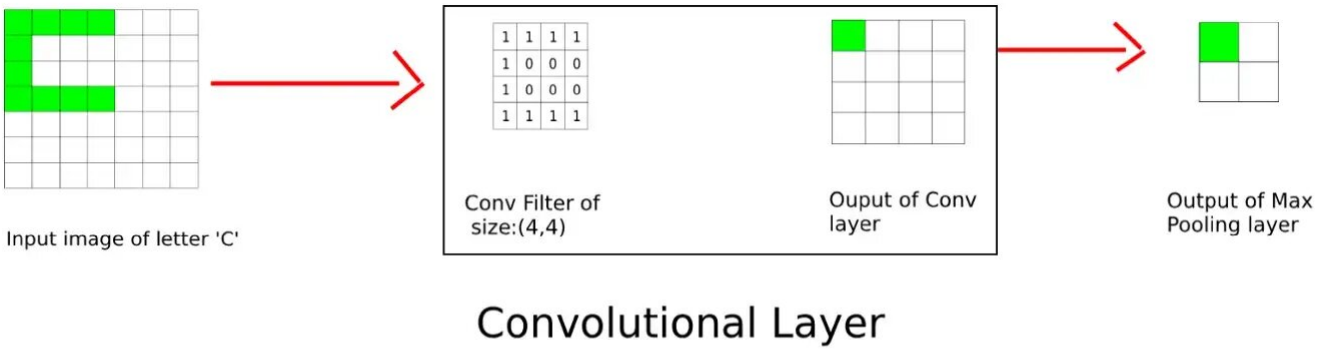
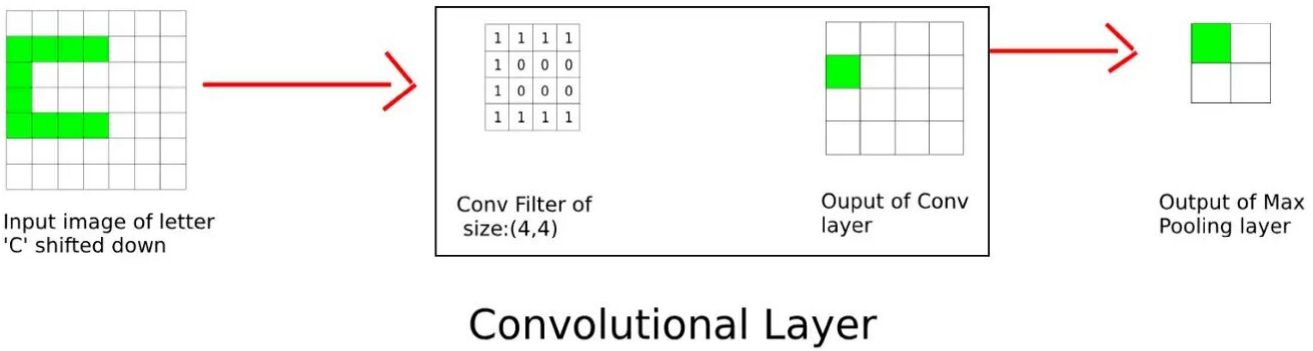


Figure 2. Visualization of features in a fully trained model. For layers 2-5 we show the top 9 activations in a random subset of feature maps across the validation data, projected down to pixel space using our deconvolutional network approach. Our reconstructions are *not* samples from the model: they are reconstructed patterns from the validation set that cause high activations in a given feature map. For each feature map we also show the corresponding image patches. Note: (i) the the strong grouping within each feature map, (ii) greater invariance at higher layers and (iii) exaggeration of discriminative parts of the image, e.g. eyes and noses of dogs (layer 4, row 1, cols 1). Best viewed in electronic form.

CNNs : remark

- Due to convolution+pooling, CNNs are (approximately) translation-invariant : moving the object around does not change the output $h(\tau(x)) = h(x)$.





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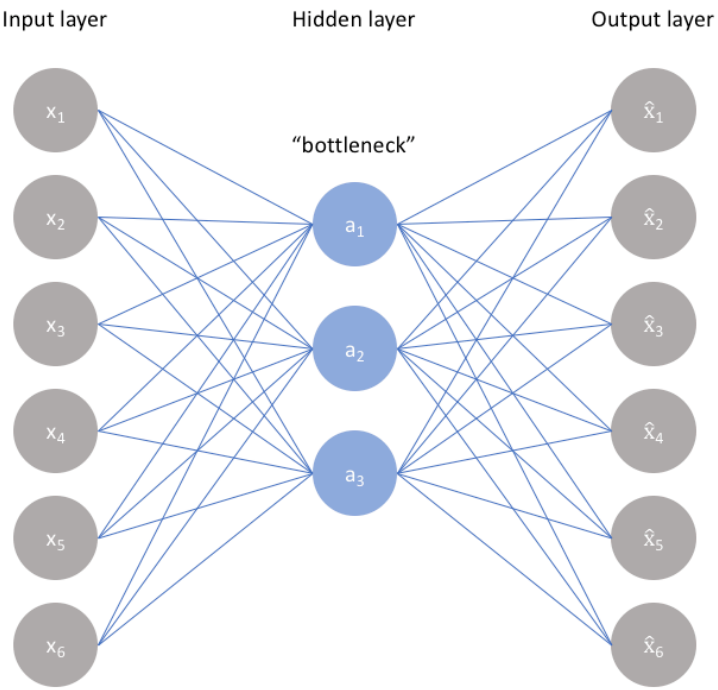
- Autoencoders are Unsupervised Neural Networks, designed for representation learning and/or dimension reduction
- Two parts : an encoder $f_\theta : x \to z$, and a decoder $g_\pi : z \to \tilde{x} \approx x$
- main idea : impose a bottleneck in the network to compressed knowledge representation of the input.

Rk : This assumes that the data are structured (like images !), otherwise such compression will be very difficult if not impossible without loosing much information.

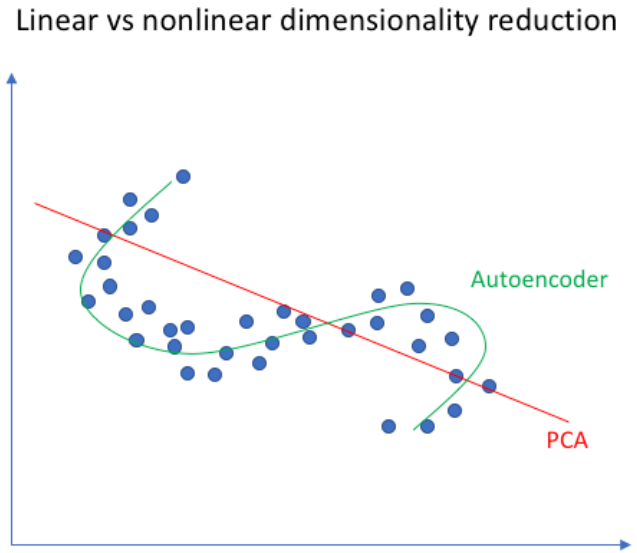


AutoEncoder principle

$\Rightarrow$ Formulate the problem as a supervised learning problem whose output is $\{x_\ell\}$

$\Rightarrow$ The empirical risk to minimize is thus $L(f(x), x)$: the bottleneck plays a key role (otherwise the network simply passes the values to the output.)

$\Rightarrow$ if linear activation function were used, that would perform PCA like dimension reduction

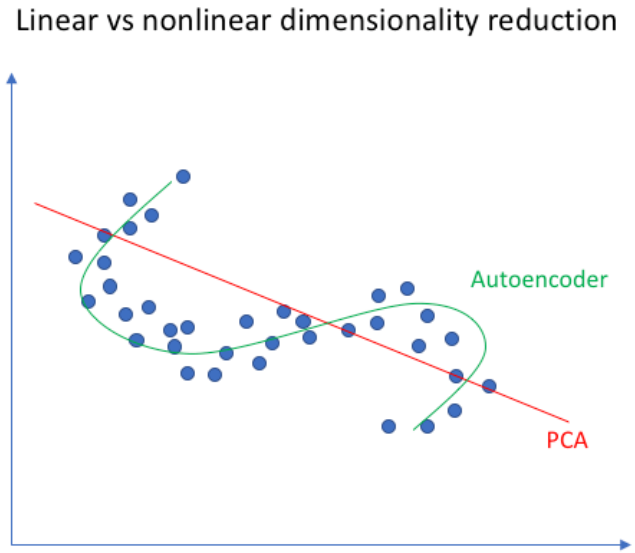


AutoEncoder principle

$\Rightarrow$ Formulate the problem as a supervised learning problem whose output is $\{x_\ell\}$

$\Rightarrow$ The empirical risk to minimize is thus $L(f(x), x)$: the bottleneck plays a key role (otherwise the network simply passes the values to the output.)

$\Rightarrow$ if linear activation function were used, that would perform PCA like dimension reduction

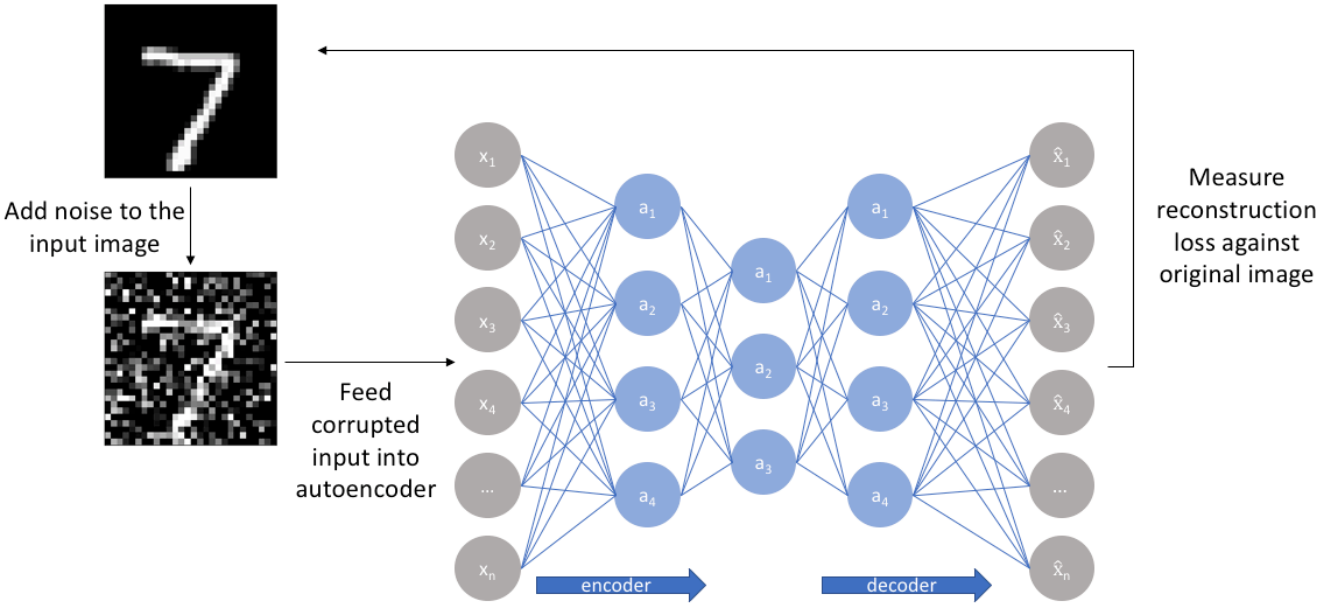


The AutoEncoder must be :

- sensitive enough to the inputs, to built an accurate reconstruction
- insensitive enough to the inputs to avoid overfitting

This requires to regularize the loss function of the form $L(f(x), x) + \textit{regularization}$

Example of application : AE for denoising



The low-dimensional representation has a regularizing effect (like wavelet thresholding).

Sparse AE

How many nodes ?

- If too many nodes, the AE may be capable of learning a way to simply memorize the data.

Sparse AE

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- If too many nodes, the AE may be capable of learning a way to simply memorize the data.

- Taking inspiration from ℓ_1 sparse regularization (like LASSO) : keep the number of nodes in hidden layers quite large, but regularize the loss function by penalizing activations within a layer. For layer k :

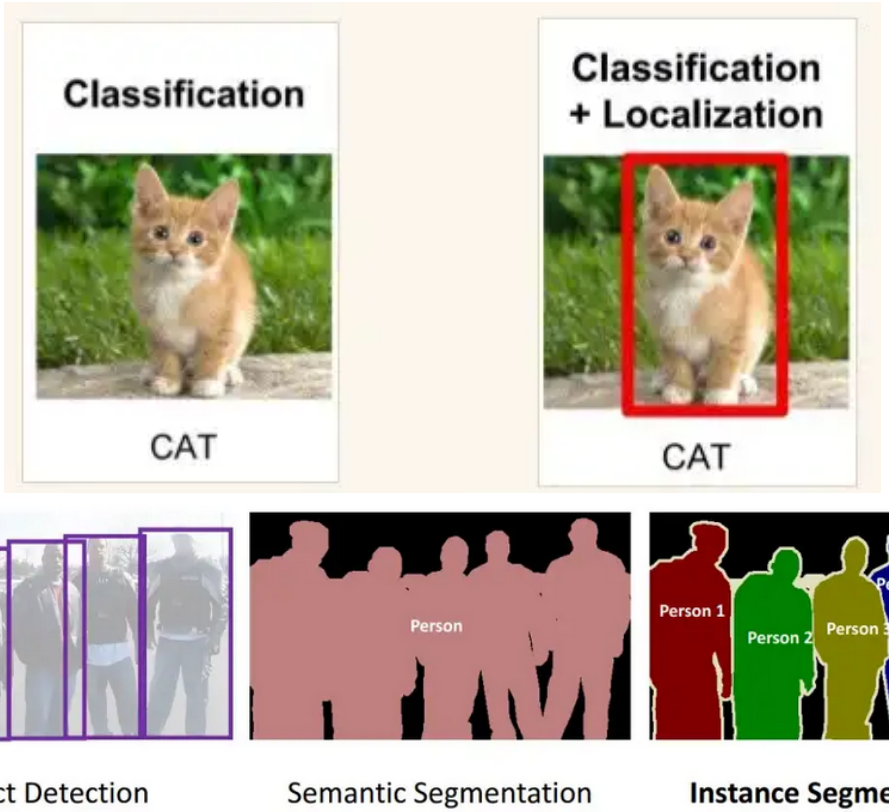
$$L(f(x), x) + \lambda \sum_{j=1}^{r_k} |o_j^k|$$

Table of Contents

U-Net

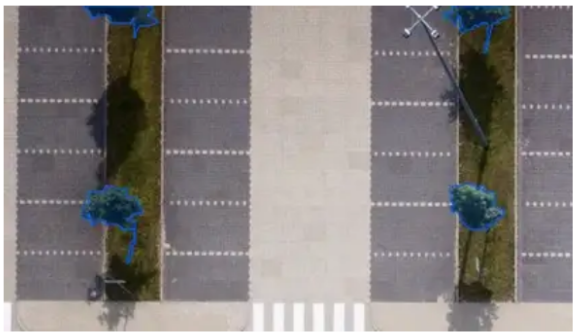
https://towardsdatascience.com/understanding-semantic-segmentation-with-unet-6be4f42d4b47

- U-Net is a popular architecture for image-to-image tasks such as localization, segmentation...

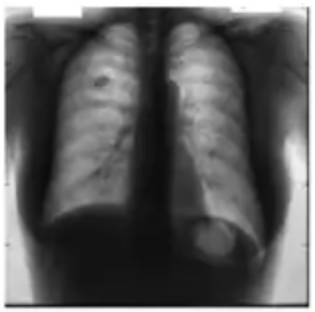


Why U-net ?

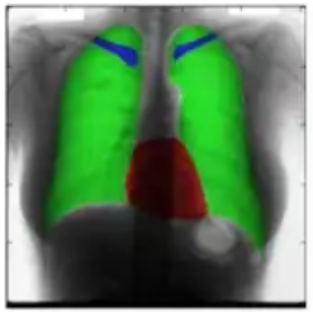
- Why not CNNs ?



Source: https://blog.playment.io/semantic-segmentation/



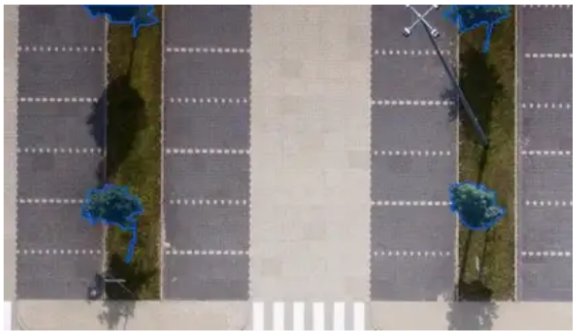
Input Image



Segmented Image

Why U-net ?

- Why not CNNs ? They include pooling



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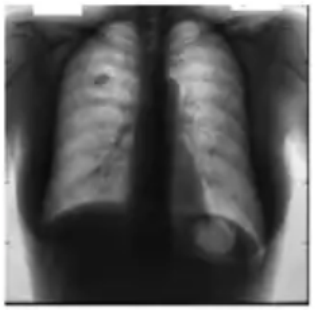

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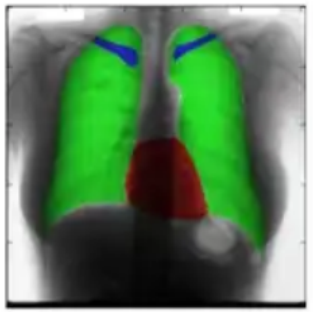

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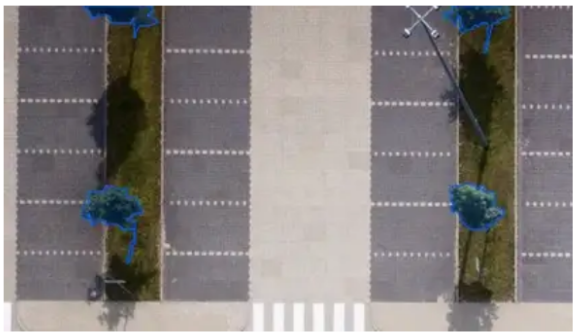
- Why not CNNs ? They include pooling
- Why not regular AE ?



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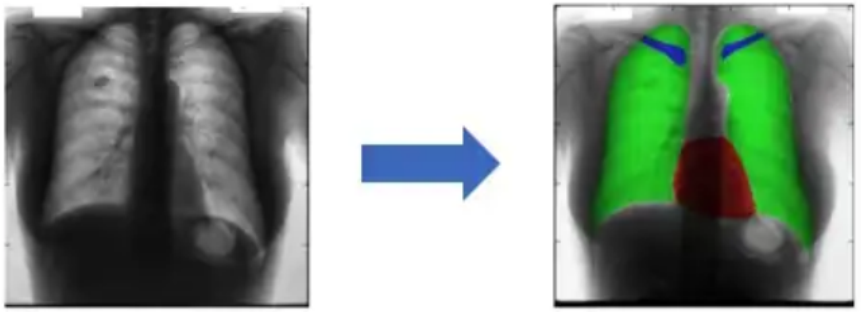

Why U-net ?

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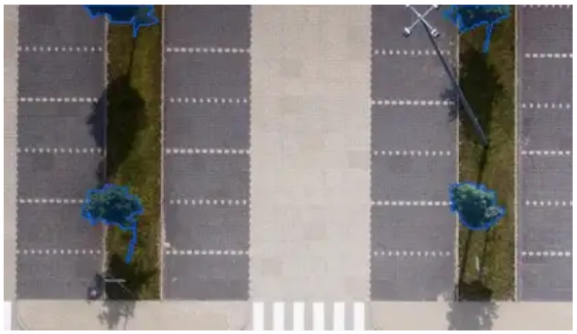

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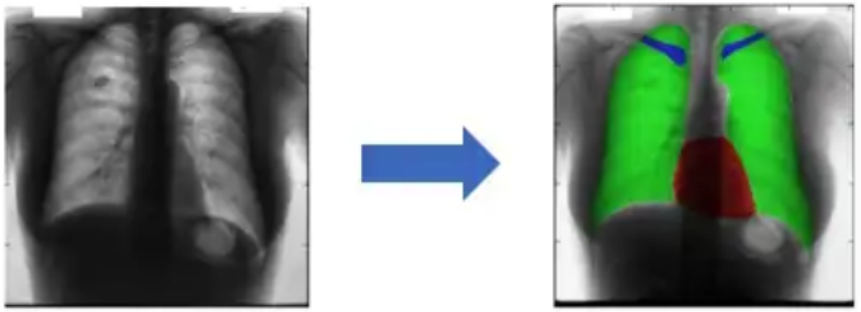
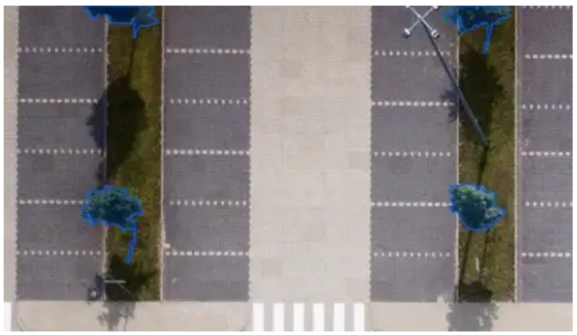


Why U-net ?

- Why not CNNs ? They include pooling
- Why not regular AE ? They are made to reconstruct the same image, and do not detect and localize high-level structure
- "Combine" the two ? U-Net



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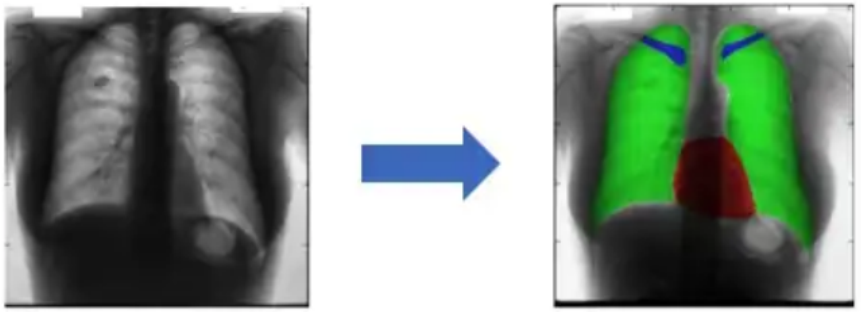

- The pooling is important to detect WHAT is in the image, but loses WHERE it is since the resolution is crushed
- There are ways to upscale and restore the resolution (similar to AE), but the WHERE information is still lost

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At each scale, the output of the corresponding encoder layer is simply concatenated to the output of the corresponding decoder layer, before being passed to the next decoder layer. *Disarmingly simple !*

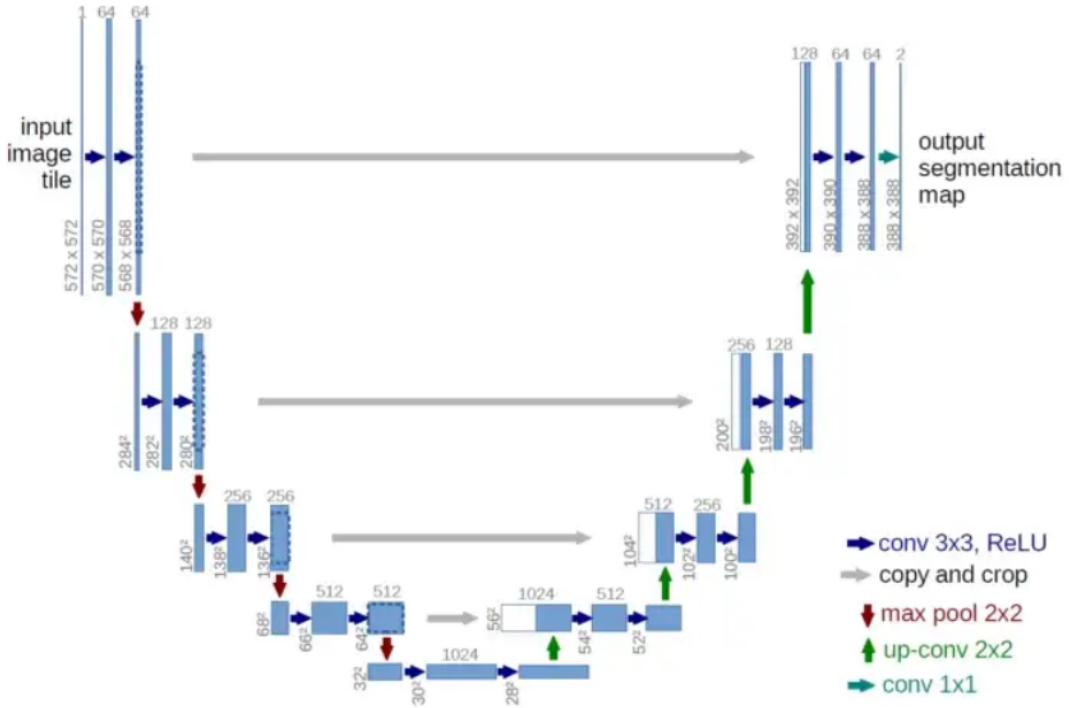

Fig. 1. U-net architecture (example for 32x32 pixels in the lowest resolution). Each blue box corresponds to a multi-channel feature map. The number of channels is denoted on top of the box. The x-y-size is provided at the lower left edge of the box. White boxes represent copied feature maps. The arrows denote the different operations.