

Deep Learning 101

Flatiron Wide Algorithms and Mathematics (FWAM!)

Gabriella Contardo (Flatiron Institute, Center for Computational Astrophysics)
gcontardo@flatironinstitute.org

Outline of tutorial part I

- Machine learning principles
- What is *deep learning*?
- Neural networks:
 - Components
 - Training
 - Fully Connected / Multi-Layer Perceptron (MLP)
 - Convolutional neural networks

A bit of definitions

Machine Learning (ML) :

- Relying on data analysis to automate model building to perform certain tasks.
- Model learns from data, extracts patterns, and makes some ‘prediction’
- Learning can be **supervised**, **unsupervised**, or **semi-supervised**.
- Various type of models: SVM, Random Forest, KNN, neural networks....

Deep Learning :

- Subgroup of ML based on artificial neural networks
- Strongly rely on “pattern” extraction and representation learning
- Very good ability to approximate complex functions + generalize
- Needs (lots of) (labeled) data

Some Machine Learning principles

3 main “components”:

- Data
- Machine or model
- Criterion (learning and evaluation)

Goal : Automatically extract relevant information from the data that *generalize* well to infer on new data (‘test’ data from similar distribution, but different from training examples)

Learn a model on training data to optimize some criterion, select the best on validation data, then infer on test data.

Supervised Learning

Training data is composed of

- Examples (“inputs”)
- ‘Targets’ --or label(s)-- (i.e outputs) for each example.

E.g. image classification.

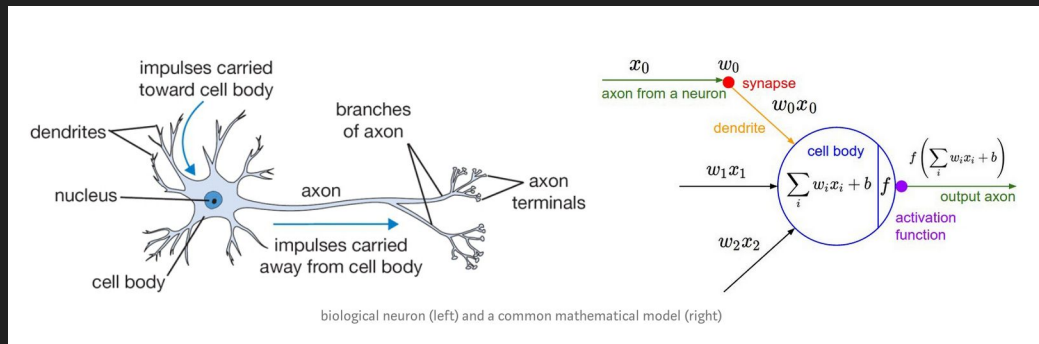
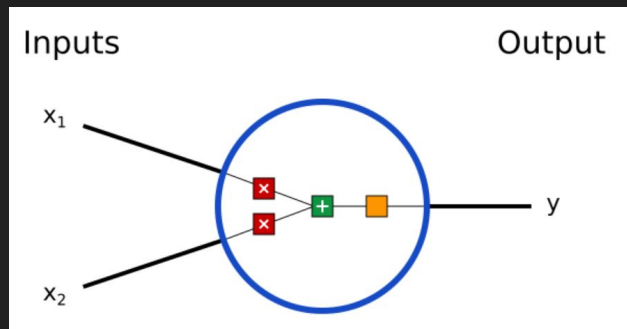
Different type of targets => different learning problem:

- Limited set of values, categorical : classification (multi-class, multi-label,...)
- Continuous values : regression
- Other type e.g. noisy targets, weak supervision etc.

Goal: Find an approximation of the labeling process.

What are neural networks?

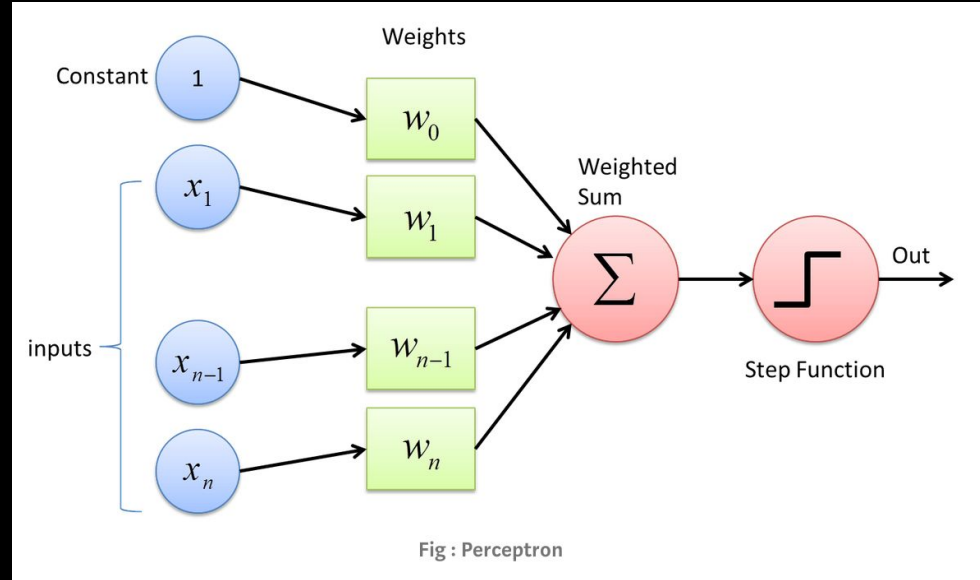
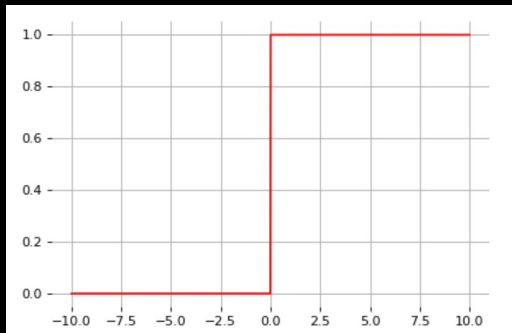
- Non-linear, highly parametric, functions' approximators
- Loosely inspired from brain : network of interconnected neurons that “activate” or not.
- Composition of stacked ‘*layers*’ of weights (parameters) producing *neurons*.



Let's start with a very simple one: Perceptron

- Like linear regression: $\sum_i w_i x_i$
- But with an additional **activation function**

Here : “step” function, threshold to obtain binary outputs.



'Vanilla' Neural Networks : Multi Layer Perceptron (MLP)

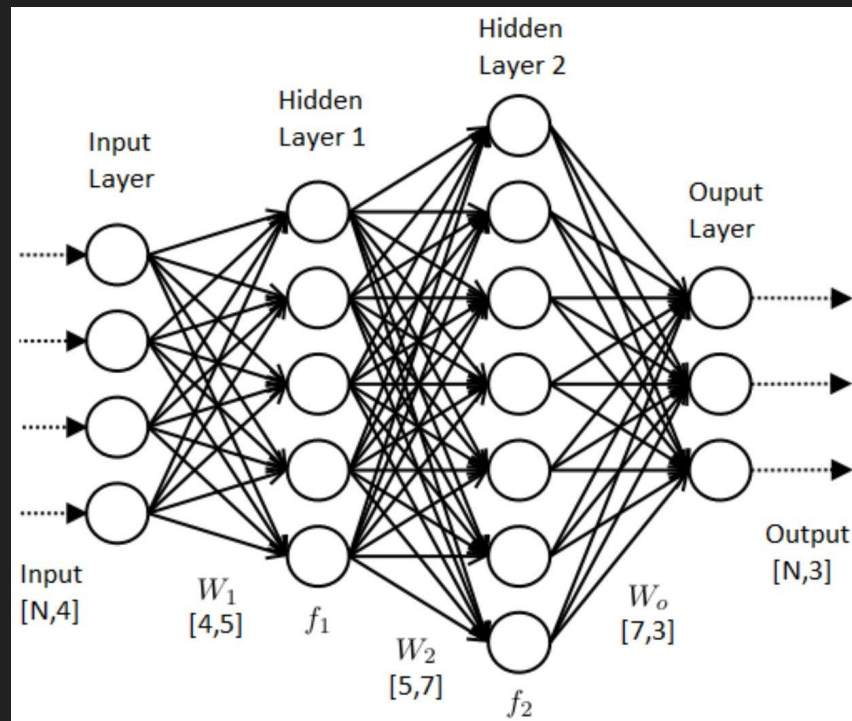
- Also called '**fully-connected**' **feed-forward** neural networks.
- Stack 'perceptron' on several *layers*.
- Composition of functions:

$$\begin{aligned} out &= \sigma(W_H * l_{H-1} + b_H) \\ l_h &= \sigma(W_h * l_{h-1} + b_h) \\ out &= \sigma(W_H * \sigma(W_{H-1} * \sigma(\dots \sigma(W_1 * \\ input + b_1) + \dots) + b_{H-1}) + b_H) \end{aligned}$$

- Each *hidden layer* has a *latent size* (output size)

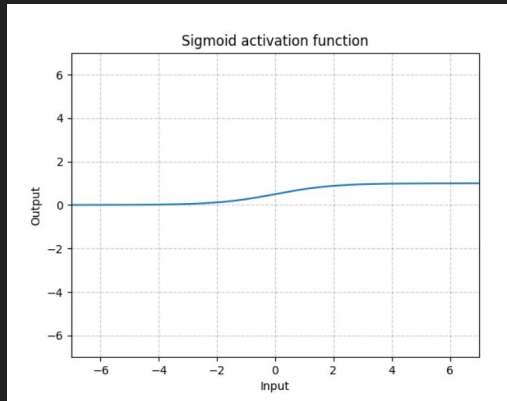
Glossary:

- Input nodes, Output nodes
- Connections / weights
- Activation function
- Hidden layers

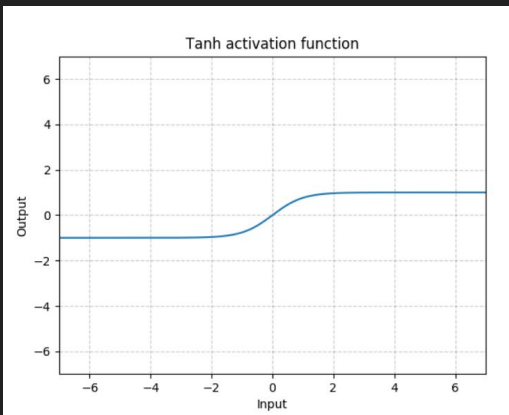


(Some) Activation Functions:

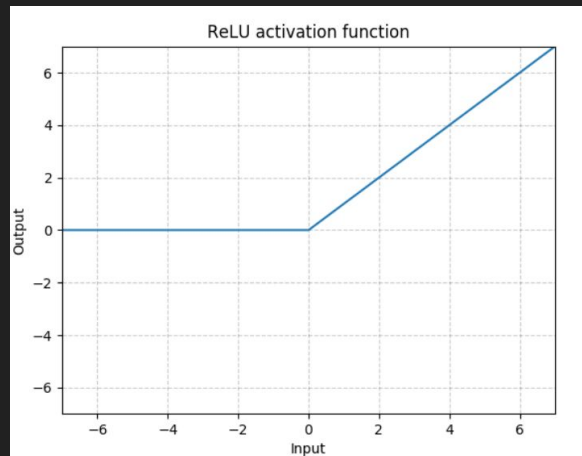
- Sigmoid:



- Tanh



- Rectified Linear Unit (ReLU) / LeakyReLU:



- Softmax : all neurons in $[0,1]$ and sum to 1 (good for probability distribution).

Training : Finding the “best” weights (= parameters)

Remember that ‘cost’ function (criterion) ?

=> Goal is to minimize that

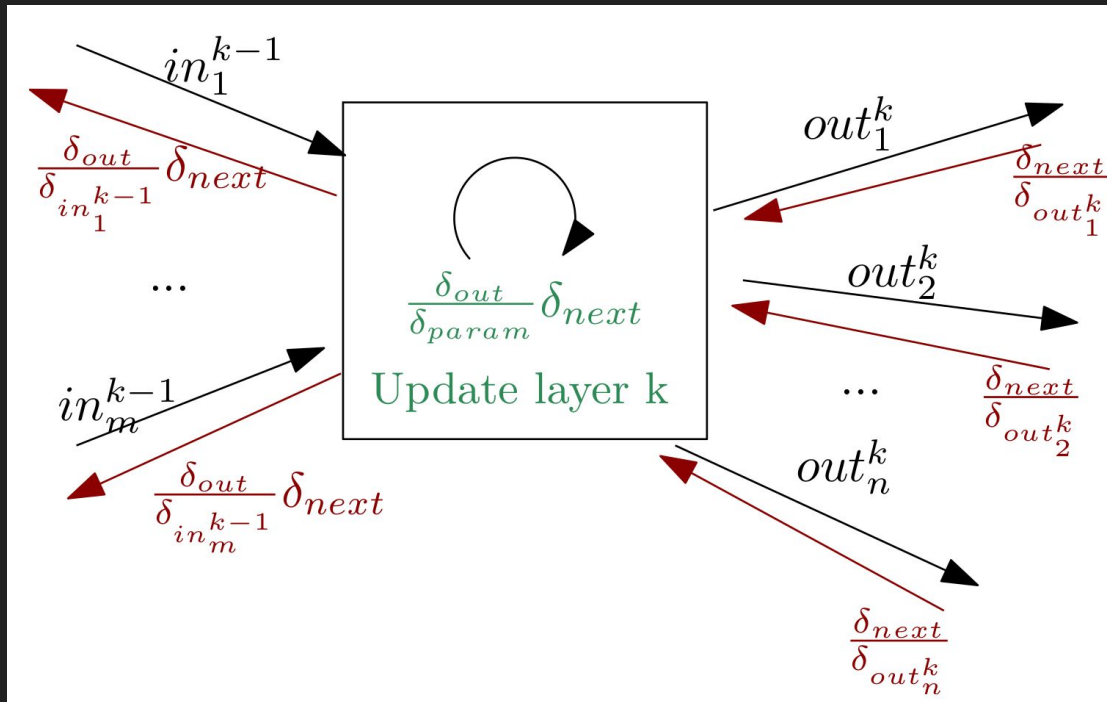
How ? Using gradient descent and backpropagation of the gradients !

Learning algorithm

- “Forward pass”: Feed an example (or more) to the network
- Compute error with regard to your criterion (compared to expected targets)
- Compute gradients
- Update weights
- Repeat until stopping criterion

Backpropagation ?

- Goal of gradient : update the weights in the “right” direction
 - Which weight is responsible for the error and on what ‘amount’ ?
- Backpropagation relies on the chain rules to compute the gradients of a layer’s weight using the delta’s of next layer.
- Pytorch / Tensorflow : auto-diff

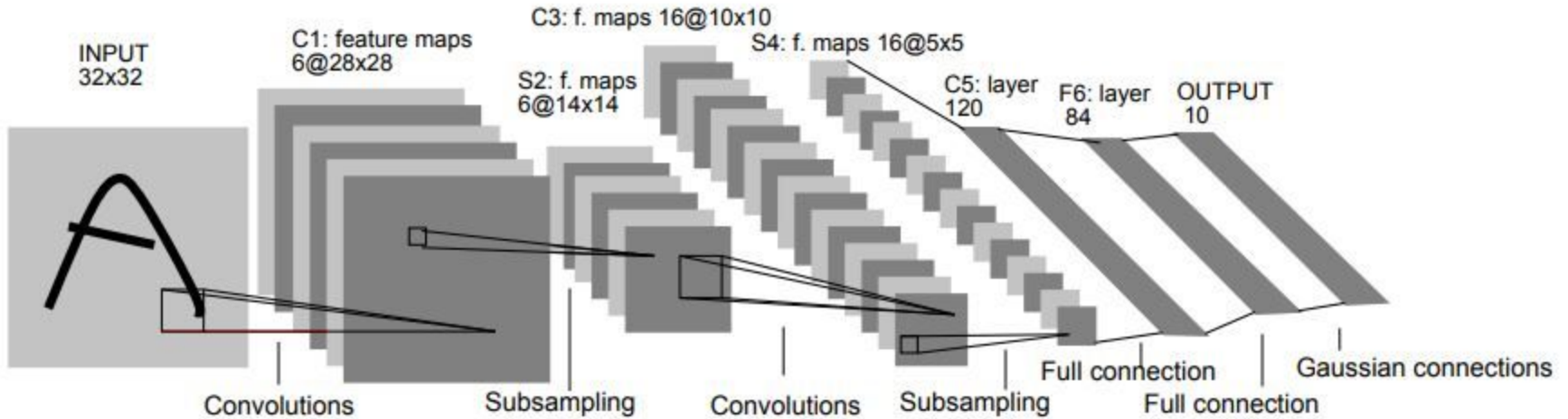


Different Losses

- Regression :
 - Mean-square error (MSE)
 - (Smooth) L1-Loss
- Classification :
 - Negative Log-Likelihood
 - Cross-Entropy
- And many others defined for specific problems e.g. semi supervised embeddings, generative methods, etc.
- + add some regularization constraint on the parameters of the network

<https://playground.tensorflow.org/>

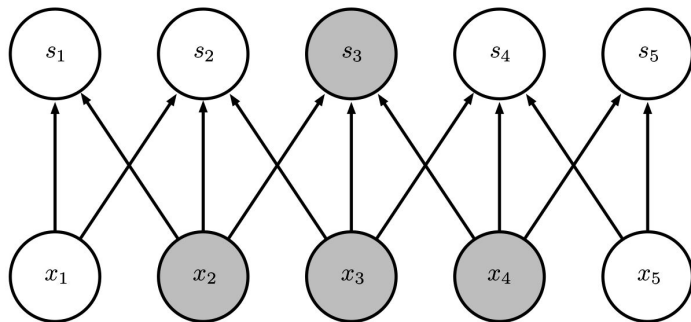
Convolutional Neural Networks



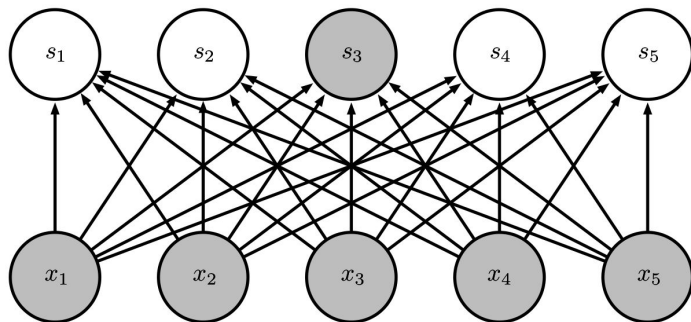
Convolutional Neural Networks

- Use local connections instead of fully-connected

Sparse
connections
due to small
convolution
kernel



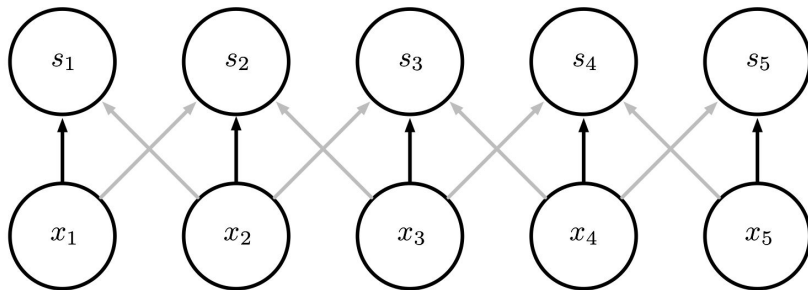
Dense
connections



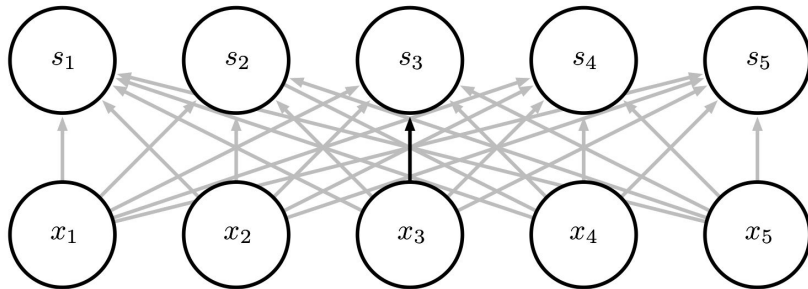
Convolutional Neural Networks

- Share weights (parameters)

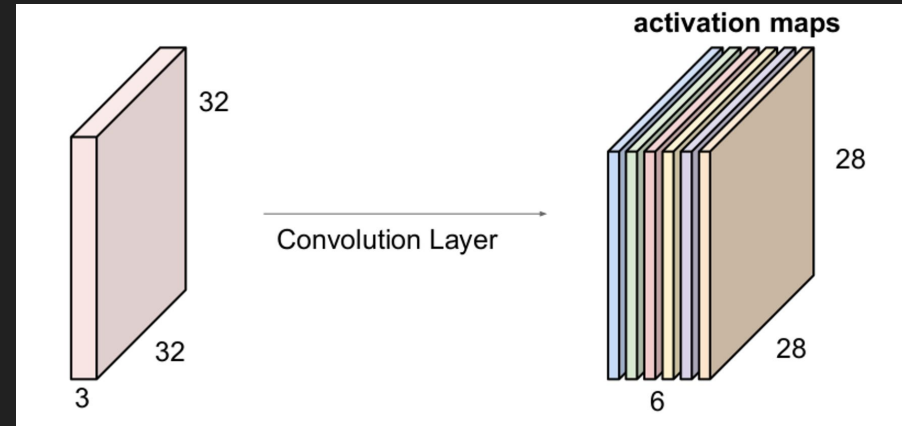
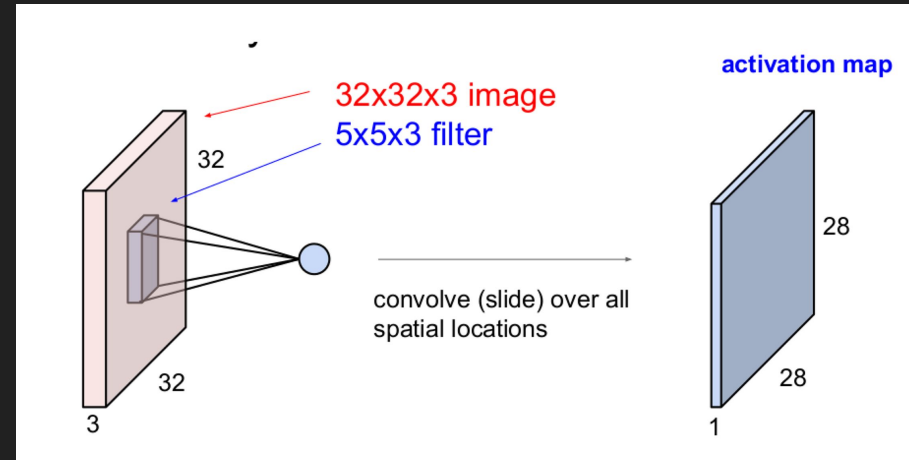
Convolution
shares the same
parameters
across all spatial
locations



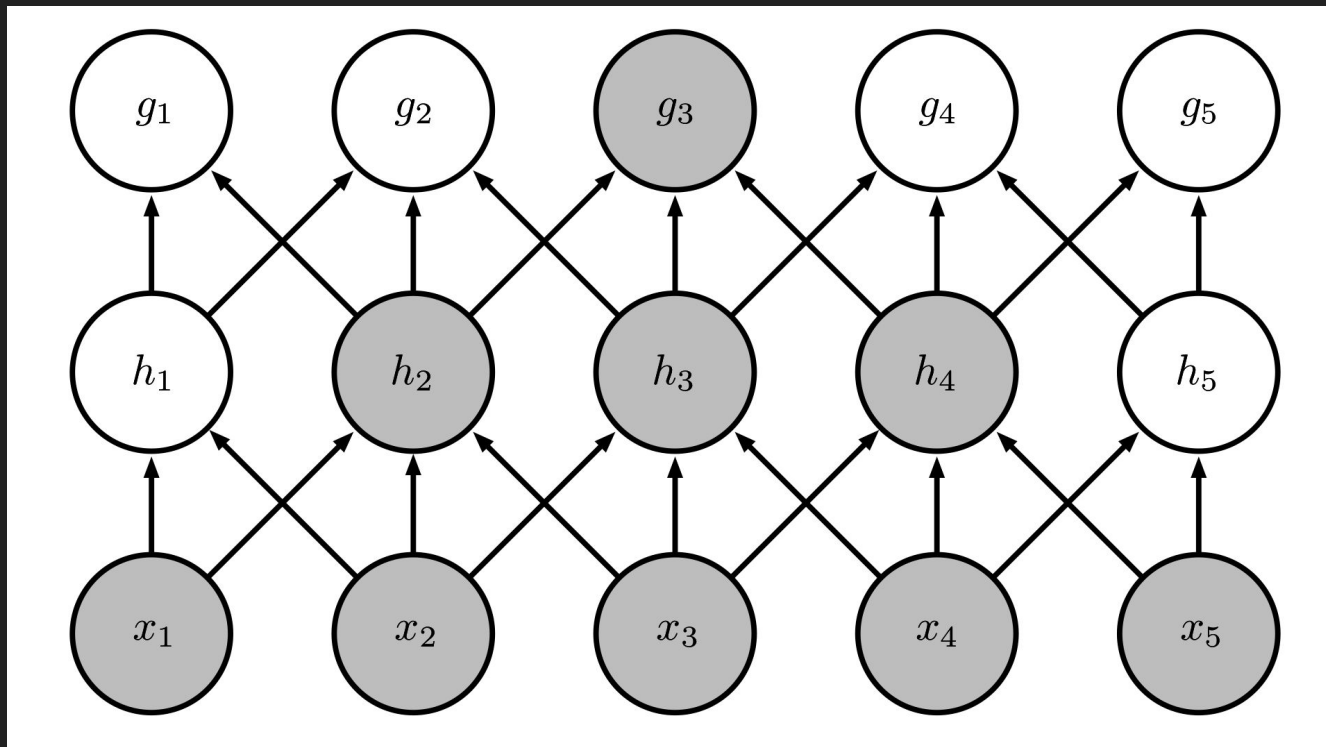
Traditional
matrix
multiplication
does not share
any parameters



- Filters extend the full depth of the input volume
- Convolve the filter with the image: Slide over the image spatially, computing dot products.
- Each layer can train several convolution filters : channels
- Stack the activation map produced by each filter; repeat.

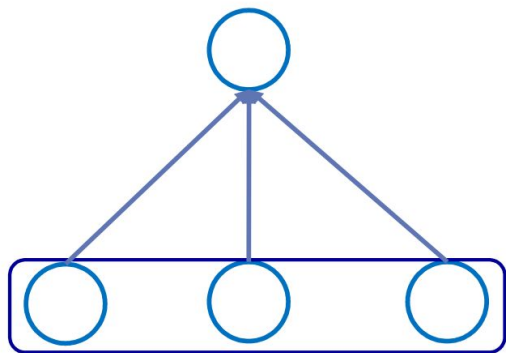


Growing receptive field



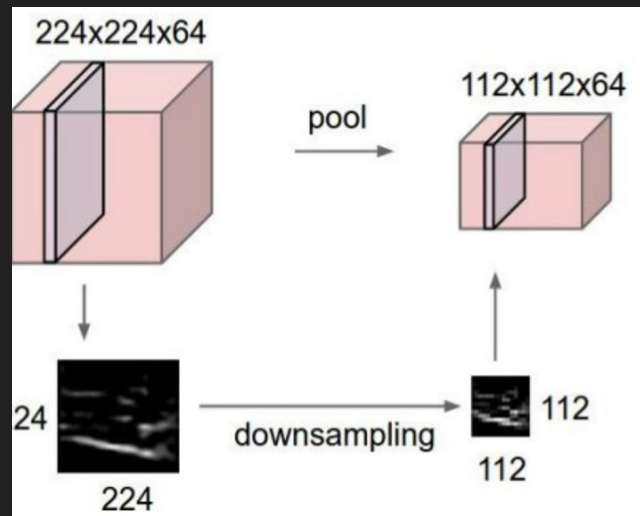
Pooling

- Number of features extracted can be very large (increasing number of channels / filters)
- To reduce the size of the activation maps, one can :
 - Use strides
 - Downsample using Max or AveragePooling - applied on each channel independently



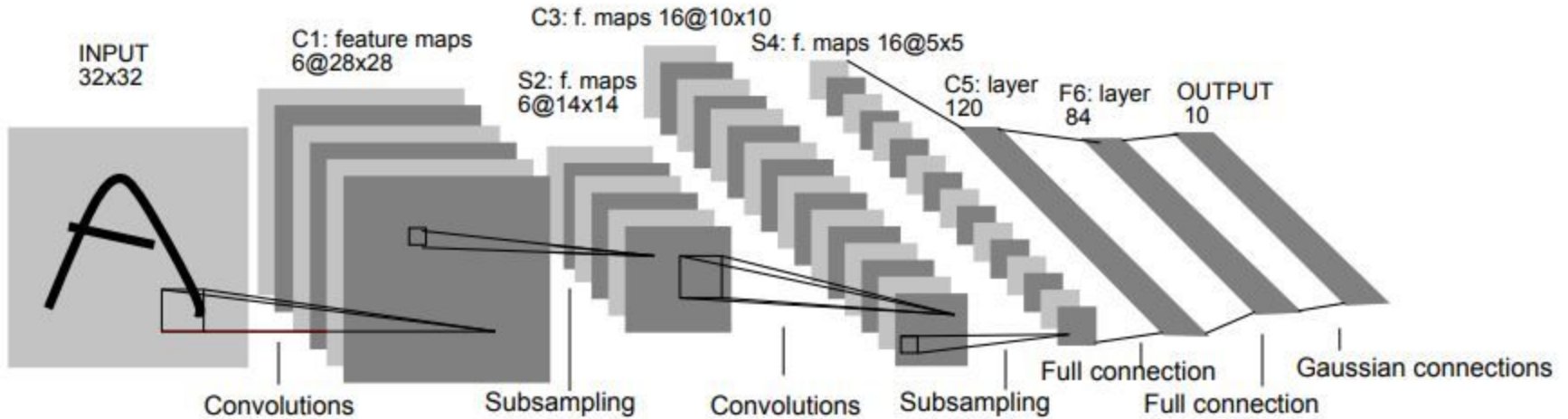
Pooled feature (max
or mean operator)

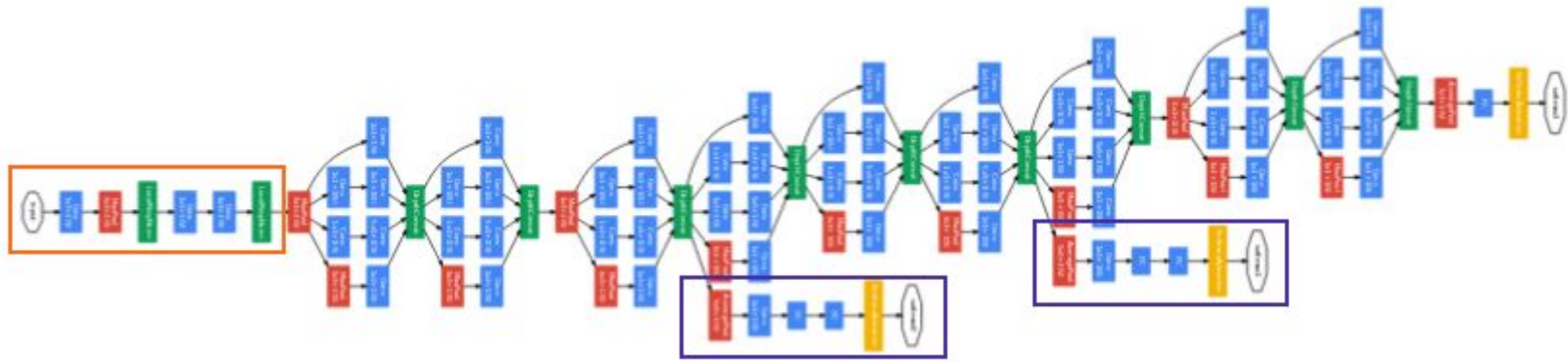
Convolutional features



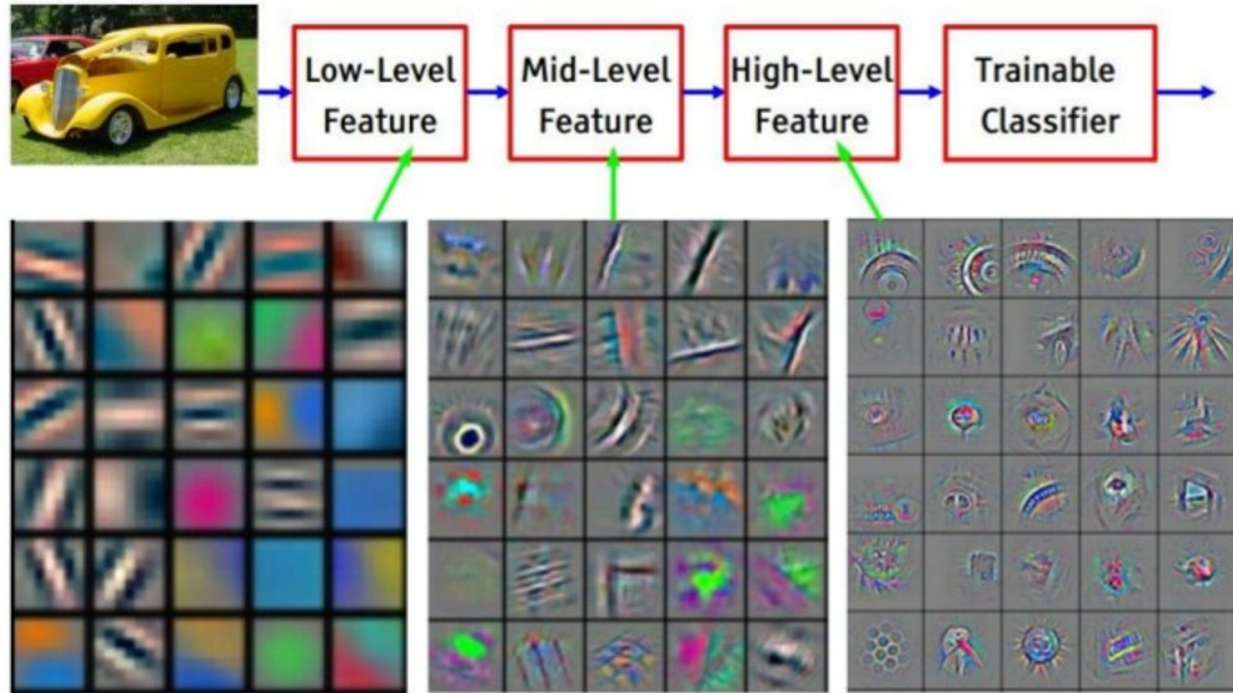
Credit Fei-Fei Li's course

Convolutional Neural Networks



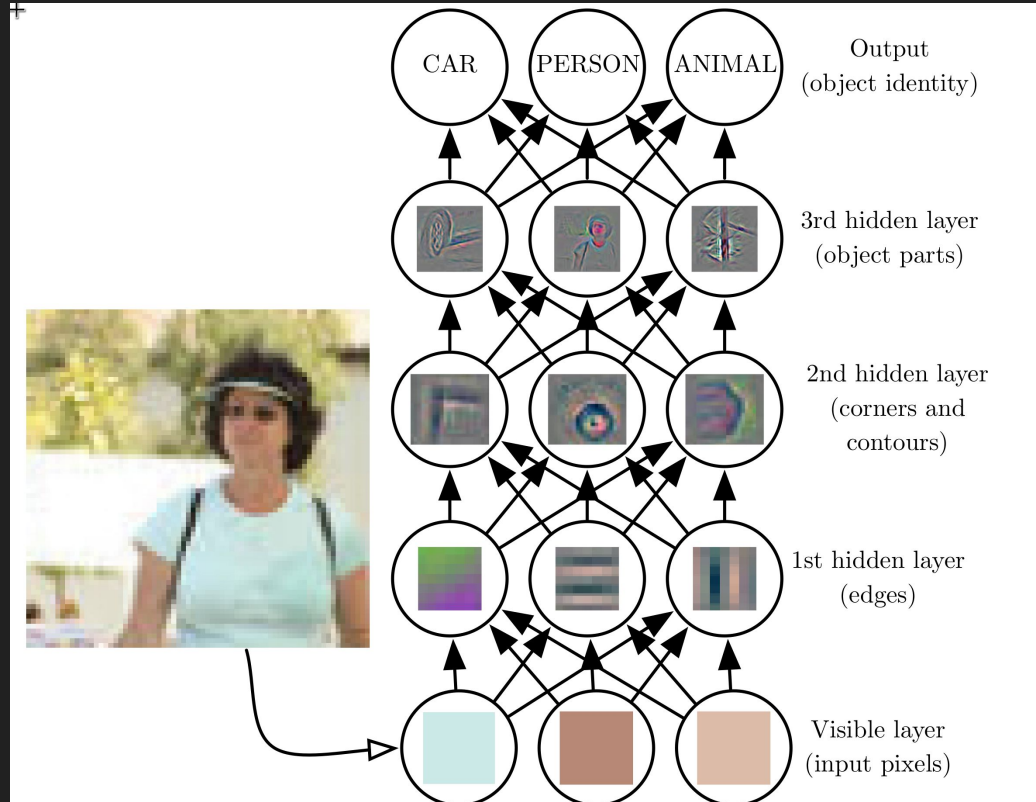


“Inside” deep learning : Representation Learning



Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

“Inside” deep learning : Representation Learning



Neural Networks

©2016 Fjodor van Veen - asimovinstitute.org

Backfed Input Cell

Input Cell

Noisy Input Cell

Hidden Cell

Probabilistic Hidden Cell

Spiking Hidden Cell

Output Cell

Match Input Output Cell

Recurrent Cell

Memory Cell

Different Memory Cell

Kernel

Convolution or Pool

Perceptron (P)



Feed Forward (FF)



Radial Basis Network (RBF)



Deep Feed Forward (DFF)



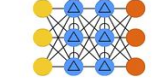
Recurrent Neural Network (RNN)



Long / Short Term Memory (LSTM)



Gated Recurrent Unit (GRU)



Auto Encoder (AE)



Variational AE (VAE)



Denoising AE (DAE)



Sparse AE (SAE)



Markov Chain (MC)



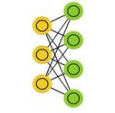
Hopfield Network (HN)



Boltzmann Machine (BM)



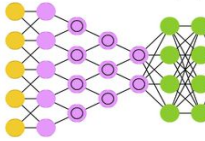
Restricted BM (RBM)



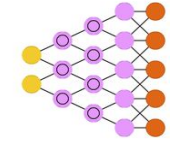
Deep Belief Network (DBN)



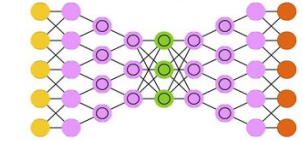
Deep Convolutional Network (DCN)



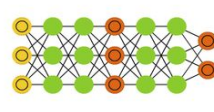
Deconvolutional Network (DN)



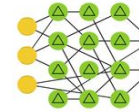
Deep Convolutional Inverse Graphics Network (DCIGN)



Generative Adversarial Network (GAN)



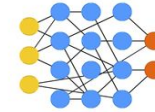
Liquid State Machine (LSM)



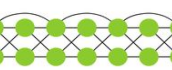
Extreme Learning Machine (ELM)



Echo State Network (ESN)



Deep Residual Network (DRN)



Kohonen Network (KN)



Support Vector Machine (SVM)



Neural Turing Machine (NTM)



Summary

- Neural nets are composition of functions and extract high levels representations of the data.
- Good tool to approximate 'functions' on complex / high dim data.
- ... if you have the right data + give the model the right information.
 - Pre-processing data correctly + calibrating the problem is most of the work...
- Can lack 'interpretability' at first glance / in vanilla mode...but some tricks and tools exist (e.g. saliency maps, heatmap backprop,...)
- Practical: Pytorch / Tensorflow
- Go beyond 'just' classification / regression:
 - unsupervised / weakly supervised x representation learning, disentanglement, generative models, transfer learning, etc.

Some Resources

- Pattern Recognition and Machine Learning by Bishop
- Machine Learning Andrew Ng's class on coursera
<https://www.coursera.org/learn/machine-learning>
- Deep Learning Book by Goodfellow, Bengio and Courville, online version
<http://www.deeplearningbook.org/> + lectures available on several chapters
- On Computer Vision / CNN, Li & Karpathy's course
<http://cs231n.stanford.edu/>
- PyTorch / Tensorflow - Keras tutorials