

Introduction to (Deep) Neural Networks

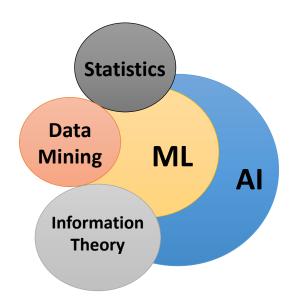
Davide Bacciu bacciu@di.unipi.it



Outline

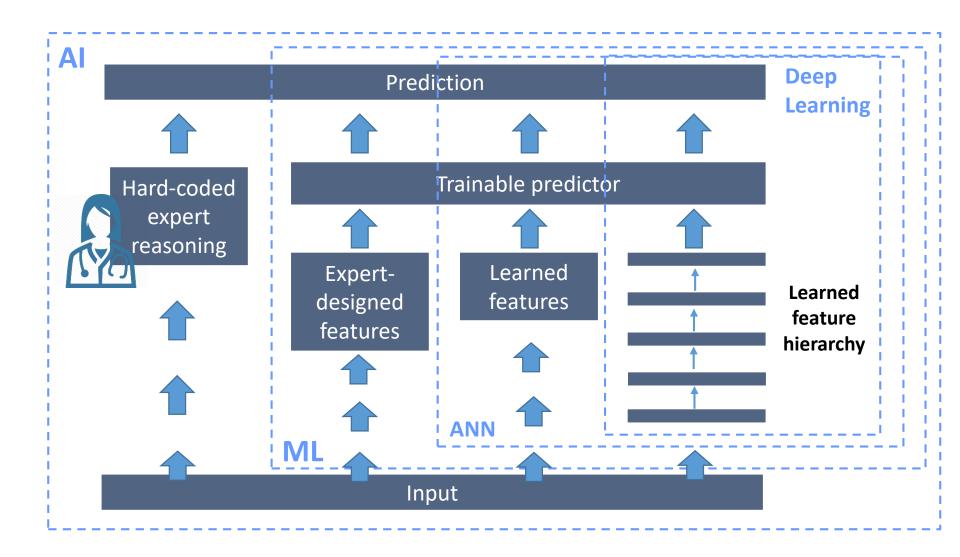
- Introduction
- Machine learning preliminaries
- Neural Networks basics
 - Neuron model
 - Architectural aspects
 - Training
- Deep learning
 - Convolutional neural networks (images)
 - Recurrent neural networks (sequences)

Machine Learning (ML)



Machine Learning is a field of artificial intelligence dealing with models and methods that allow computer to learn from data

Deep Learning



Machine Vision



"A cat is sitting on a toilet seat" (NeuralTalk)

...some evident open issues..

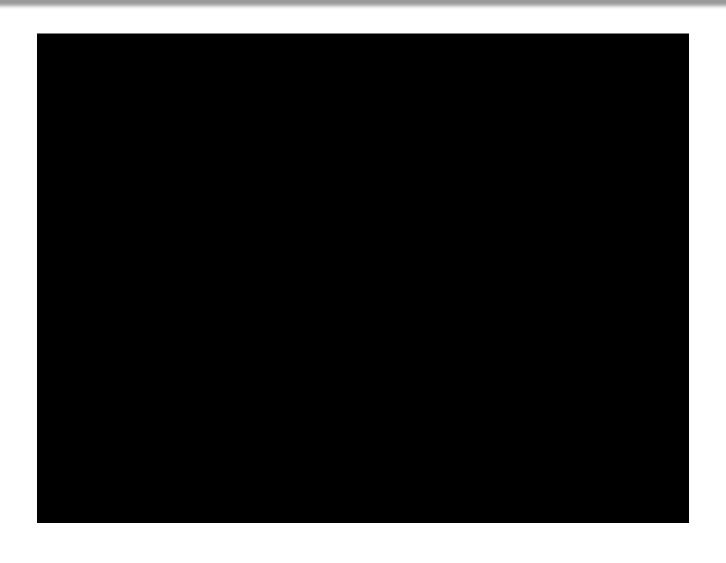


"A woman holding a teddy bear in front of a mirror"

Autonomous Driving



Deep Reinforcement Learning



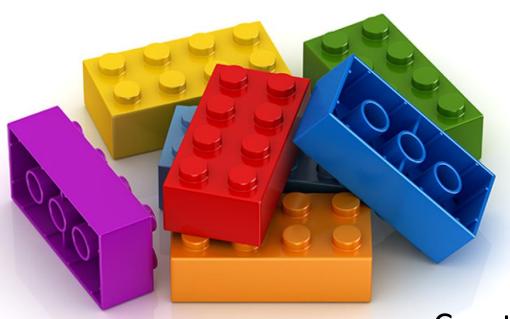
Using Machine Learning to Generate Images



Generative Adversarial Networks

Create faces of non-existing people

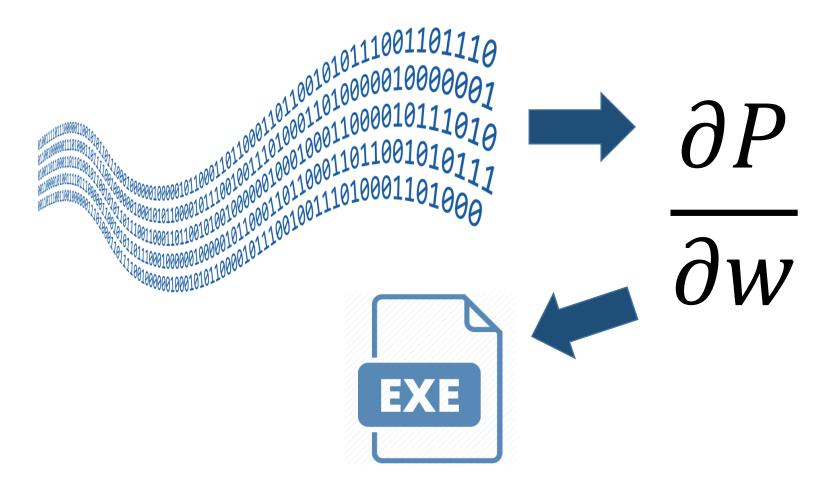
The Deep Learning Lego



Creating applications by putting together various combinations of basic types of neural networks

Differentiable Programming

Software development as a data-driven process



Python

- Support for vectorization and GPU (at the price of some swearing at installation time)
- Loads of useful libraries for Machine learning Deep learning Machine vision

The reference language for machine learning



ML preliminaries



Learning from examples

- Acquisition (inference/induction) from data (examples) of the rules, models or representations which enable the production of a desired behaviour
- The goal is not to memorize but to generalize the acquired knowledge
 - More than simply fitting the data
 - Estimating the value of function for unseen examples
- Given a set of N examples

$$(x_1, y_1); (x_2, y_2) ... (x_N, y_N)$$

find a function $f(\cdot)$ such that it is a good predictor of y for a future input x

ML – Tasks & Data



Supervised Learning

Learn an unknown function predicting an output in response to an input

 Predicting credit risk given customer profile

(x, y)



Unsupervised Learning

Identification of structures, regularities associations and anomalies in the data

 Signaling anomalous transactions

(x)



Reinforcement Learning

Learning of a policy or complex behaviour while being allowed to observe only partial responses from the interaction with the environment or the user

Autonomous agents

(s, a, r)

Empirical Error (Supervised Case)

Suppose we have a finite set

$$D = (x_1, y_1); (x_2, y_2) \dots (x_N, y_N)$$

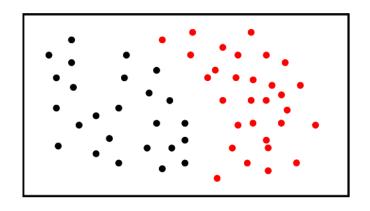
providing the target values y_i over N samples

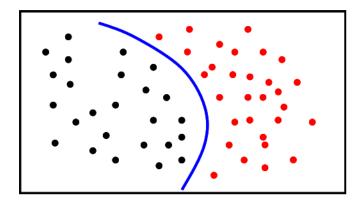
The empirical (sample) error of model *M* with respect to the sample *D* is

$$Err_D(M) = \sum_{(x_i, y_i)} J(M(x_i), y_i)$$

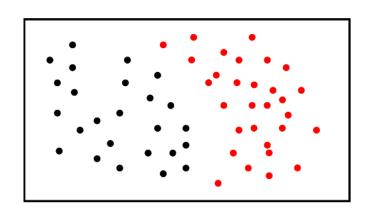
where $J(M(x_i), y_i)$ is the loss, i.e. a function measuring the discrepancy between the predicted $M(x_i)$ and the target value y_i

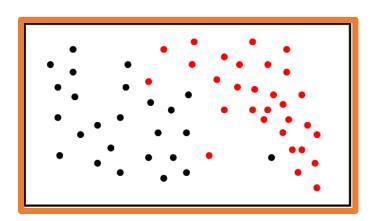
Empirical Risk & Model Complexity



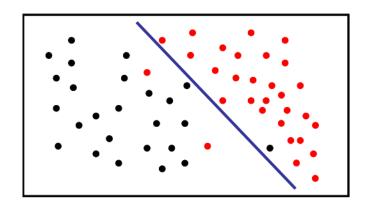


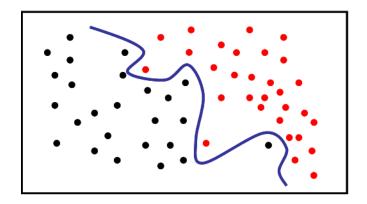
Empirical Risk & Model Complexity



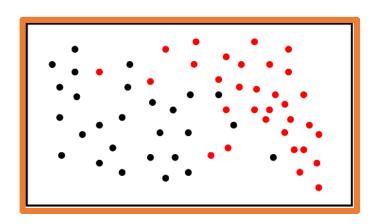


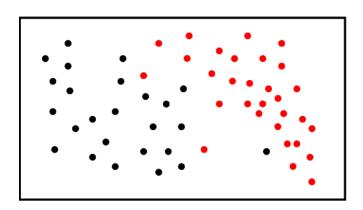
Best model now?



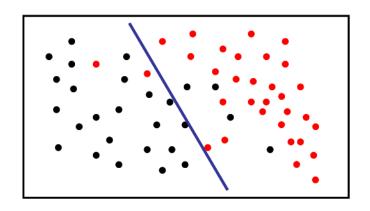


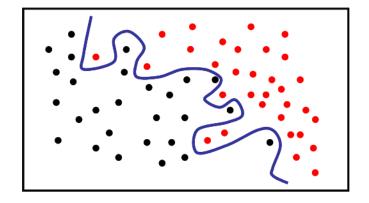
Empirical Risk & Model Complexity





Bias-Variance Dilemma





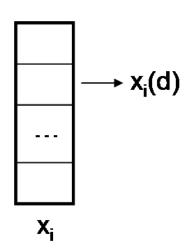
Key Ingredients of Machine Learning

- Data
- Tasks
- Learning Machinery
 - Computational model how knowledge is represented
 - Linear regression
 - Bayesian Classifier
 - Neural Networks
 - Learning algorithm how knowledge is adapted to the observations (examples)
 - Backpropagation
 - Expectation-Maximization
- Validation: measures of learning quality and performance

ML – Information Representation

Vectorial data

- The *i*-th input sample x_i is a *D*-dimensional numerical vector
 - Continuous, categorical or mixed values
 - Describes an individual of our world of interest,
 e.g. patients in a biomedical application
- ullet The single dimensions d are called features and numerically represent an attribute of the individual
 - E.g. if x_i describes a patient, $x_i(d)$ can be his/her age
- Also output samples y_i are D'-dimensional numerical vectors

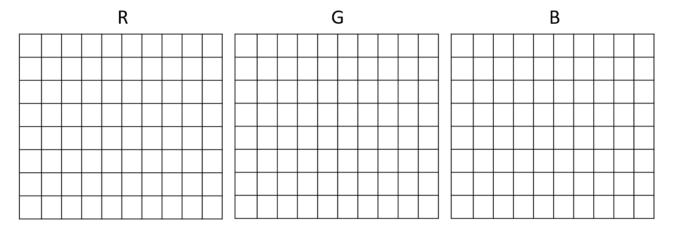


ML – Information Representation

Images

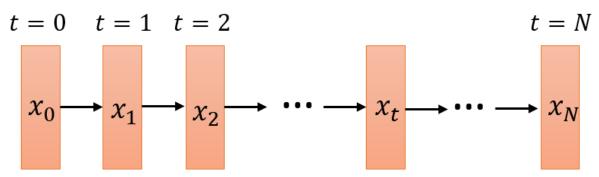
Images are matrices of pixels intensity





ML – Information Representation

Sequential data



- Variable size data characterized by sequentially dependent information
- Examples: financial timeseries, sequences of operations, natural language sentences, ...
- Each element of the sequence is a vector
- In ML can be used both as input and output information

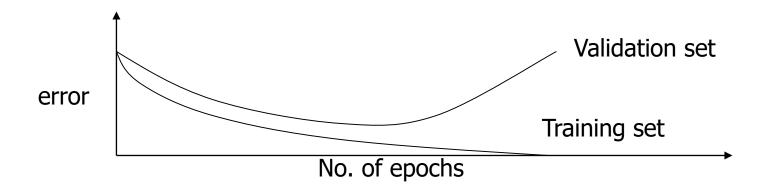
Dataset Preparation

Dataset should normally be split into three sets as follows:

- Training set use to update the weights. Patterns in this set are repeatedly in random order. The weight update equation are applied after a certain number of patterns.
- Validation set use to decide when to stop training only by monitoring the error and to select the best model configuration
- Test set Use to test the performance of the neural network. It should not be used as part of the neural network development and model selection cycle

Model Selection

- Statistically sound validation techniques should be used to determine model hyperparameters
 - Non-adaptive user-chosen model parameters
 - E.g. architecture of neural networks, penalty weighting, optimization algorithm setup...
- Use validation error to select the best model configuration



Regularization

- Constrain the learning model to avoid overfitting and help improving generalization
- Add penalization terms to the error function that punishes the model for excessive use of resources
 - Limit the amount of parameters that are used to learn a task
 - Limit the total activation of neurons in the network

$$J' = J(y, y^*) + \lambda R(\cdot)$$
 Hyperparameter to be chosen in model selection
$$||A||_1 = \sum_{ij} |a_{ij}|$$

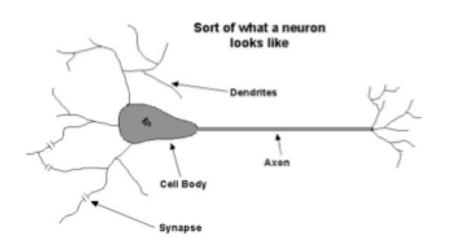
$$||A||_2 = \sqrt{\sum_{ij} a_{ij}^2}$$

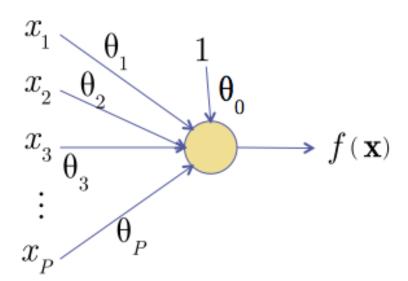
Neural Networks



The Neuron Metaphor

- Neurons
 - accept information from multiple inputs,
 - transmit information to other neurons.
- Multiply inputs by weights along edges
- Apply some function to the set of inputs at each node





Characterizing the Artificial Neuron (I)

- Input/Output signal may be.
 - Real value.
 - Unipolar {0, 1}.
 - Bipolar {-1, +1}.
- Weight : ϑ_{ij} strength of connection from unit **unit** j to unit i
- Learning amounts to adjusting the weights ϑ_{ij} by means of an optimization algorithm aiming to minimize a cost function

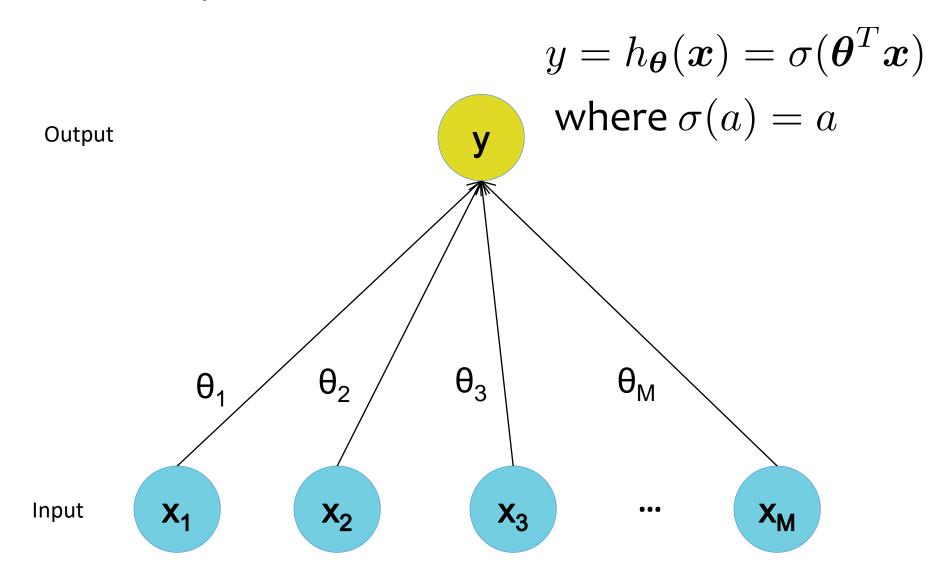
Characterizing the Artificial Neuron (II)

• The bias b is a constant that can be written as $\vartheta_{i0}x_0$ with $x_0 = 1$ and $\vartheta_{i0} = b$ such that

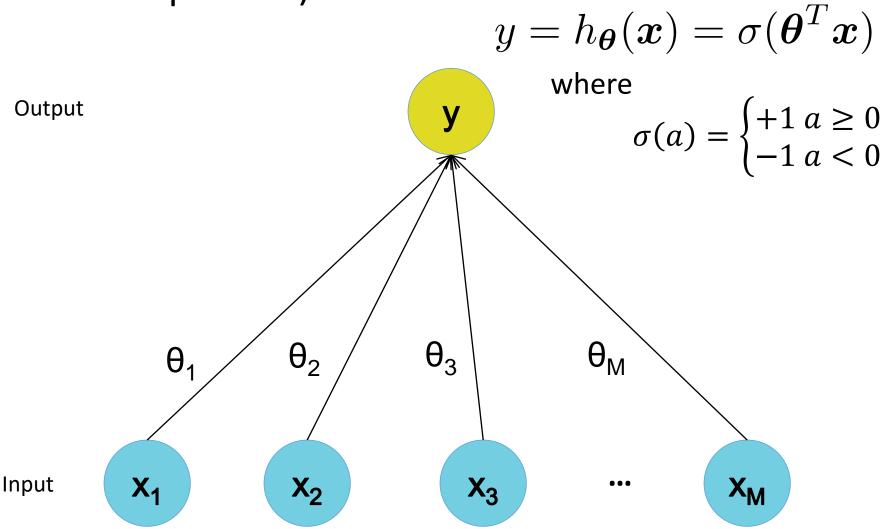
$$net_i = \sum_{j=0}^n \vartheta_{ij} x_j$$

The function f(net_i(x)) is the unit's activation function. In the simplest case, f is the identity function, and the unit's output is just its net input.
 This is called a linear unit

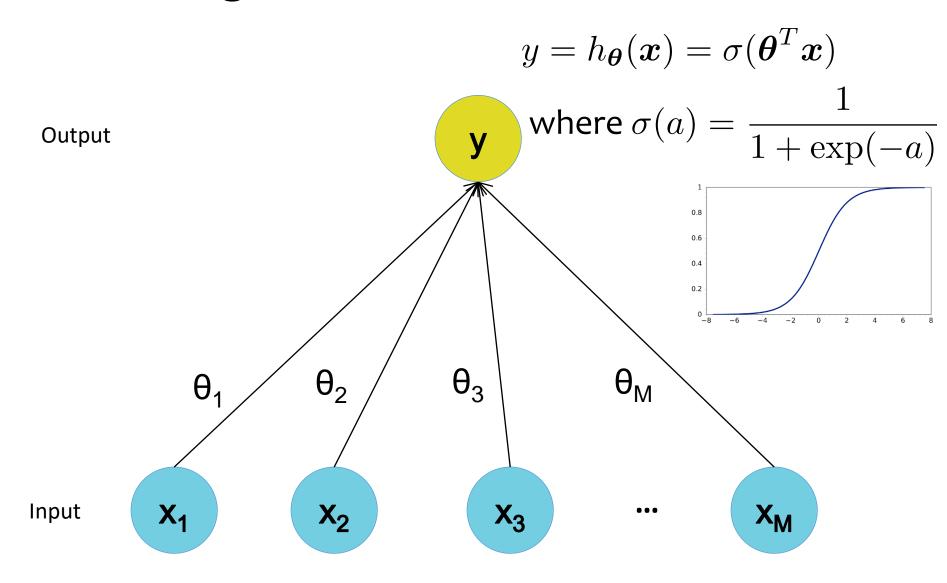
A Simple Linear Neuron



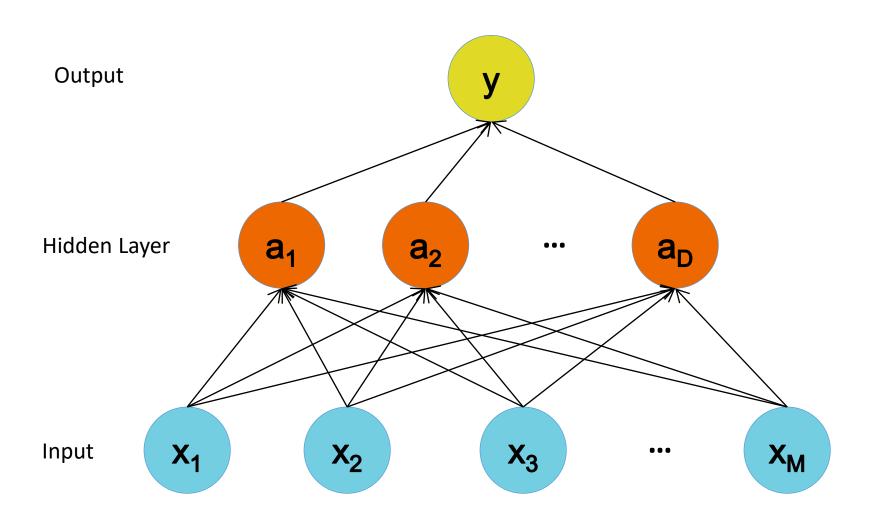
Linear Threshold Unit (a.k.a. Perceptron)



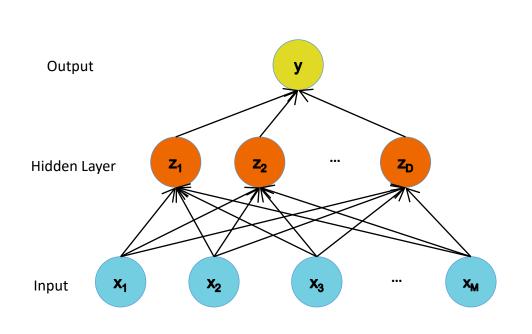
The Logistic Neuron

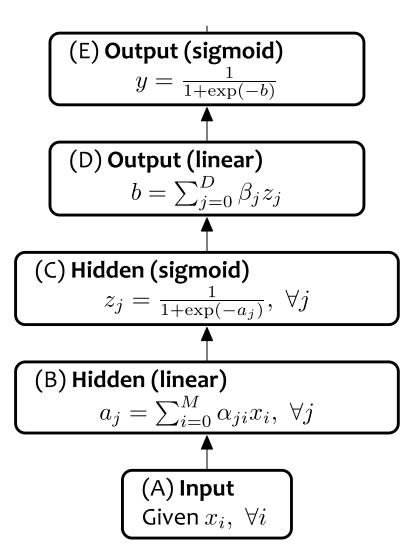


Multilayer Perceptron

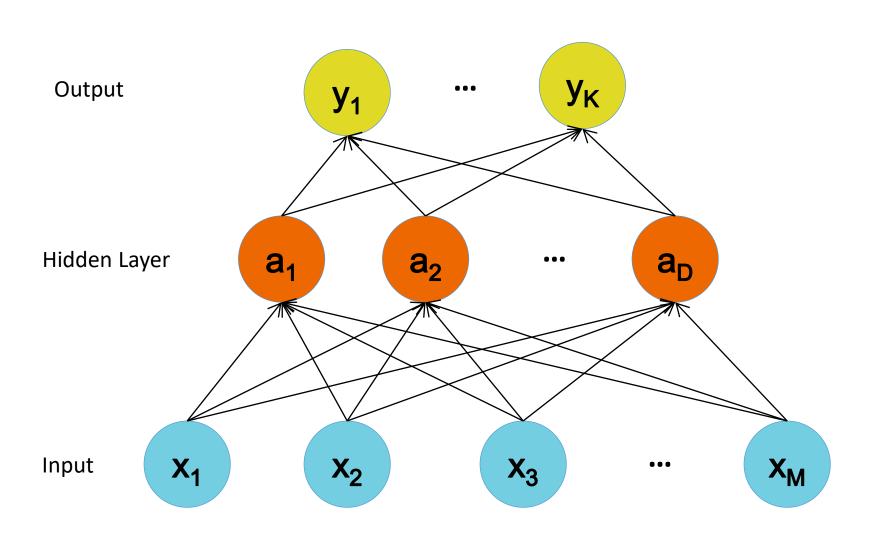


Multilayer Perceptron



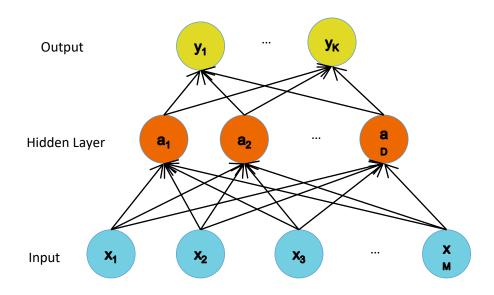


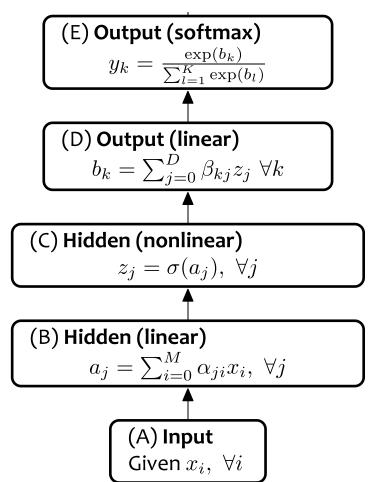
Multiple-Multiclass Outputs



Multi-Class Output Softmax:

$$y_k = \frac{\exp(b_k)}{\sum_{l=1}^K \exp(b_l)}$$





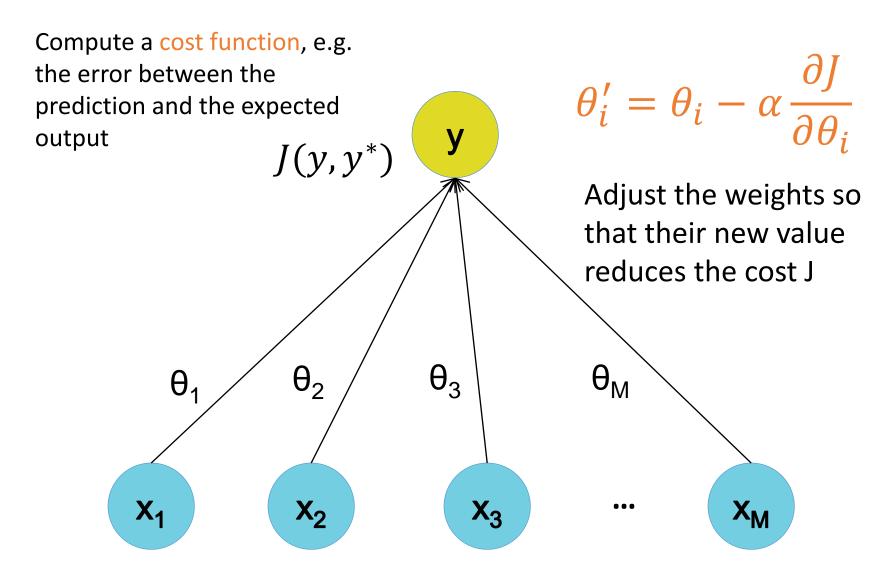
Neural Network Architectures

Even for a basic Neural Network, there are many design decisions to make:

- 1. # of hidden layers (depth)
- # of units per hidden layer (width)
- 3. Type of activation function for each layer
- 4. Loss function
- 5. Connectivity patterns
- 6. Weight sharing

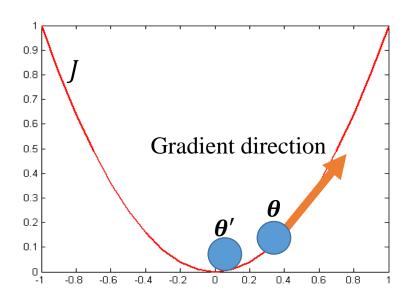
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Training NNs – Cost minimization



Gradient Descent

Weights are updated in the opposite direction of the gradient of the loss function



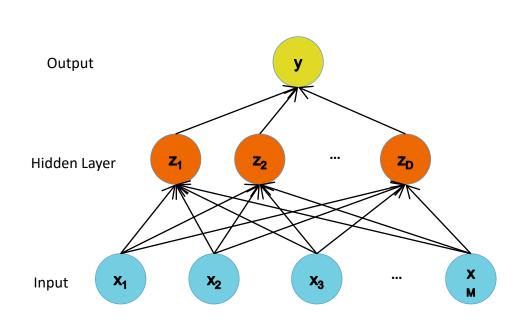
$$\theta_i' = \theta_i - \alpha \frac{\partial J}{\partial \theta_i}$$

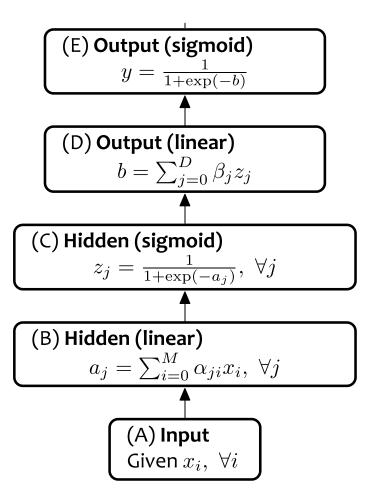
Gradient direction is the direction of uphill of the error function.

By taking the negative we are going downhill

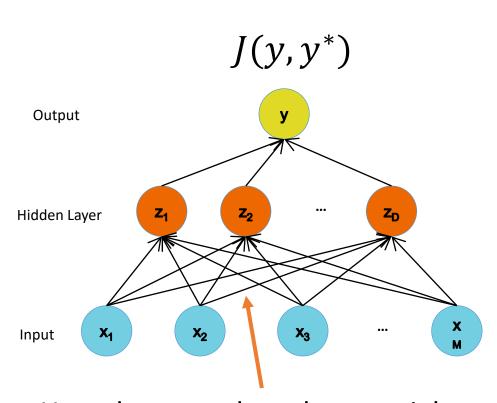
Hopefully to a minimum of the error

Training Multilayer NNs

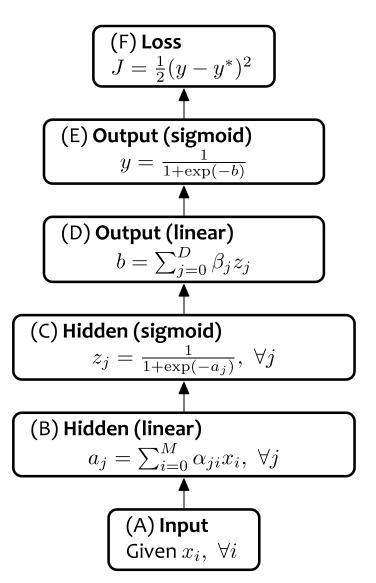




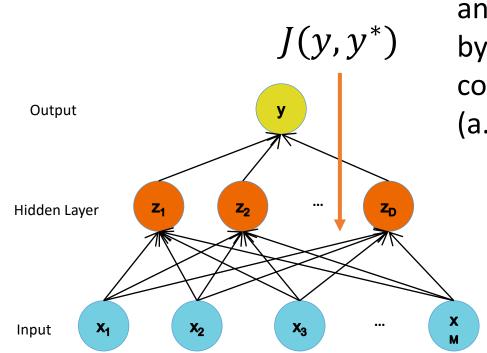
Training Multilayer NNs



How do we update these weights given the loss is available only at the output unit?



Error Backpropagation



Error is computed at the output and propagated back to the input by chain rule to compute the contribution of each weight (a.k.a. derivative) to the loss

A 2-step process

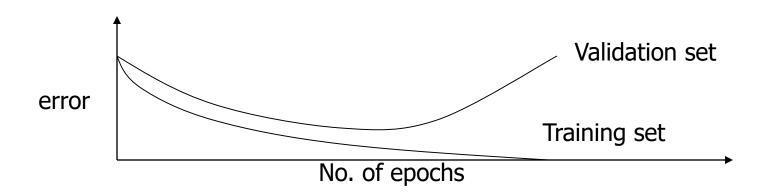
- Forward pass Compute the network output (model.predict())
- Backward pass –
 Compute the loss function gradients and update (model.fit())

Convergence Criteria

- Learning is obtained by repeatedly supplying training data and adjusting by backpropagation
 - Typically 1 training set presentation = 1 epoch
- We need a stopping criteria to define convergence
 - Euclidean norm of the gradient vector reaches a sufficiently small value
 - Absolute rate of change in the average squared error per epoch is sufficiently small
 - Validation for generalization performance: stop when generalization performance reaches a peak

Early Stopping

- Running too many epochs may overtrain the network and result in overfitting and perform poorly in generalization
- Keep a hold-out validation set and test accuracy after every epoch. Maintain weights for best performing network on the validation set and stop training when error increases beyond this
- Always let the network run for some epochs before deciding to stop (patience parameter), then backtrack to best result



Neural Network in 1 Slide

1. Given training data:

$$\{oldsymbol{x}_i, oldsymbol{y}_i\}_{i=1}^N$$

2. Choose each of these:

Decision function

$$\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

Loss function

$$\ell(\hat{m{y}},m{y}_i)\in\mathbb{R}$$

- Penalty (optional) $\lambda R(\cdot)$

3. Define goal:

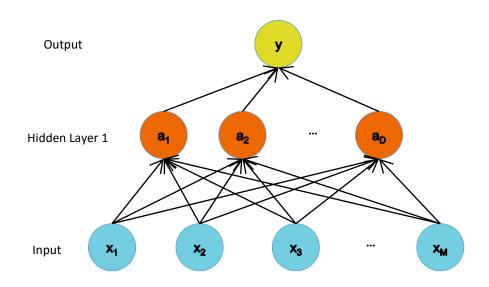
$$oldsymbol{ heta}^* = rg\min_{oldsymbol{ heta}} \sum_{i=1}^N \ell(f_{oldsymbol{ heta}}(oldsymbol{x}_i), oldsymbol{y}_i)$$

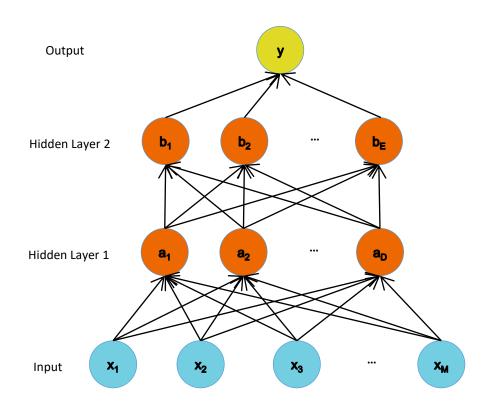
4. Train with SGD:

(take small steps opposite the gradient)

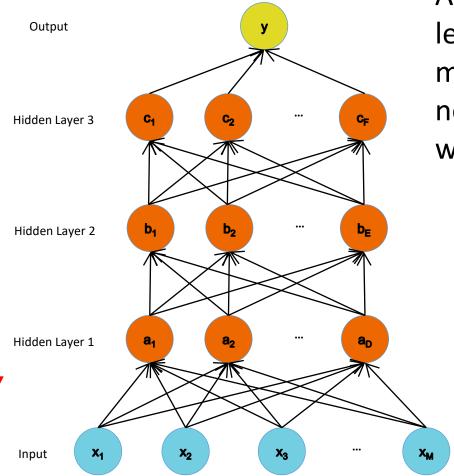
$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$







Backpropagation through many layers has numerical problems that makes learning notstraightforward (Gradient Vanish/Esplosio n)

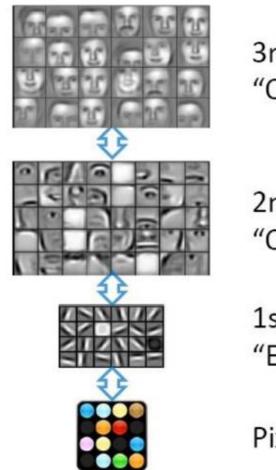


Actually deep learning is way more than having neural networks with a lot of layers

Representation learning

- We don't know the "right" levels of abstraction of information that is good for the machine
- So let the model figure it out!

Feature representation



3rd layer "Objects"

2nd layer "Object parts"

1st layer "Edges"

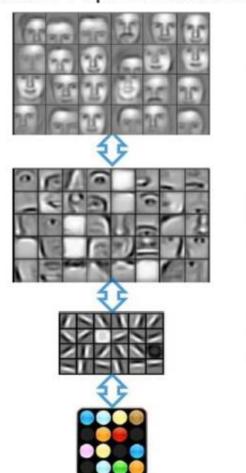
Pixels

Representation learning

Face Recognition:

- Deep Network can build up increasingly higher levels of abstraction
- Lines, parts, regions

Feature representation



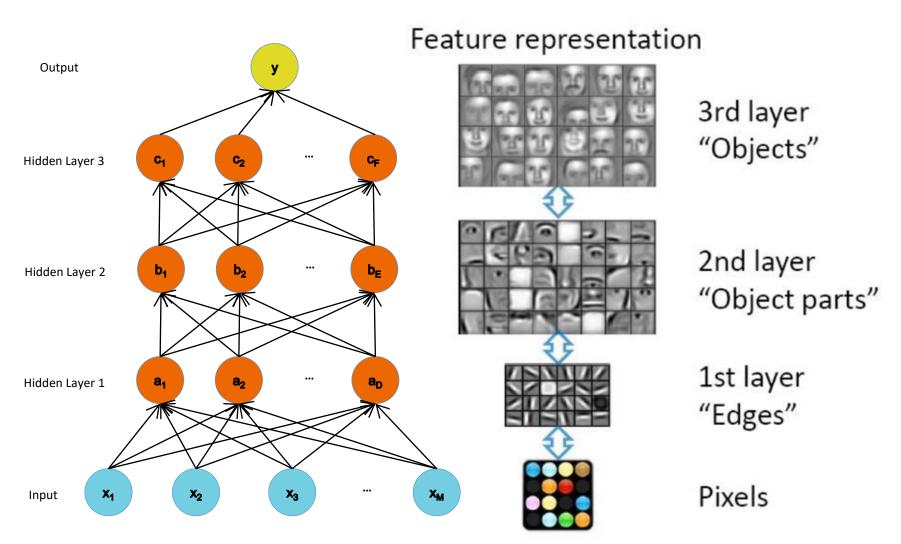
3rd layer "Objects"

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1st layer "Edges"

Pixels

Representation learning

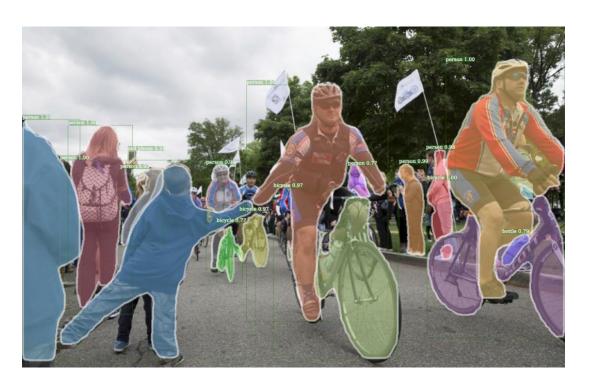


Convolutional Neural Networks



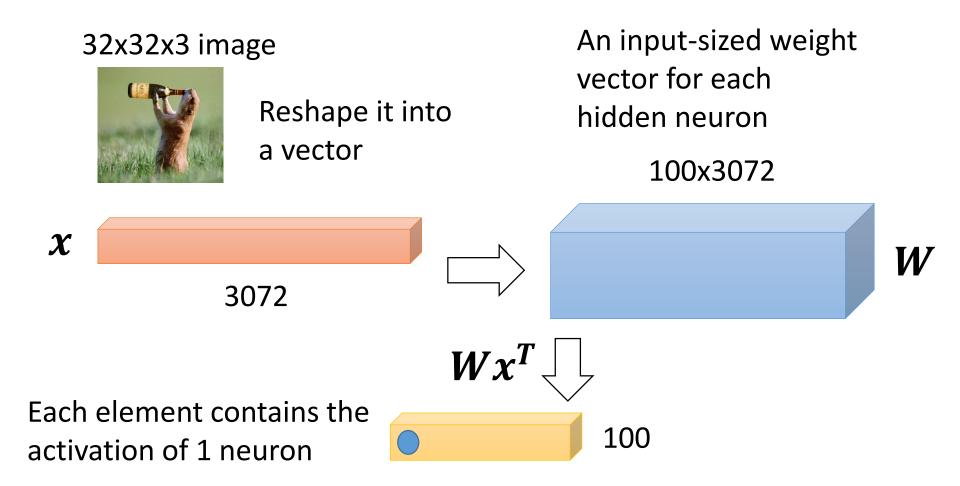
Introduction

Convolutional Neural Networks

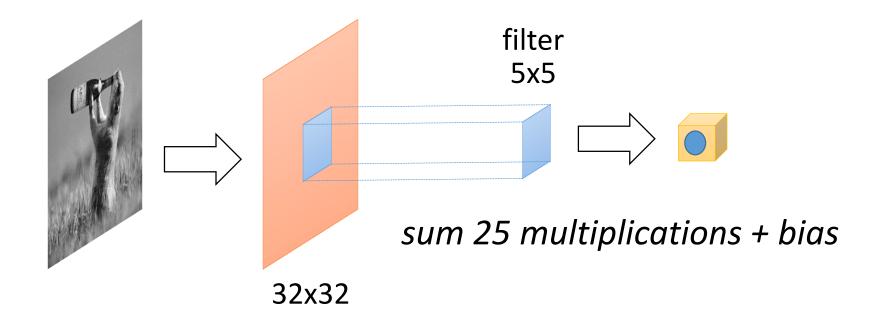


Dense Vector Multiplication

Processing images: the dense way

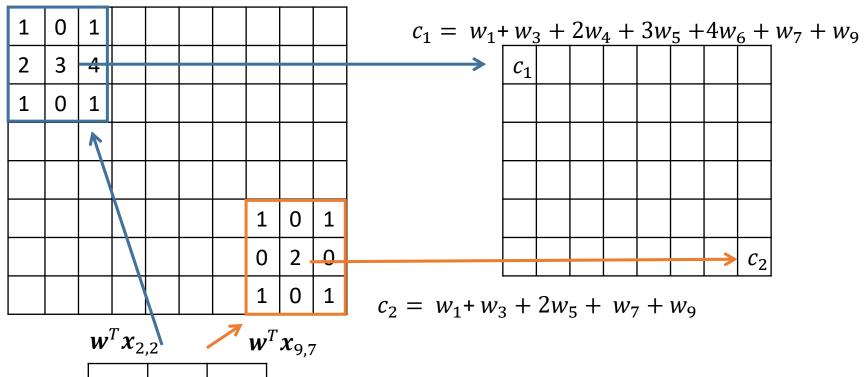


Convolution Operator



Matrix input preserving spatial structure

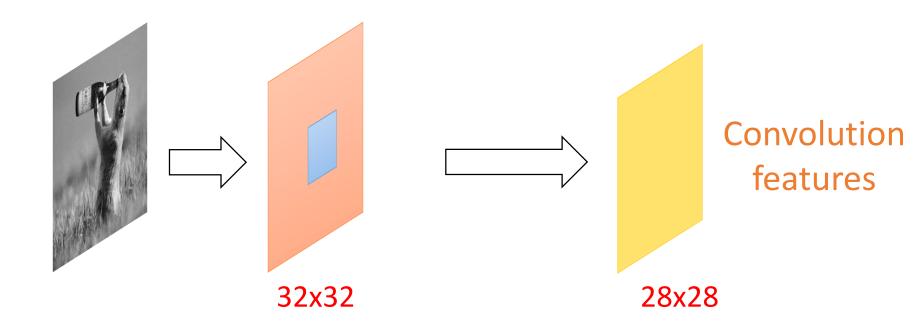
Adaptive Convolution



w_1	w_2	W_3
W_4	w_5	w_6
w_7	w_8	W ₉

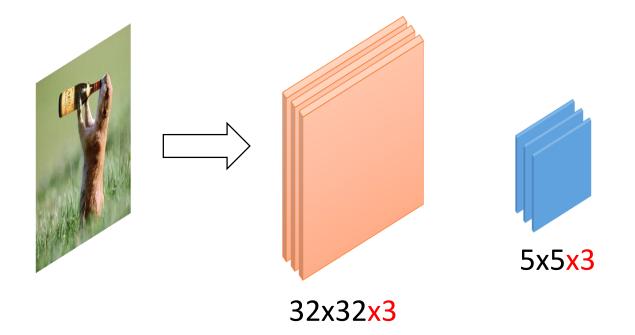
Convolutional filter (kernel) with (adaptive) weights w_i

Convolutional Features



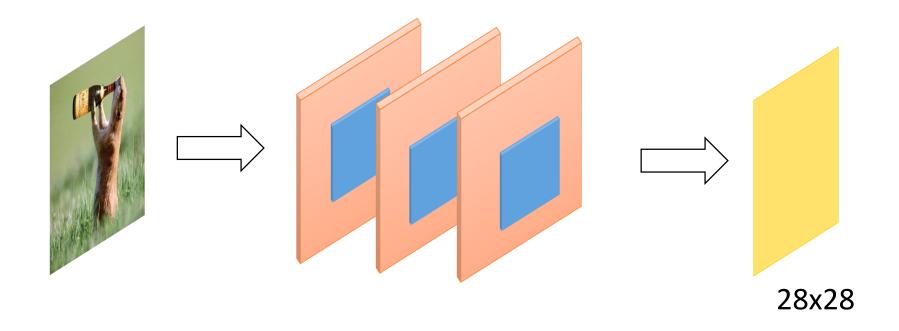
Slide the filter on the image computing elementwise products and summing up

Multi-Channel Convolution



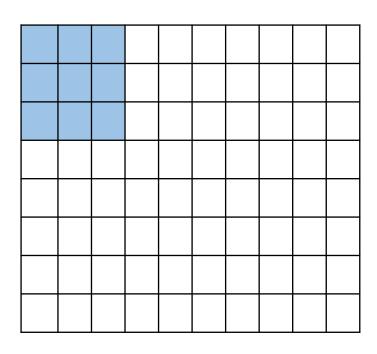
Convolution
filter has a
number of
slices equal to
the number of
image channels

Multi-Channel Convolution

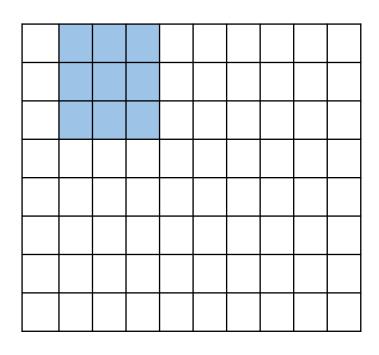


All channels are typically convolved together

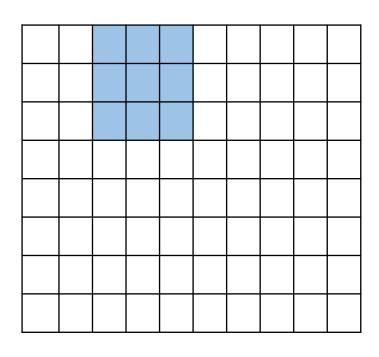
- They are summed-up in the convolution
- The convolution map stays bi-dimensional



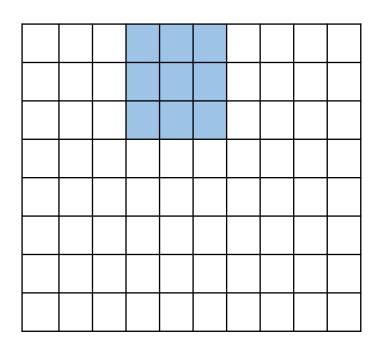
- Basic convolution slides the filter on the image one pixel at a time
 - Stride = 1



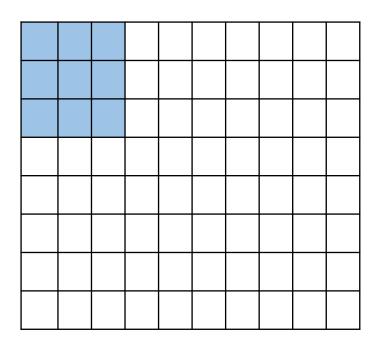
- Basic convolution slides the filter on the image one pixel at a time
 - Stride = 1



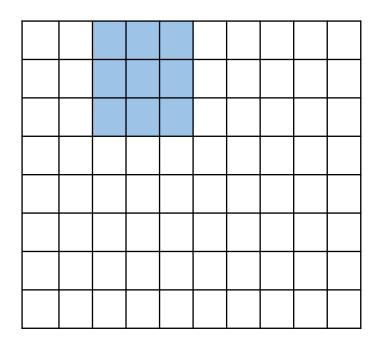
- Basic convolution slides the filter on the image one pixel at a time
 - Stride = 1



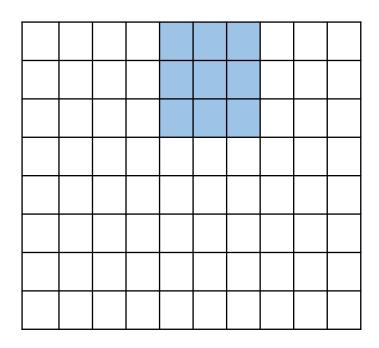
- Basic convolution slides the filter on the image one pixel at a time
 - Stride = 1



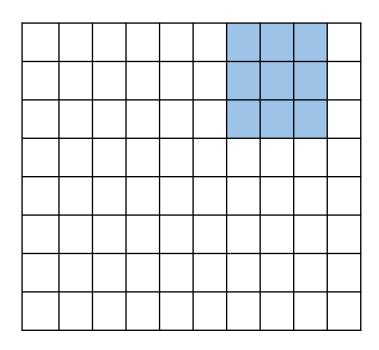
- Basic convolution slides the filter on the image one pixel at a time
 - Stride = 1
- Can define a different stride
 - Hyperparameter



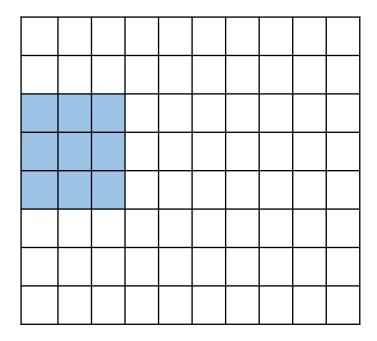
- Basic convolution slides the filter on the image one pixel at a time
 - Stride = 1
- Can define a different stride
 - Hyperparameter



- Basic convolution slides the filter on the image one pixel at a time
 - Stride = 1
- Can define a different stride
 - Hyperparameter



- Basic convolution slides the filter on the image one pixel at a time
 - Stride = 1
- Can define a different stride
 - Hyperparameter



stride = 2

Works in both directions!

- Basic convolution slides the filter on the image one pixel at a time
 - Stride = 1
- Can define a different stride
 - Hyperparameter
- Stride reduces the number of multiplications
 - Subsamples the image

Zero Padding

Add columns and rows of zeros to the border of the image

$$W=7 (P=1)$$

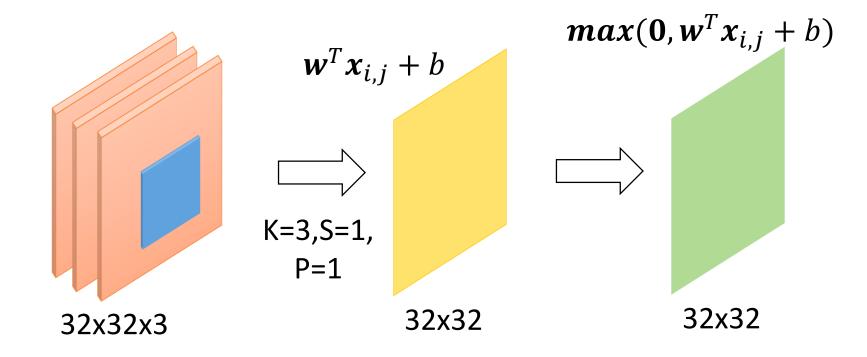
H=7 P = 1)	0	0	0	0	0	0	0	0	0
	0								
	0								
	0								
	0								
	0								
	0								
	0								
	0								

Zero padding serves to retain the original size of image

$$P = \frac{K - 1}{2}$$

Pad as necessary to perform convolutions with a given stride S

Feature Map Transformation

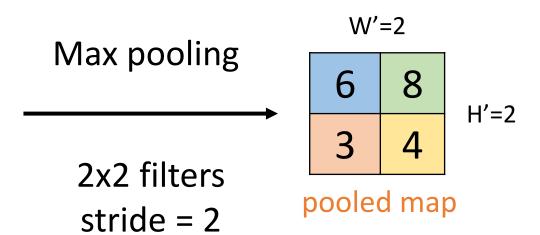


- Convolution is a linear operator
- Apply an element-wise nonlinearity to obtain a transformed feature map

Pooling

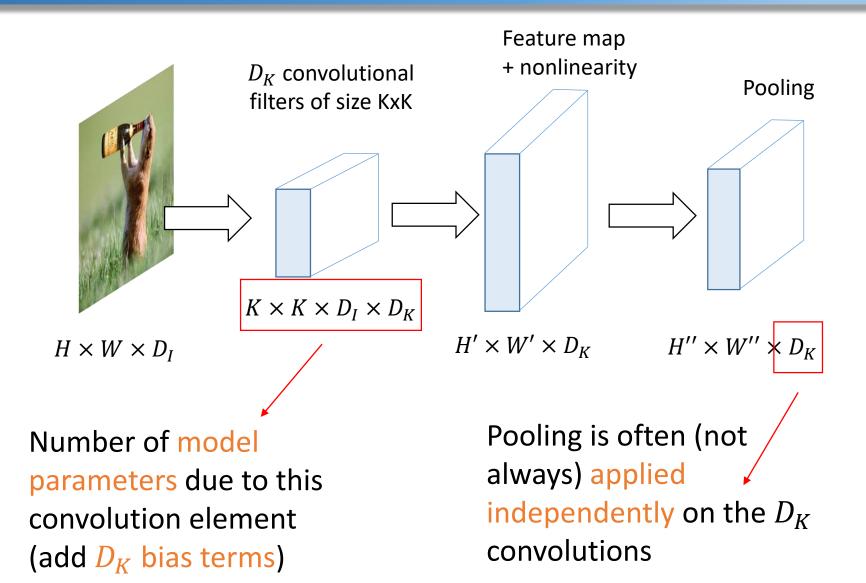
- Operates on the feature map to make the representation
 - Smaller (subsampling)
 - Robust to (some) transformations

W=4



feature map

Convolutional Filter Banks



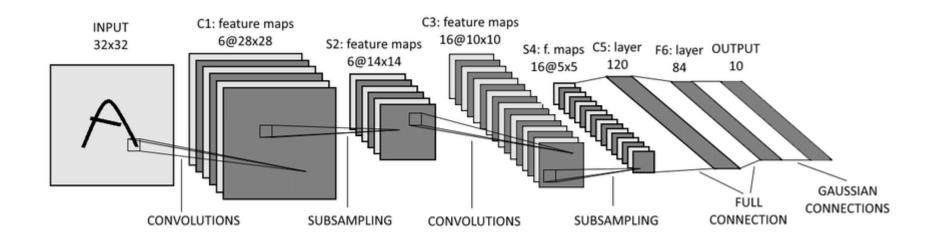
Specifying CNN in Code (Keras)

Number of convolution filters D_k

Define input size (only first hidden layer)

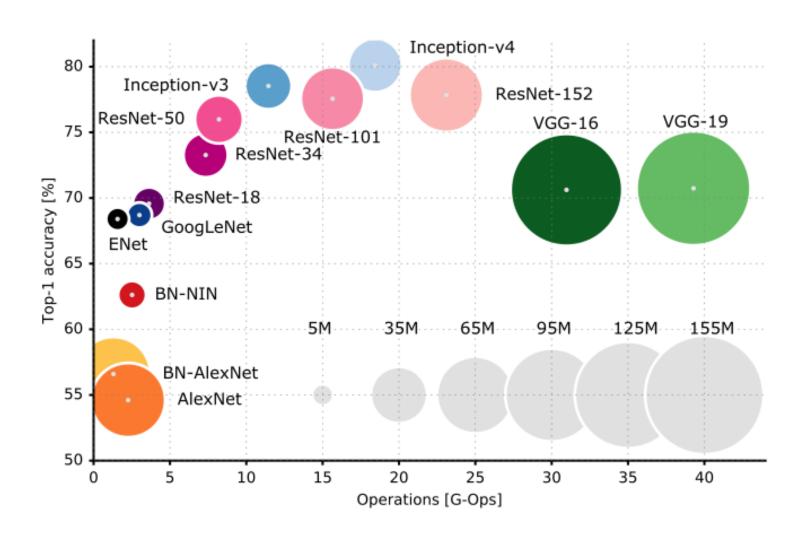
Does for you all the calculations to determine the final size to the dense layer (in most frameworks, you have to supply it)

LeNet-5 (1989)

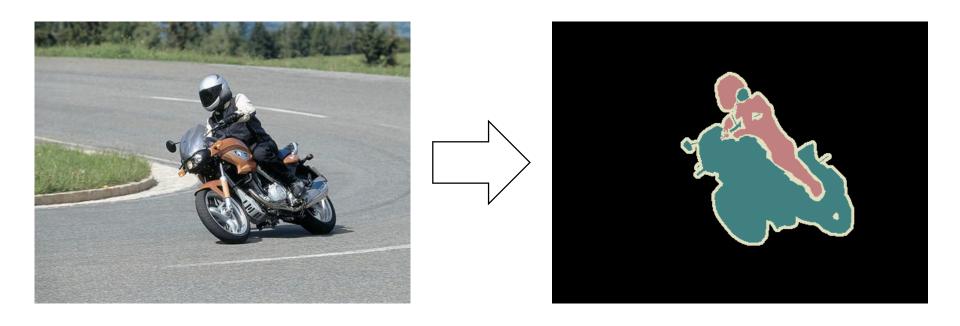


- Grayscale images
- Filters are 5x5 with stride 1 (sigmoid nonlinearity)
- Pooling is 2x2 with stride 2
- No zero padding

CNN Architecture Evolution

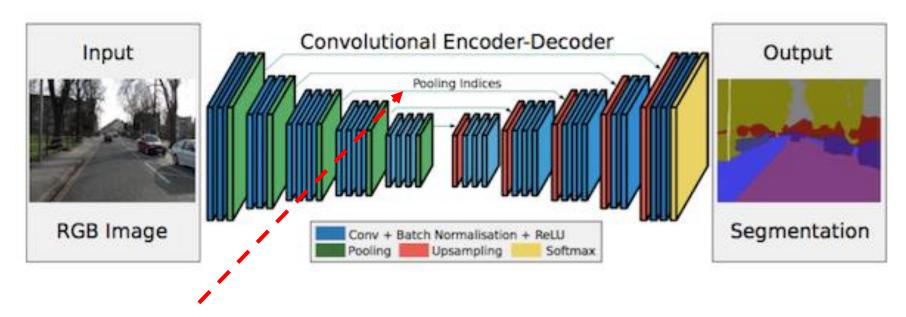


Semantic Segmentation



Traditional CNN cannot be used for this task due to the downsampling of the striding and pooling operations

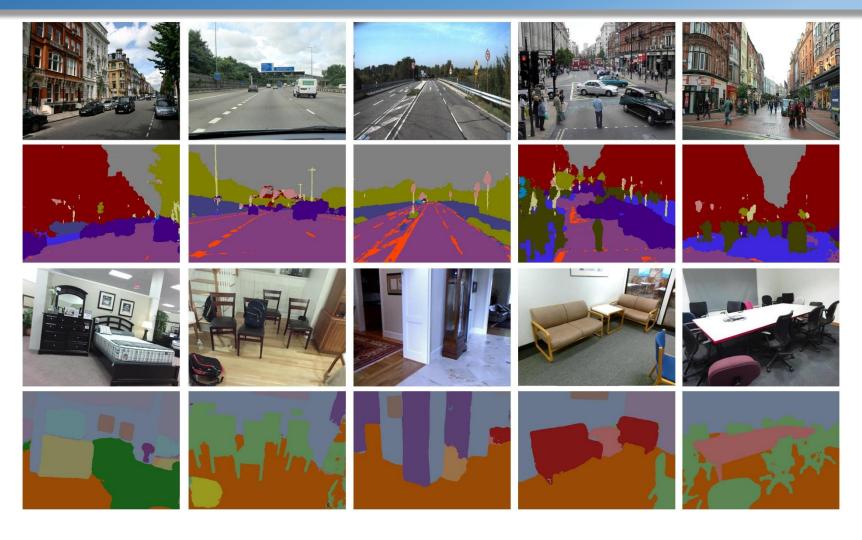
Deconvolution Architecture



Maxpooling indices transferred to decoder to improve the segmentation resolution.

Badrinarayanan et al, SegNet: A Deep Convolutional Encoder-Decoder Architecture for Image Segmentation, PAMI 2017

SegNet Segmentation



Demo here: http://mi.eng.cam.ac.uk/projects/segnet/

Software

- CNN are supported by any deep learning framework (TF, Torch, Pytorch, MS Cognitive TK, Intel OpenVino)
- Caffe was one of the initiators and basically built around CNN
 - Introduced protobuffer network specification
 - ModelZoo of pretrained models (LeNet, AlexNet, ...)
 - Support for GPU
- Caffe2 is Facebook's extensions to Caffe
 - Less CNN oriented
 - Support from large scale to mobile nets
 - More production oriented than other frameworks

Other Software

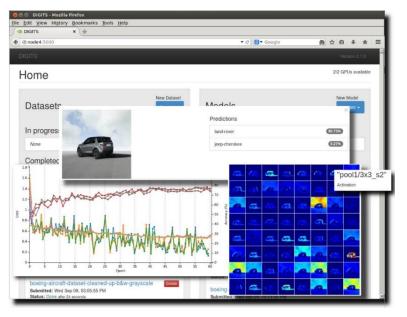
- Matlab distributes its Neural Network Toolbox which allows importing pretrained models from Caffe and Keras-TF
- Matconvnet is an unofficial Matlab library specialized for CNN development (GPU, modelzoo, ...)
- Want to have a CNN in your browser?
 - Try ConvNetJS
 (https://cs.stanford.edu/people/karpathy/convnetjs/)

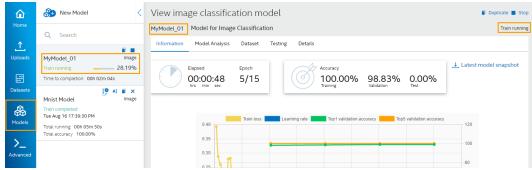
GUIs

Major hardware producers have GUI and toolkits wrapping Caffe, Keras and TF to play with CNNs

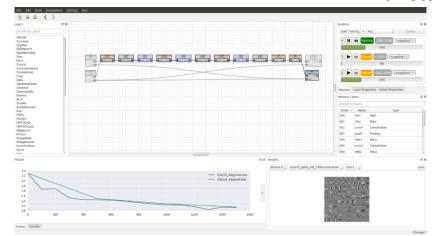
Intel OpenVino

NVIDIA Digits





Barista

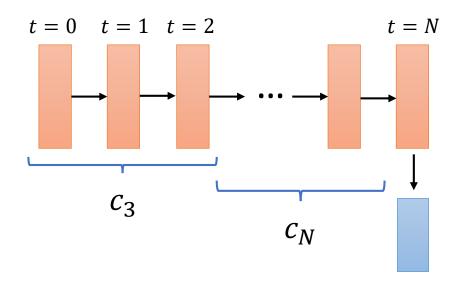


Plus others...

Recurrent Neural Networks



Dealing with Sequences in NN



Variable size data describing sequentially dependent information

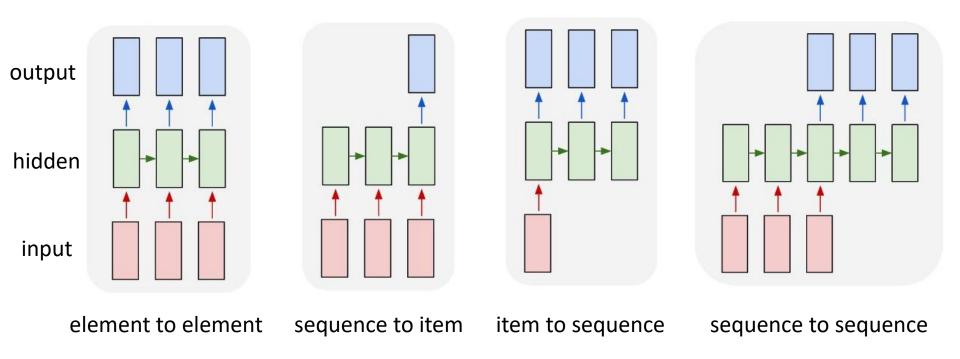
Neural models need to capture dynamic context c_t to perform predictions

- Recurrent Neural Network
 - Fully adaptive (Elman, SRN, ...)
 - Randomized approaches (Reservoir Computing)
 - Gated recurrent networks

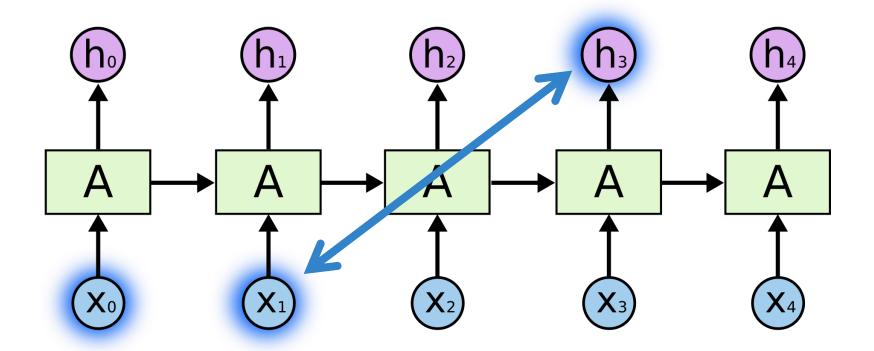
Unfolding RNN (Forward Pass)

By now you should be familiar with the concept model of model unfolding/unrolling on the data data unfolding (Xt) memory encoding Map an arbitrary length sequence $x_0 \dots x_t$ to fixedlength encoding h_t

Supervised Recurrent Tasks

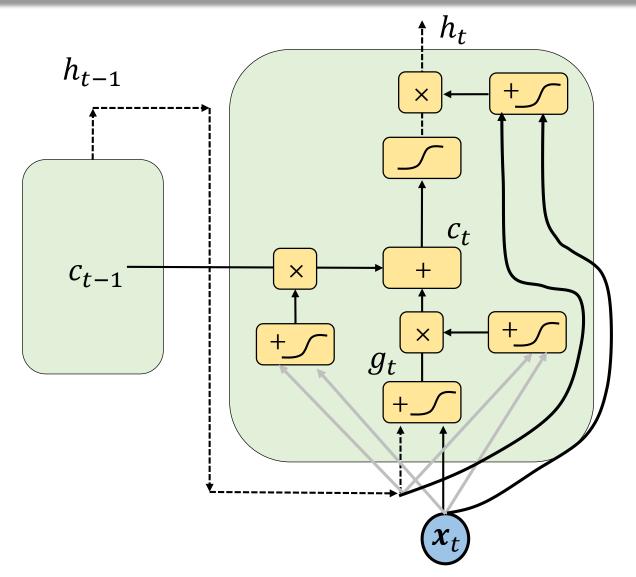


Learning to Encode Input History



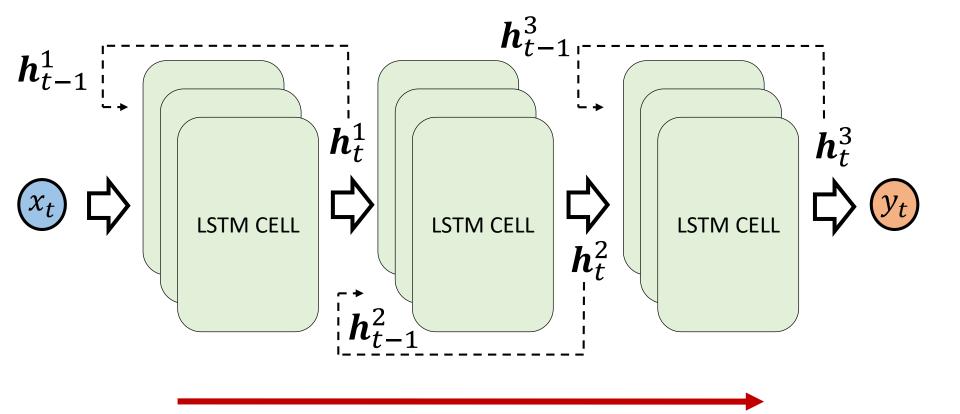
Hidden state h_t summarizes information on the history of the input signal up to time t

Long Short Term Memory – The Cell



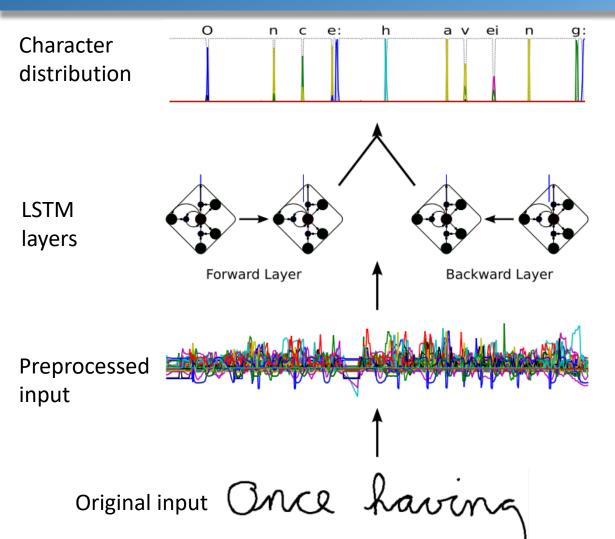
Using gates to control memory access

Deep LSTM



LSTM layers extract information at increasing levels of abstraction (enlarging context)

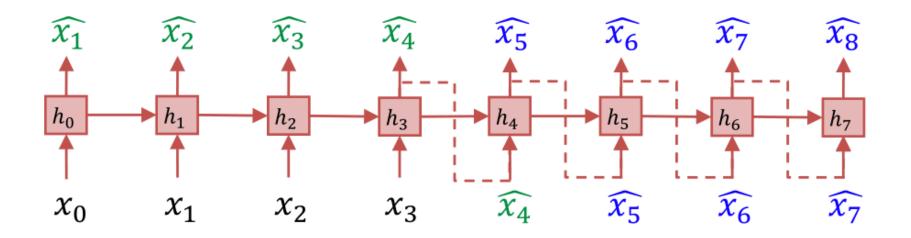
Bidirectional LSTM – Character Recognition

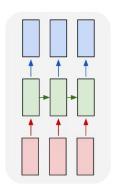


1 output for each character plus no output symbol

A. Graves, A novel connectionist system for unconstrained handwriting recognition, TPAMI 2009

Predicting the future with RNNs





■: RNN Cell

 x_i : ground-truth $(0 \le i < 4)$

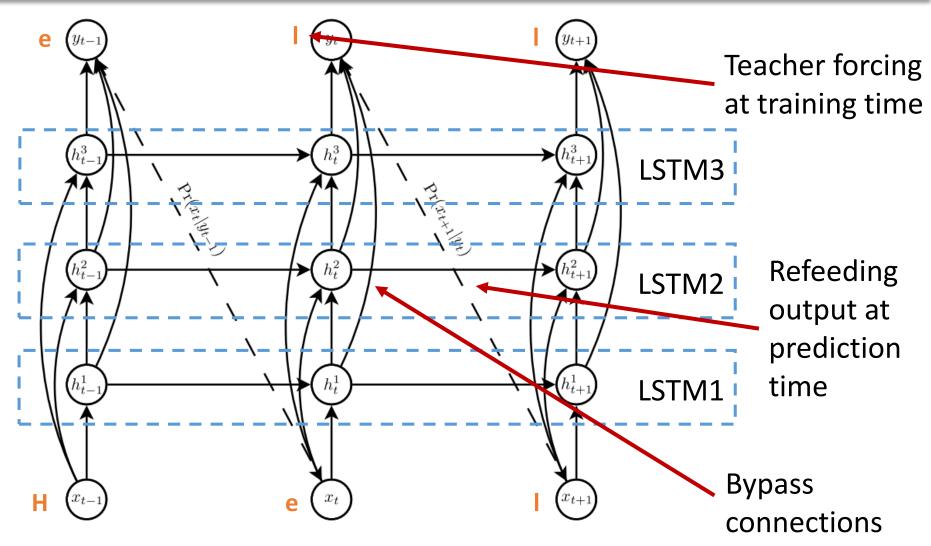
 $\hat{x_i}$: 1-step prediction $(1 \le i < 5)$

 $\hat{x_i}$: multi-step prediction (5 \le i < 9)

 h_i : hidden state $(0 \le i < 9)$

Element-to-element

Generative Use of LSTM/GRU



A. Graves, Generating Sequences With Recurrent Neural Networks, 2013

Character Generation Fun

Shakespeare

PANDARUS:

Alas, I think he shall be come approached and the day

When little srain would be attain'd into being never fed,

And who is but a chain and subjects of his death,

I should not sleep.

Second Senator:

They are away this miseries, produced upon my soul,

Breaking and strongly should be buried, when I perish

The earth and thoughts of many states.

Character Generation Fun

Linux Kernel Code

```
* If this error is set, we will need anything right after that BSD.
static void action new function(struct s stat info *wb)
 unsigned long flags;
 int lel idx bit = e->edd, *sys & \sim((unsigned long) *FIRST_COMPAT);
 buf[0] = 0xFFFFFFF & (bit << 4);
 min(inc, slist->bytes);
 printk(KERN WARNING "Memory allocated %02x/%02x, "
  "original MLL instead\n"),
  min(min(multi run - s->len, max) * num data in),
  frame pos, sz + first seg);
 div u64 w(val, inb p);
 spin unlock(&disk->queue lock);
 mutex unlock(&s->sock->mutex);
 mutex unlock(&func->mutex);
 return disassemble(info->pending bh);
```

Generate Sad Jokes

A 3-LSTM layers neural network to generate English jokes character by character

Why did the boy stop his homework? Because they're bunny boo!

What do you get if you cross a famous California little boy with an elephant for players?
Market holes.

Q: Why did the death penis learn string?

A: Because he wanted to have some

roasts case!

Software

- Standard gated RNN are available in all deep learning frameworks (Python et al) as well as in Matlab's Neural Network Toolbox
- If you want to play with one-element ahead sequence generation try out char-RNN implementations
 - https://github.com/karpathy/char-rnn (ORIGINAL)
 - https://github.com/sherjilozair/char-rnn-tensorflow
 - https://github.com/crazydonkey200/tensorflow-char-rnn
 - http://pytorch.org/tutorials/intermediate/char rnn generation tutorial.html

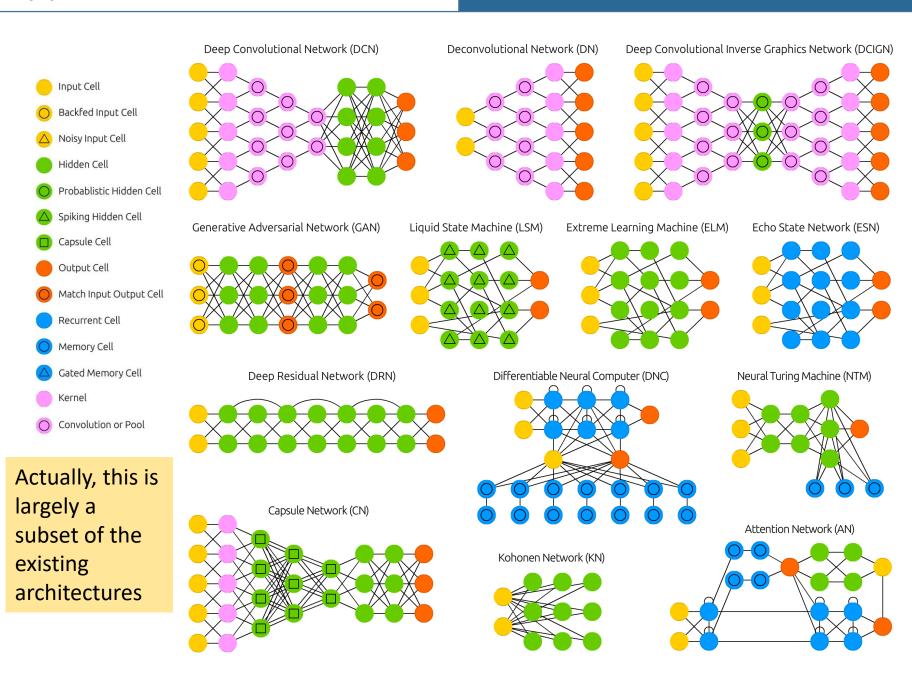
Wrap-Up



Things to Remember

- Vectorial data: feedforward neural networks
- Image data: convolutional neural networks
- Sequential data: recurrent neural networks
- Need to chose:
 - Activation and loss functions
 - Optimization algorithms
- Model selection
 - Train-valid-test
 - Data preprocessing
 - Regularization

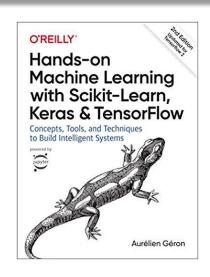
A mostly complete chart of Neural Networks Input Cell Deep Feed Forward (DFF) Backfed Input Cell ©2019 Fjodor van Veen & Stefan Leijnen asimovinstitute.org Noisy Input Cell Perceptron (P) Feed Forward (FF) Radial Basis Network (RBF) Hidden Cell Probablistic Hidden Cell Spiking Hidden Cell Recurrent Neural Network (RNN) Long / Short Term Memory (LSTM) Gated Recurrent Unit (GRU) Capsule Cell Output Cell Match Input Output Cell Recurrent Cell Auto Encoder (AE) Variational AE (VAE) Denoising AE (DAE) Sparse AE (SAE) Memory Cell Gated Memory Cell Kernel Convolution or Pool Markov Chain (MC) Hopfield Network (HN) Boltzmann Machine (BM) Restricted BM (RBM) Deep Belief Network (DBN)

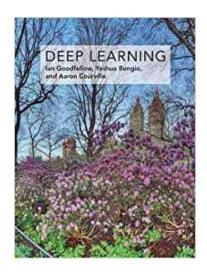


References

A practical handbook to start wrestling with Machine Learning models (2nd ed)

1st edition content is outdated on the NN part!





The reference book for deep learning models

Also freely available online

Advanced ML course @ UNIPI: bit.ly/2rzREqb