Machine learning and physical modelling-2

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NERSC/Sorbonne University

https://github.com/brajard/Geilo-Winter-school

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Steps of a machine learning process

Steps

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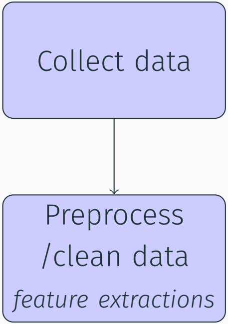

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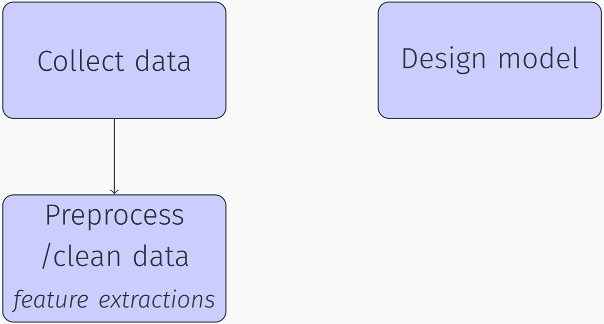

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feature extractions

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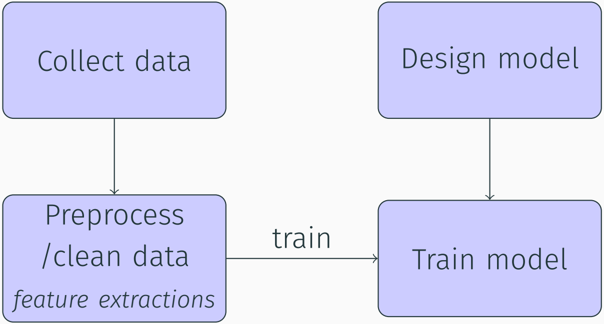
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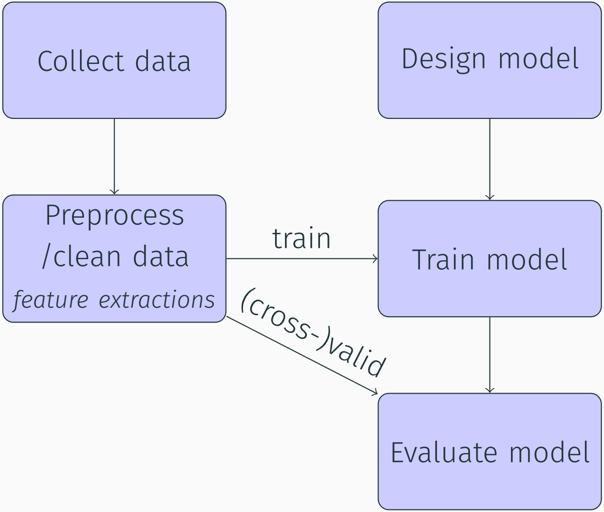

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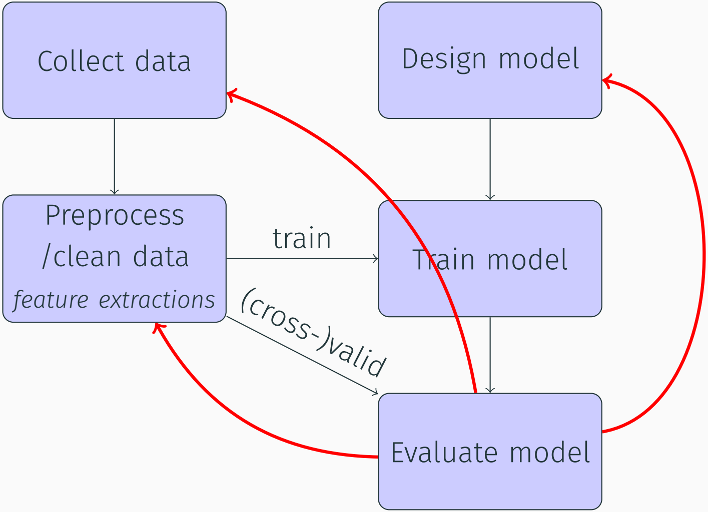
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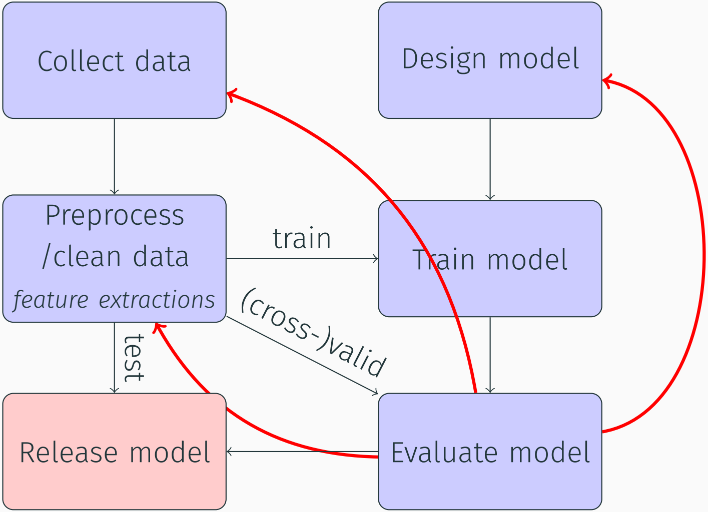
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In summary

From one dataset, 3 sub-datasets have to be extracted:

- A training dataset
- A validation dataset

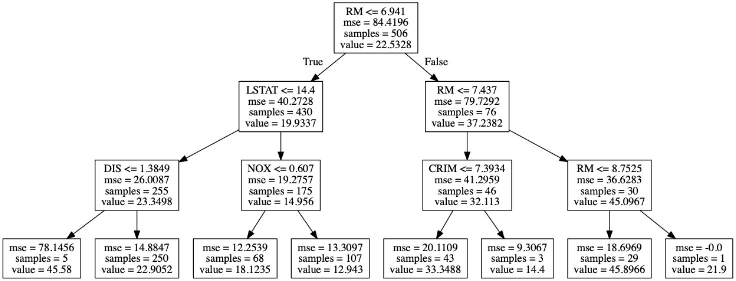
Can be done iteratively in a cross-validation procedure. Some parameters of the model (e.g. polynomial order in a polynomial regression) were determined from the validation dataset.

- A test dataset (independent from the two other) to estimate the final performance of the model.

A standard Machine learning model: Random Forests

A decision tree

Predict house price (in $1000's) from 13 features:



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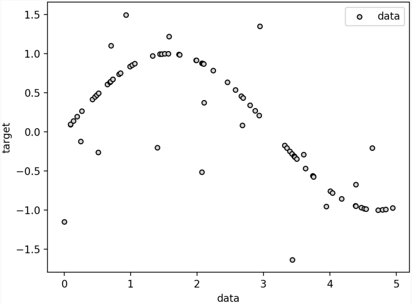
Uni-variate example



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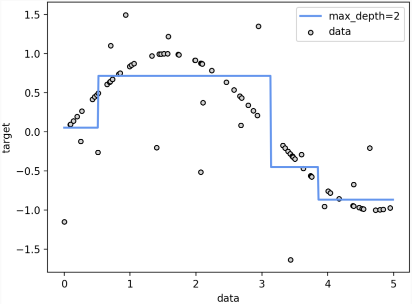

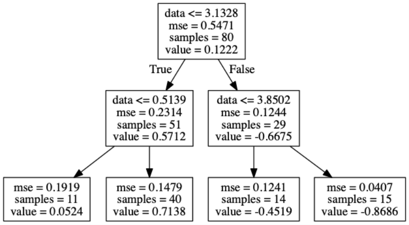

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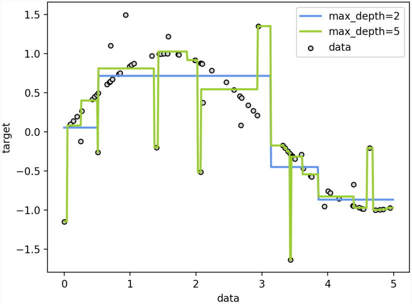

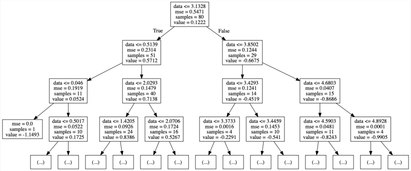

From tree to forest

Disadvantages of regression tree:

- Can overfit the data

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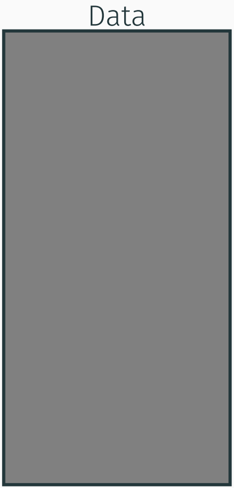
One extension of Regression Tree: Random Forest

The (over simplified) principle of Random Forest



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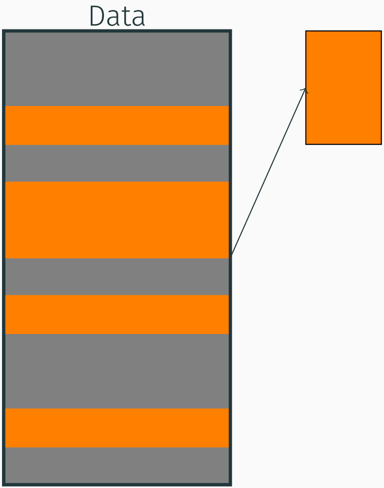

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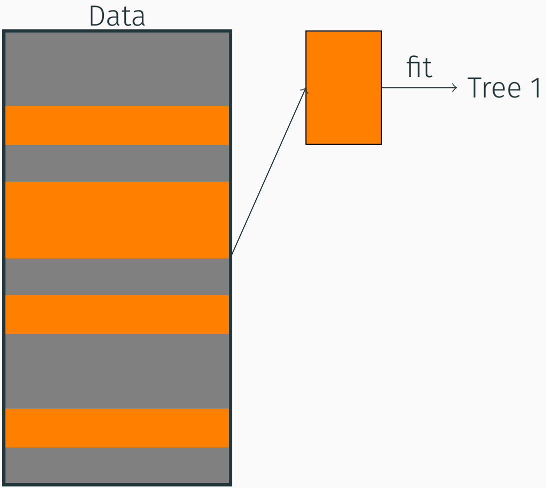

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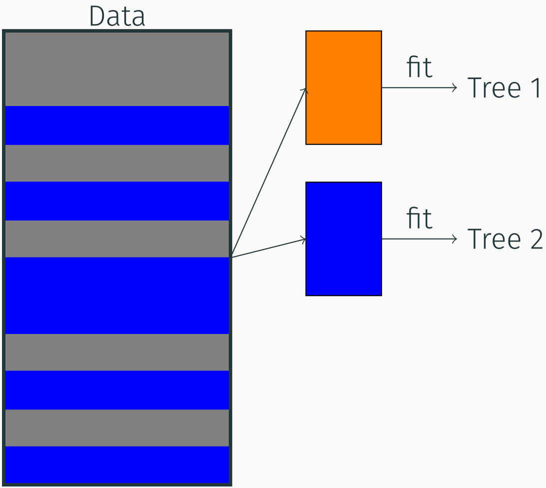

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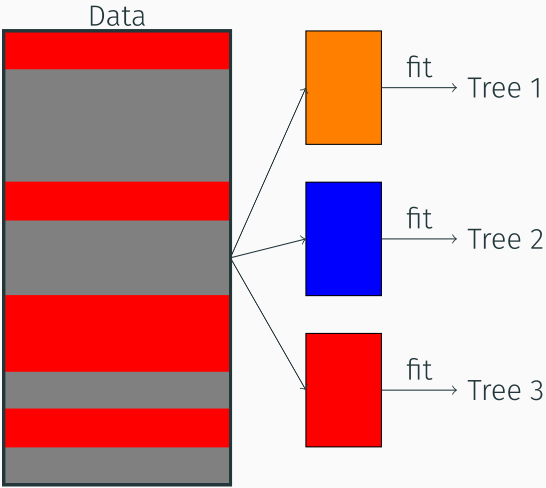

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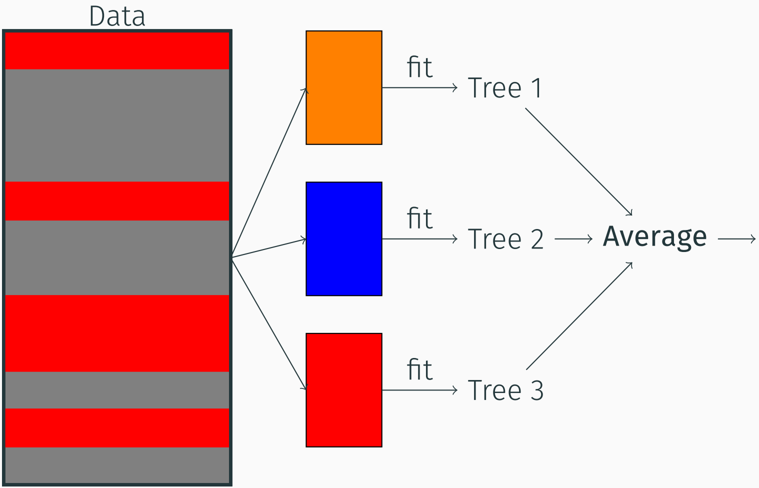
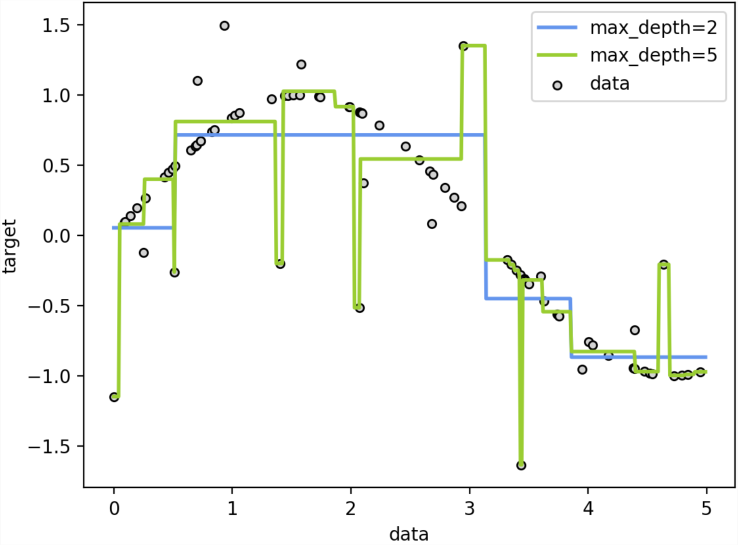


Results on the univariate experiment

Prediction of Randoms trees



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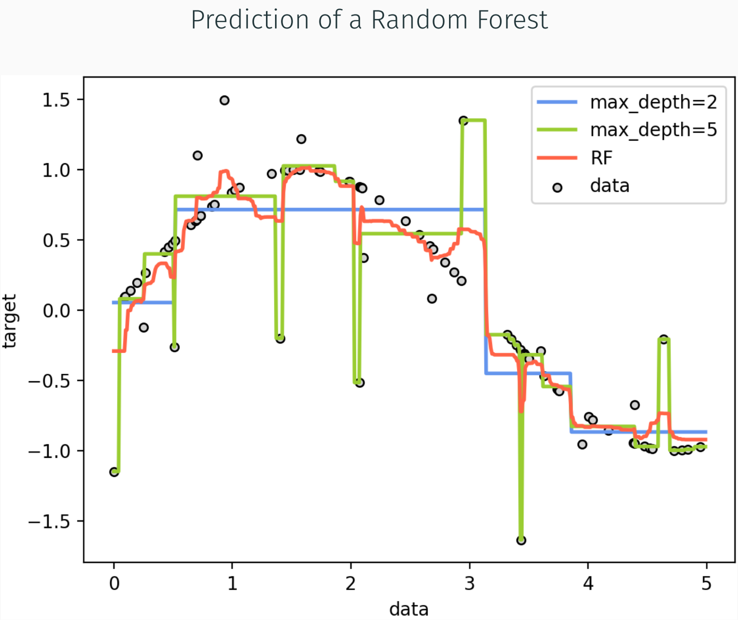

Some key parameters

```python
from sklearn.ensemble import RandomForestClassifier

rf = RandomForestRegressor(n_estimators=n, max_features=
    maxf, min_samples_split=min_split, ...)
```

- `n_estimators`: number of trees (generally the larger is the better)

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- `min_samples_fit`: number of features to consider at each split. The minimum value of 2 means that the tree is fully developed (small bias but great variance).

Determination of the parameters

- Parameters that are not optimized during the training are called hyper parameters.

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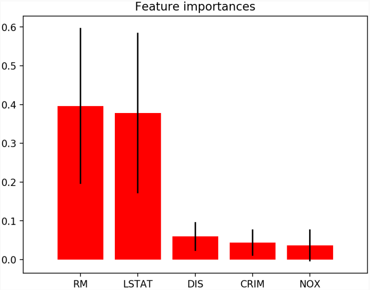
- They can be determined using a score on the validation dataset or using a cross-validation procedure.
- A convenient (but very costly) procedure in scikit-learn: gridsearch.

Example on notebook

Feature importance

```
rf = RandomForestRegressor(n_estimators=1000,
    max_features=10,random_state=10)
rf.fit(X,y)
importances = rf.feature_importances_
```

Indicates the impact of a feature in predicting the target.



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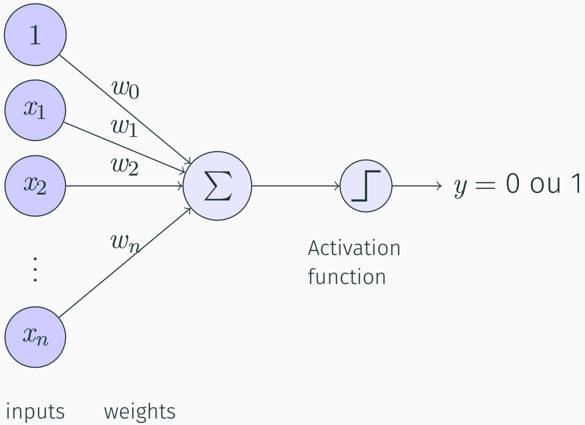
Neural Networks

The perceptron : an artificial neuron



Computation

$$y = f(w_0 + w_1.x_1 + w_2.x_2 + \cdots + w_n.x_n) = f(w_0 + \sum_{i=1}^{n} w_i.x_i)$$

Some remarks

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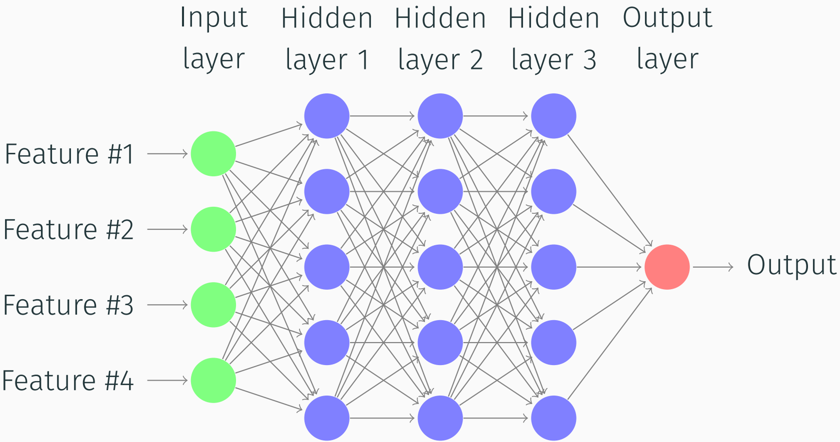
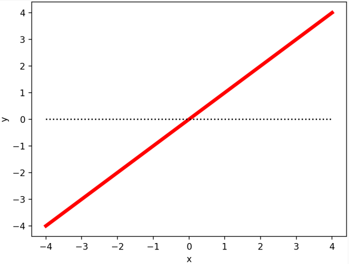
> More complexe models are build by combining several perceptrons

Multi-layer perceptron

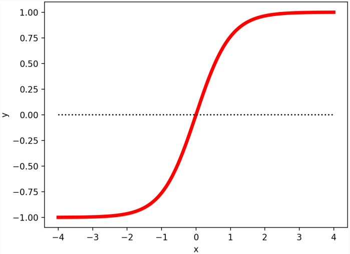


More usual activation functions

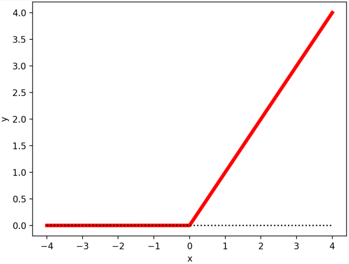
Linear



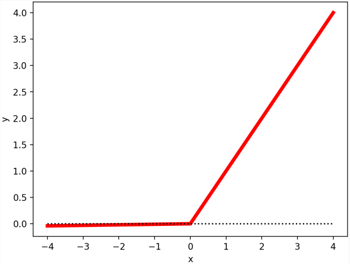
Hyperbolic tangent



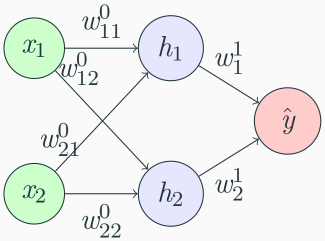
ReLU



Leaky-ReLU



Training a neural-net: gradient backpropagation



Objective

Determination of the best set of weights $\mathbf{w}$ to minimize the Loss function $L = ||\hat{y} - y||$.
Gradient descent algorithms based on $\partial L / \partial w$

1. Given a couple (x, y)

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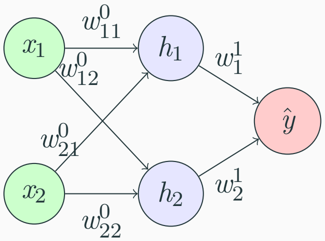

1. Given a couple (x, y)
2. Forward computation:
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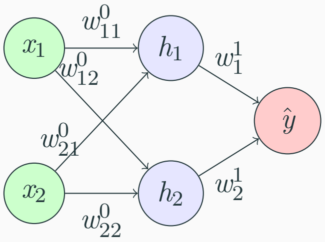

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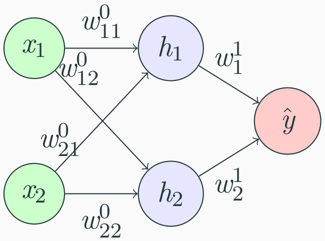

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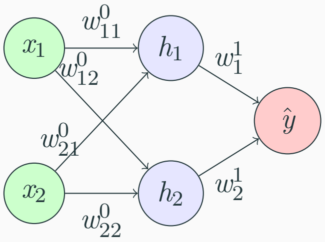

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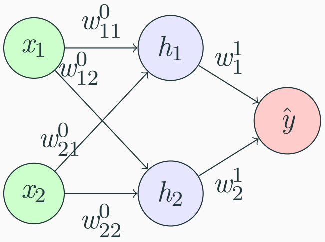

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   - Layer 0
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Classification and regression loss

Regression

- Last layer:
  linear or hyperbolic
  tangent
- Loss function:

$$L(\hat{y}, y) = \sum_i (\hat{y}_i - y_i)^2$$

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Regression

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$$L(\hat{y}, y) = \sum_i (\hat{y}_i - y_i)^2$$

Classification

- Last layer:
  Soft-max

$$p_j = f_j(\mathbf{h}) = \frac{e^{h_j}}{\sum_k e^{h_k}}$$

- Loss function:
  Negative crossentropy

$$L(p, y) = -\sum_i \sum_j y_{i,j}. \log p_{i,j}$$

Batch/Stochastic training

Dataset: (X, y) with N samples, $\mathbf{w}$: initial weights

Batch Training:

- For i from 1 to N:
    1. $L = L + L(f(x_i), y_i)$
- Calculate $\partial L / \partial w$
- update weights:$\mathbf{w}$

1 Update is performed after N forward passes of the neural net.

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Stochastic Training:

- For i from 1 to N:
  1. Compute $L(f(x_i), y_i)$
  2. Calculate $\partial L / \partial w$
  3. update weights:$\mathbf{w}$

N Updates are performed after N forward passes of the neural net.

Batch training

Dataset: (X, y) with N samples, $\mathbf{w}$: initial weights

- for k from 1 to $N//B$:
  - for i from $B(k-1)+1$ to Bk:
    1. Compute $L(f(x_i), y_i)$
  - Calculate $\partial L/\partial w$
  - update weights:$\mathbf{w}$

N//B updates are performed after N forward passes of the neural net

B is the batchsize

- B=1: stochastic training
- B=N: batch training
- Generally B«N

Convolutional neural net

X: an image

x_{11}	x_{12}	x_{13}	x_{14}	x_{15}	x_{16}
x_{21}	x_{22}	x_{23}	x_{24}	x_{25}	x_{26}
x_{31}	x_{32}	x_{33}	x_{34}	x_{35}	x_{36}
x_{41}	x_{42}	x_{43}	x_{44}	x_{45}	x_{46}
x_{51}	x_{52}	x_{53}	x_{54}	x_{55}	x_{56}
x_{61}	x_{62}	x_{63}	x_{64}	x_{65}	x_{66}

$$\begin{matrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{matrix}$$

$\mathbf{w}$

h: first feature

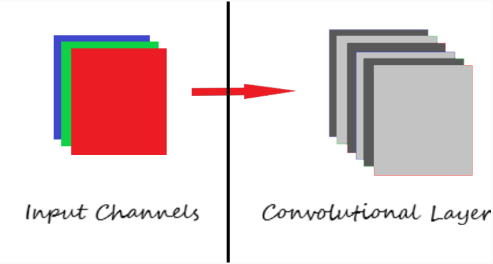
h_{11}	h_{12}	h_{13}	h_{14}
h_{21}	h_{22}	h_{23}	h_{24}
h_{31}	h_{32}	h_{33}	h_{34}
h_{41}	h_{42}	h_{43}	h_{44}

Perform a standard convolution

$$h_{i,j} = \sum_{k=1}^{3} \sum_{l=1}^{3} x_{i+k-1,j+l-1} \cdot w_{k,l}$$

Convolutional layer

A convolutional layer is composed of p convolutions (size of layer) extracting p features from the data.



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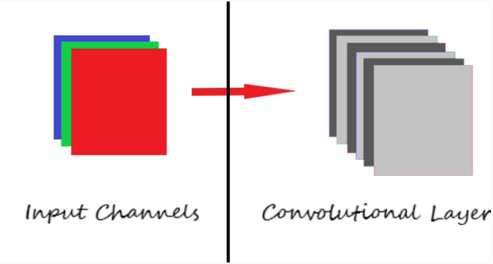
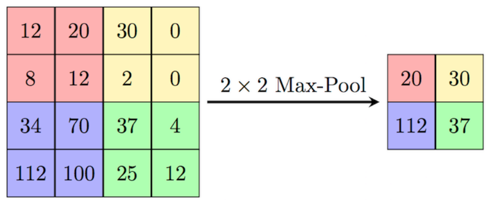


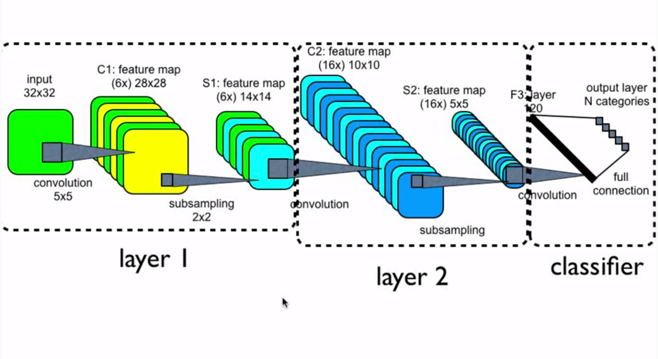
The size of the feature space is generally very big

Max-Pooling

In order to reduce the size of the feature space, a common operation is to perform a max-pooling.



A traditionnal CNN architecture



Example of AlexNet

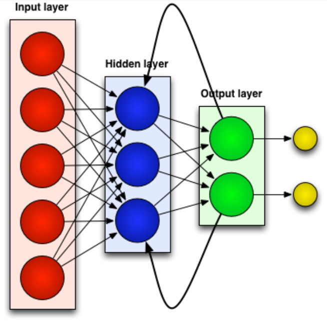
AlexNet is the first Deep architecture used on ImageNet challenge in 2012 and achieved an error of 15.3% (10% better than the previous best classifier). The paper was cited more than 34,000 times.

Alex Krizhevsky and Geoffrey E Hinton, *ImageNet Classification with Deep Convolutional Neural Networks*, Neural Information Processing Systems (2012), 1–9.

Layer		Feature Map	Size	Kernel Size	Stride	Activation
Input	Image	1	227x227x3	-	-	-
1	Convolution	96	55 x 55 x 96	11x11	4	relu
	Max Pooling	96	27 x 27 x 96	3x3	2	relu
2	Convolution	256	27 x 27 x 256	5x5	1	relu
	Max Pooling	256	13 x 13 x 256	3x3	2	relu
3	Convolution	384	13 x 13 x 384	3x3	1	relu
4	Convolution	384	13 x 13 x 384	3x3	1	relu
5	Convolution	256	13 x 13 x 256	3x3	1	relu
	Max Pooling	256	6 x 6 x 256	3x3	2	relu
6	FC	-	9216	-	-	relu
7	FC	-	4096	-	-	relu
8	FC	-	4096	-	-	relu
Output	FC	-	1000	-	-	Softmax

A quick typology of few neural nets

Recurrent Neural Networks

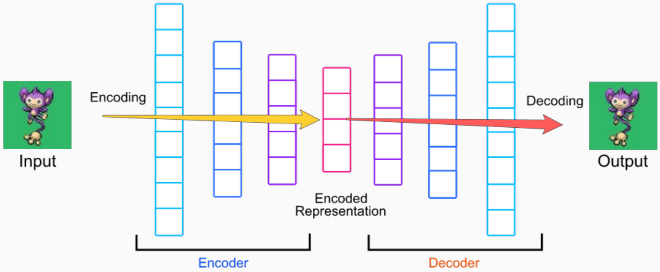


Some popular types of recurrent neural networks:

- Long short-term memory (LSTM)
- Gated Reccurent Unit (GRU)

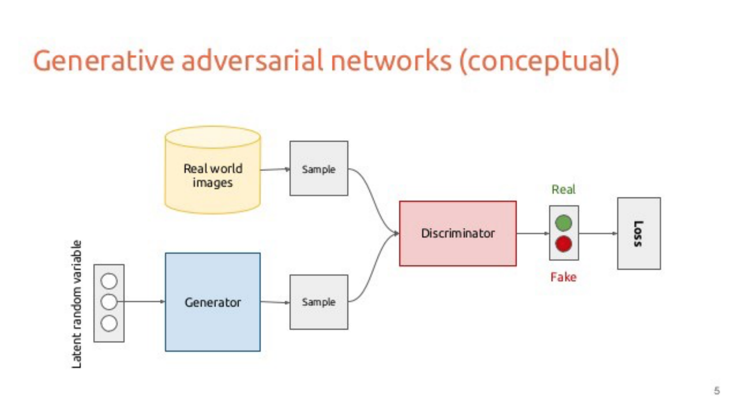
Used in machine translation and text processing

Autoencoders

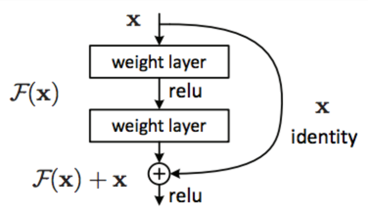


Used in image denoising, compressing, generation,...

Generative adversarial networks



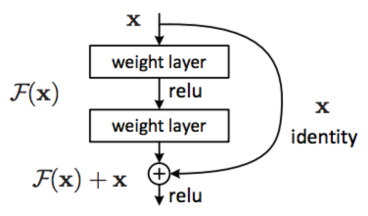
Residual Networks



x : input, y : output

$$y = x + \mathcal{F}(x)$$

Residual Networks



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