Machine learning and physical modelling-2

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NERSC

https://github.com/brajard/MAT330

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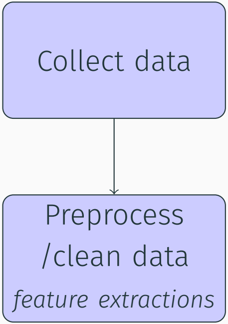
Steps of a machine learning process

Steps

Collect data

Steps



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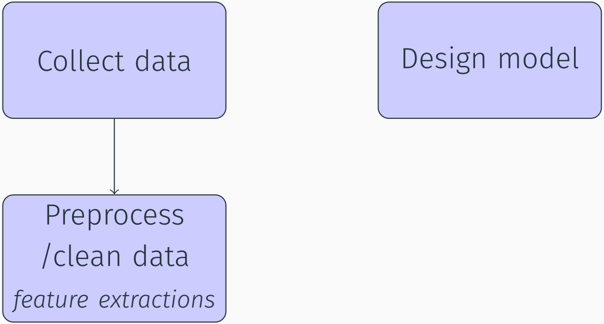
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Preprocess
/clean data
feature extractions

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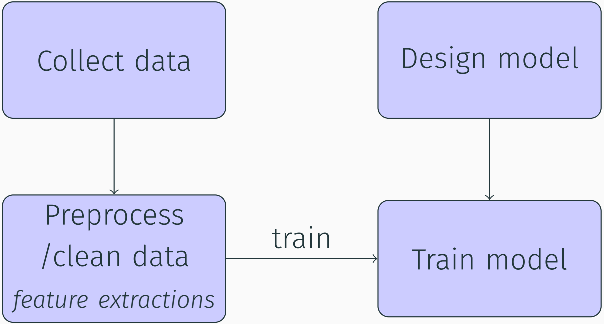

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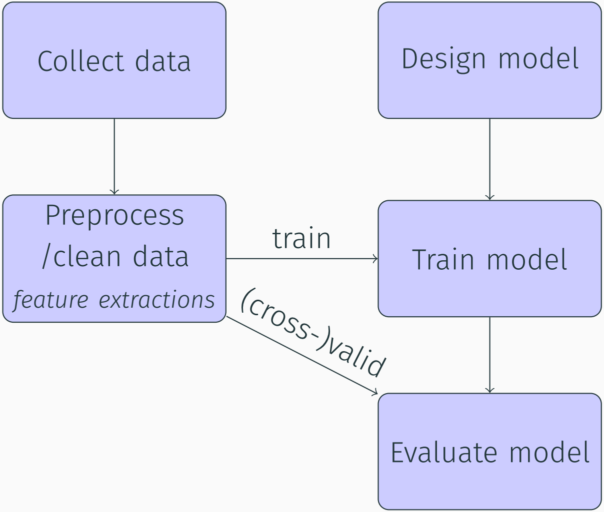

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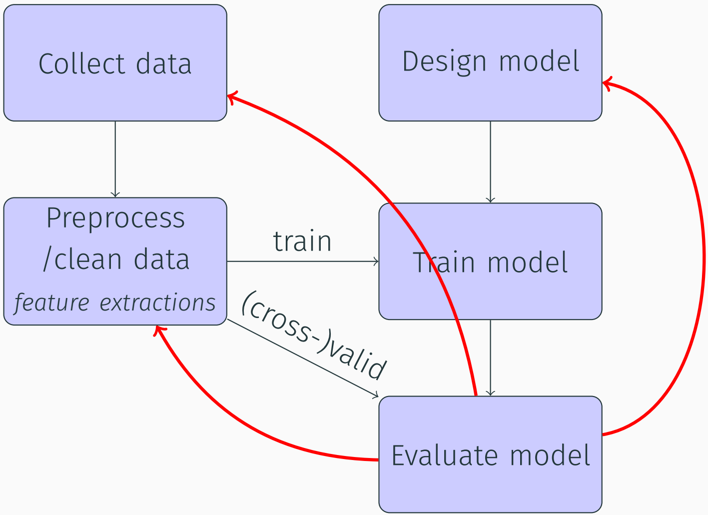
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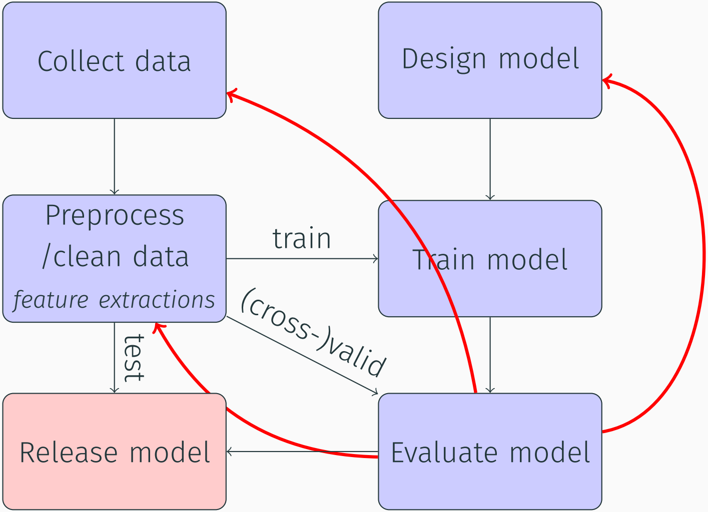
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test
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Evaluate model

In summary

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

- A training dataset
- A validation dataset

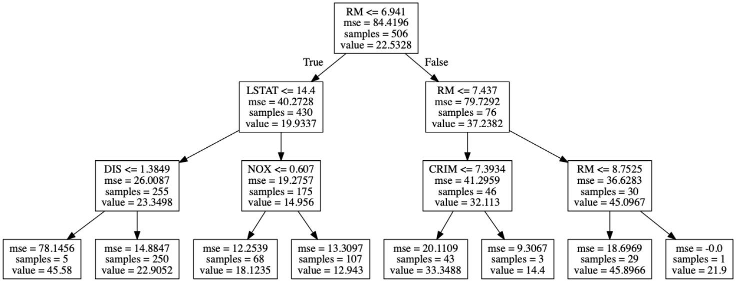
Can be done iteratively in a cross-validation procedure. Some parameters of the model (e.g. polynomial order in a polynomial regression) were determined from the validation dataset.

- 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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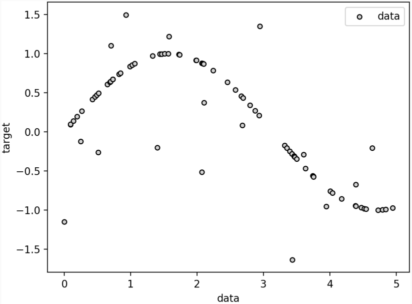
Uni-variate example



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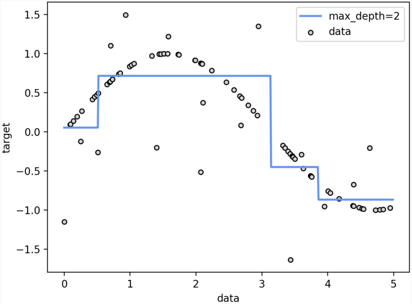

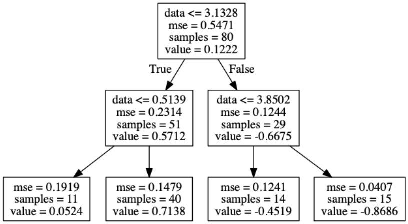

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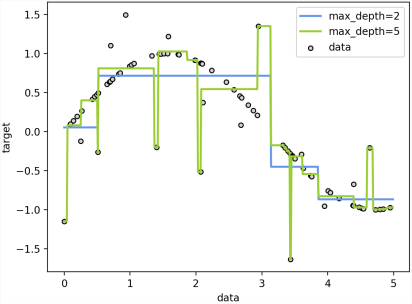

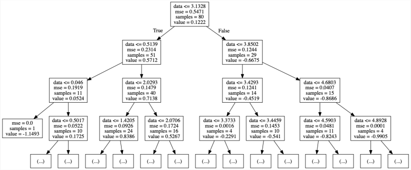

From tree to forest

Disadvantages of regression tree:

- Can overfit the data

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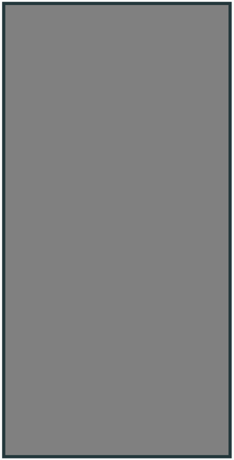
One extension of Regression Tree: Random Forest

The (over simplified) principle of Random Forest

Data



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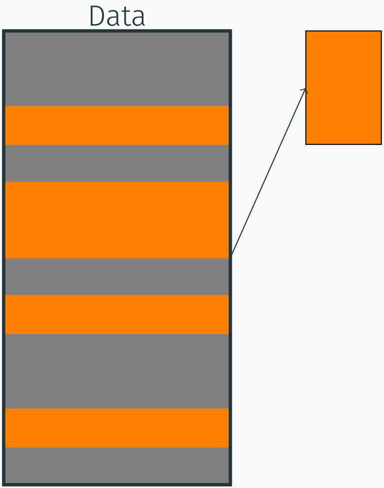

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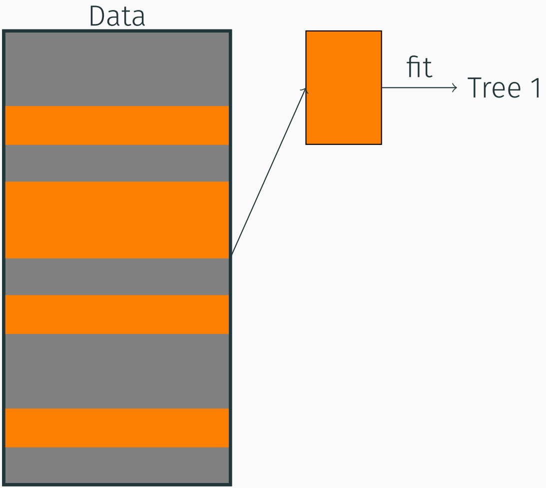

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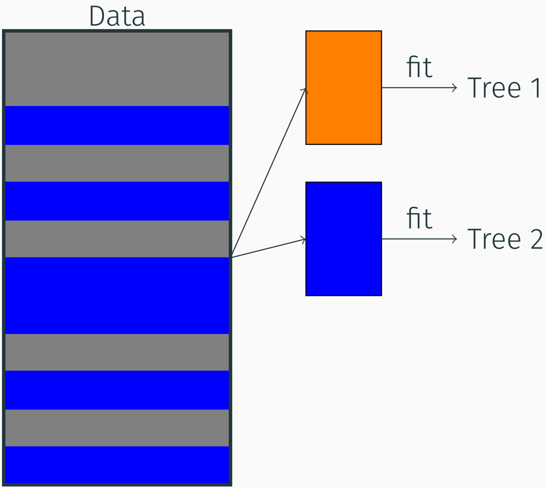

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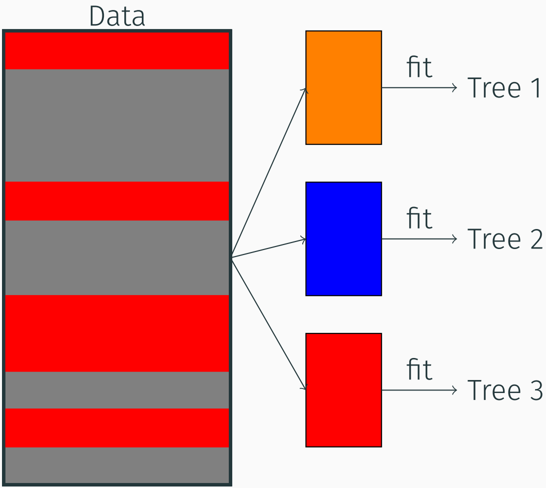

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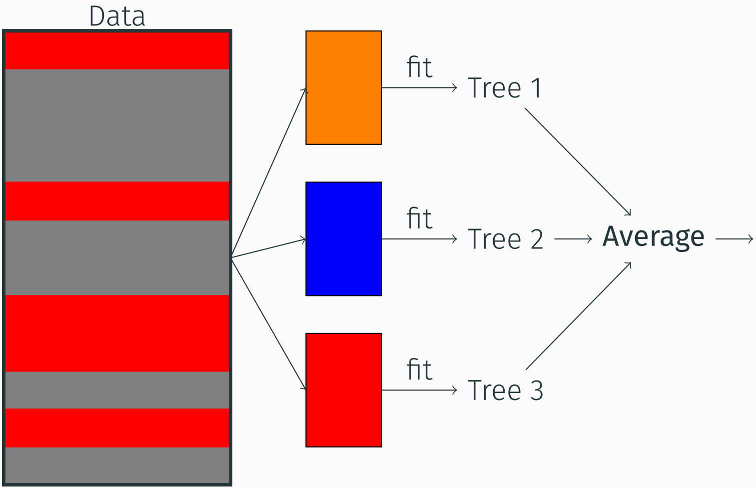
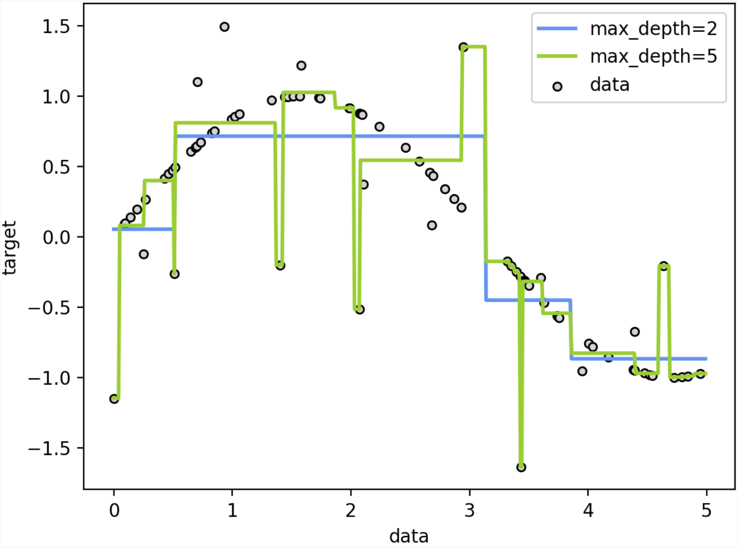


Results on the univariate experiment

Prediction of Randoms trees



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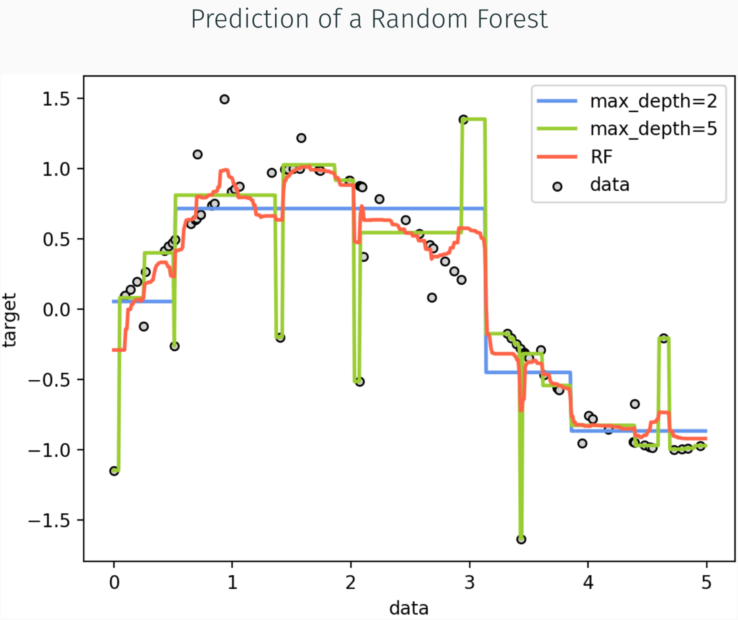

Some key parameters

```
from sklearn.ensemble import RandomForestClassifier

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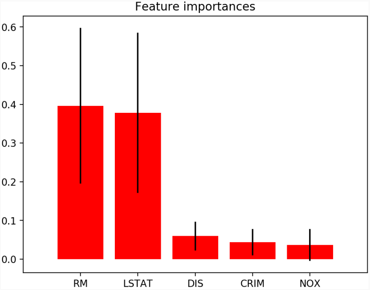
- `min_samples_fit`: number of features to consider at each split. The minimum value of 2 means that the tree is fully developed (small bias but great variance).

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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Determination of the hyperparameters

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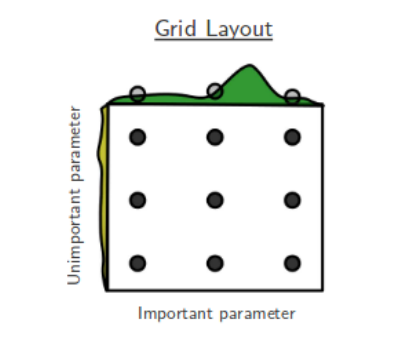
https://xkcd.com/1838/

Stir the pile: The gridsearch

1. Specify a list of hyperparameters to be tested.
2. For each of the parameters, specify a set of values to test
3. Train a model for each of the possible combinations of hyperparameters
4. Retain the best model (using, e.g., cross-validation)



`https://medium.com/@senapati.dipak97/grid-search-vs-random-search-d34c92946318`

Remarks on the gridsearch procedure

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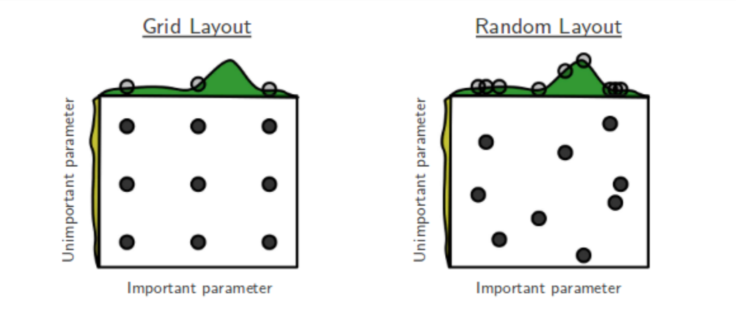
- The procedure is easy to parallelized.
- it is not naturally adapted for quantitative hyperparameters.
- it can become very costly. (e.g. 8 hyperparameters with 8 values each to test = $8^8 = 16,777,216$ trainings.

Random search

1. Specify a list of hyperparameters to be tested.
2. For each of the parameters, specify a set of values to test or a law to draw a random value.
3. Draw n combinations of the hyperparameters.
4. Train a model for each of the combinations.
5. Retain the best model (using, e.g., cross-validation)



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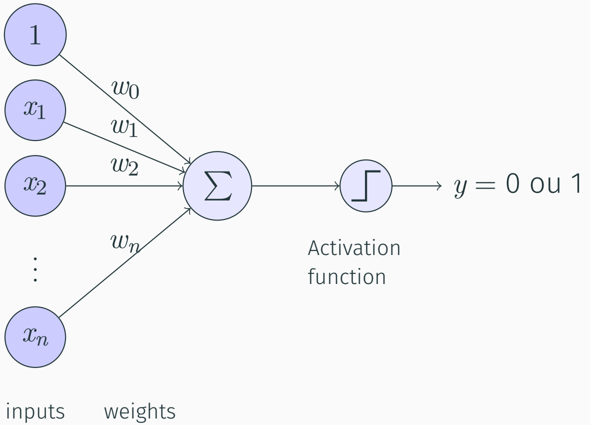
Both gridsearch and random search are implemented and easy to use in scikit-learn.

Neural Networks

The perceptron : an artificial neuron



Computation

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

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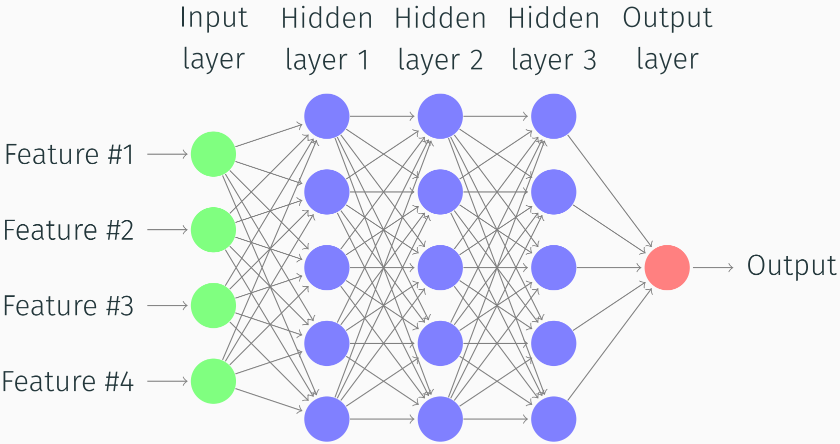
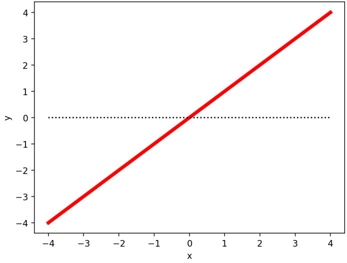
More complexe models are build by combining several perceptrons

Multi-layer perceptron (Densely connected layers)

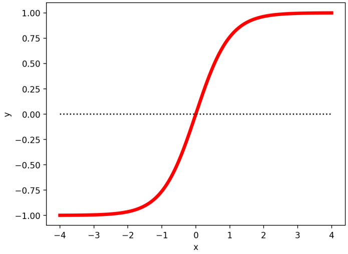


Most usual activation functions

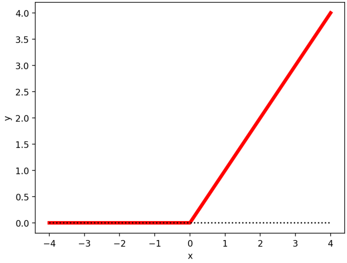
Linear



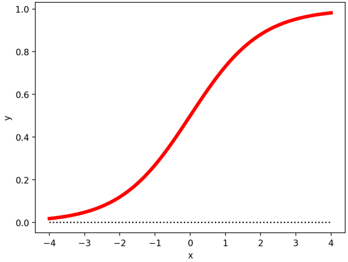
Hyperbolic tangent



ReLU

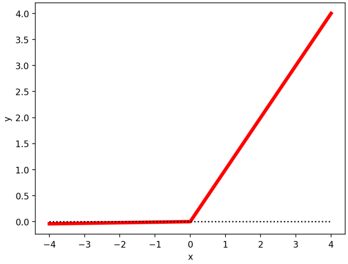


Sigmoid

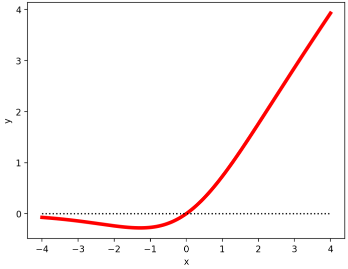


New fancy activation functions

Leaky-ReLU



Swish



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

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

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}

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

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

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

Main parameters of a convolutional layer

- Size of the filter K

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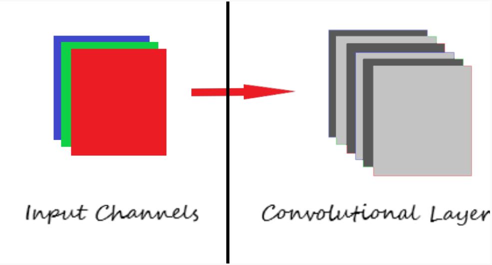
  A convolutional layer is composed of p convolutions (size of layer) extracting p features from the data.



$O = \frac{W-K+2P}{S} + 1$, where O is the output size and W the input size.

Main parameters of a convolutional layer

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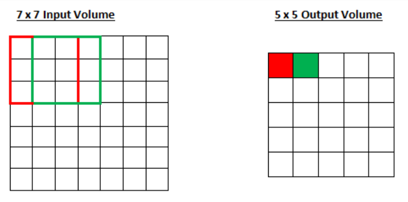
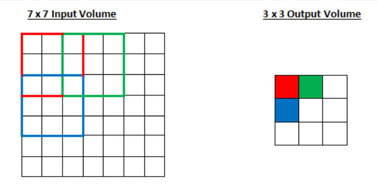
- Strides S

$S = 1$ $\qquad\qquad\qquad\qquad$ $S = 2$





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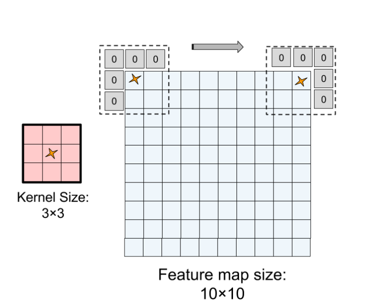
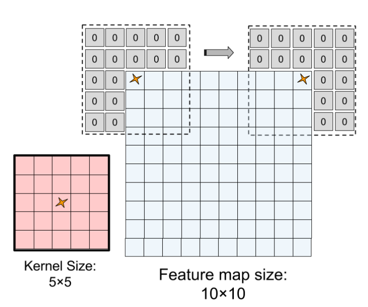
- Strides S
- Padding P

$P = 1$



$P = 2$



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Summary of Convolutional layer steps

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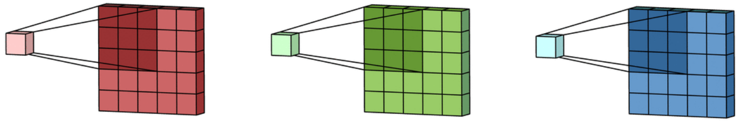

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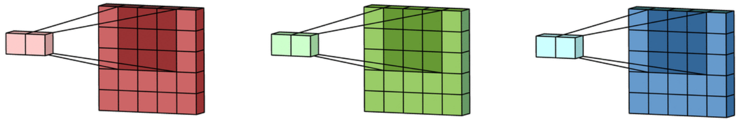

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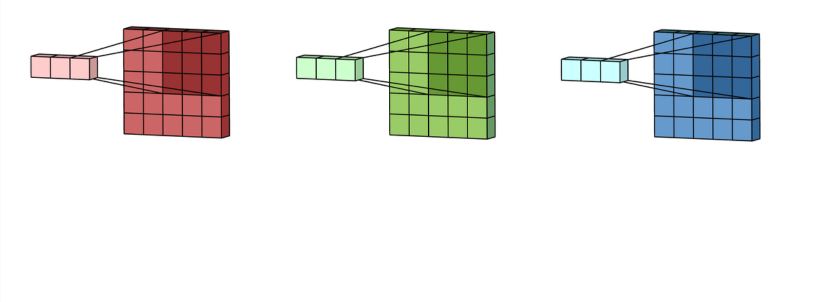

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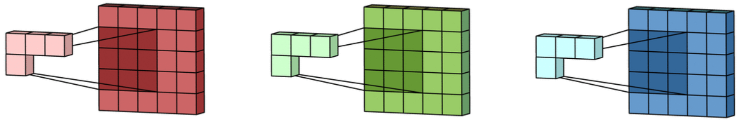

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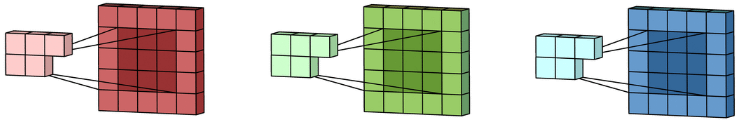

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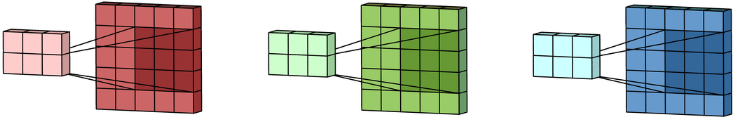

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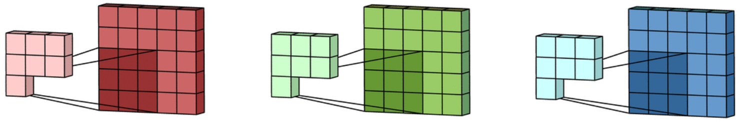

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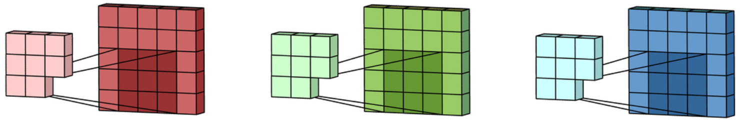

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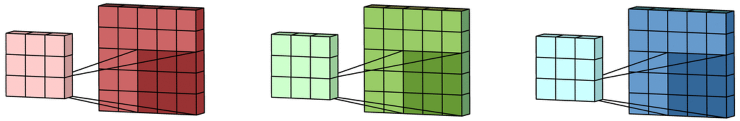

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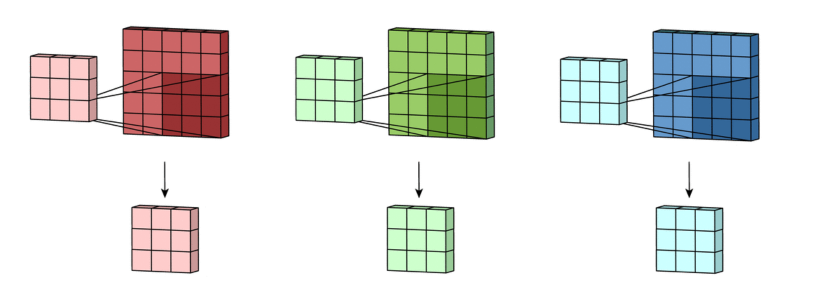

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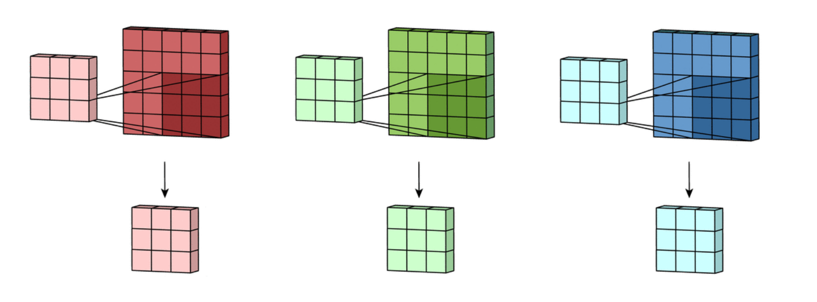

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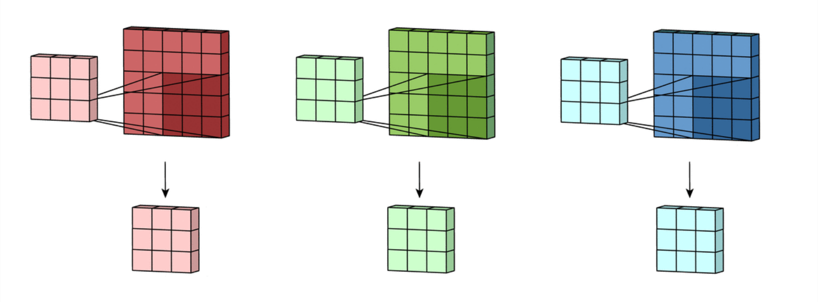
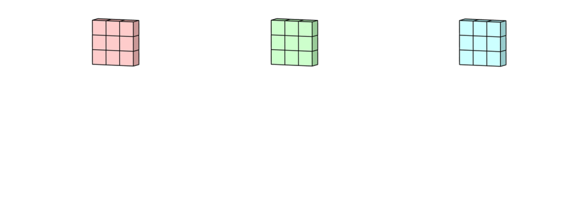
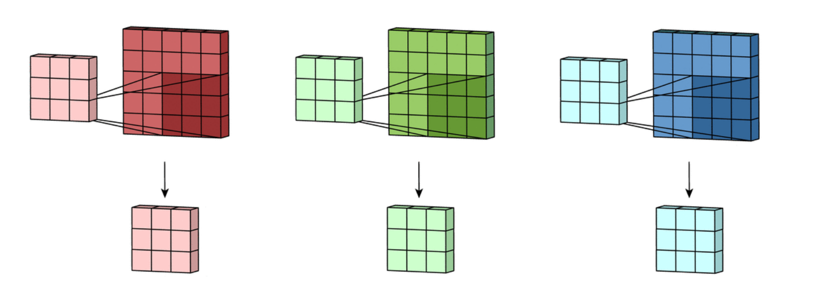


2. Addition

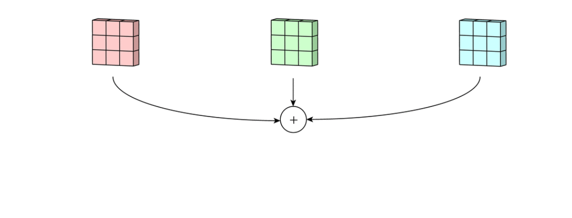


Summary of Convolutional layer steps

1. Convolution



2. Addition



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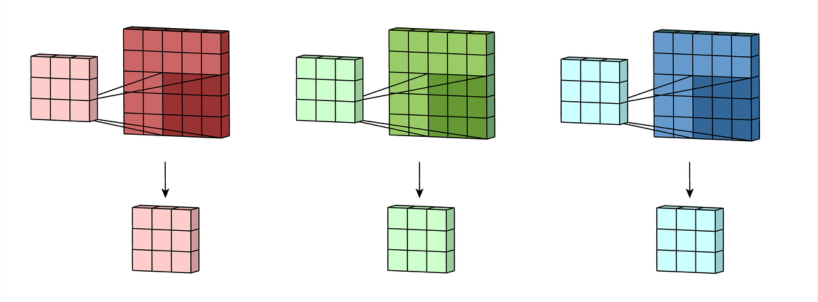

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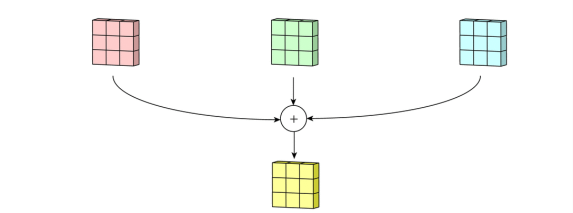

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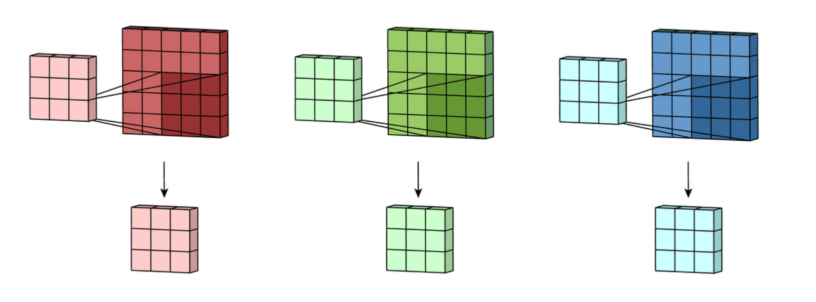

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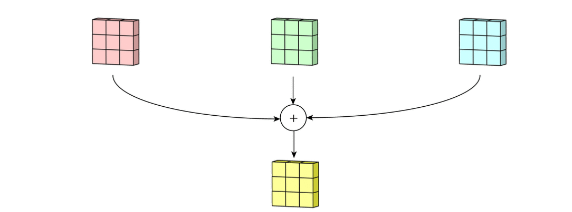

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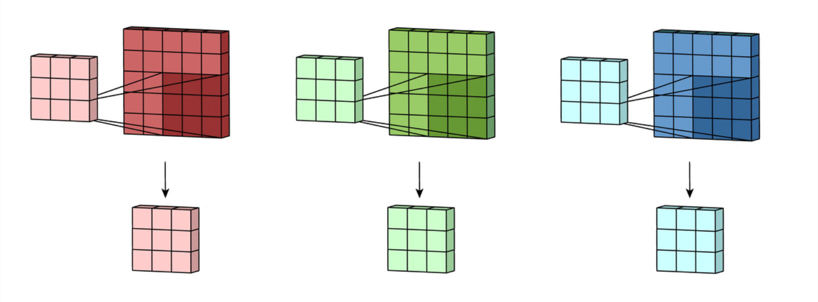

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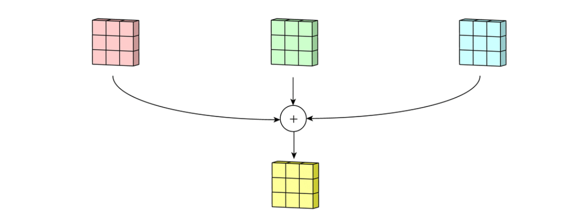
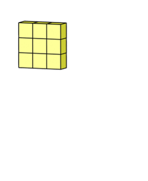


3. Bias



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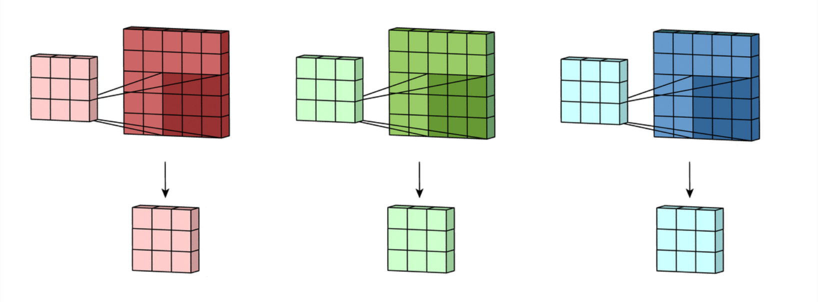

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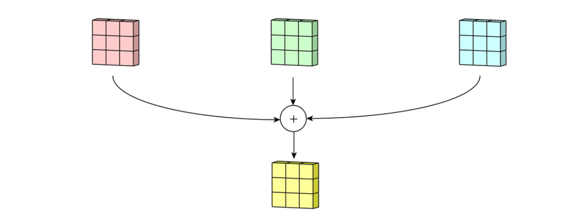

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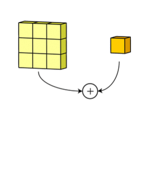

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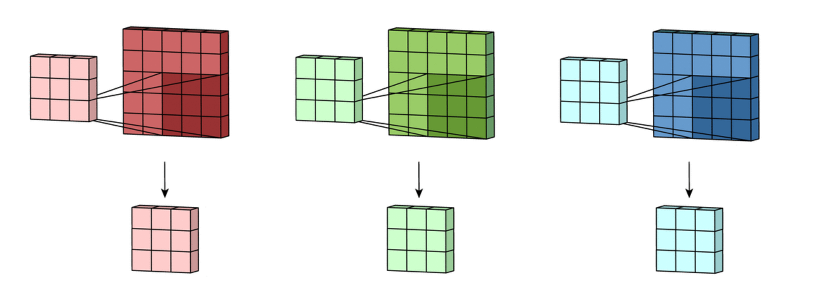

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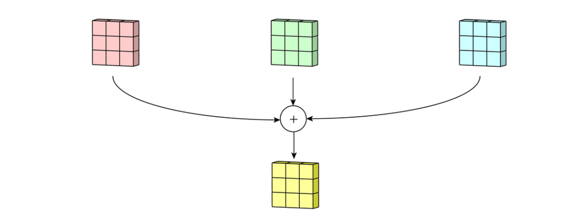

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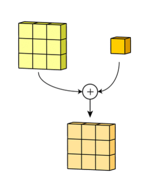
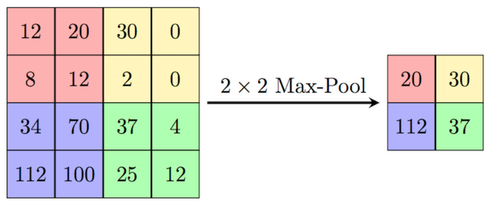


Remarks on Convolutional layers

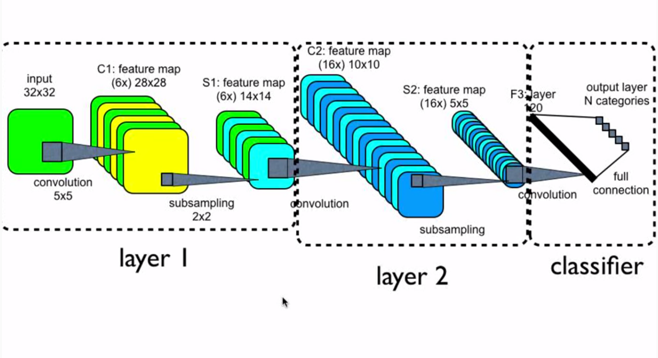
- Convolutional layers are acting locally on the image (But you can still use large scale information by adding more layers)
- Convolutions are invariant by translation (the weights do not depend on the location on the image).
- They can handle images of different sizes.

Max-Pooling

In order to reduce the size of the feature space (en to enhance the gradients), a common operation is to perform a max-pooling.



A traditionnal CNN architecture



Example of AlexNet

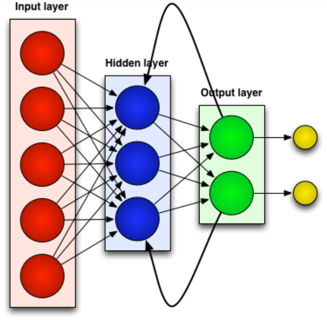
AlexNet is the first Deep architecture used on ImageNet challenge in 2012 and achieved an error of 15.3% (10% better than the previous best classifier). The paper was cited more than 34,000 times.

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

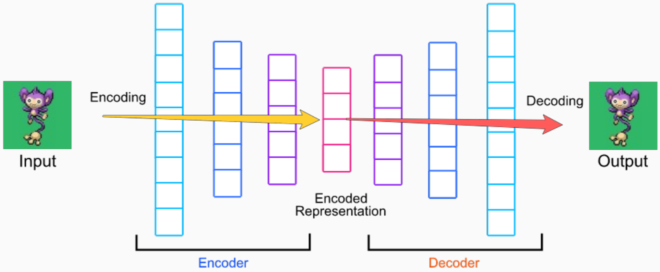


Some popular types of recurrent neural networks:

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

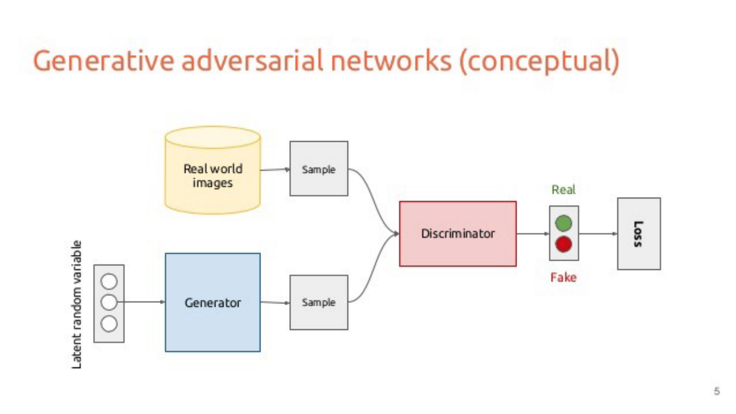
Used in machine translation and text processing

Autoencoders

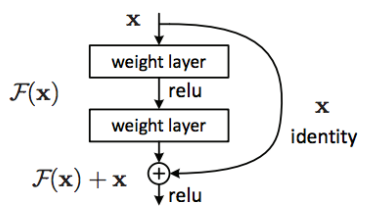


Used in image denoising, compressing, generation,...

Generative adversarial networks



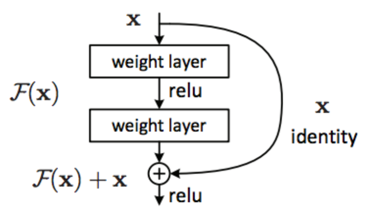
Residual Networks

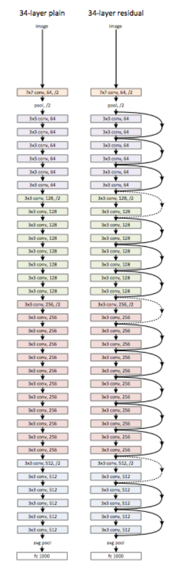


x : input, y : output

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

Residual Networks





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Questions addressed in this lecture

- What are the steps of a machine learning process?
- What is the principle of the Random Forests? [Van16,5.8]
- How to determine the hyperparamters? [Van16,5.3]
- What is a artificial neural network? [GBC16,6]
- What is a convolutive layers [GBC16,9]
- What are the main types of neural networks? [GBC16,10, 14, 20]

https://towardsdatascience.com/intuitively-understanding-convolutions-for-deep-learning-1f6f42faee1

Refs

[Van16,n]: Jake VanderPlas, *Python Data Science Handbook*, section n
[GBC16,n]: Goodfellow etal., Deep Learning, chapter n