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

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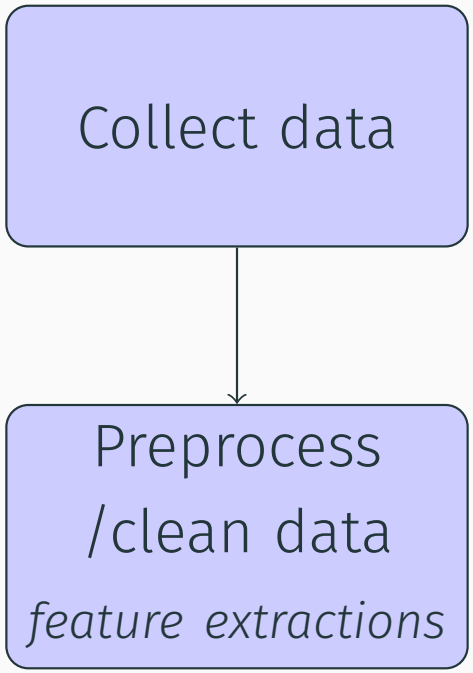

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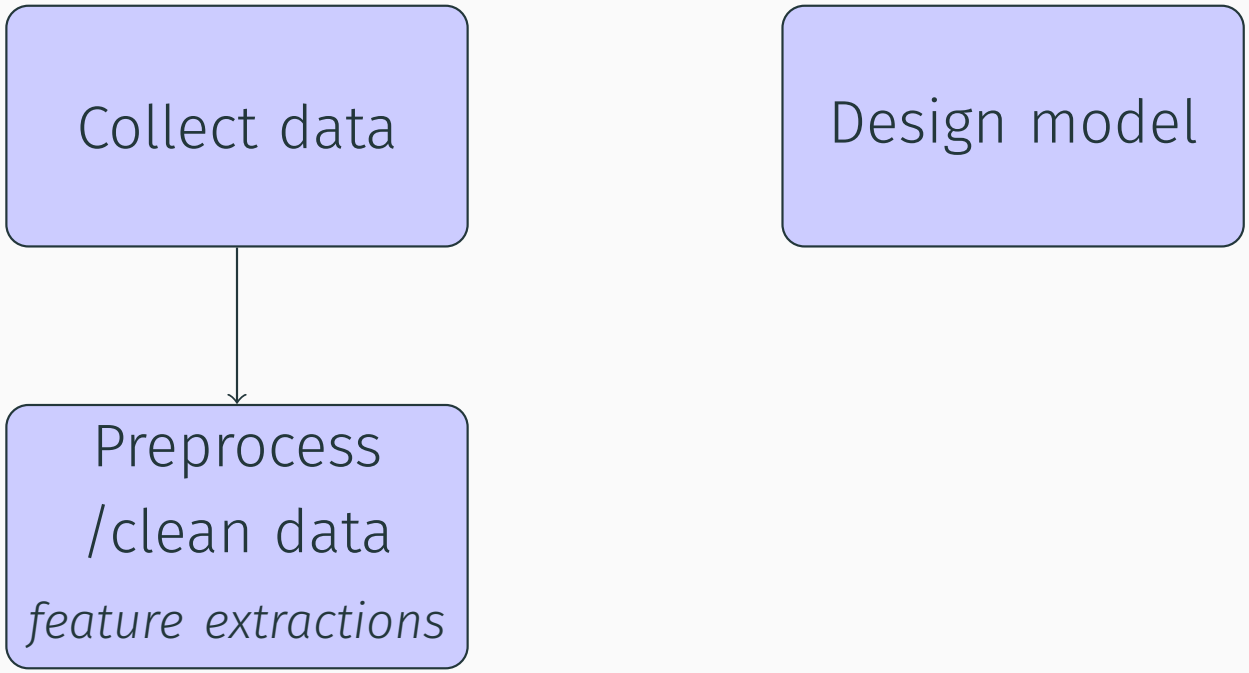
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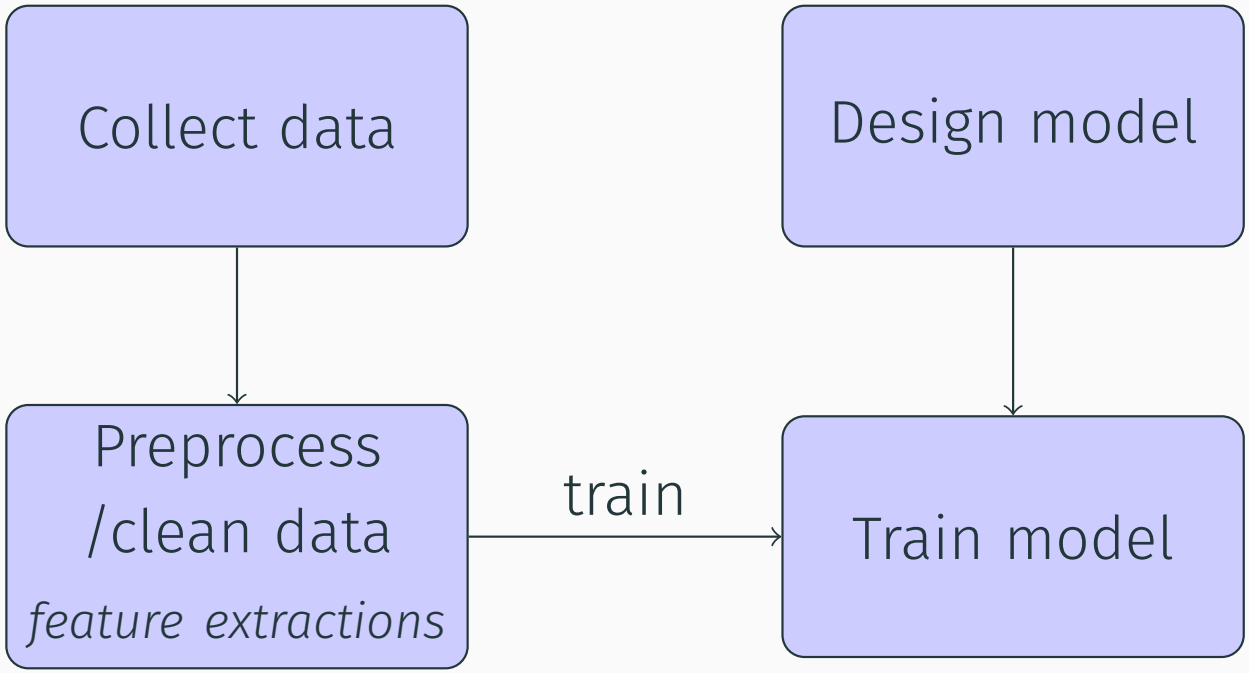
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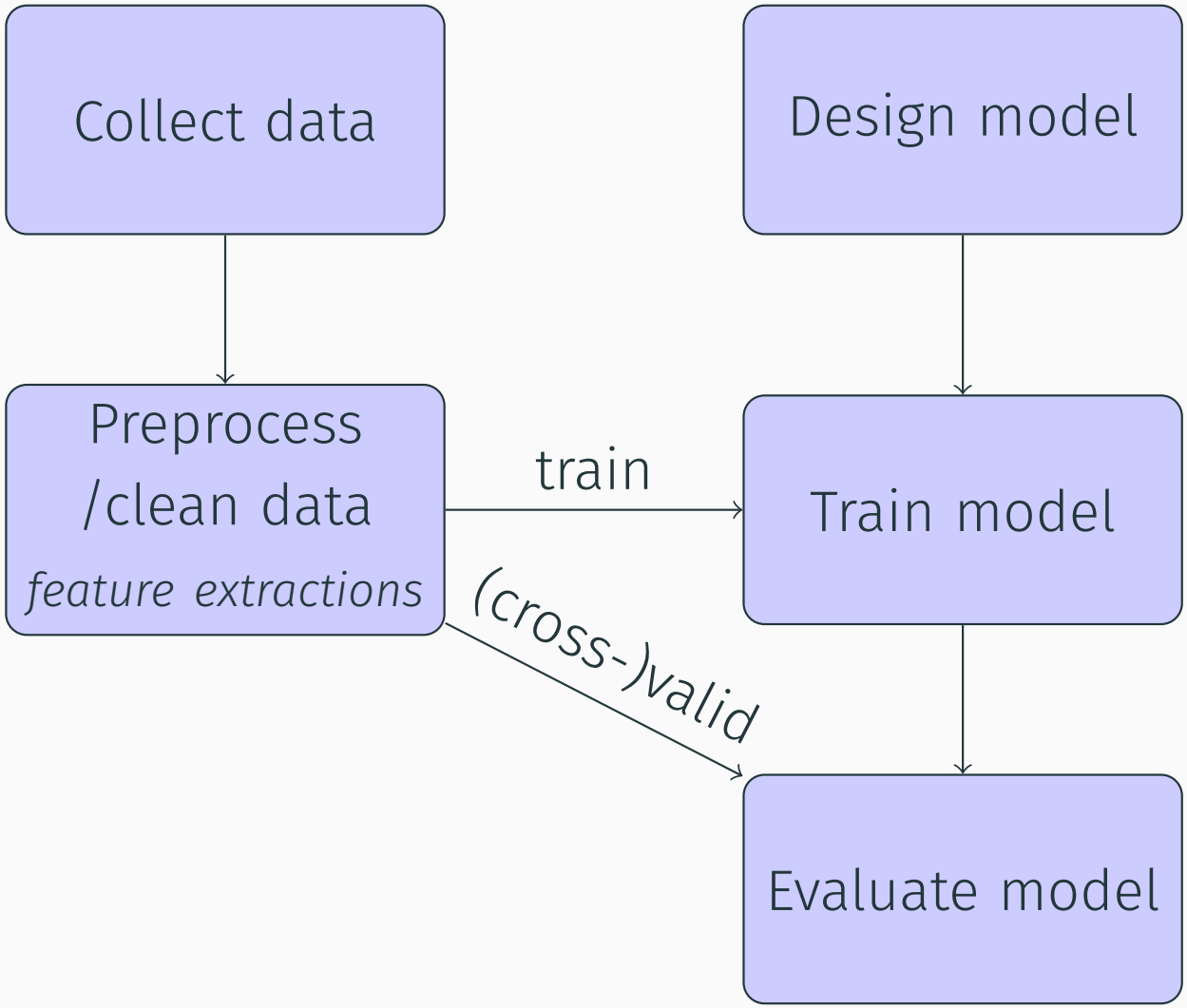
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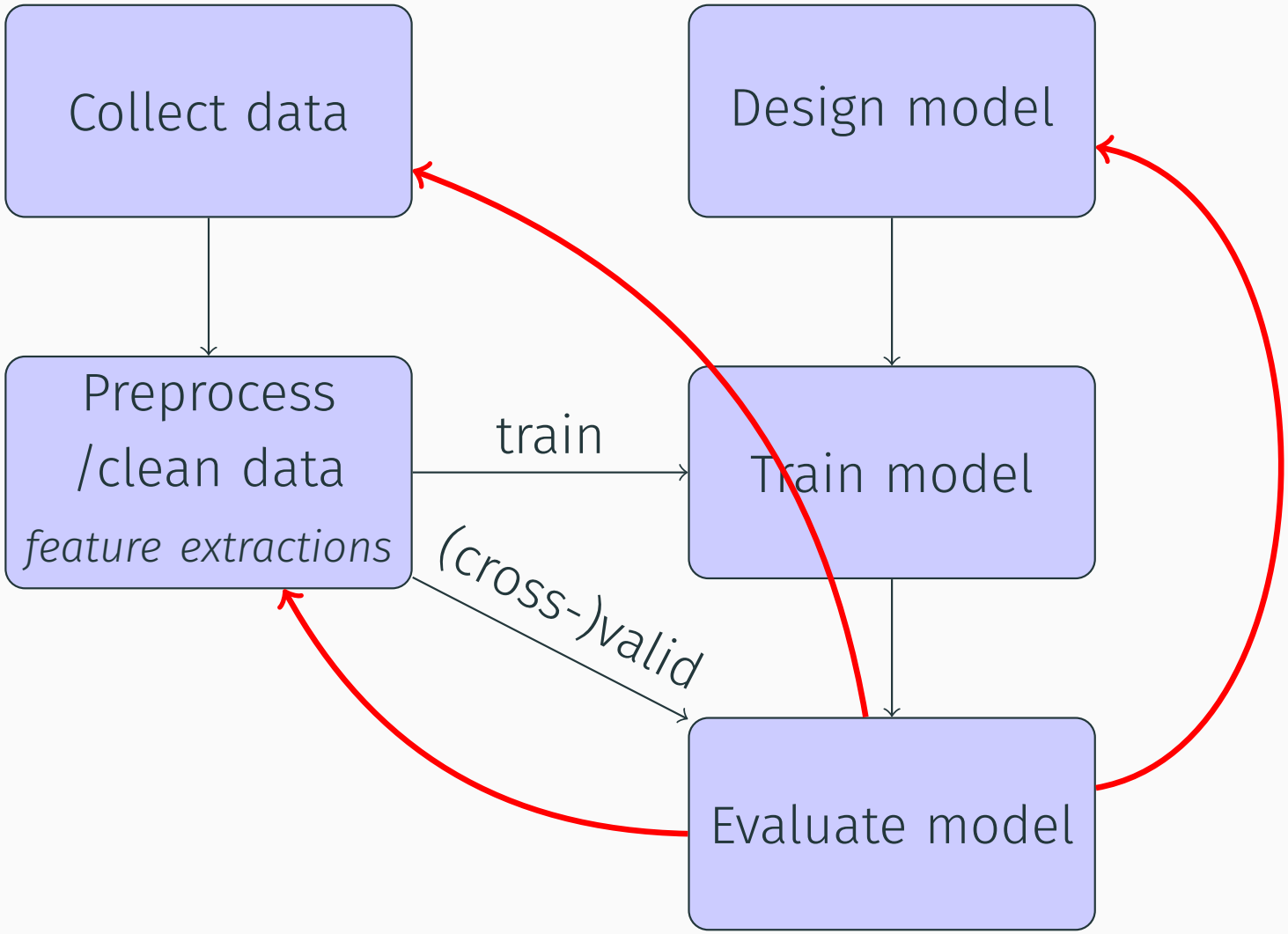
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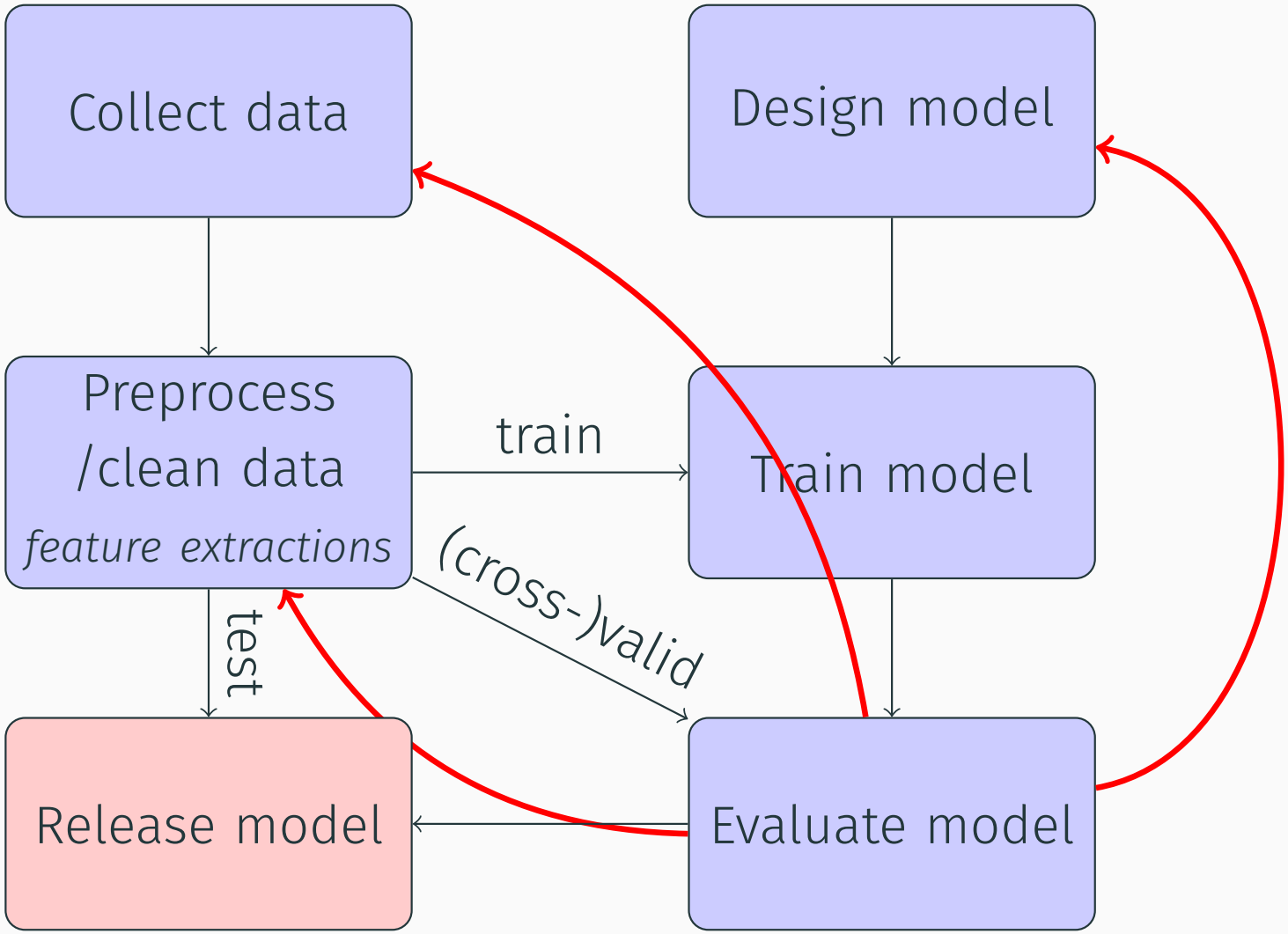
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Train model
(cross-)valid
test
Release model
Evaluate model

In summary

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

- A training dataset
- A validation dataset

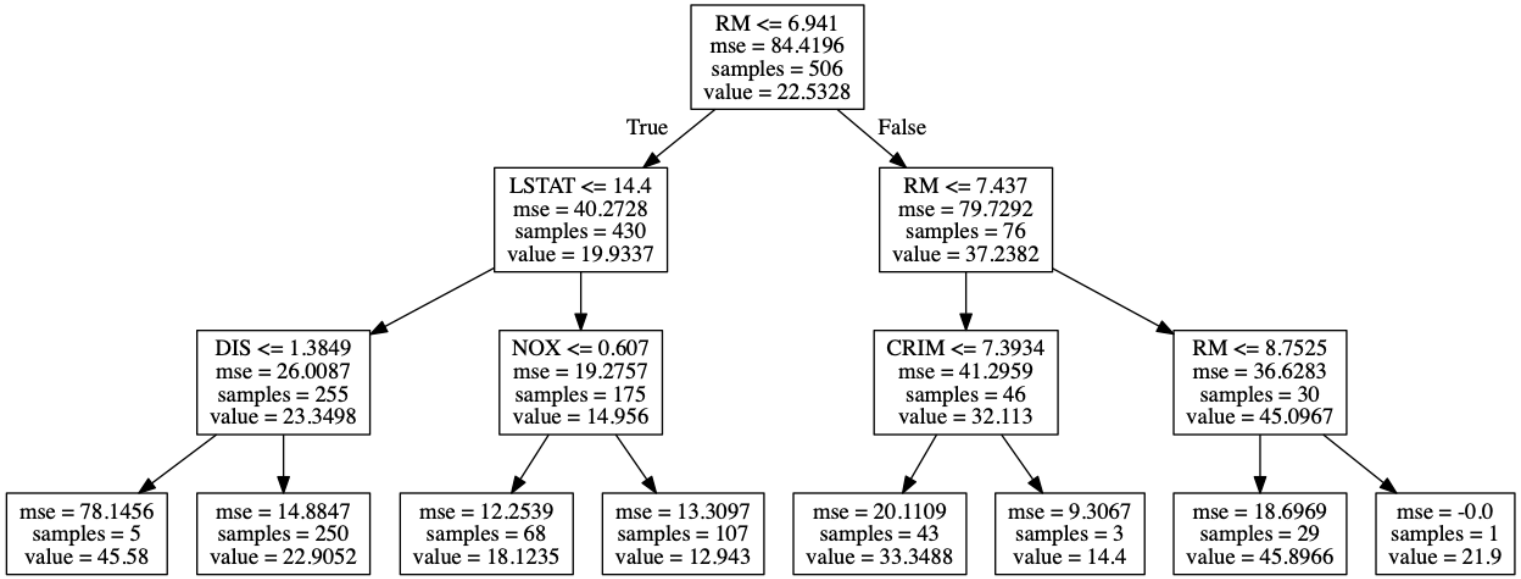
Can be done iteratively in a cross-validation procedure.
Some parameters of the model (e.g. polynomial order in a polynomial regression) were determined from the validation dataset.

- 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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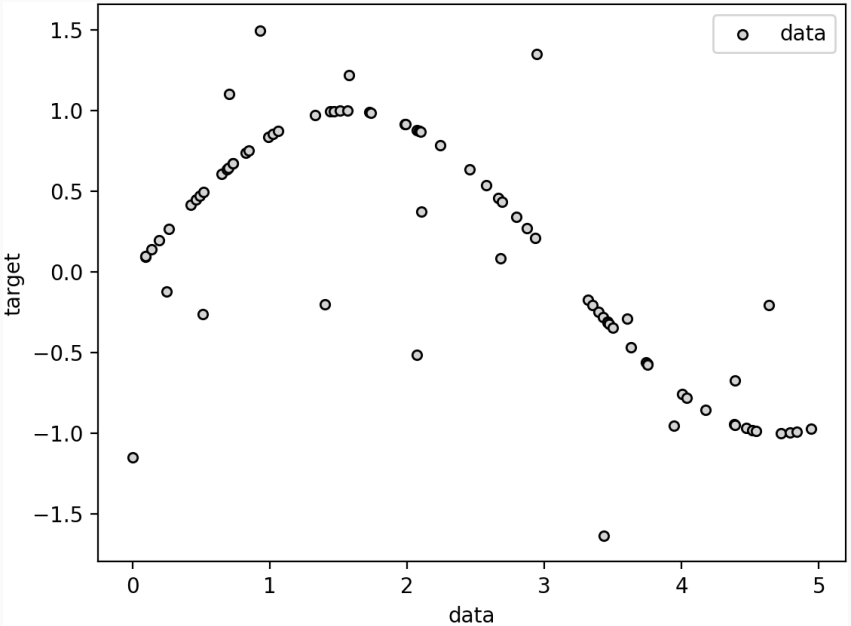
LSTAT	lower status of the population

Uni-variate example



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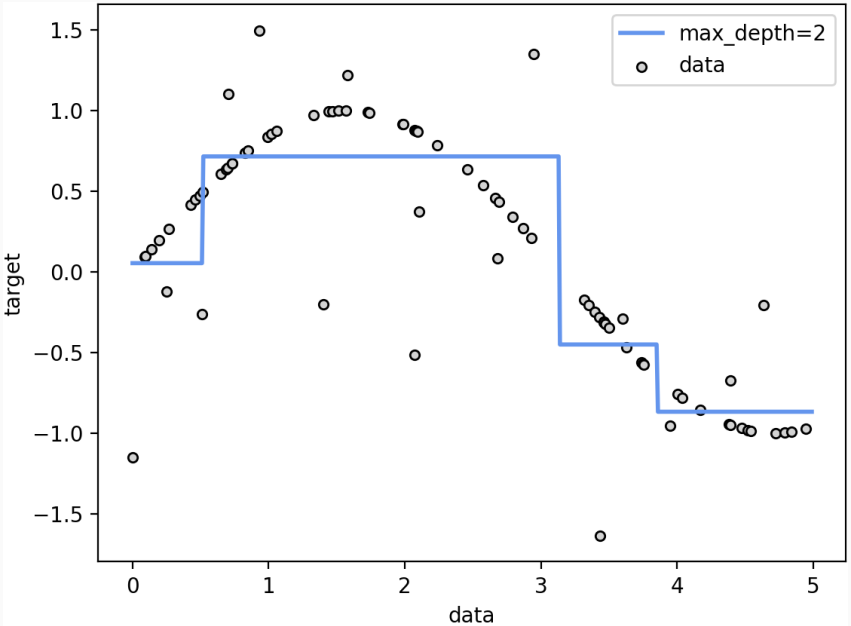

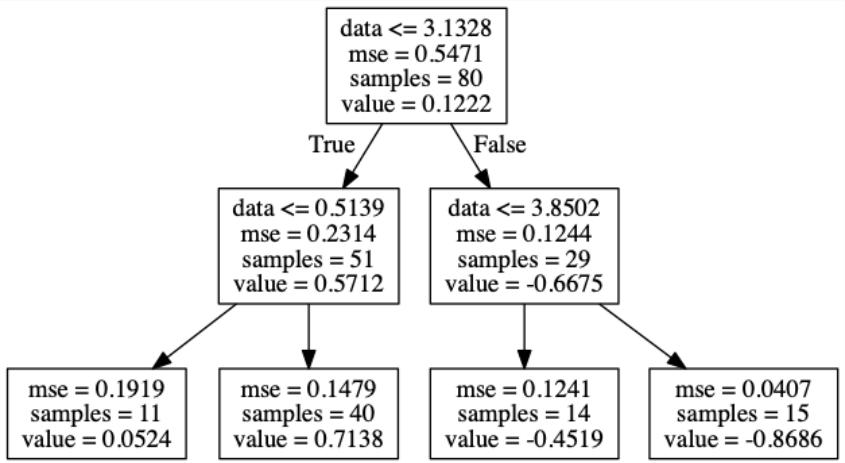

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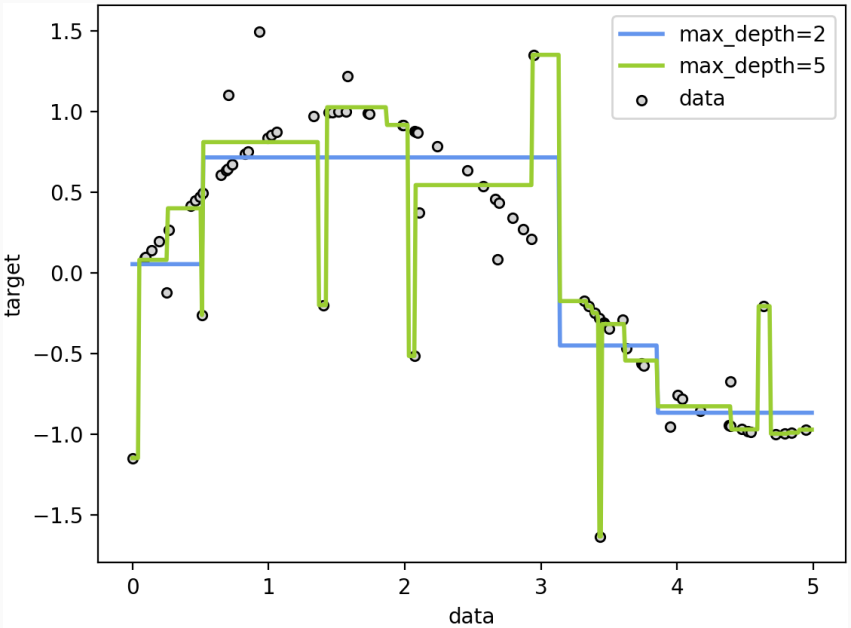

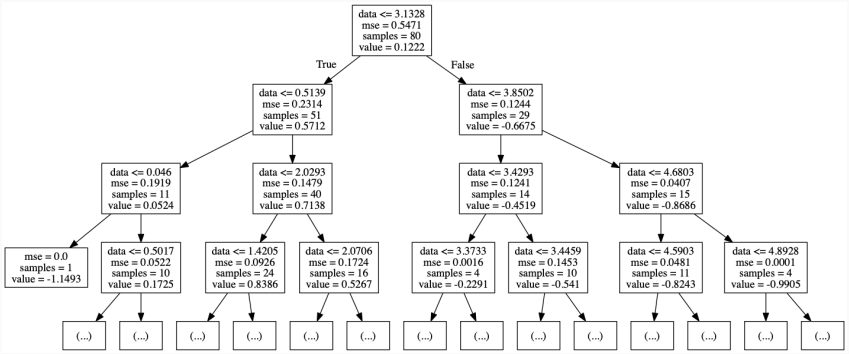

From tree to forest

Disadvantages of regression tree:

- Can overfit the data

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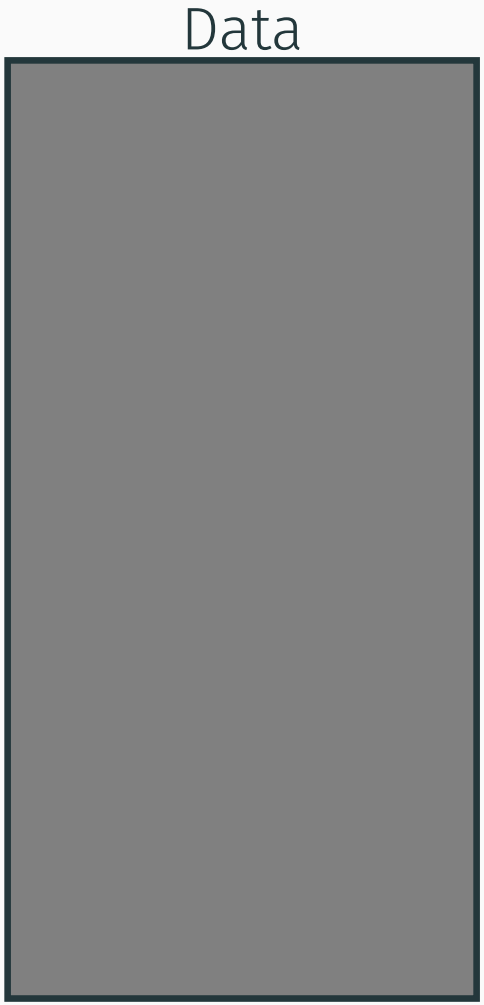
One extension of Regression Tree: Random Forest

The (over simplified) principle of Random Forest



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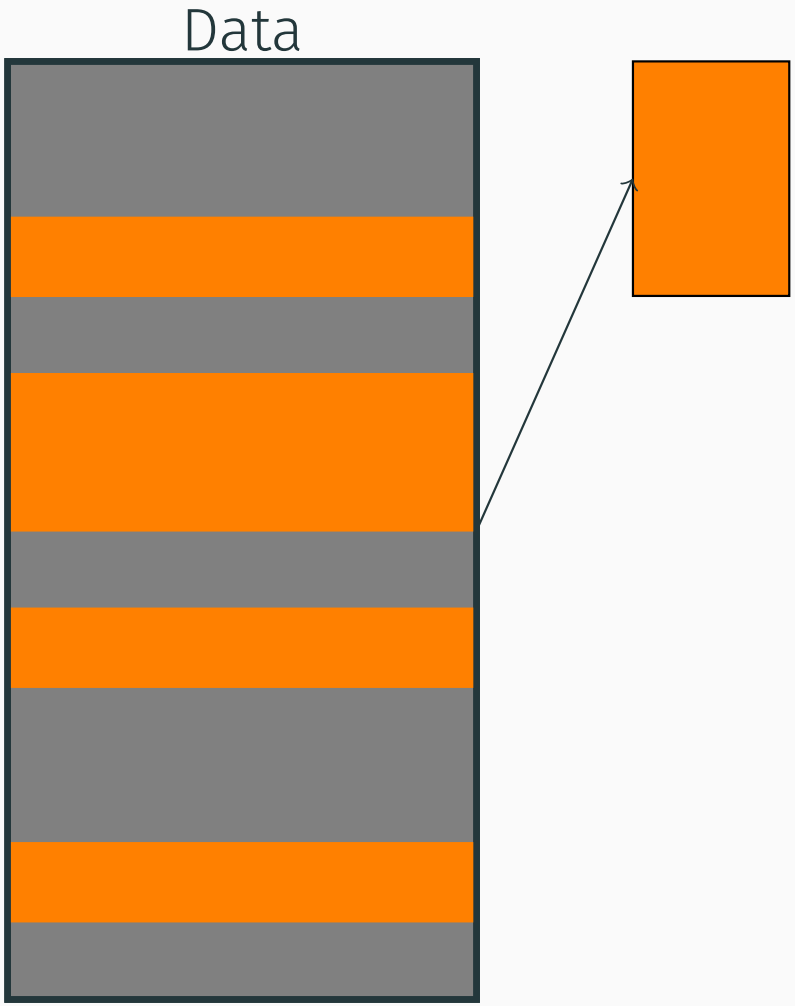

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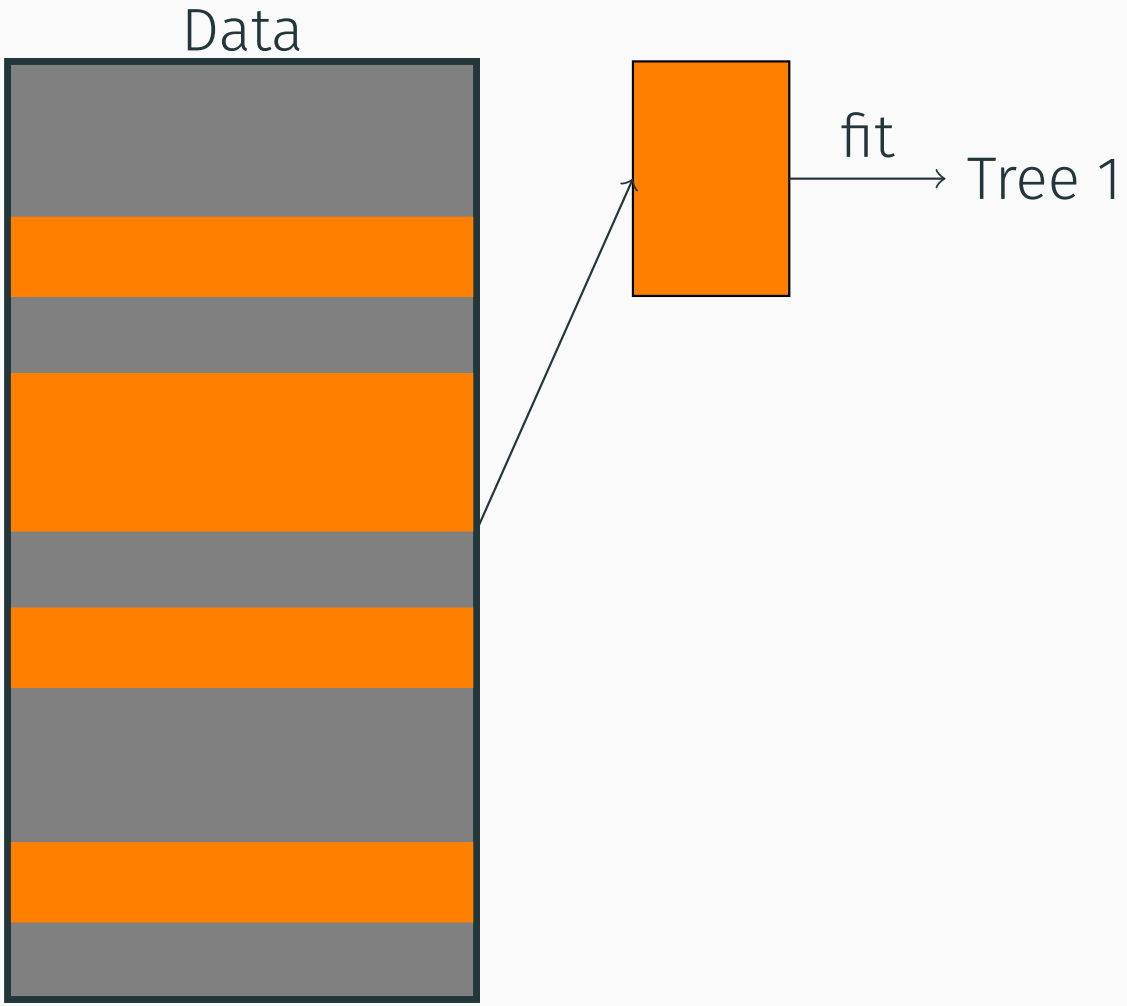

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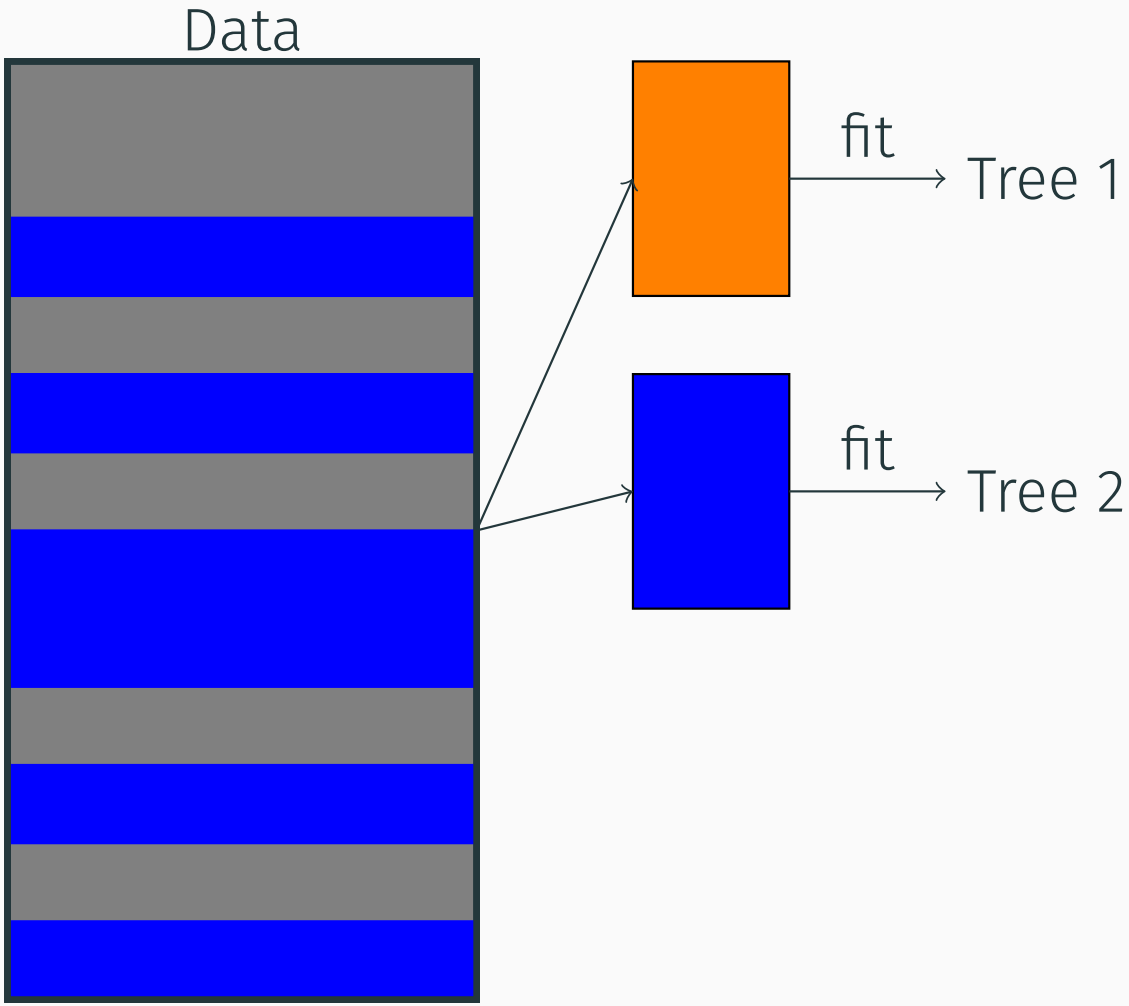

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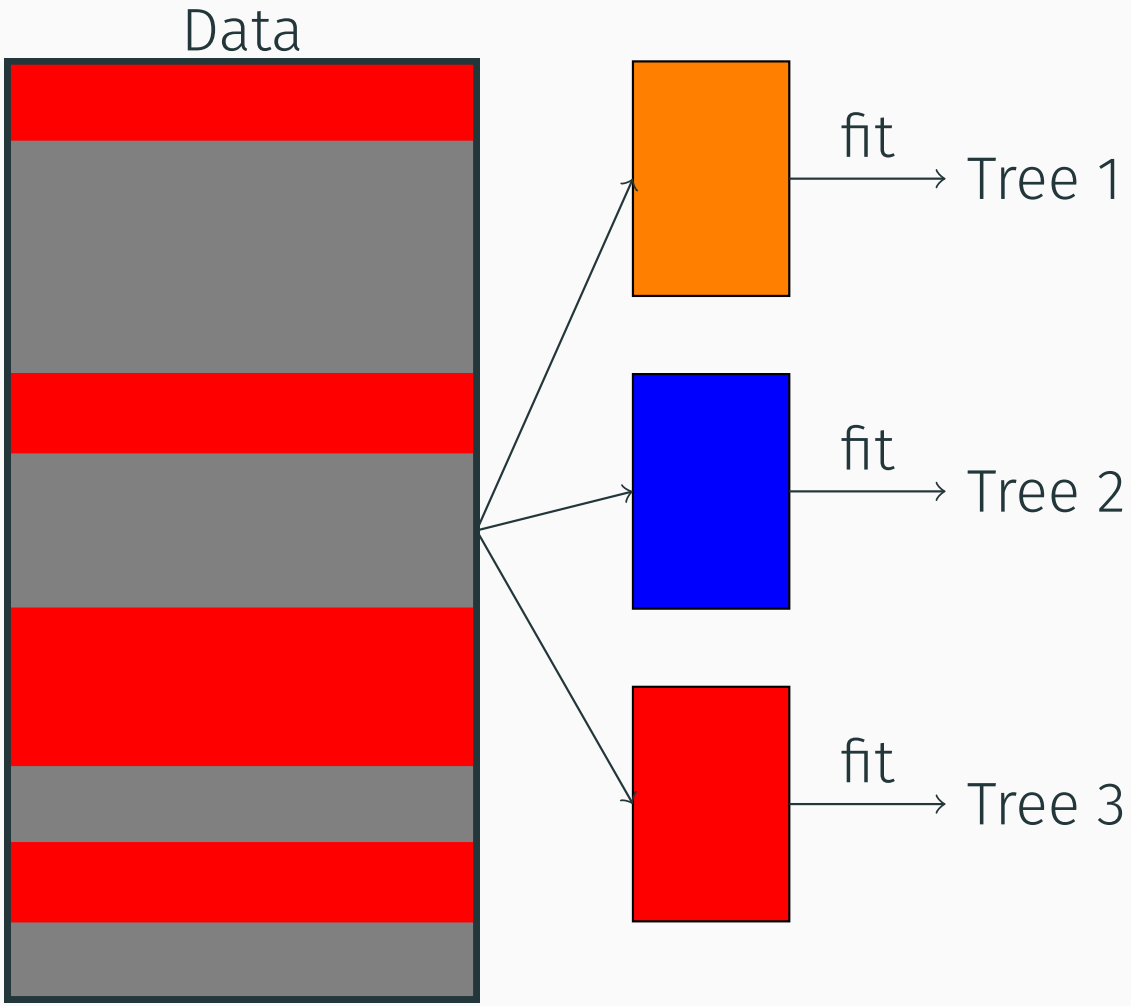

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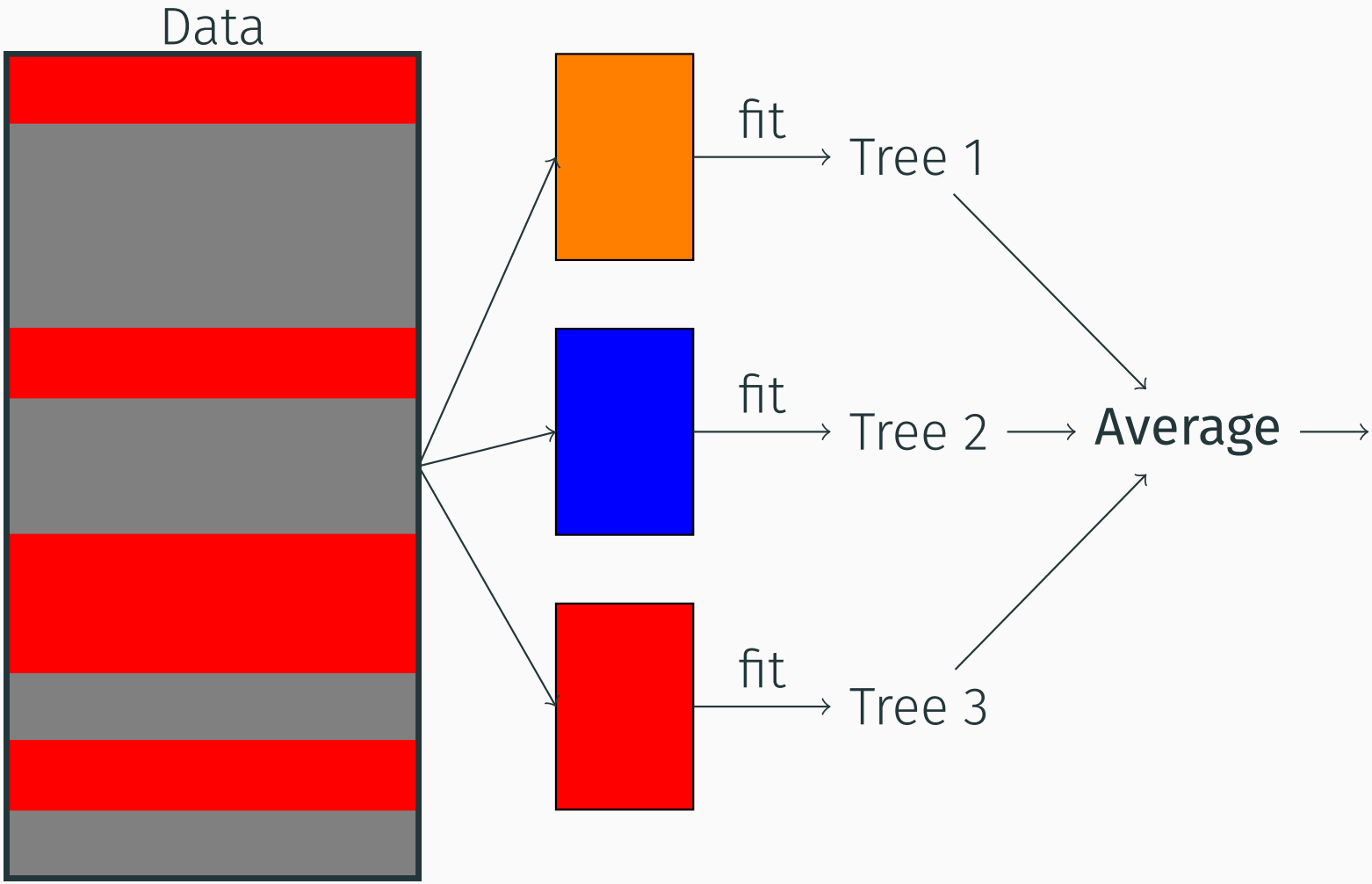
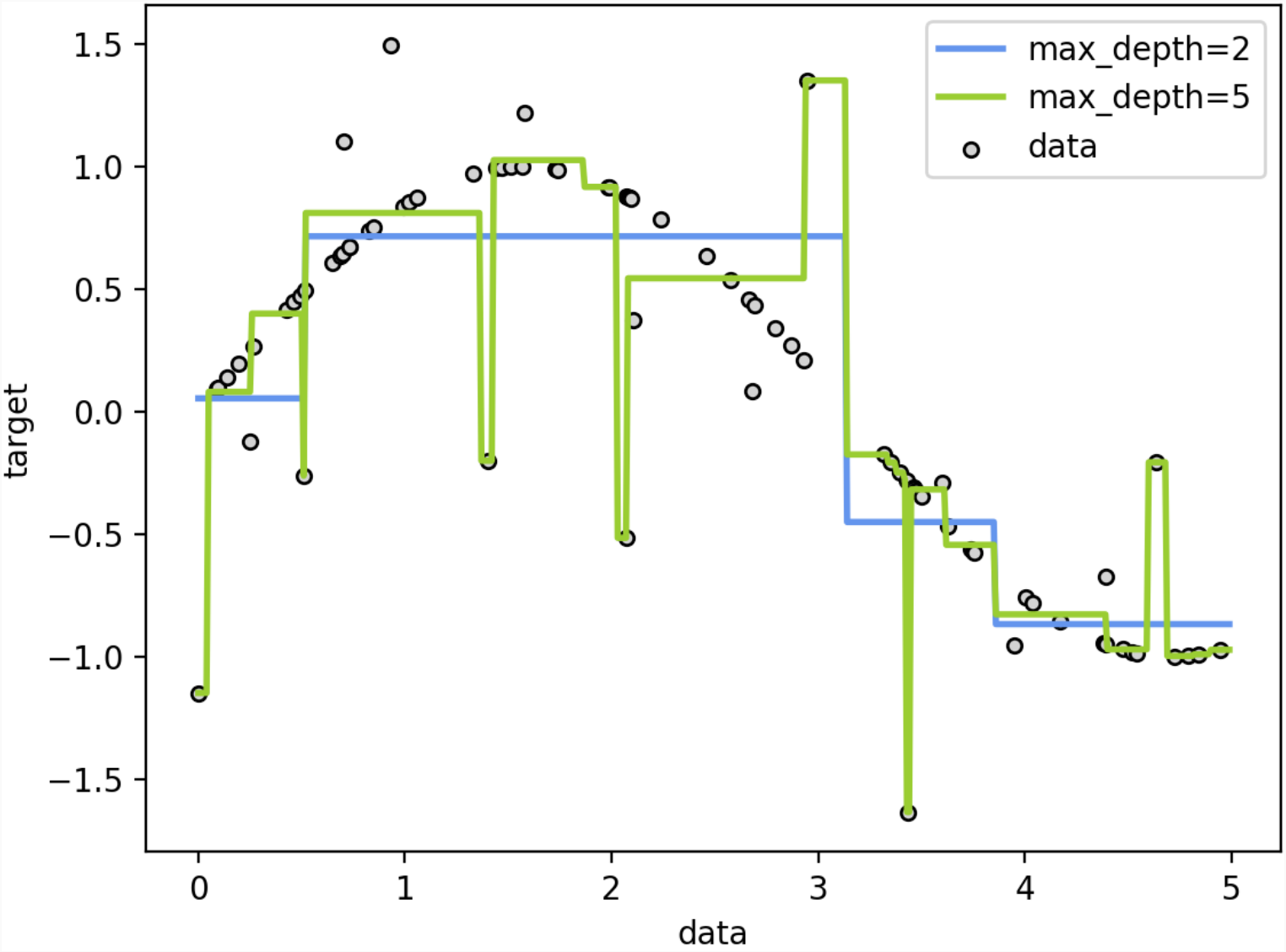


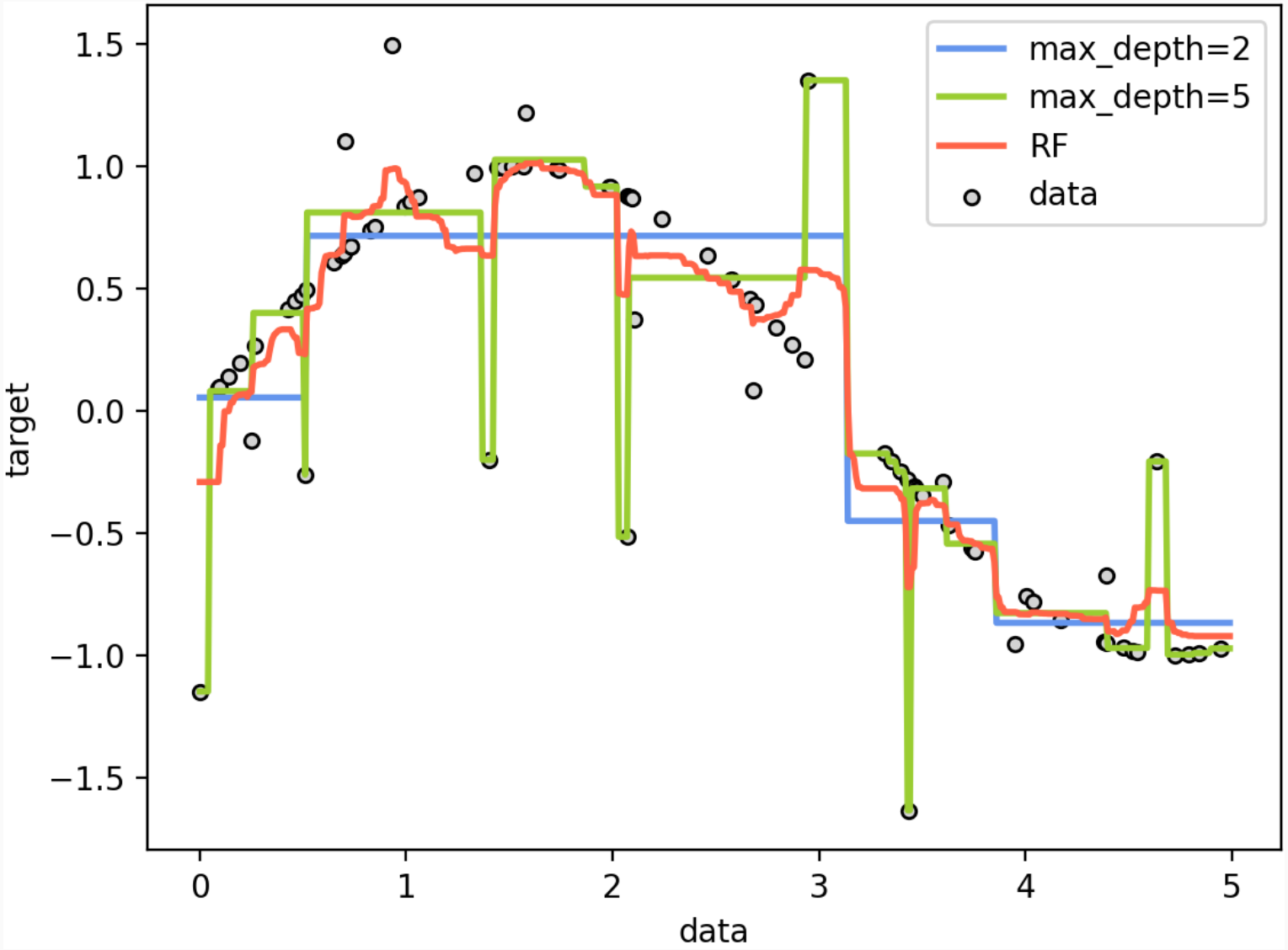
Results on the univariate experiment

Prediction of Randoms trees



Results on the univariate experiment

Prediction of a Random Forest



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).

Determination of the hyperparameters

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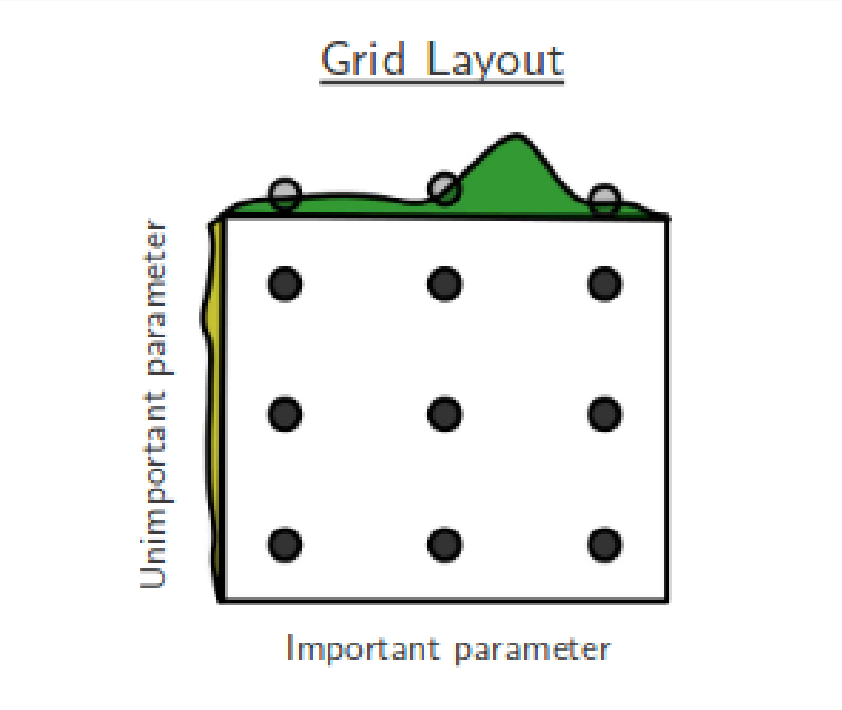
https://xkcd.com/1838/

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

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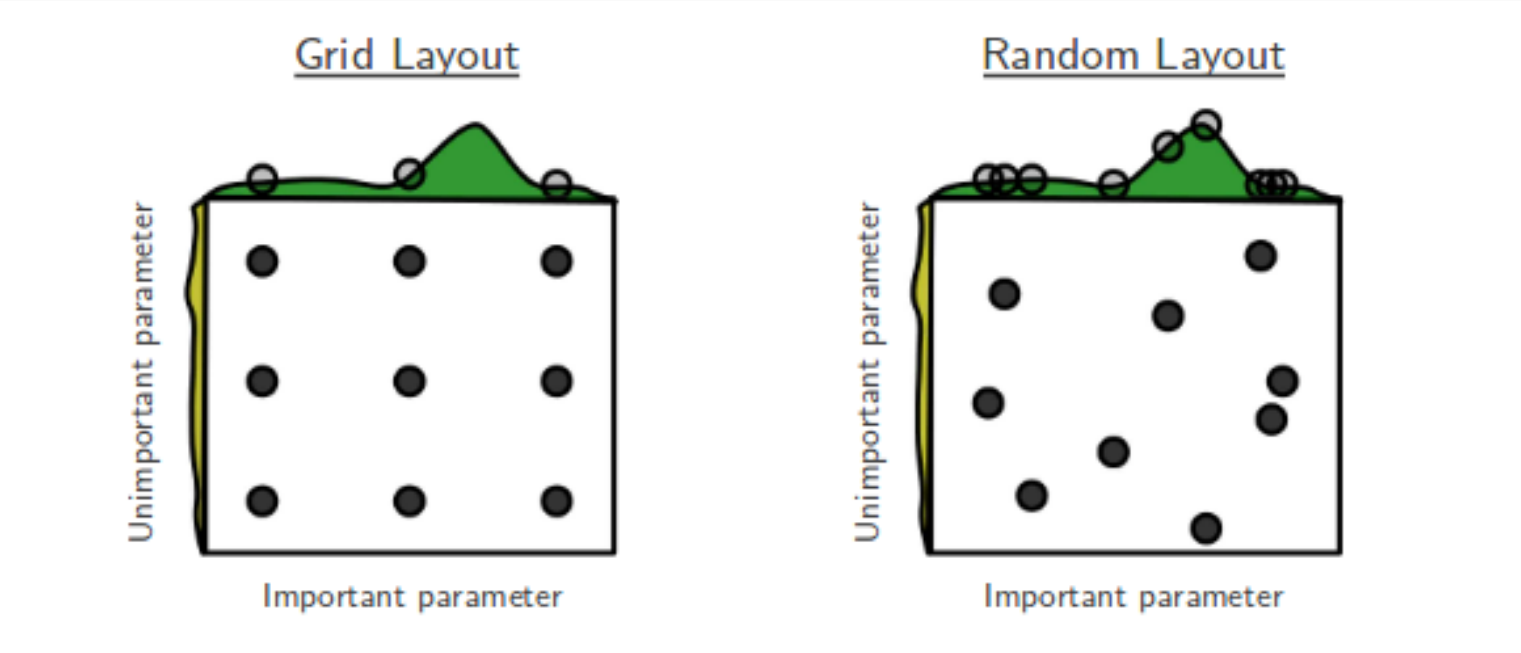
- The procedure is easy to parallelized.
- it is not naturally adapted for quantitative hyperparameters.
- it can become very costly. (e.g. 8 hyperparameters with 8 values each to test = $8^8 = 16,777,216$ trainings.

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)



Remarks on the random search procedure

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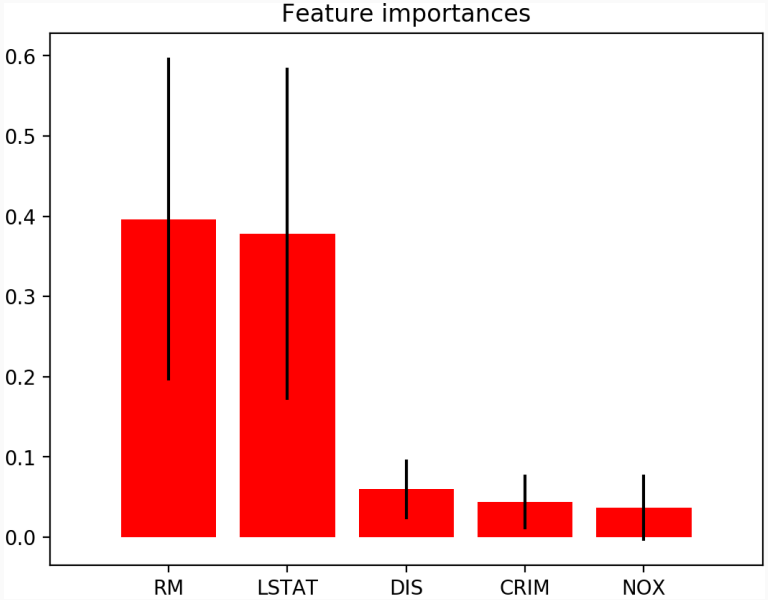
Both gridsearch and random search are implemented and easy to use in scikit-learn.

Feature processing

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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Type of features

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Encoding of the features?

Feature encoding

Type	Examples		Encoding
Quantitative	distance	$\{1.2, 2.3, 0.1\}$	$\{1.2, 2.3, 0.1\}$
Ordinal	rooms	$\{2, 3, 4\}$	$\{2, 3, 4\}$
Qualitative	Ocean	$\{\text{Atlantic}, \text{Indian}, \text{Pacific}\}$	$\{[1, 0, 0], [0, 1, 0], [0, 0, 1]\}$

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Qualitative variable: one-hot encoding.

- You must not encode qualitative features with integer $1, 2, 3$, it would mean that Pacific > Indian > Atlantic.
- In $\mathrm{sklearn}$ there is a function that makes the one-hot encoding: $\mathrm{OneHotEncoder}()$
- If the number of modalities (number of different features) is high, encoding qualitative feature produce a big-sized vector.

Embedding

A common way to deal with features with a lot of modalities : Embedding

Principle of embedding

Let's consider a qualitative variable with n modalities, represented by the n-dimensional binary vector $\mathbf{x}$

Embedding consists in representing this variable by a vector $\mathbf{v} \in \mathbb{R}^p, p << n$

The embedding is represented by a matrix $\mathbf{M} \in \mathbb{R}^{n \times p}$ such as:

$$\mathbf{v} = \mathbf{M} \cdot \mathbf{x}$$

Coefficients of $\mathbf{M}$ have to be optimized given an objective criteria (that depends on your problem)

one example: word cloud

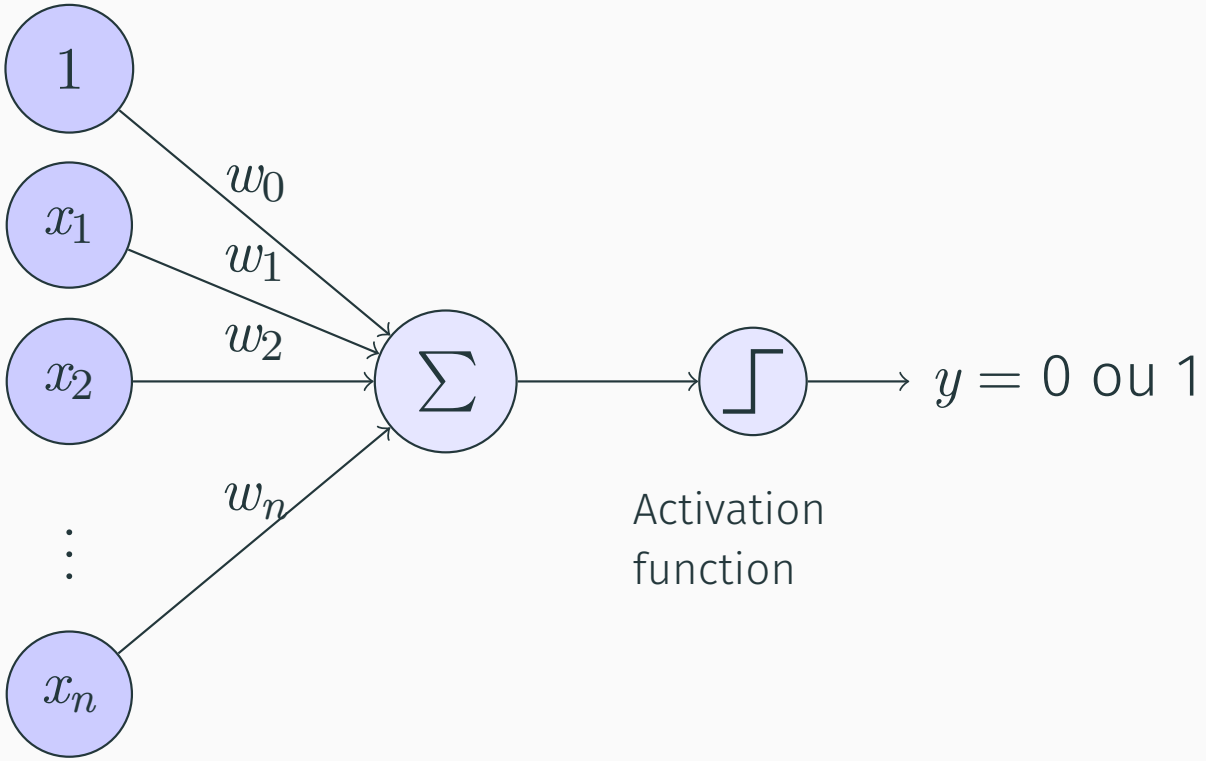
On the introduction of the *Goodfellow et al.* book.

$\mathbf{v}$ is 3-dimensional (x,y,size)

https://www.wordclouds.com

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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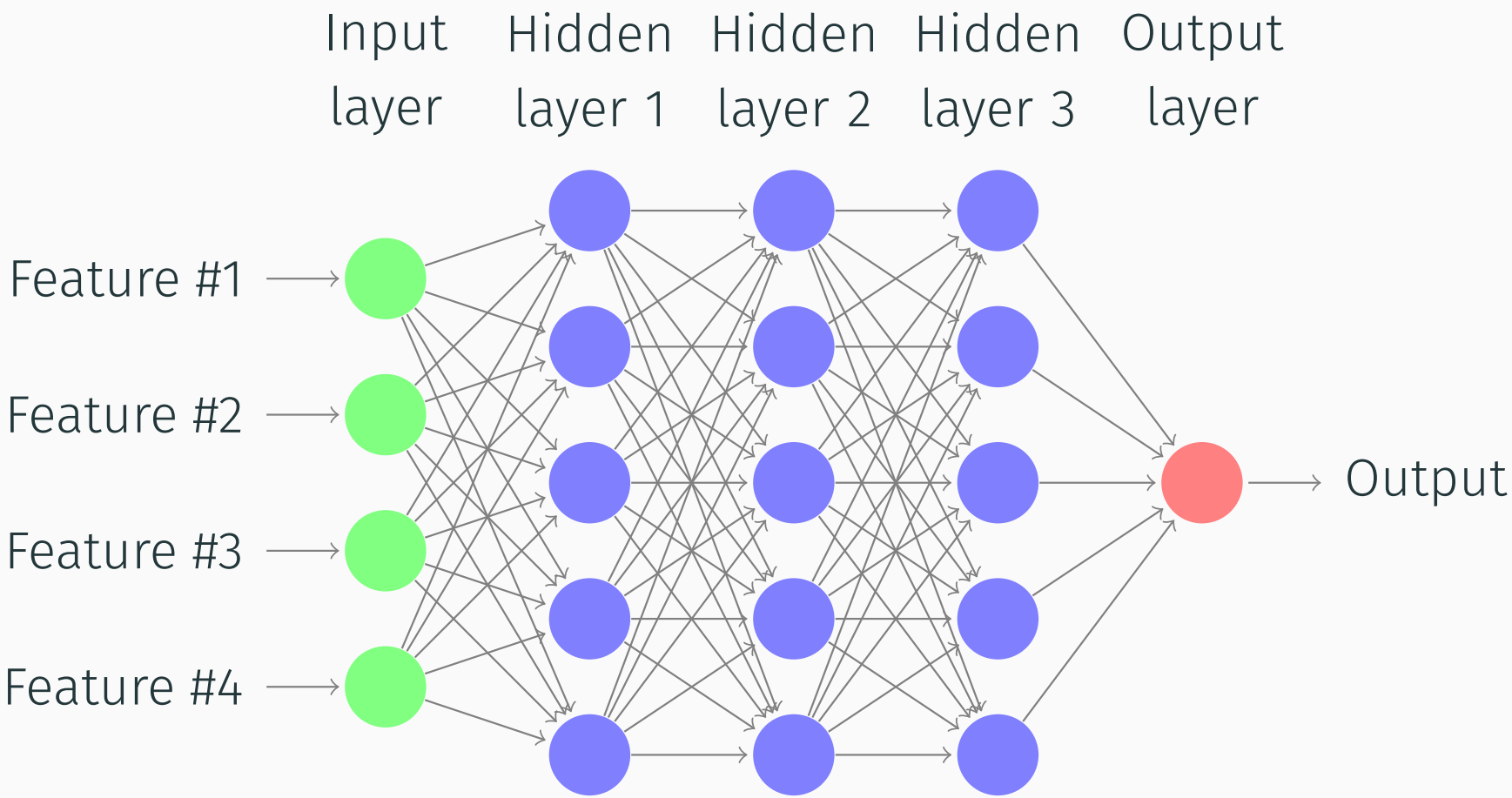
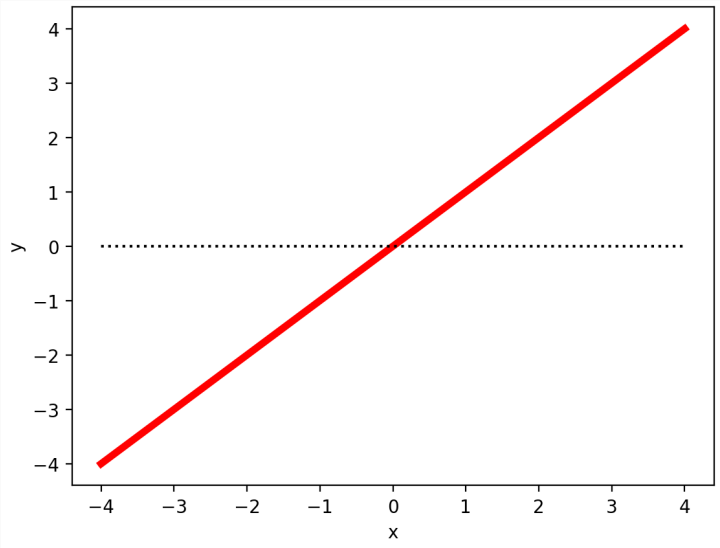
More complexe models are build by combining several perceptrons

Multi-layer perceptron (Densely connected layers)

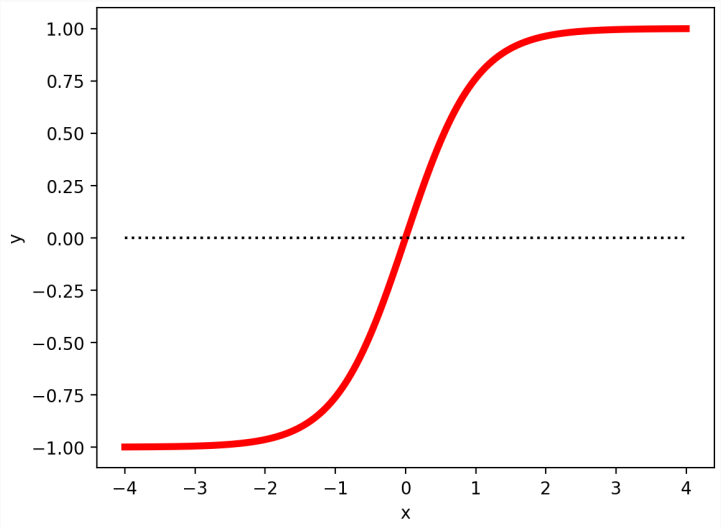


Most usual activation functions

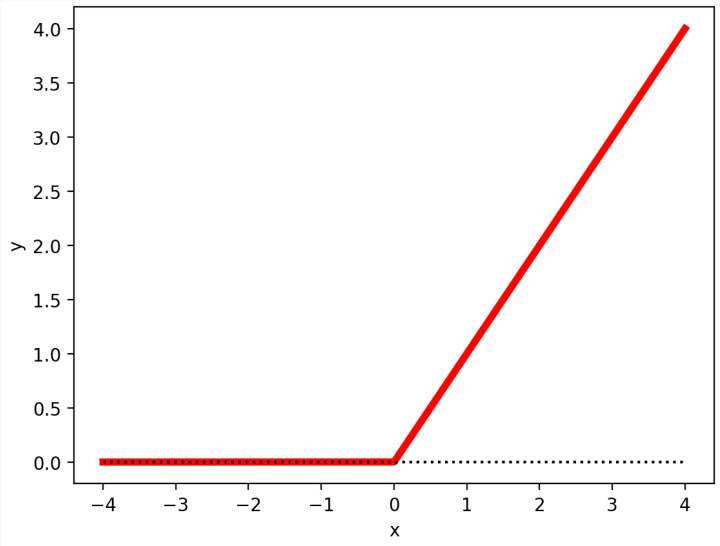
Linear



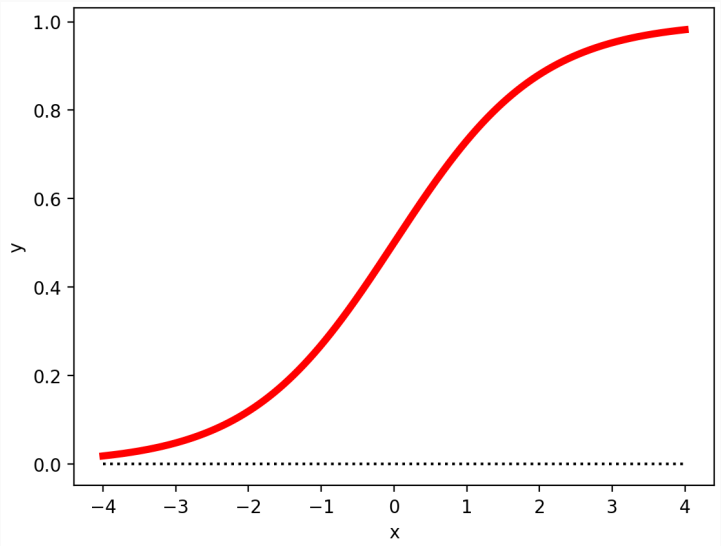
Hyperbolic tangent



ReLU

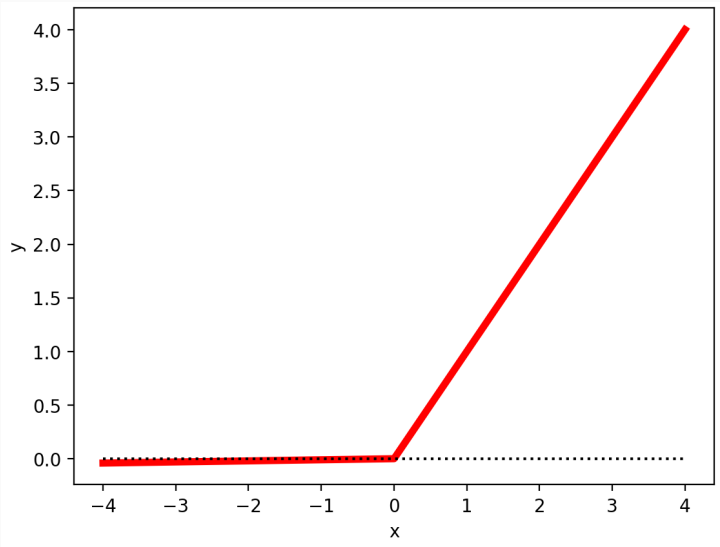


Sigmoid

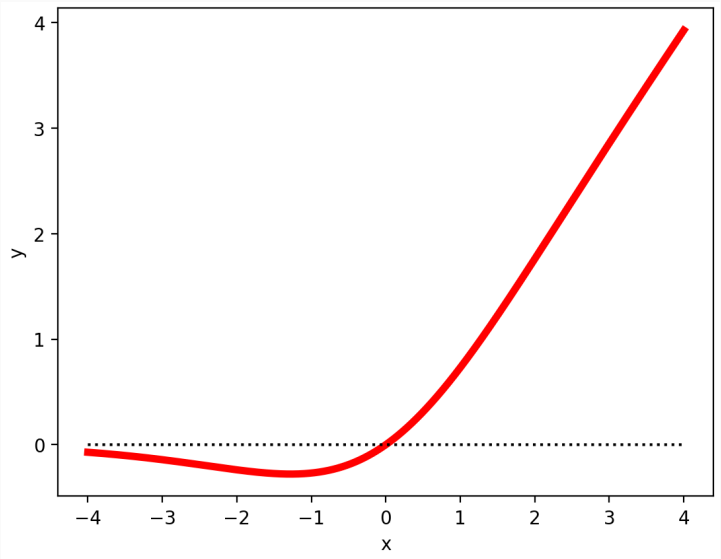


New fancy activation functions

Leaky-ReLU



Swish



Classification and regression loss

Regression

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

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

Classification and regression loss

Regression

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

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

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}

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

$\mathbf{w}$

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

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

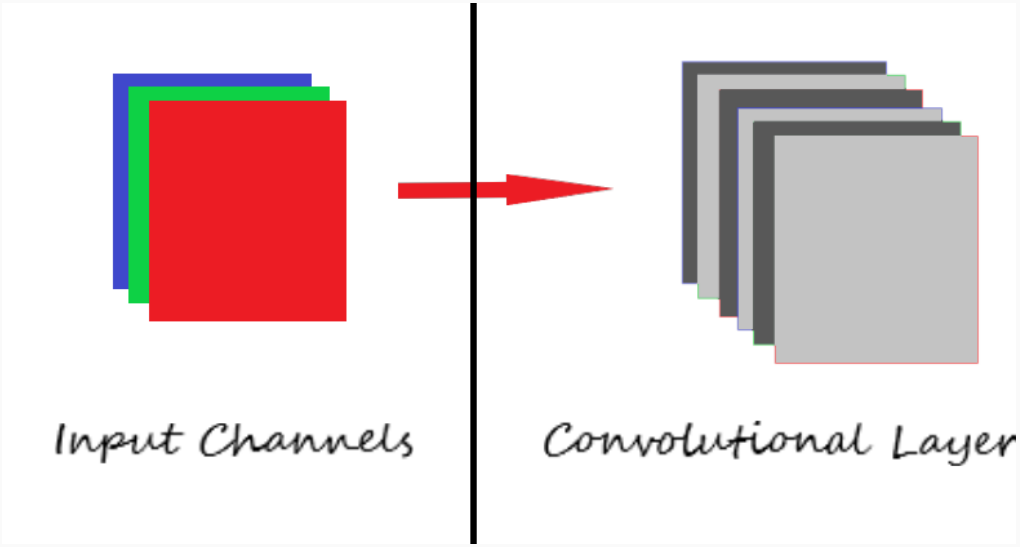
Main parameters of a convolutional layer

- Size of the filter K

Main parameters of a convolutional layer

- Size of the filter K
- Number of filters p

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

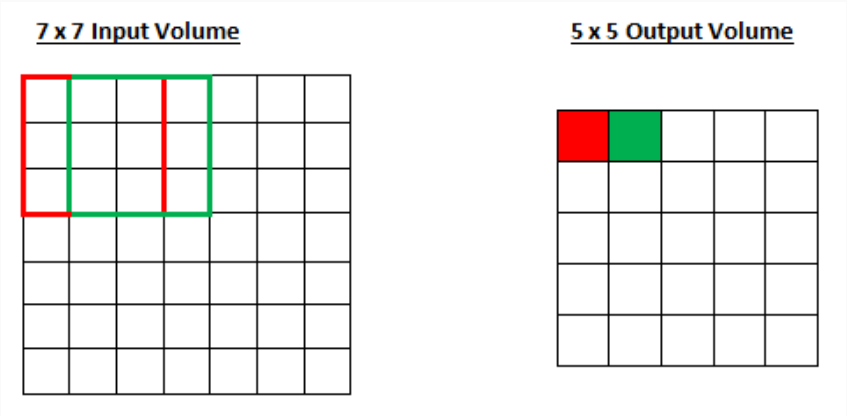


$O = \frac{W-K+2P}{S} + 1$, where O is the output size and W the input size.

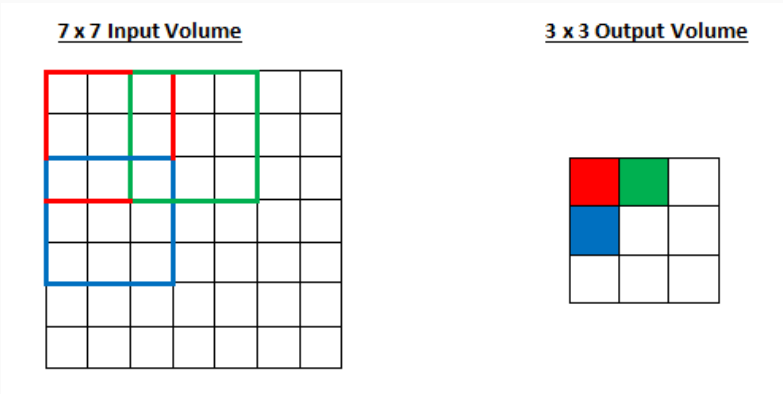
Main parameters of a convolutional layer

- Size of the filter K
- Number of filters p
- Strides S

$S = 1$



$S = 2$

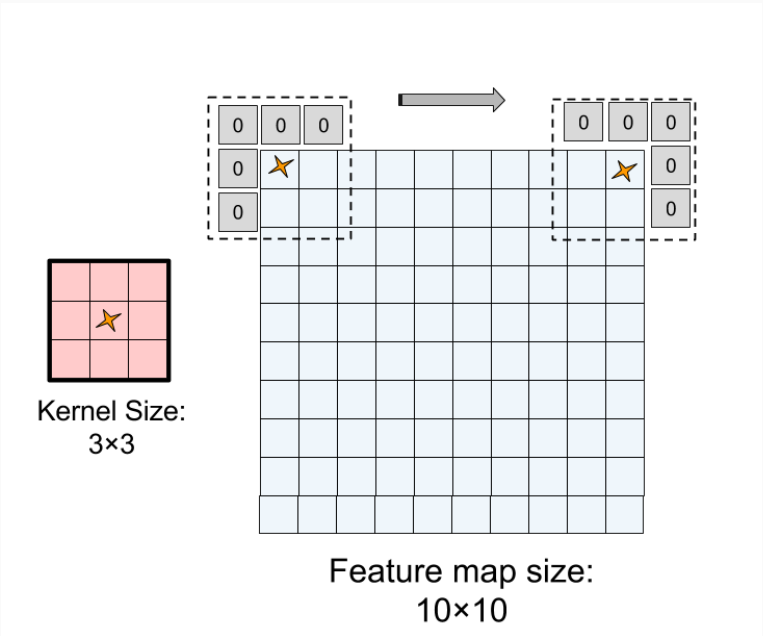


$O = \frac{W-K+2P}{S} + 1$, where O is the output size and W the input size.

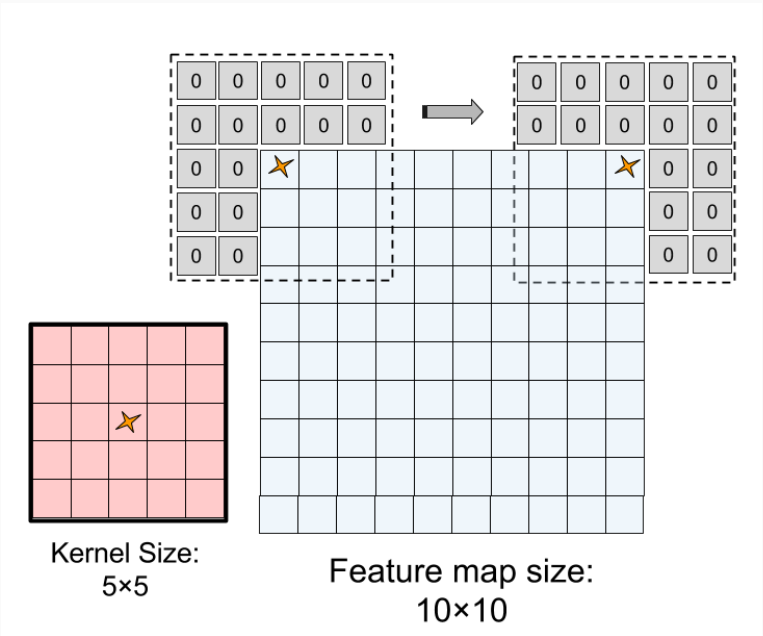
Main parameters of a convolutional layer

- Size of the filter K
- Number of filters p
- Strides S
- Padding P

$P = 1$



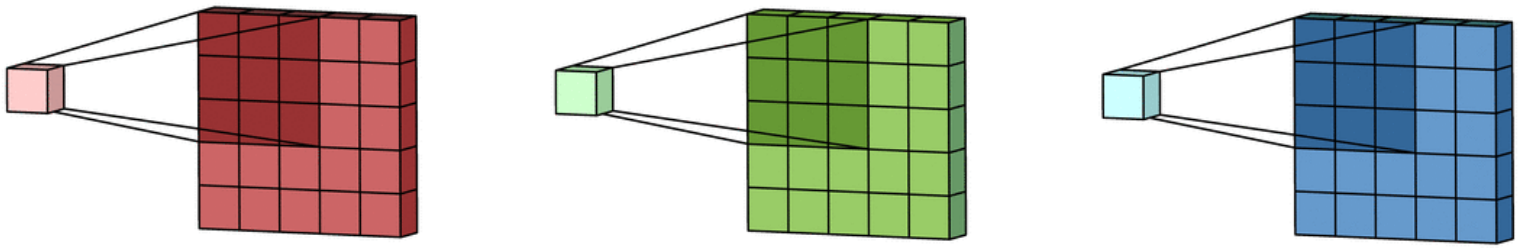
$P = 2$



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

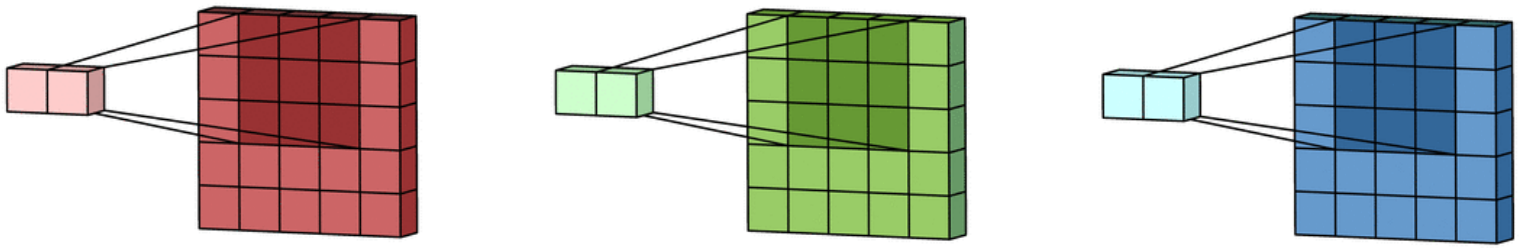
Summary of Convolutional layer steps

1. Convolution



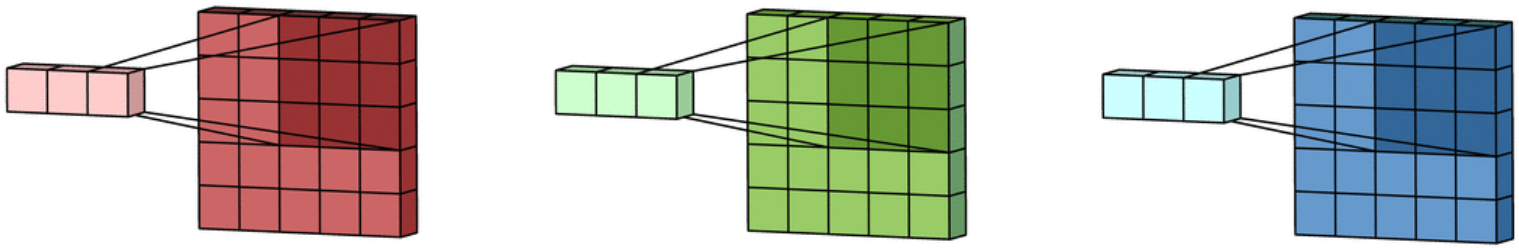
Summary of Convolutional layer steps

1. Convolution



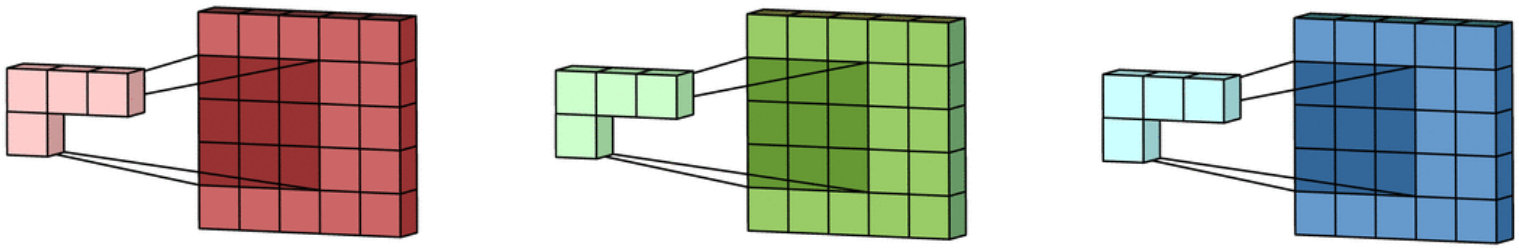
Summary of Convolutional layer steps

1. Convolution



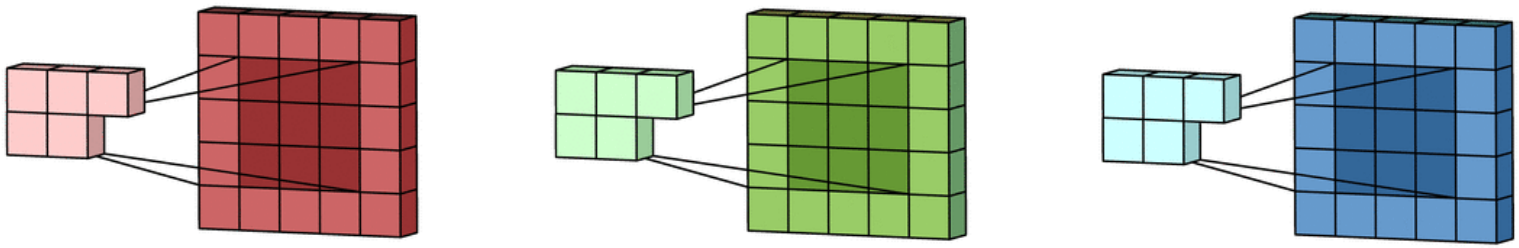
Summary of Convolutional layer steps

1. Convolution



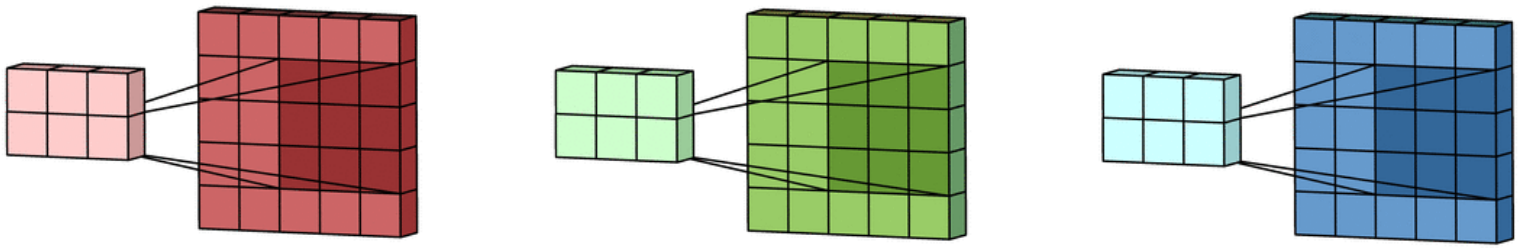
Summary of Convolutional layer steps

1. Convolution



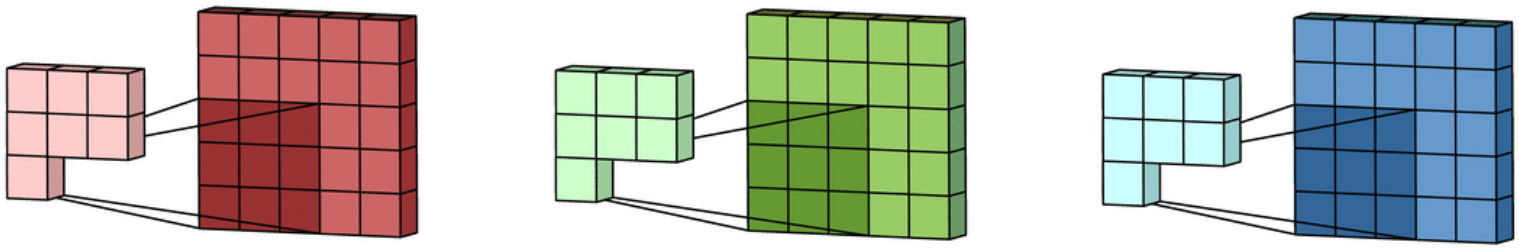
Summary of Convolutional layer steps

1. Convolution



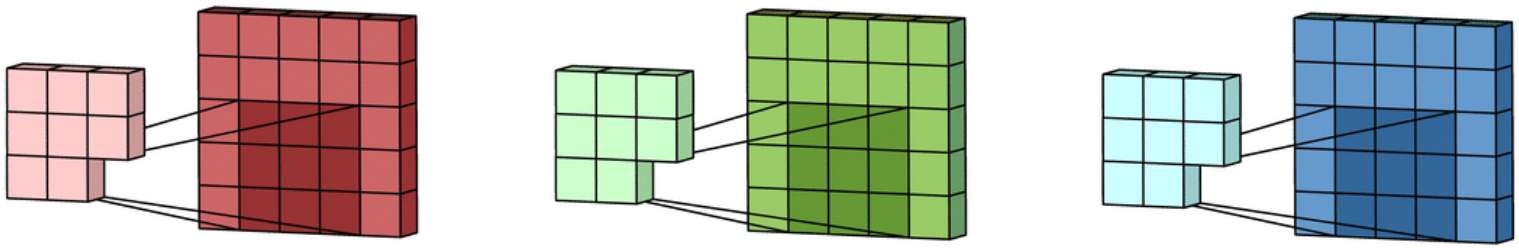
Summary of Convolutional layer steps

1. Convolution



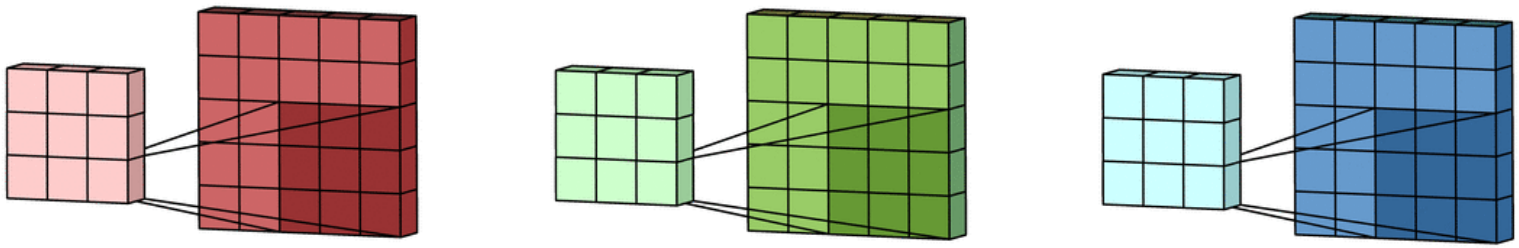
Summary of Convolutional layer steps

1. Convolution



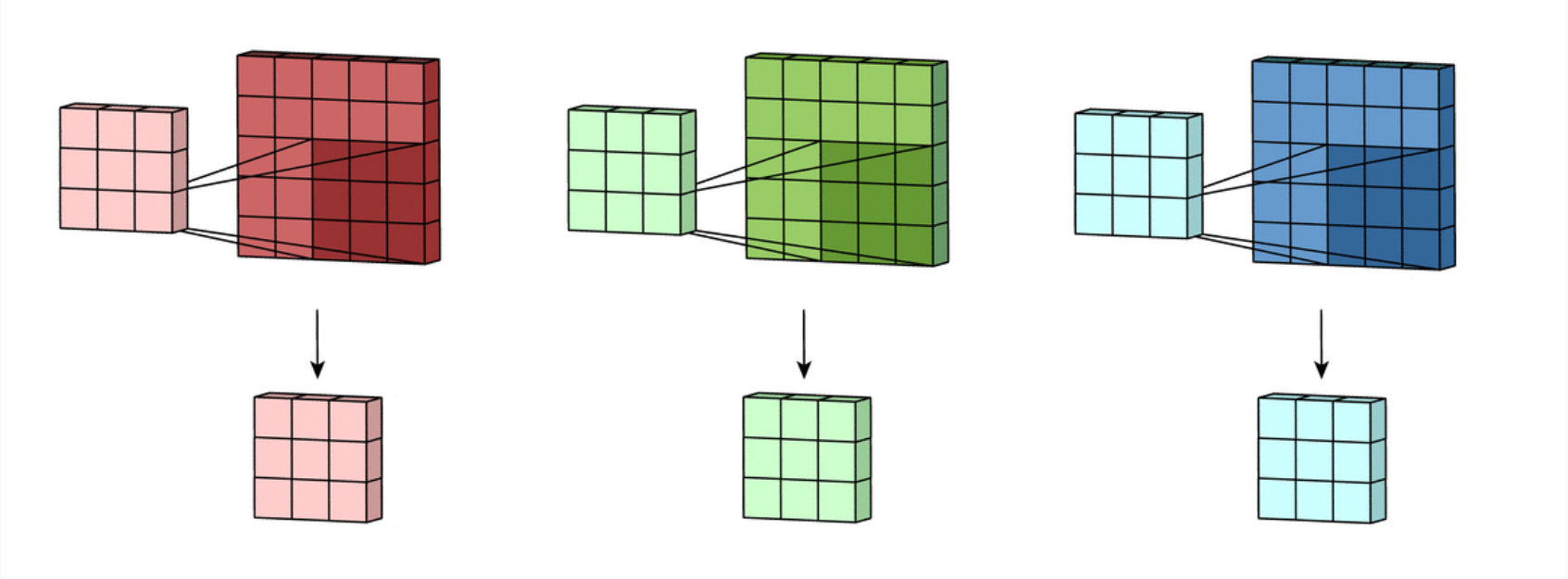
Summary of Convolutional layer steps

1. Convolution



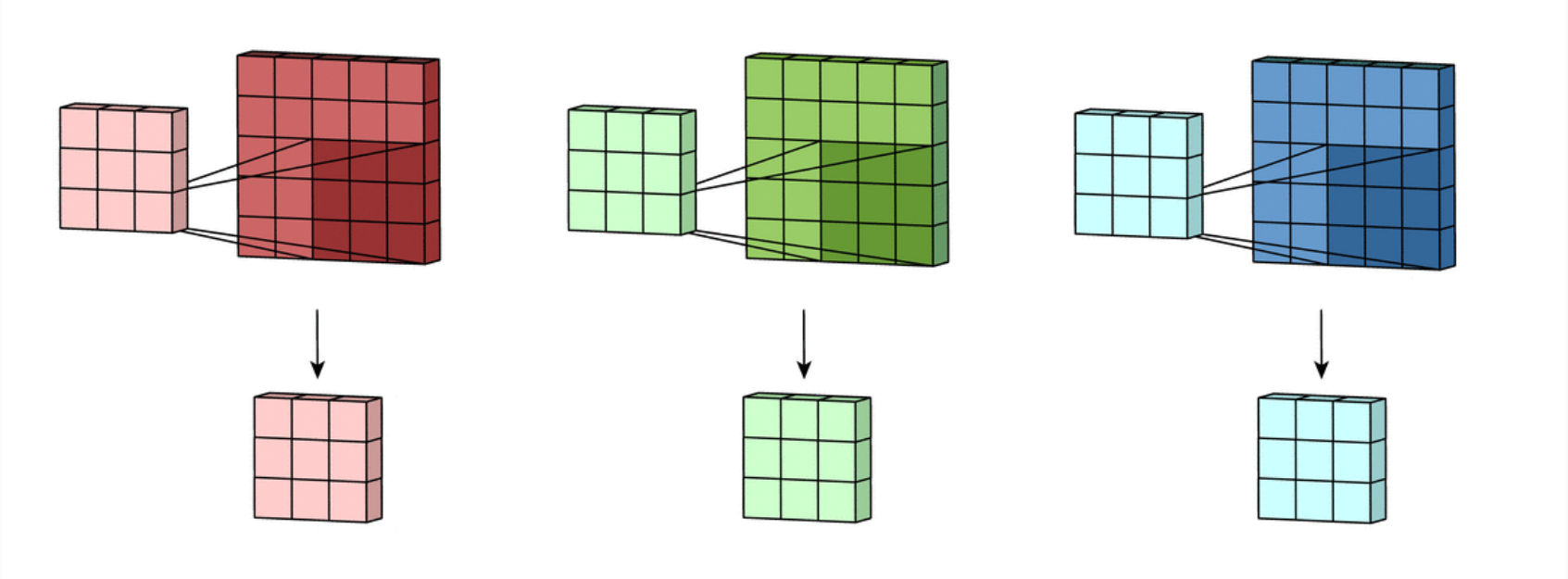
Summary of Convolutional layer steps

1. Convolution



Summary of Convolutional layer steps

1. Convolution



Summary of Convolutional layer steps

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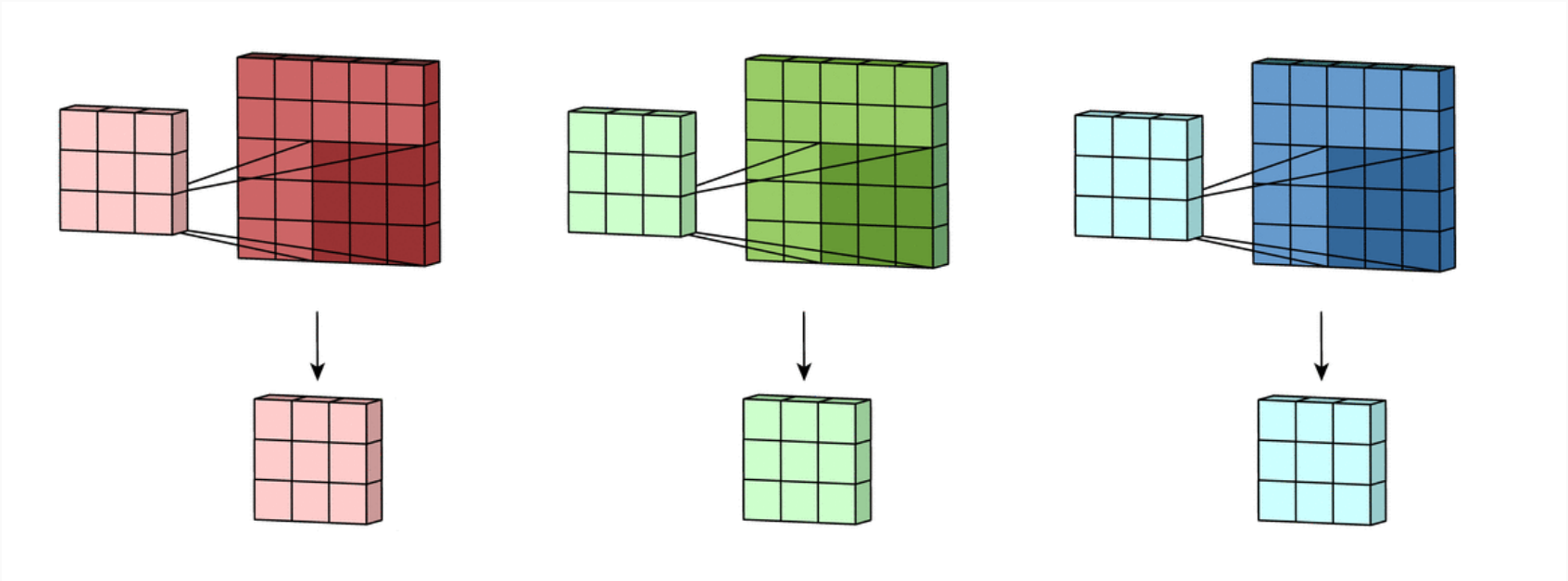
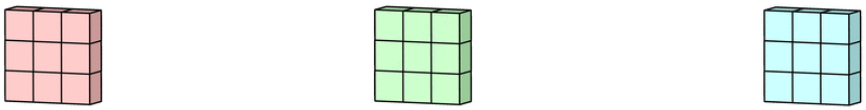
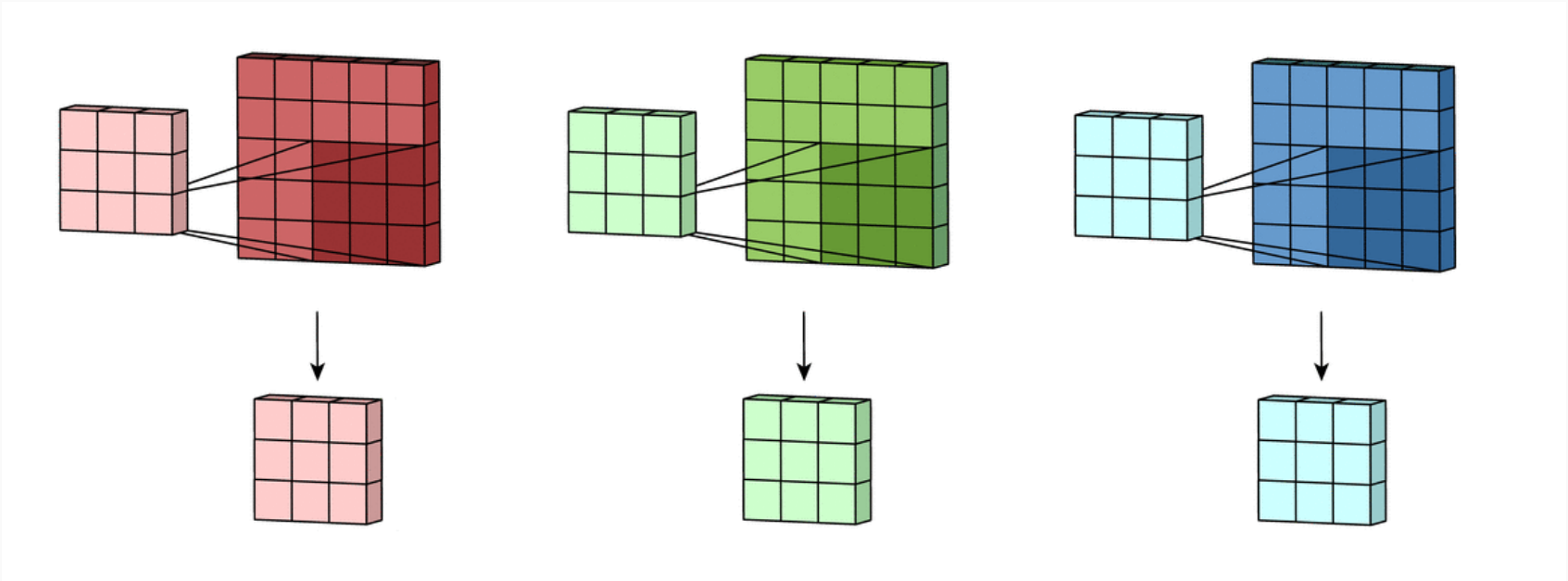


2. Addition

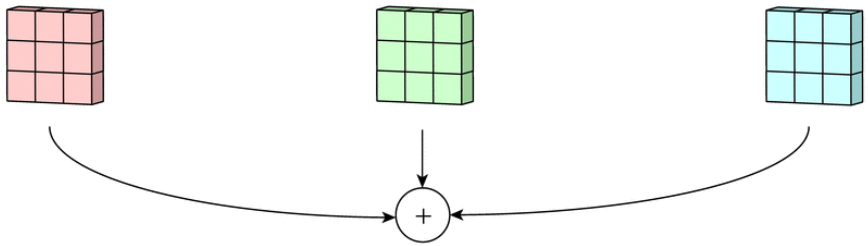


Summary of Convolutional layer steps

1. Convolution

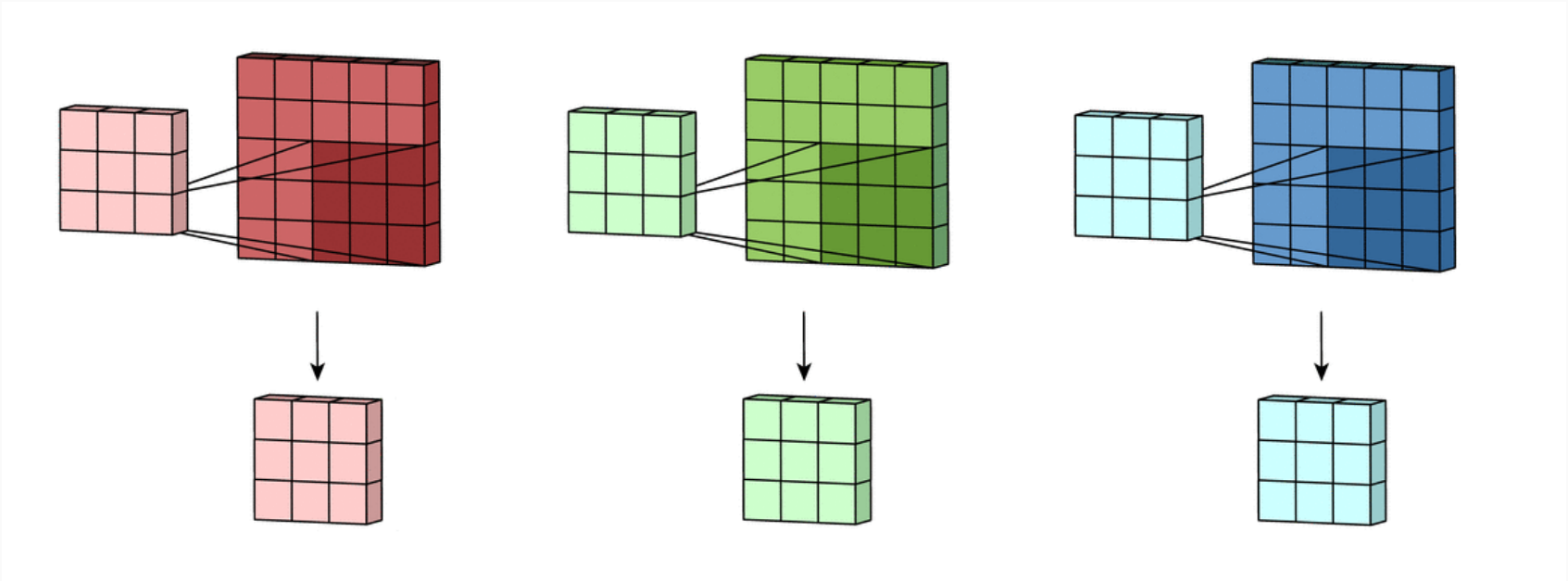


2. Addition

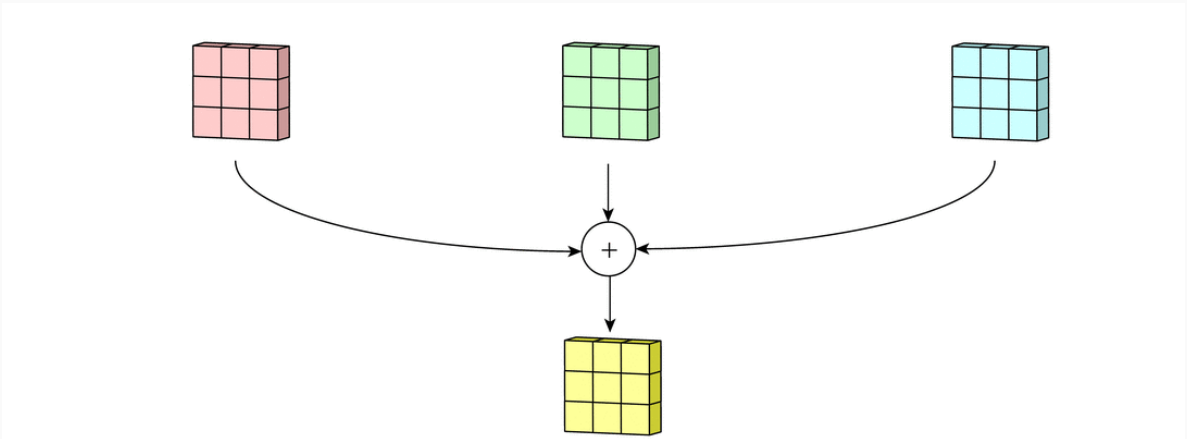


Summary of Convolutional layer steps

1. Convolution

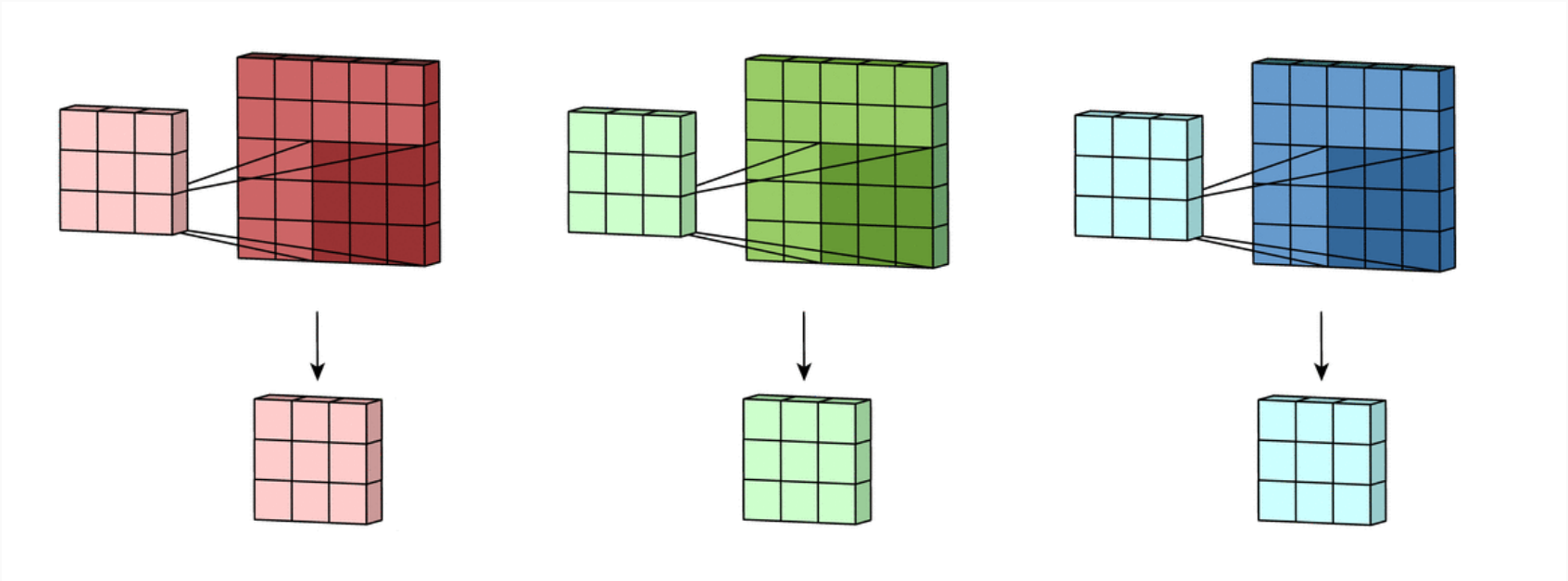


2. Addition

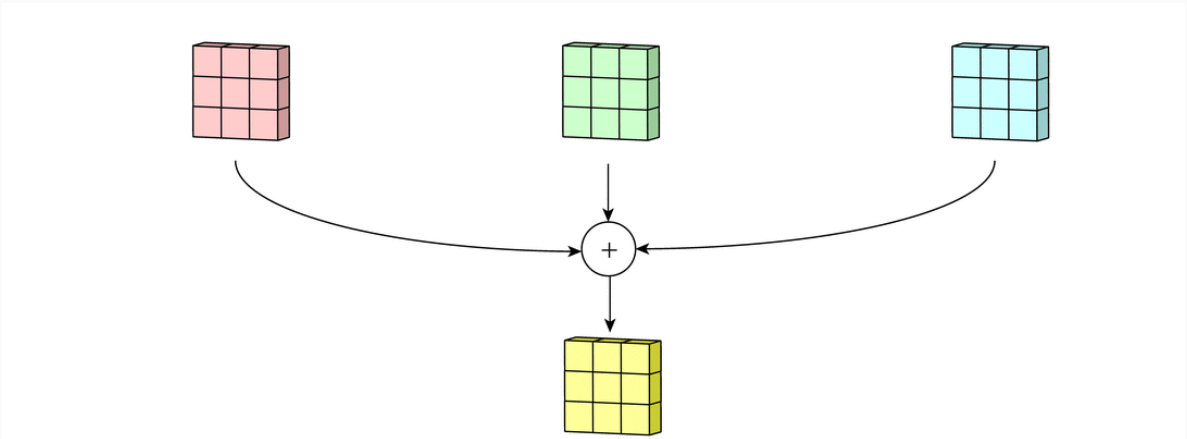


Summary of Convolutional layer steps

1. Convolution



2. Addition



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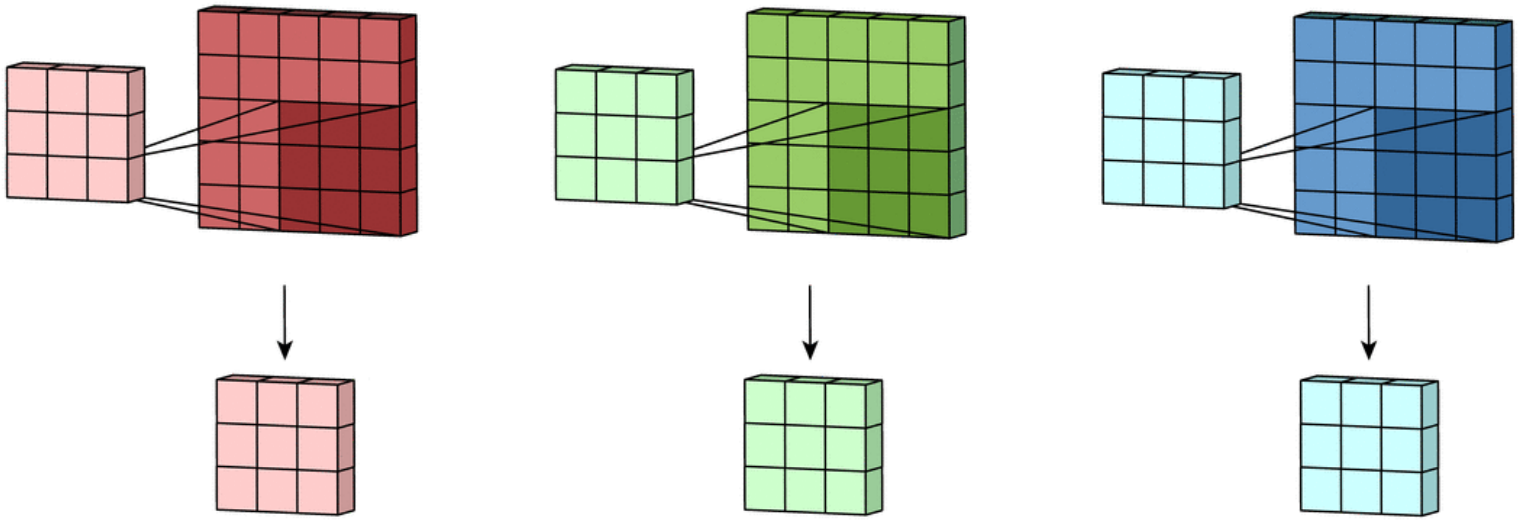
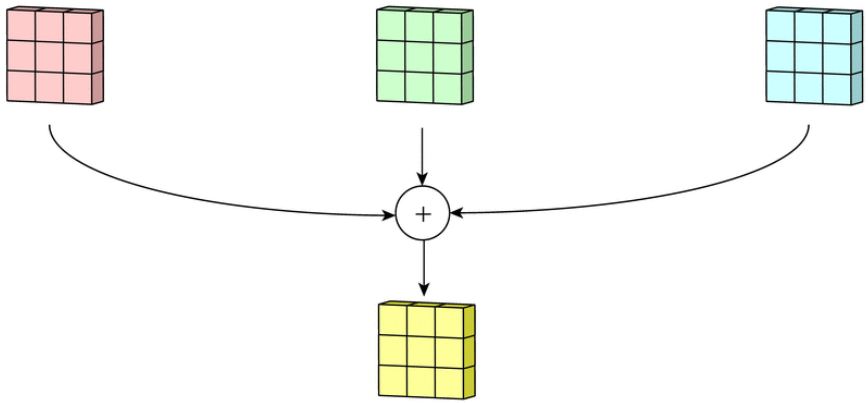
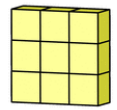


2. Addition

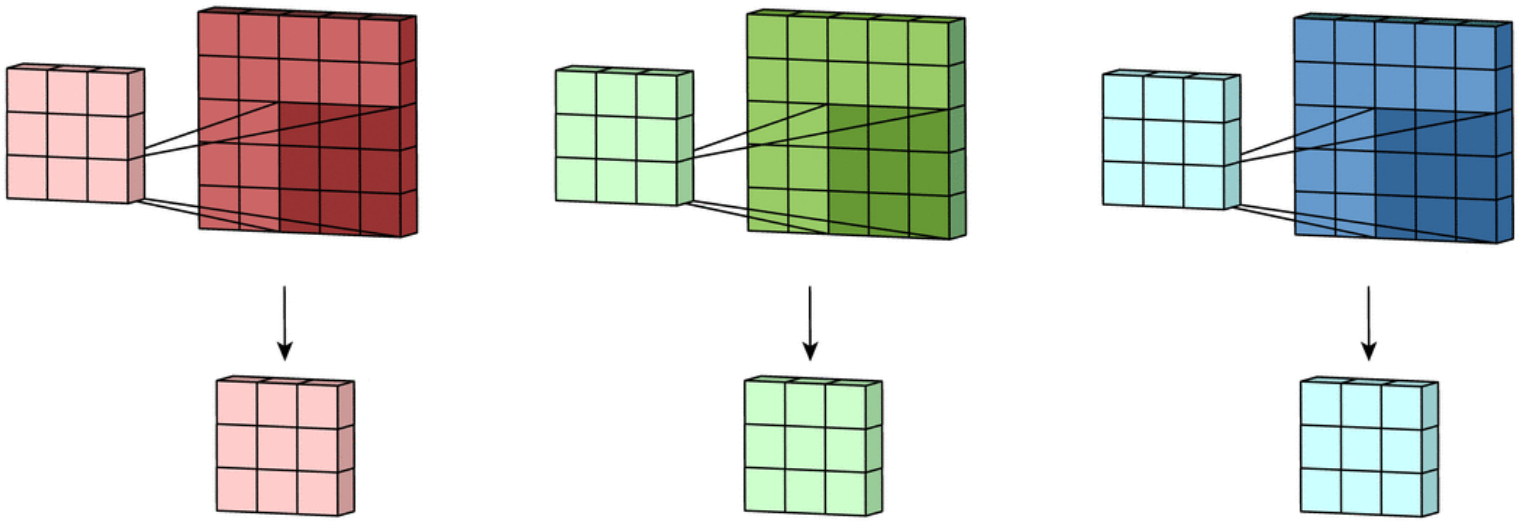


3. Bias

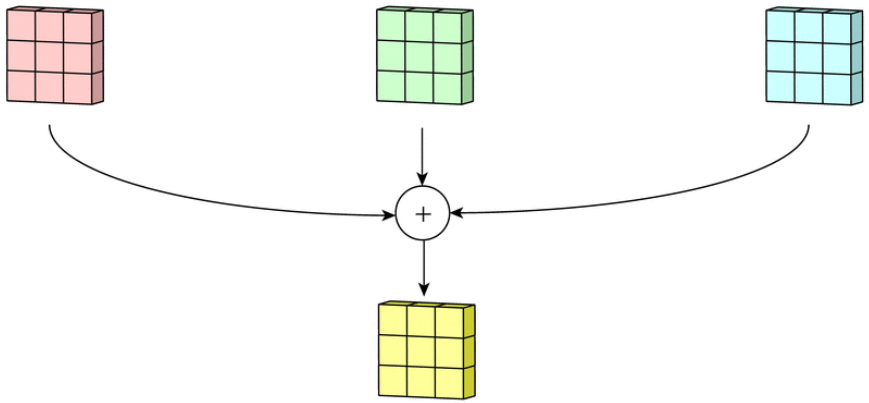


Summary of Convolutional layer steps

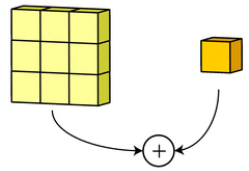
1. Convolution



2. Addition

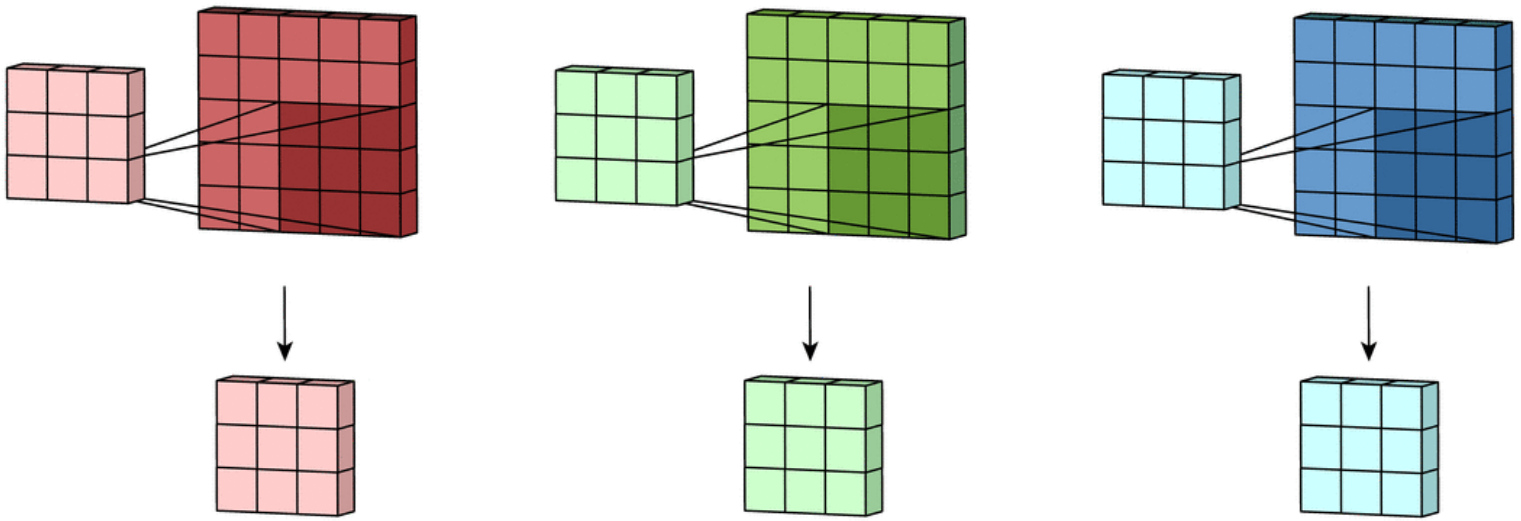


3. Bias

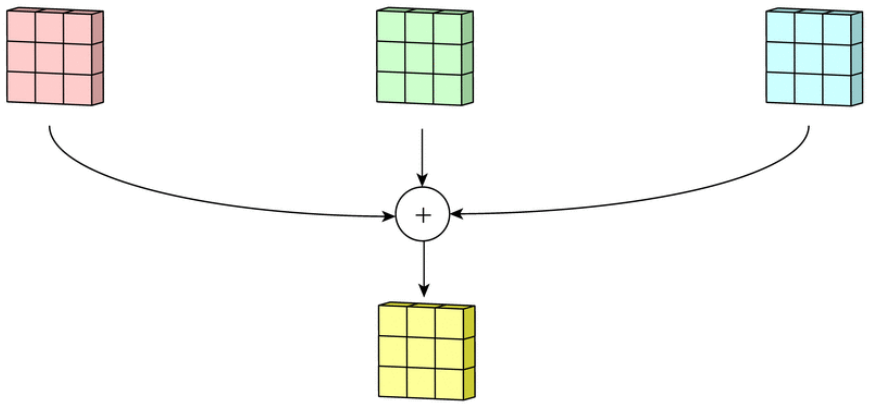


Summary of Convolutional layer steps

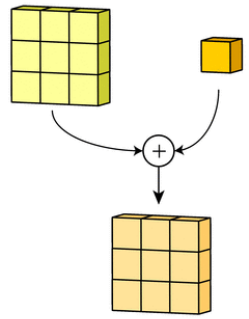
1. Convolution



2. Addition



3. Bias

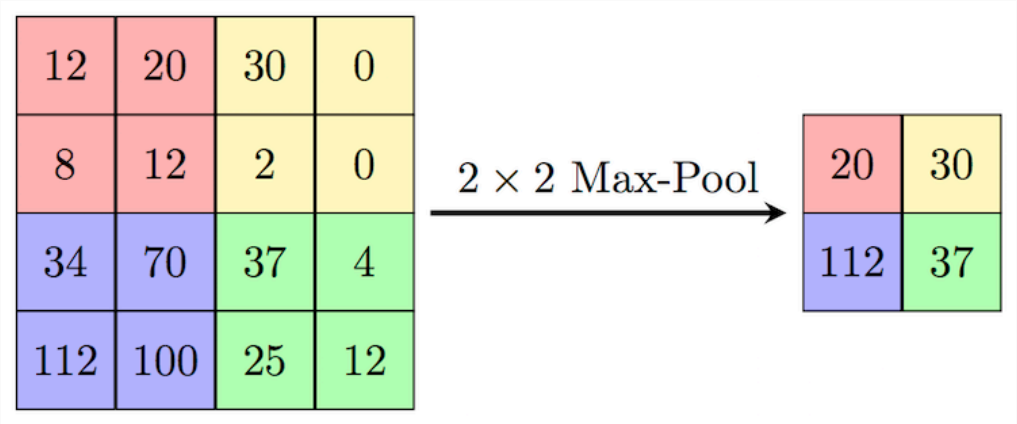


Remarks on Convolutional layers

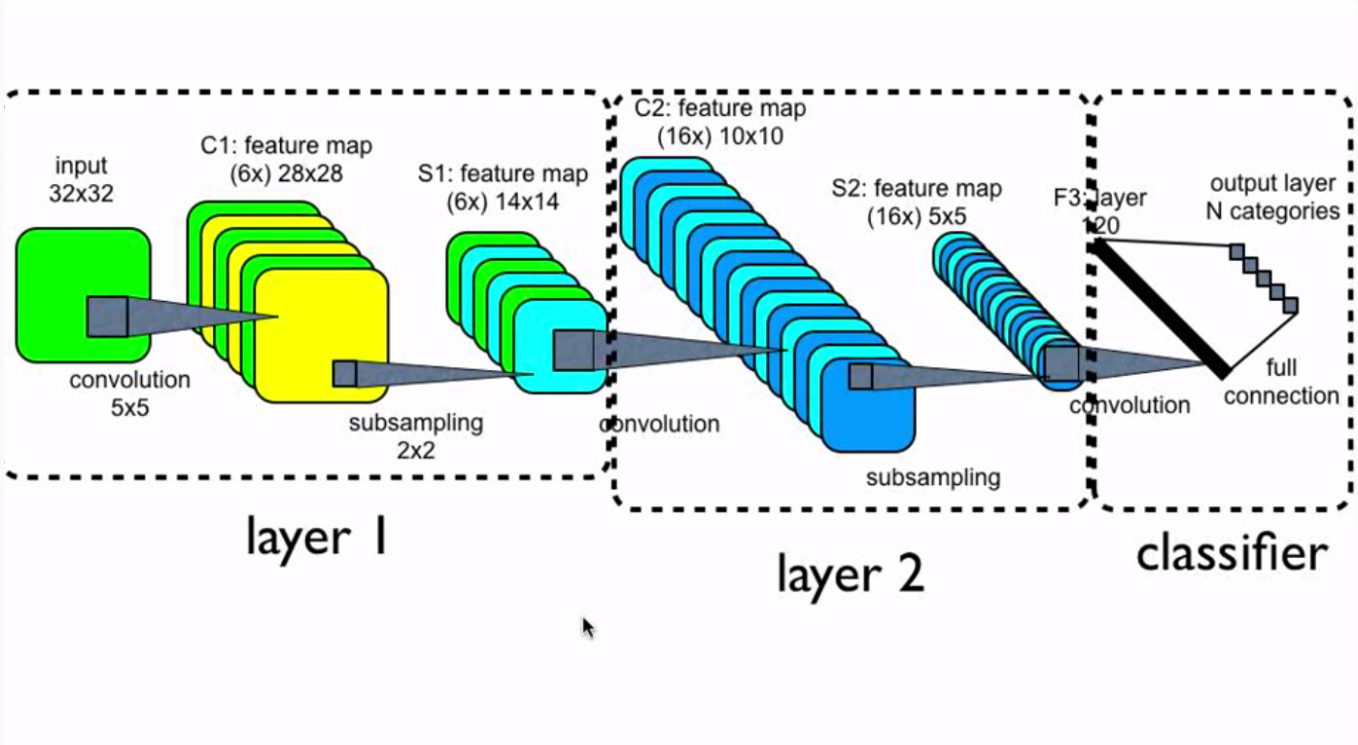
- Convolutional layers are acting locally on the image (But you can still use large scale information by adding more layers)
- Convolutions are invariant by translation (the weights do not depend on the location on the image).
- They can handle images of different sizes.

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

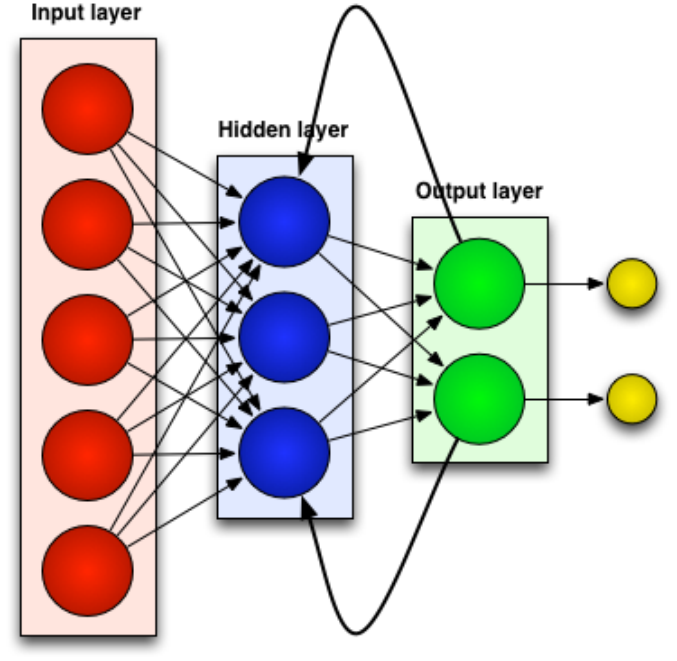
AlexNet is the first Deep architecture used on ImageNet challenge in 2012 and achieved an error of 15.3% (10% better than the previous best classifier). The paper was cited more than 34,000 times.

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

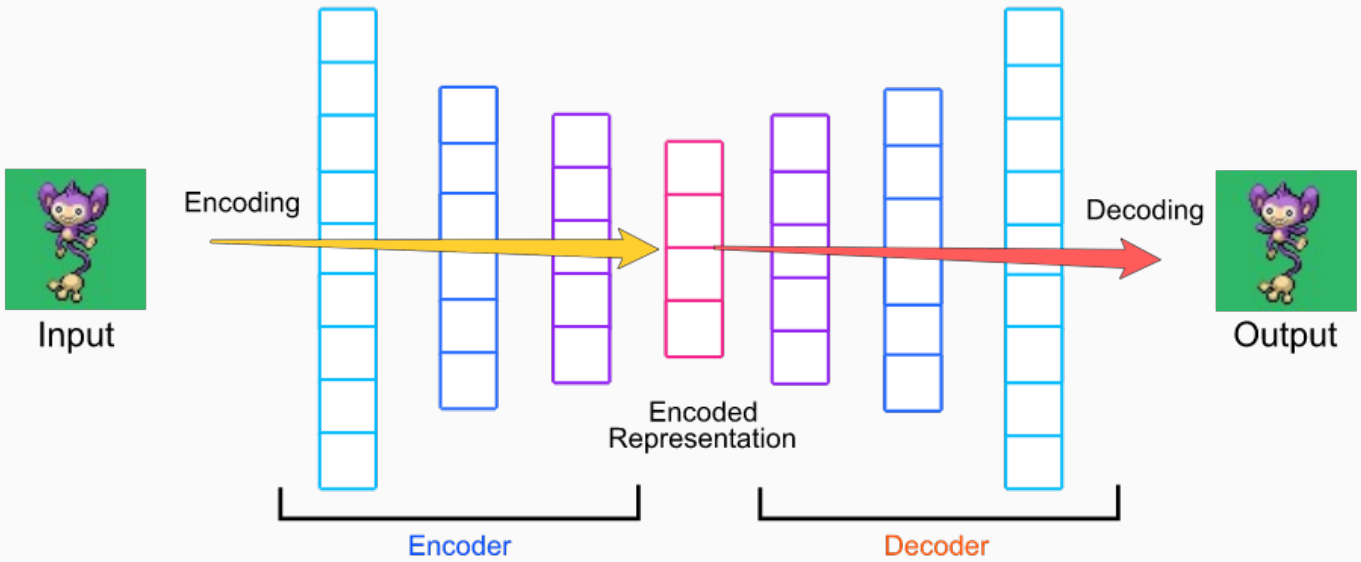


Some popular types of recurrent neural networks:

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

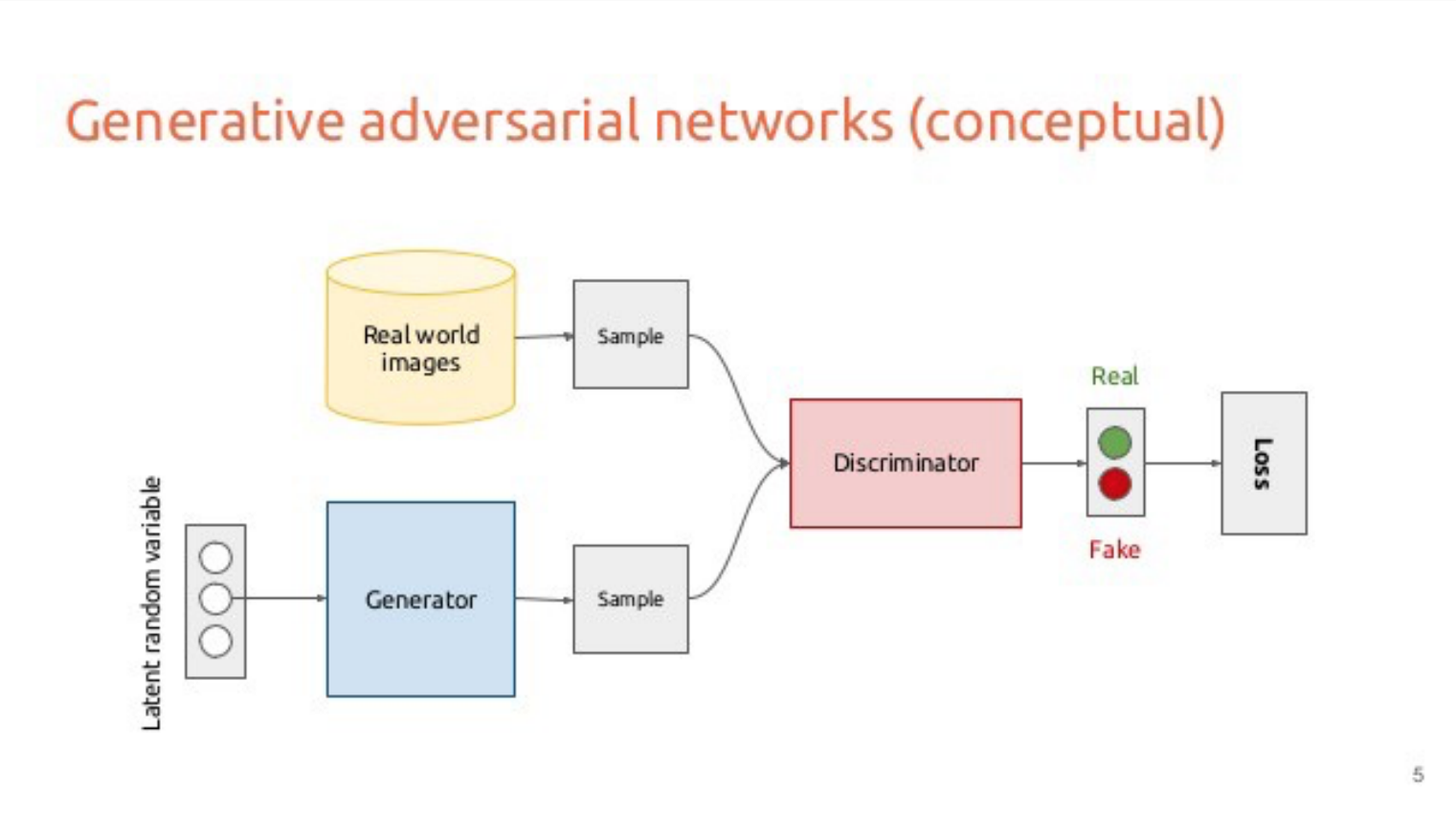
Used in machine translation and text processing

Autoencoders

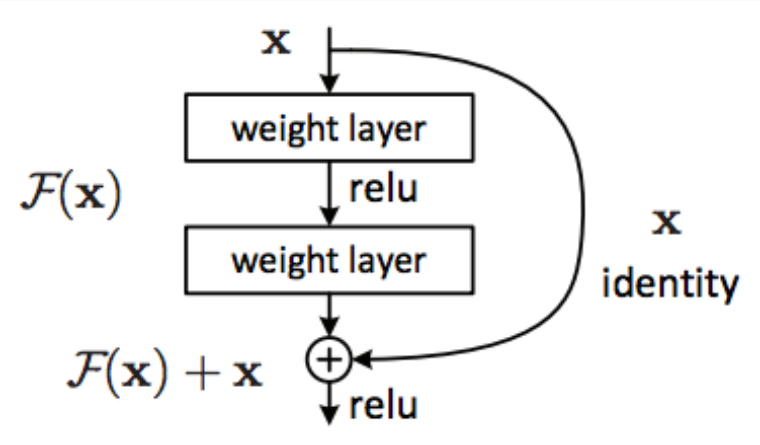


Used in image denoising, compressing, generation,...

Generative adversarial networks



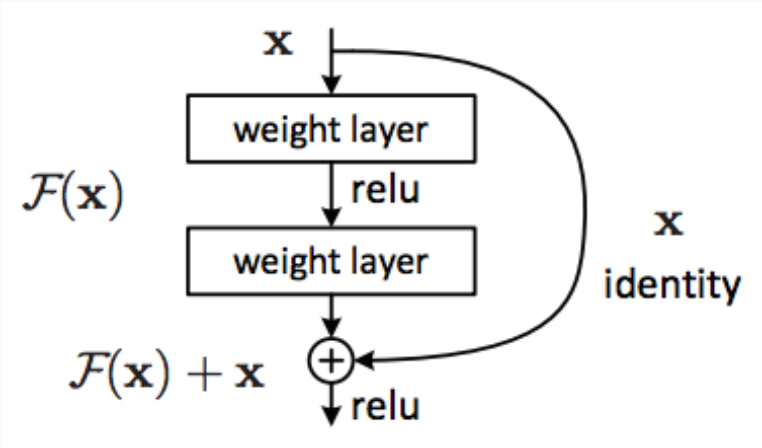
Residual Networks



x : input, y : output

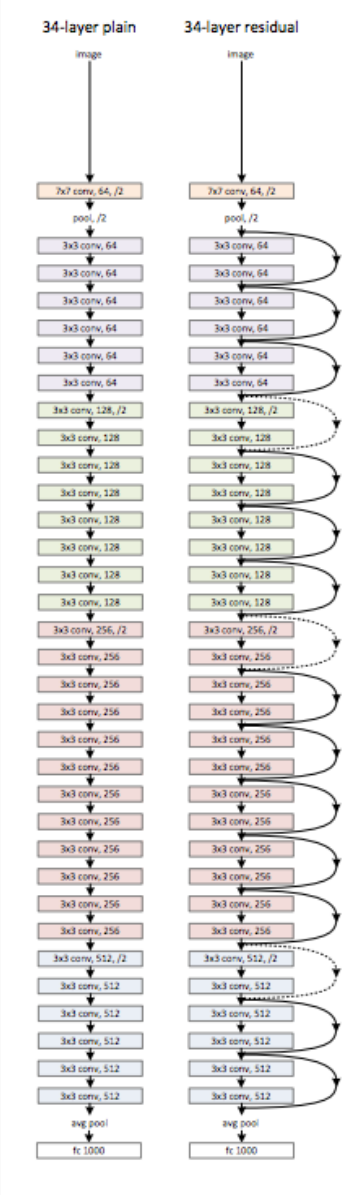
$$y = x + \mathcal{F}(x)$$

Residual Networks



x : input, y : output

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



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 encode qualitative features? [Van16,5.4]
- How to determine the hyperparamters? [Van16,5.3]
- What is a artificial neural network? [GBC16,6]
- What is a convolutive layers [GBC16,9]

  https://towardsdatascience.com/intuitively-understanding-convolutions-for-deep-learning-1f6f42faee1
- What are the main types of neural networks? [GBC16,10, 14, 20]

Refs

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