Introduction to Data Science
Supervised Learning

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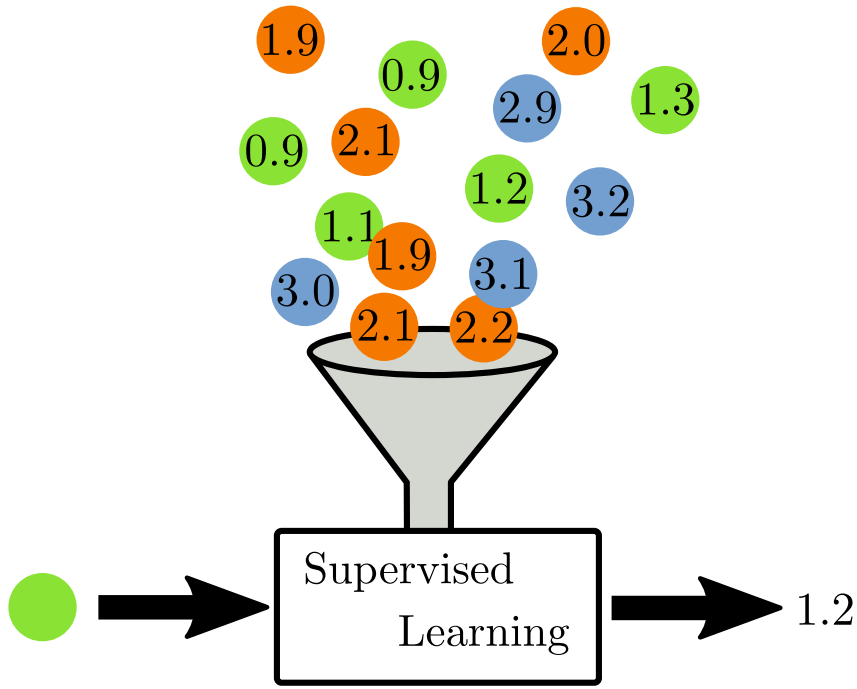
What we are talking about ?



- Learning trough examples
- Mimic human tasks (IA ?)
- Produce outputs given some inputs (functions ?)

Supervised Learning

Purpose

Given a dataset $\{(\mathbf{x}_i, y_i) \in \mathcal{X} \times \mathcal{Y}, i = 1, \ldots, N\}$, learn the dependancies between $\mathcal{X}$ and $\mathcal{Y}$.

- Example: Learn the links between cardiac risk and food habits. $\mathbf{x}_i$ is one person describe by d features concerning its food habits; y_i is a binary category (risky, not risky).
- y_i are essential for the learning process.
- Methods : K-Nearest Neighbors, SVM, Decision Tree, ...

How to Encode Data

$\mathbf{X} \in \mathbb{R}^{n \times p}$

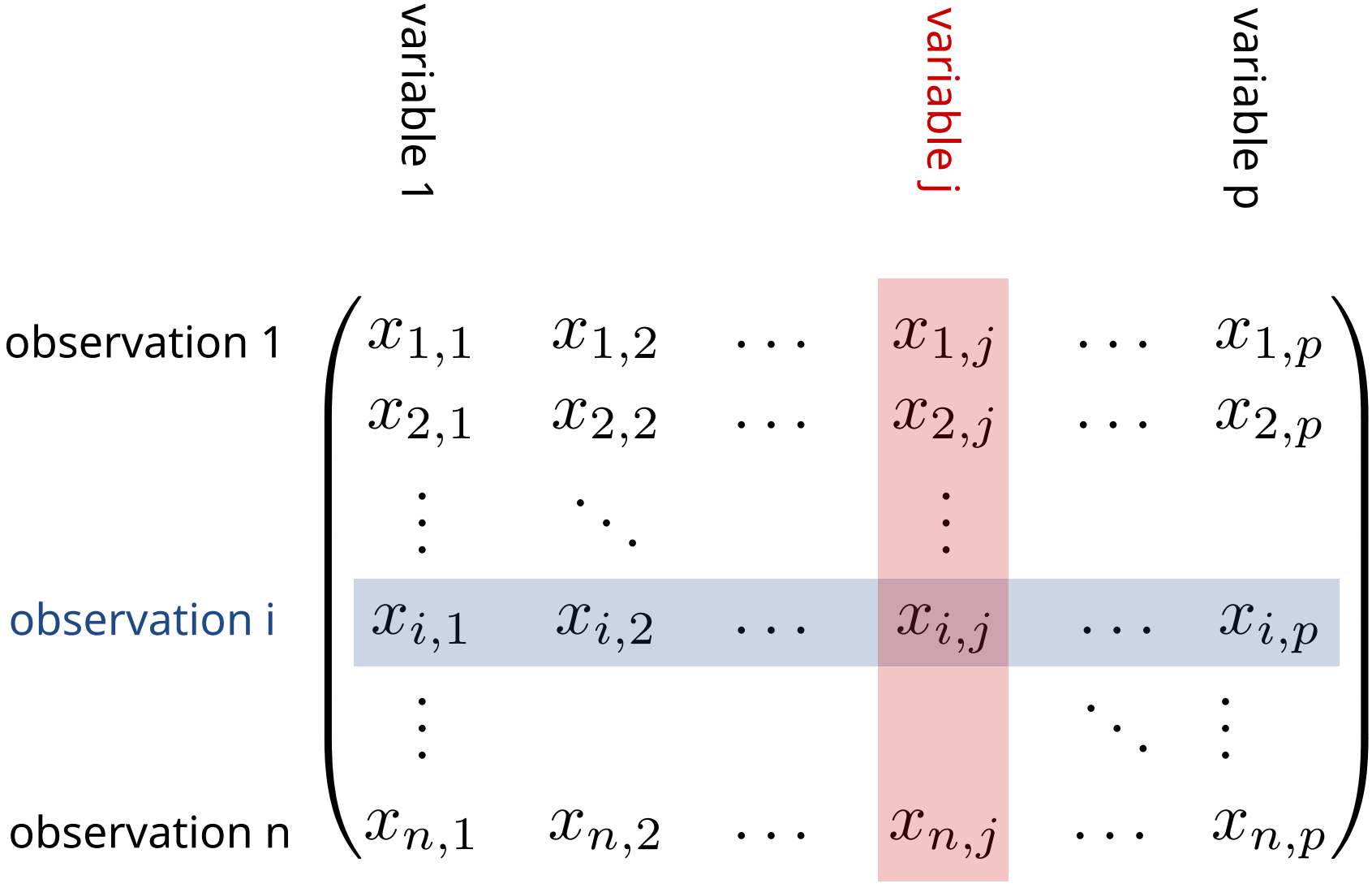
Samples

- n samples (number of lines)
- $\mathbf{X}(i,:) = \mathbf{x}_i^\top$: the i-th sample
- $\mathbf{x}_i \in \mathbb{R}^p$

Features

- p features (number of colons)
- Each sample is described by p features
- $\mathbf{X}(:,j) = \boldsymbol{x}_{\bullet j}$: The j-th feature for all sample

$\mathbf{X}(i,j)$: j-th feature of i-th sample.


variable 1
variable j
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$\begin{pmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,j} & \cdots & x_{1,p} \\ x_{2,1} & x_{2,2} & \cdots & x_{2,j} & \cdots & x_{2,p} \\ \vdots & \ddots & & \vdots & & \\ x_{i,1} & x_{i,2} & \cdots & x_{i,j} & \cdots & x_{i,p} \\ \vdots & & & & \ddots & \vdots \\ x_{n,1} & x_{n,2} & \cdots & x_{n,j} & \cdots & x_{n,p} \end{pmatrix}$

Learning Model

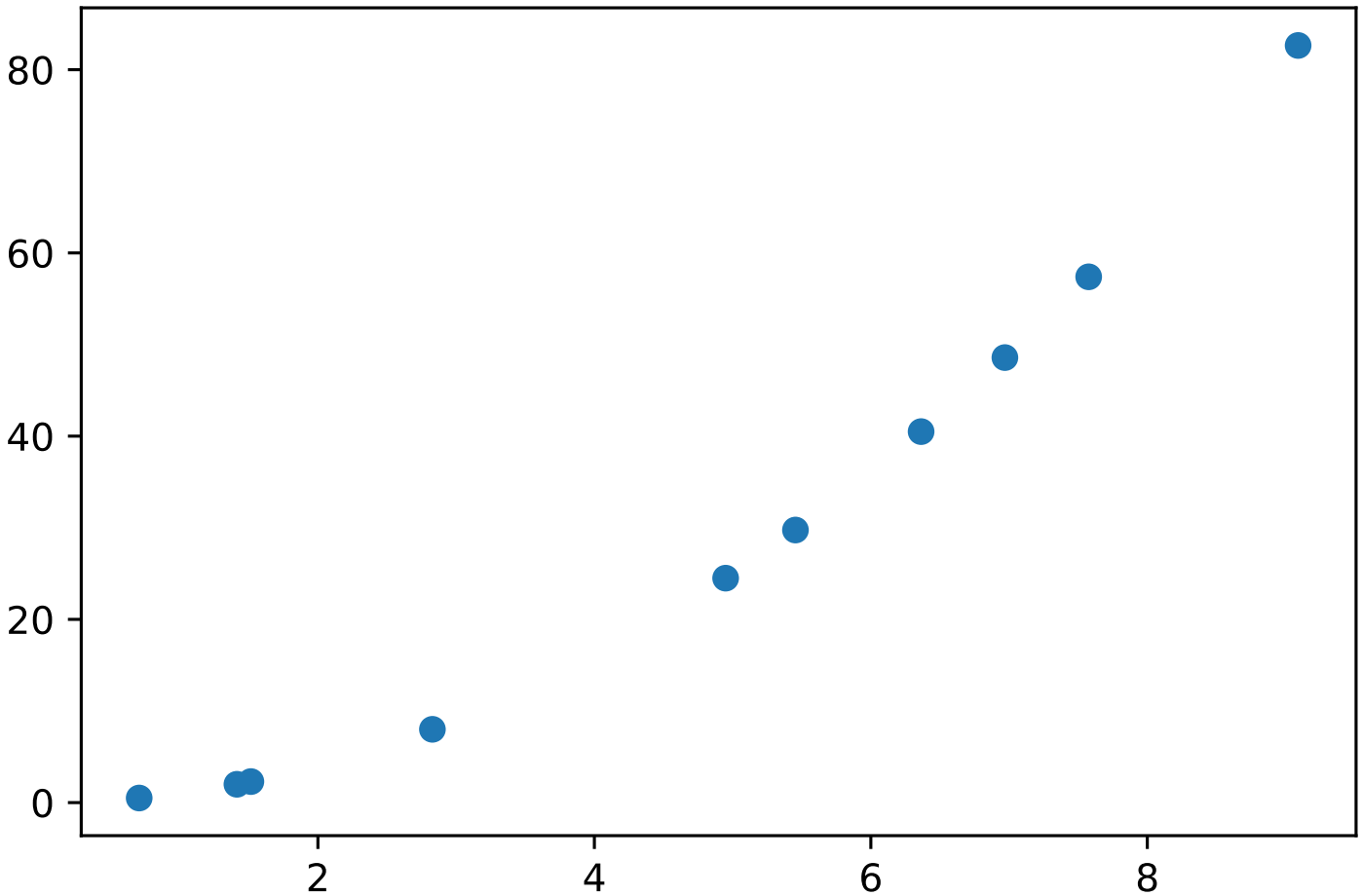
Model

$$f: \quad \mathcal{X} \to \mathcal{Y}$$
$$\mathbf{x}_i \to \hat{y}$$

We want that

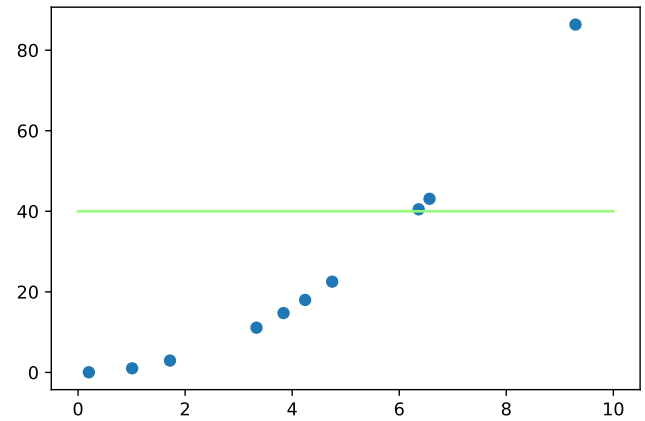
$$f(\mathbf{x}_i) \simeq y_i$$

Example



What is the underlying f function ?

Example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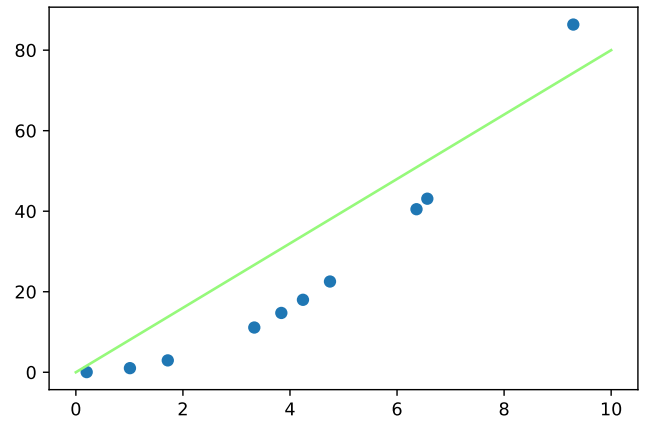
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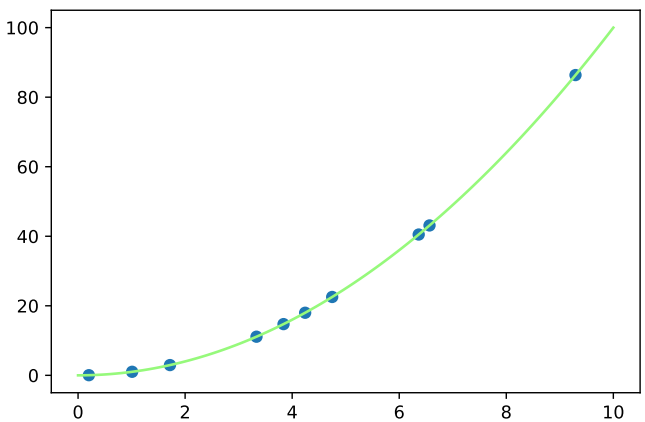
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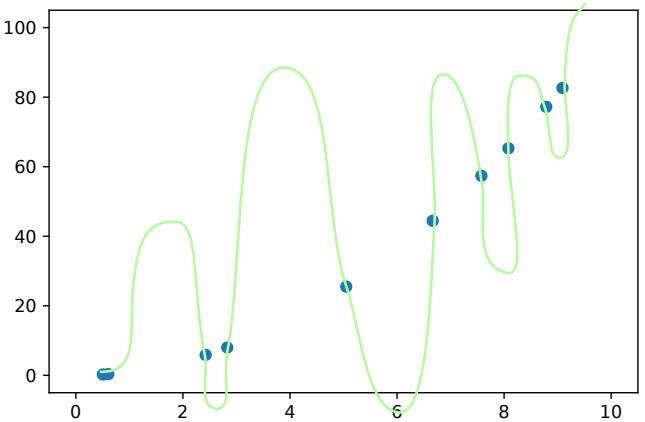
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How to find a good f ?

$$f^\star = \arg\min_f \mathcal{L}(f(\mathbf{X}), \mathbf{y}) + \lambda\Omega(f)$$

- $\mathcal{L} : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$
- $\lambda \in \mathbb{R}^+$
- $\Omega : (\mathcal{X} \to \mathcal{Y}) \to \mathbb{R}^+$

Fit to data term

$$\mathcal{L}(f(\mathbf{X}), \mathbf{y})$$

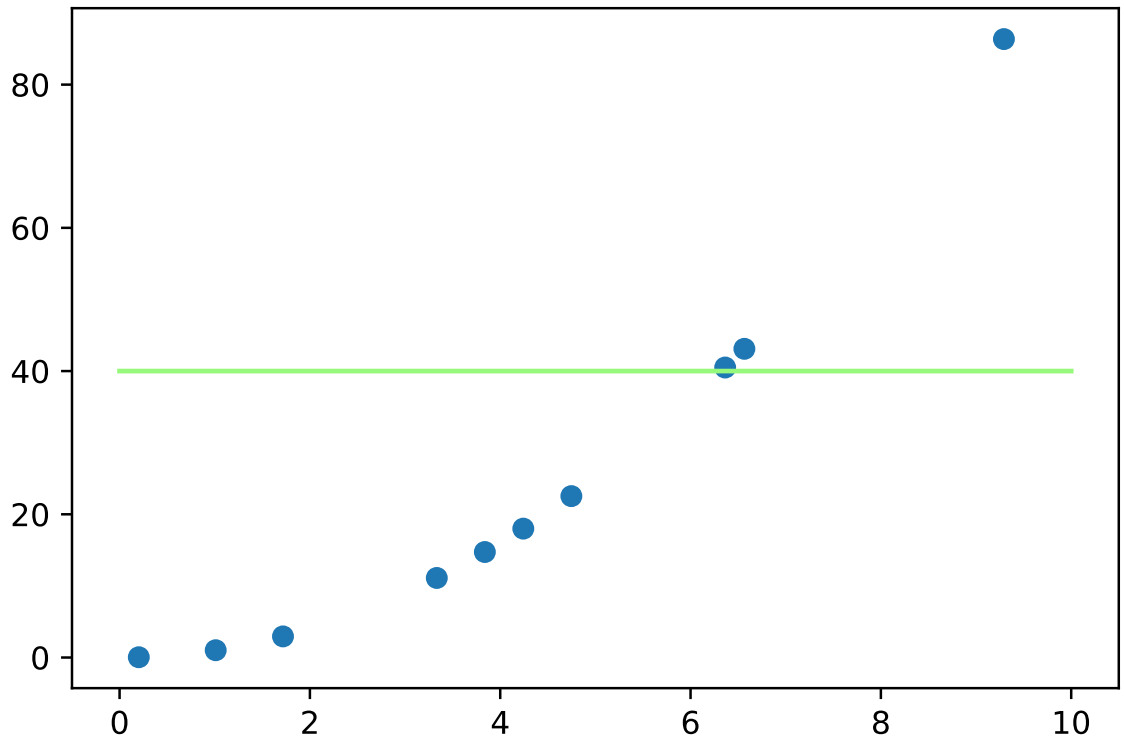
- Guarantees that the model fits the data
- Penalizes when the predicted value of $f(\mathbf{x}_i)$ is far from y_i

Regularization term

$$\Omega(f)$$

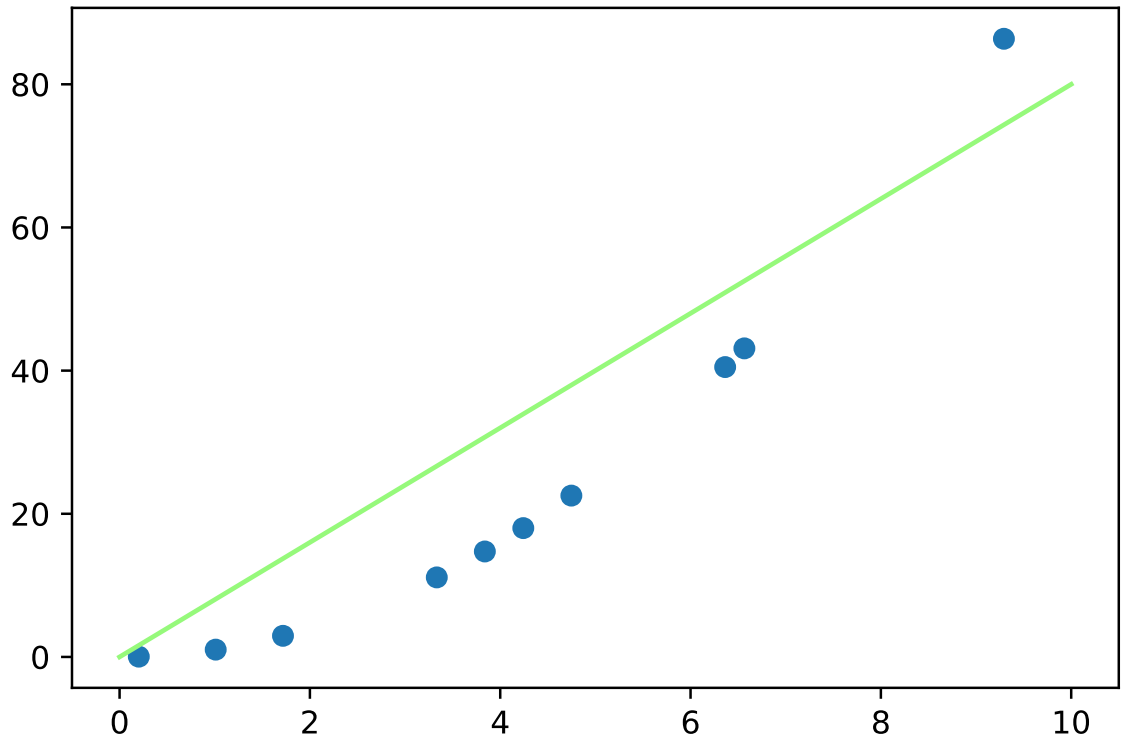
- Constrain the complexity of function f
- Occam's razor : simpler is better
- λ : Weight the balance between the two terms

Illustrations I



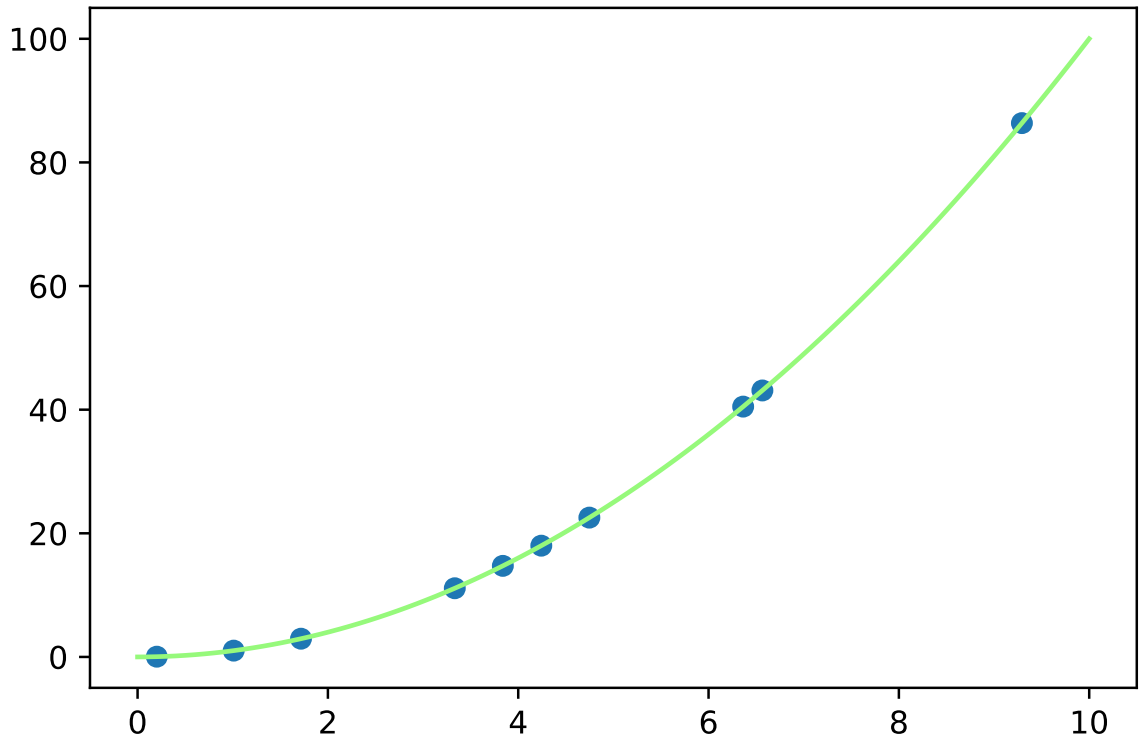
- Very high $\mathcal{L}(f(\mathbf{X}), \mathbf{y})$
- Very low $\Omega(f)$

Illustrations II



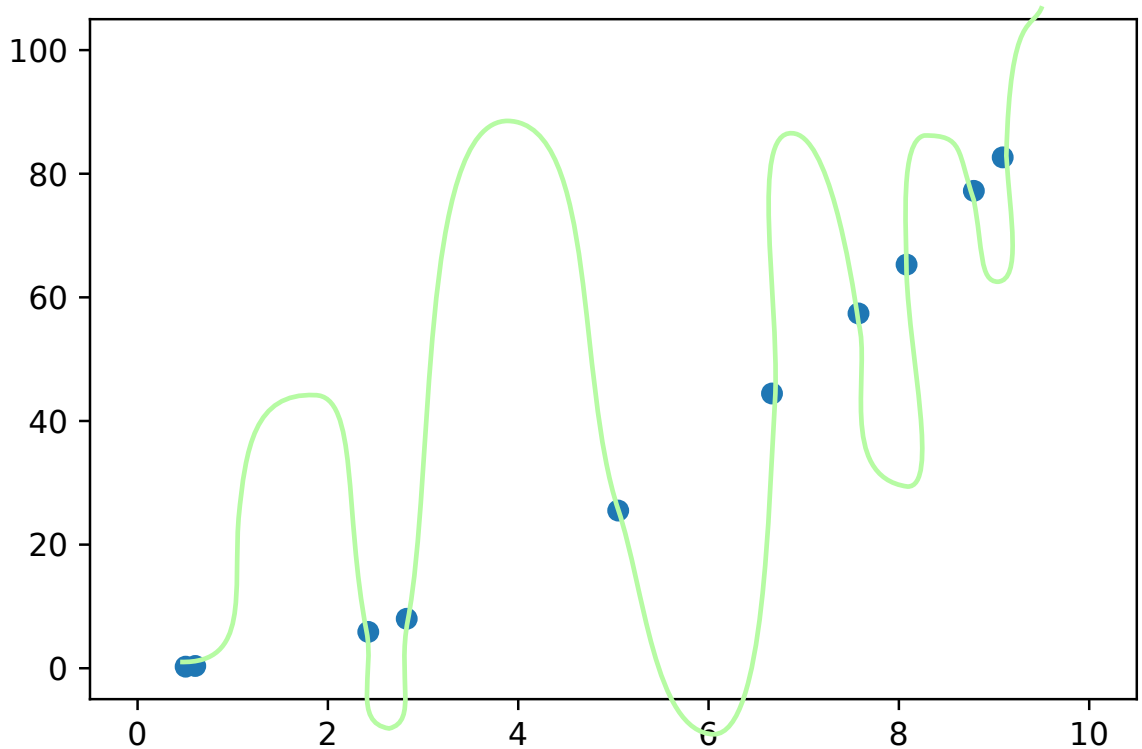
- High $\mathcal{L}(f(\mathbf{X}), \mathbf{y})$
- Low $\Omega(f)$

Illustrations III



- $\mathcal{L}(f(\mathbf{X}), \mathbf{y}) = 0$
- High $\Omega(f)$

Illustrations IV



- $\mathcal{L}(f(\mathbf{X}), \mathbf{y}) = 0$
- Very high $\Omega(f)$

Generalization

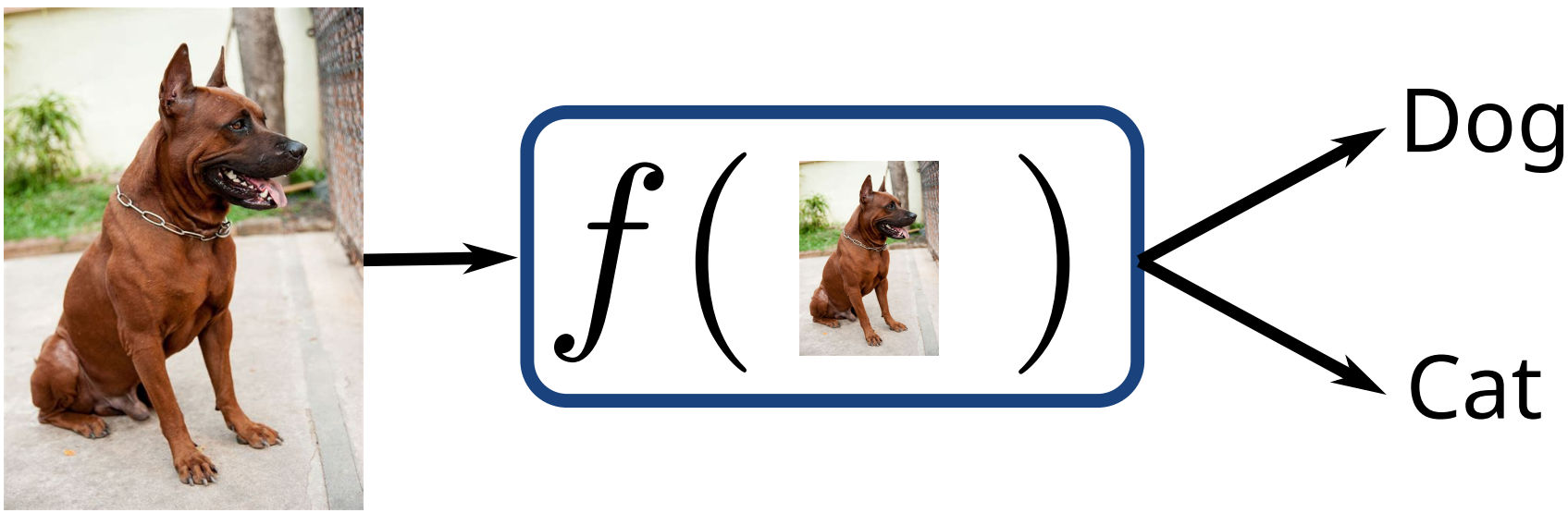
A good model generalizes well

- Good generalization : good prediction on unseen data
- Hard to evaluate without bias
-  Overfitting
- Regularization term prevents from overfitting

Supervised Learning Tasks I

Binary Classification

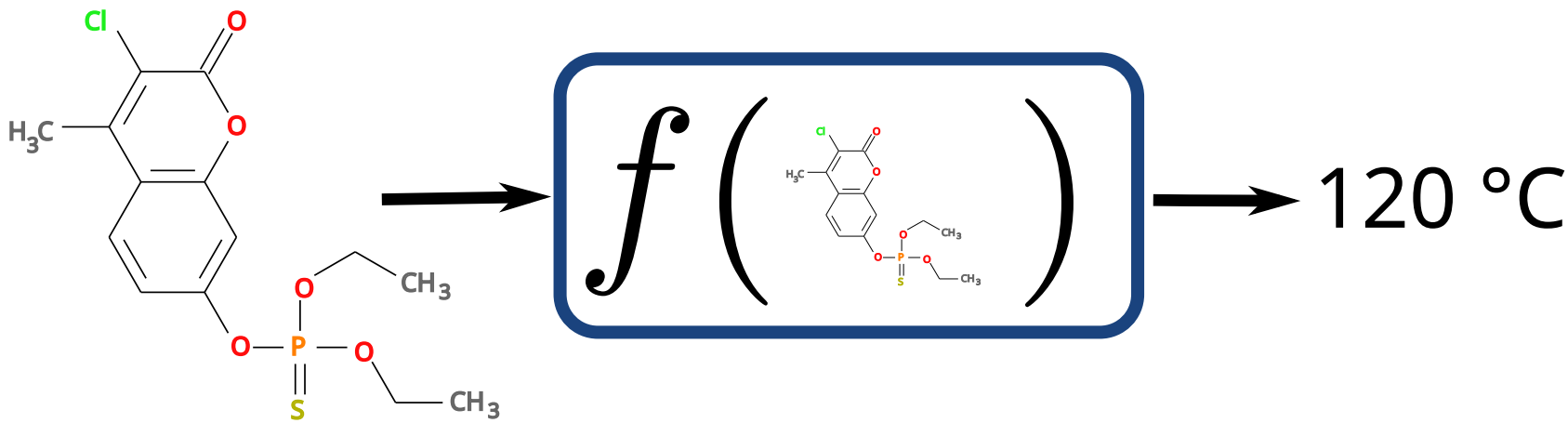
- $\mathcal{Y} = \{0, 1\}$
- Dog or cat ? Positive or Negative ?
- Performance : Accuracy, recall, precision, ...



Supervised Learning Tasks II

Regression

- $\mathcal{Y} = \mathbb{R}$
- Stock market, House price, boiling points of molecules, ...
- Performance: RMSE, MSE, MAE, ...



Supervised Learning Tasks III

And many others

- Ranking
- MultiClass classification
- Multi Labeling
- ...

Machine learning Methods for Classification

- K-nearest neighbors
- Random forests
- SVM & consorts
- Multi Layer Perceptron

k Nearest Neighbors

Principle

Determine property from the property of similar data

k Nearest Neighbors

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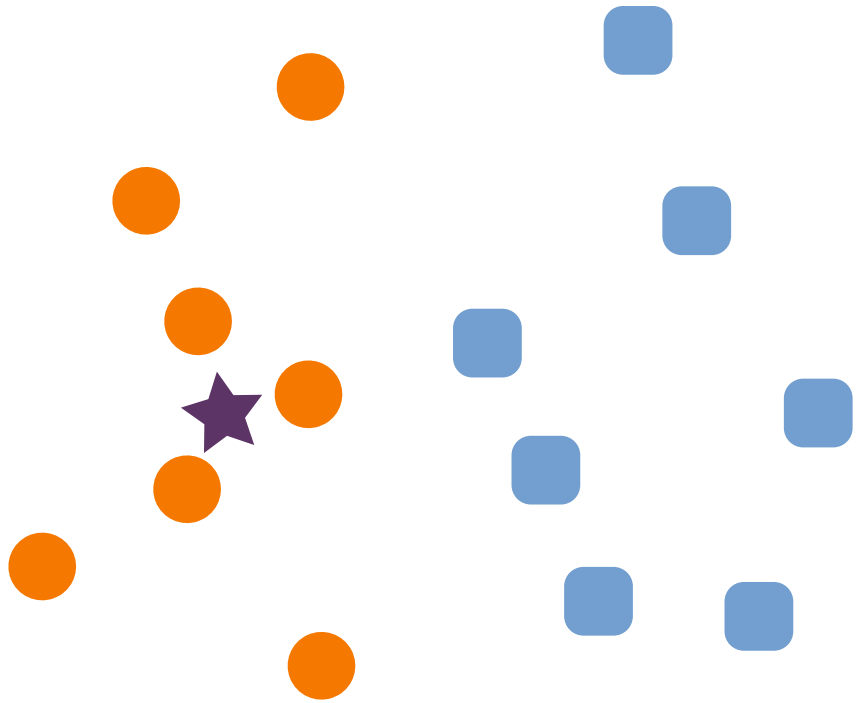

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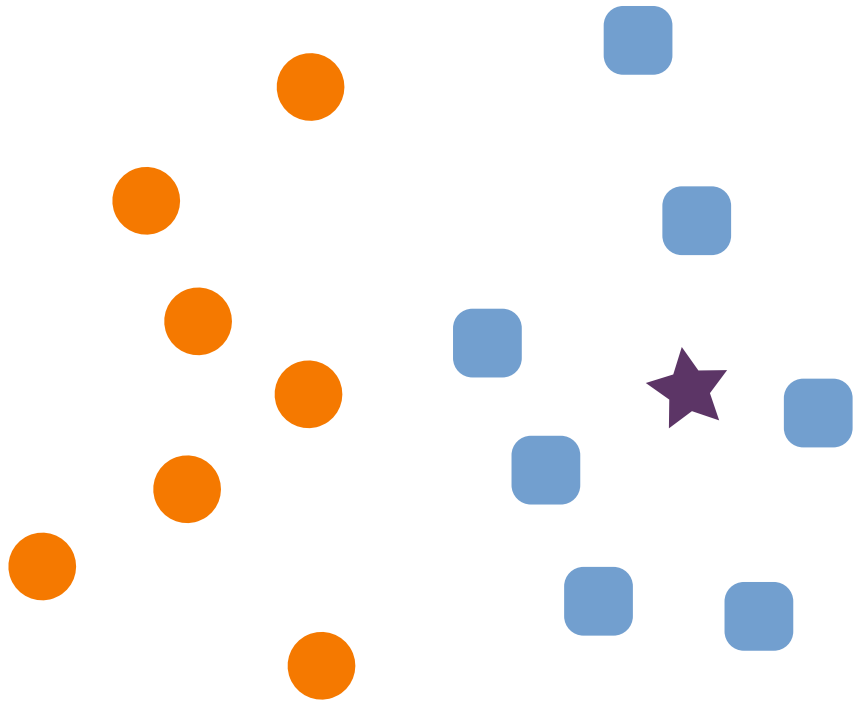

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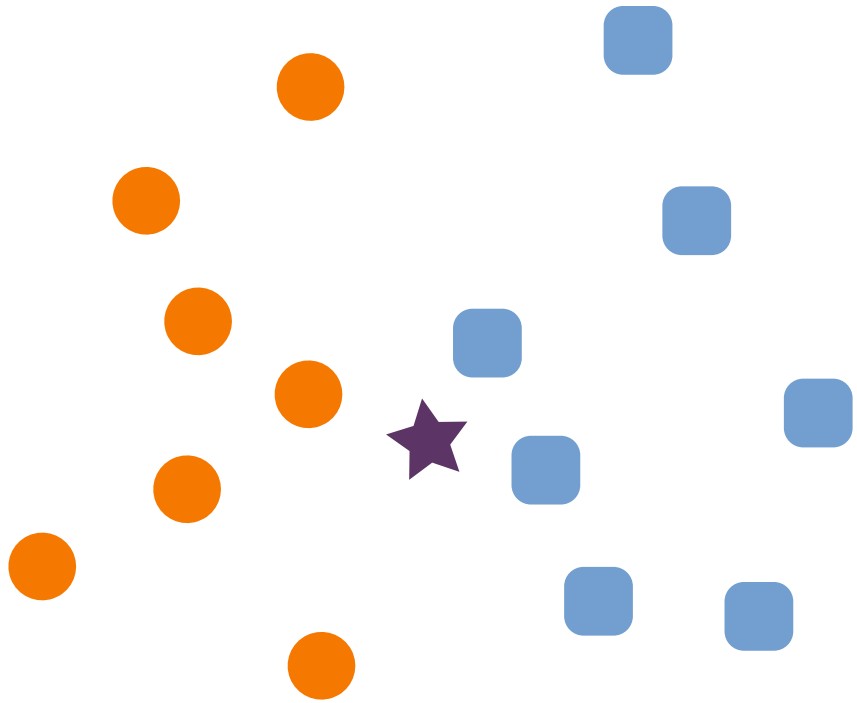

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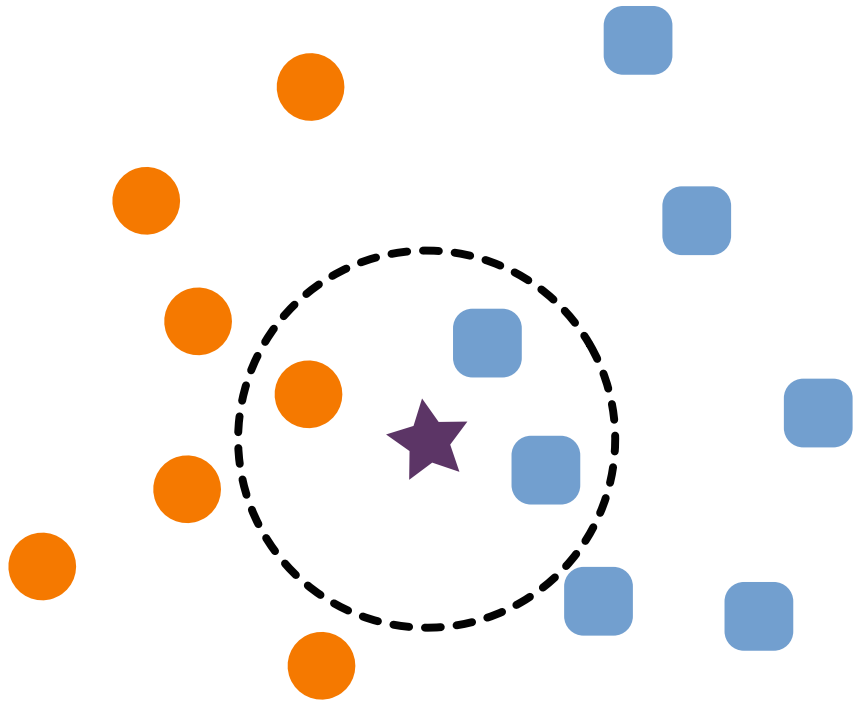

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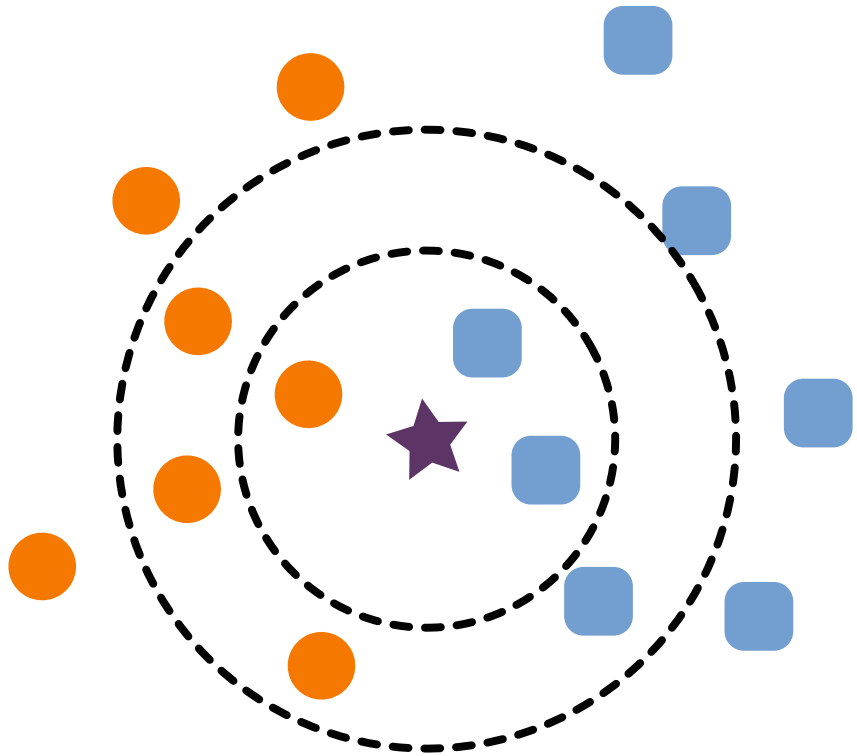

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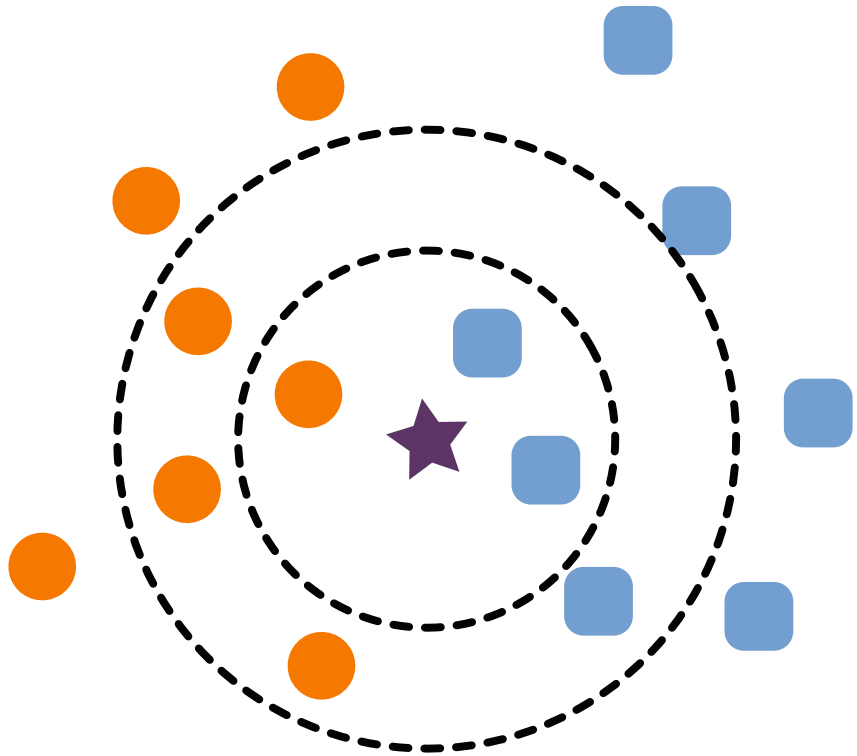


K-NN Hyperparameters

Number of neighboors k

Quantify the number of neighbors used for the decision

- Low number : high variability, high accuracy
- High number : more smooth

Distance

How the similarity is determined

- Similarity depends on data, structure, task
- Euclidean, Manhattan, ad hoc distances

KNN : the code !

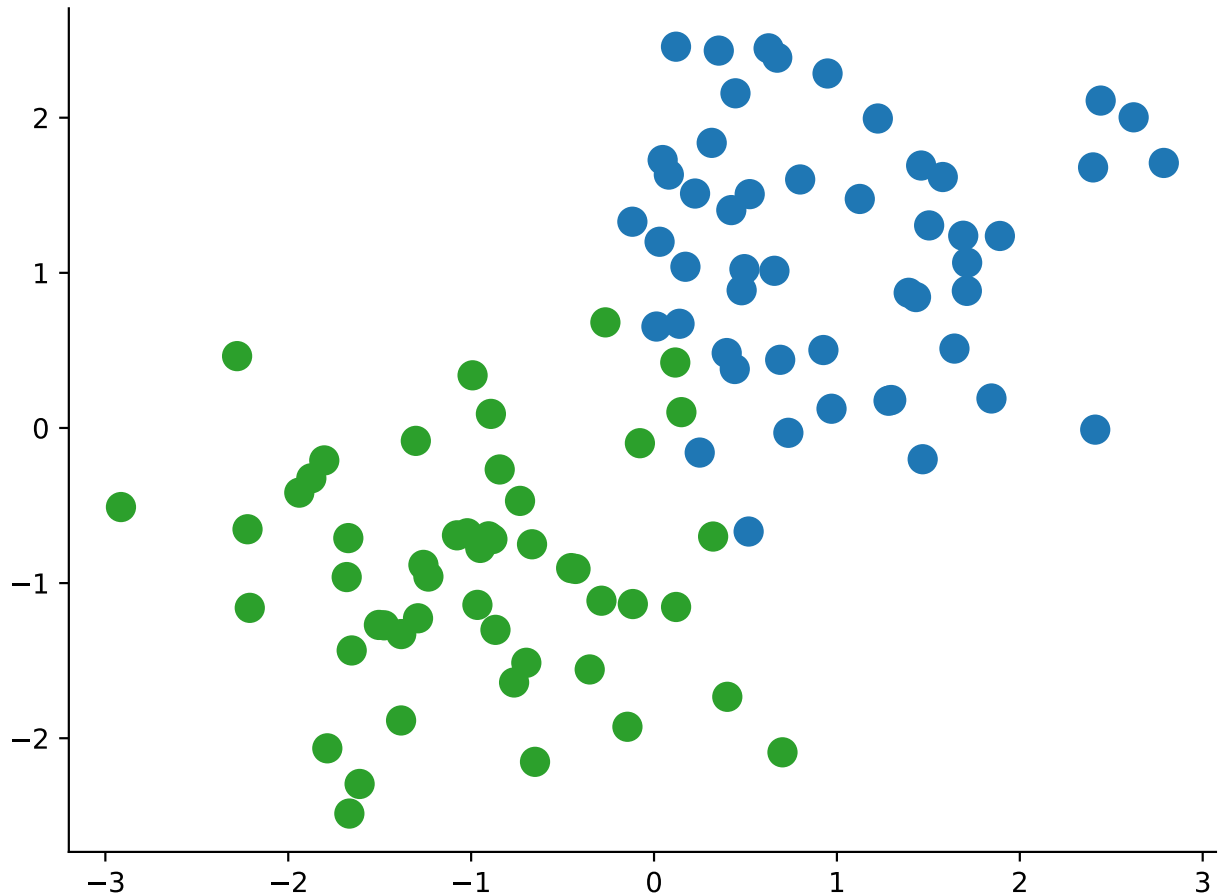
```
1  from sklearn.neighbors import KNeighborsClassifier
2  k=5
3  metric = 'manhattan'
4  knn = KNeighborsClassifier(n_neighbors=k,metric=metric)
5  knn.fit(X,y) #apprentissage
6  y_pred = knn.predict(X) # prediction
```

- Metrics : link
- $\Rightarrow$ Notebook
- the documentation

Decision Tree

Principle

Learn decision rules to separate the data.



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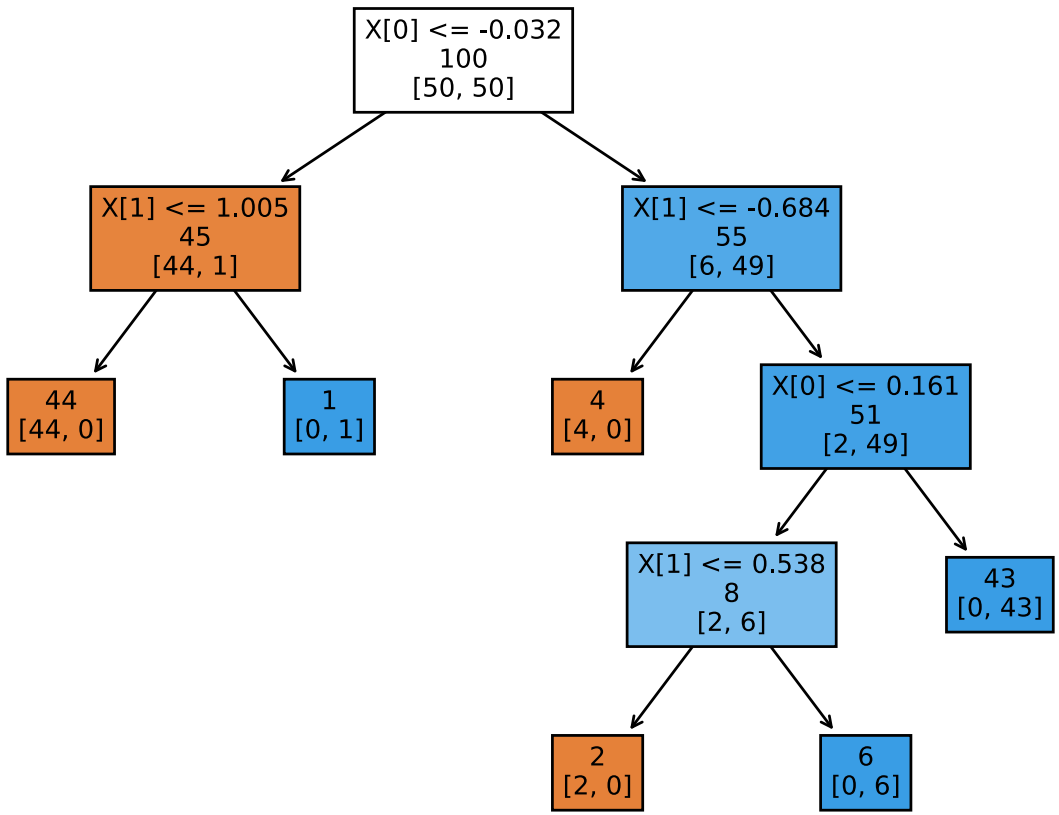

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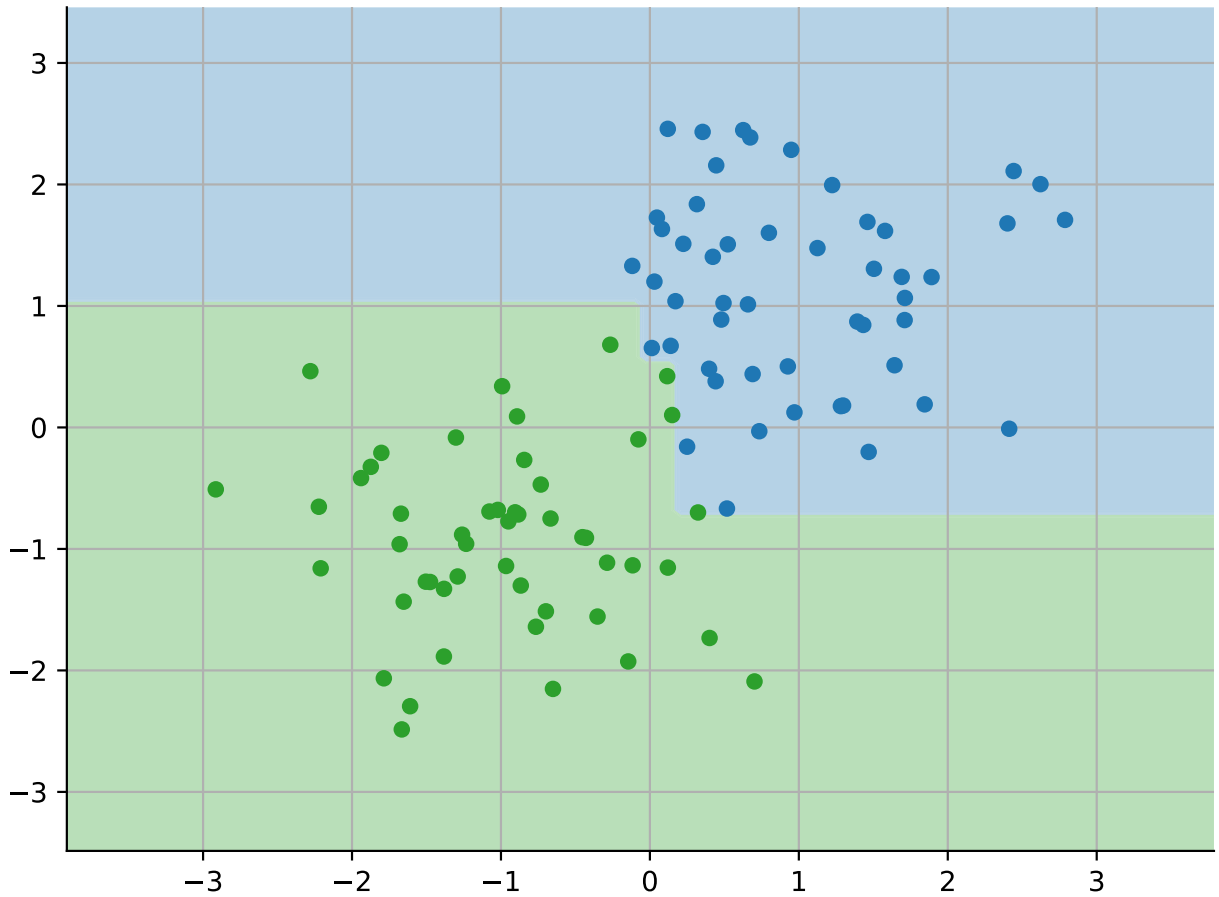
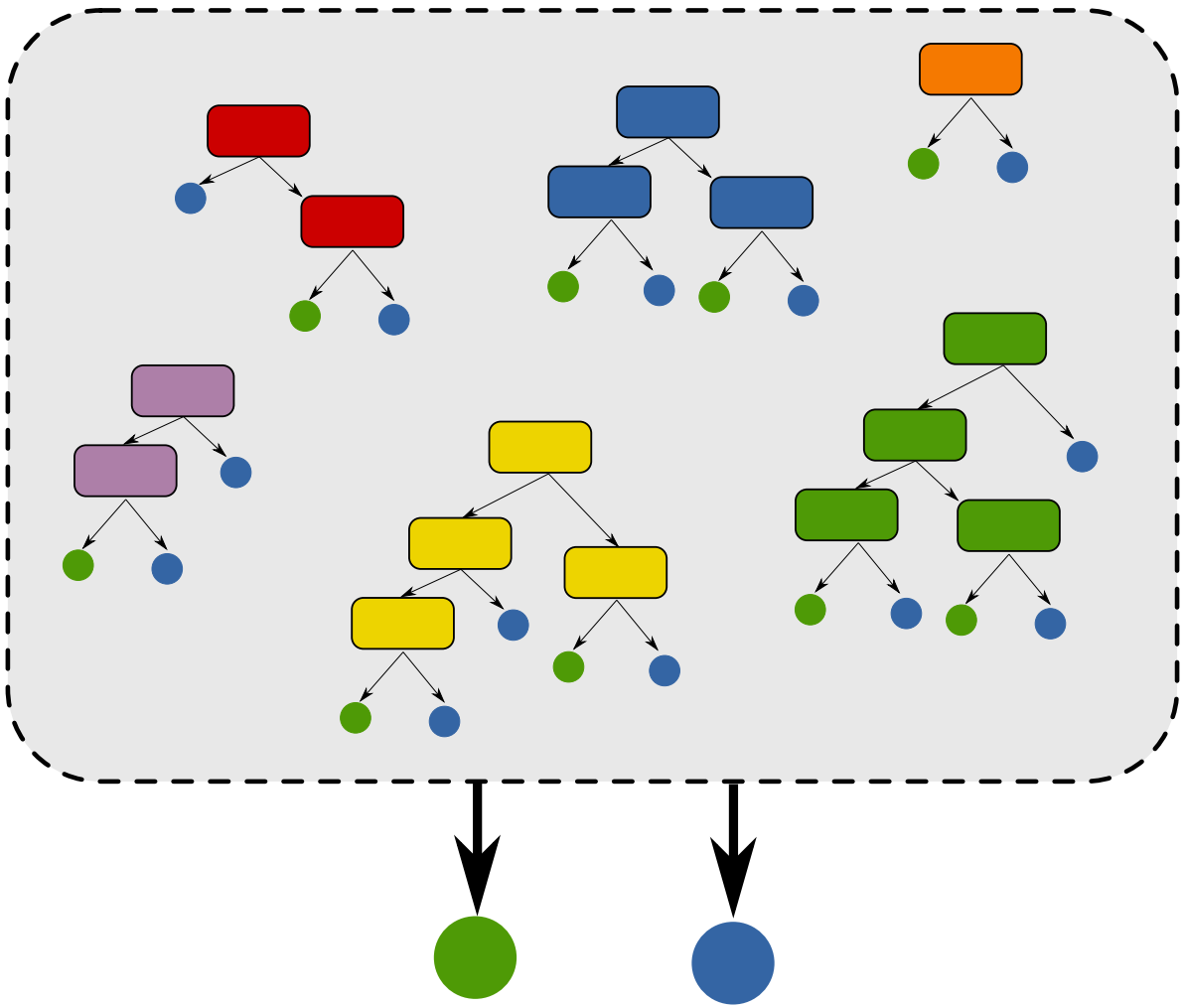


Random Forests

Principle

- Combine many decision trees to learn complex functions
- Ensemble methods, majority voting



Random Forests Hyperparameters

Number of trees

Adjust the number of trees composing the forests

- low number : fast to compute, but less accurate
- high number : slower to compute, but more accurate up to some number

Number of features

Determine the number of features to be used when splitting the data

- See the guidelines of `scikit-learn`

Tree depth

Specify the maximal depth of tree. An higher depth will make dedicate categories, but less generalizable.

Random Forests : the code !

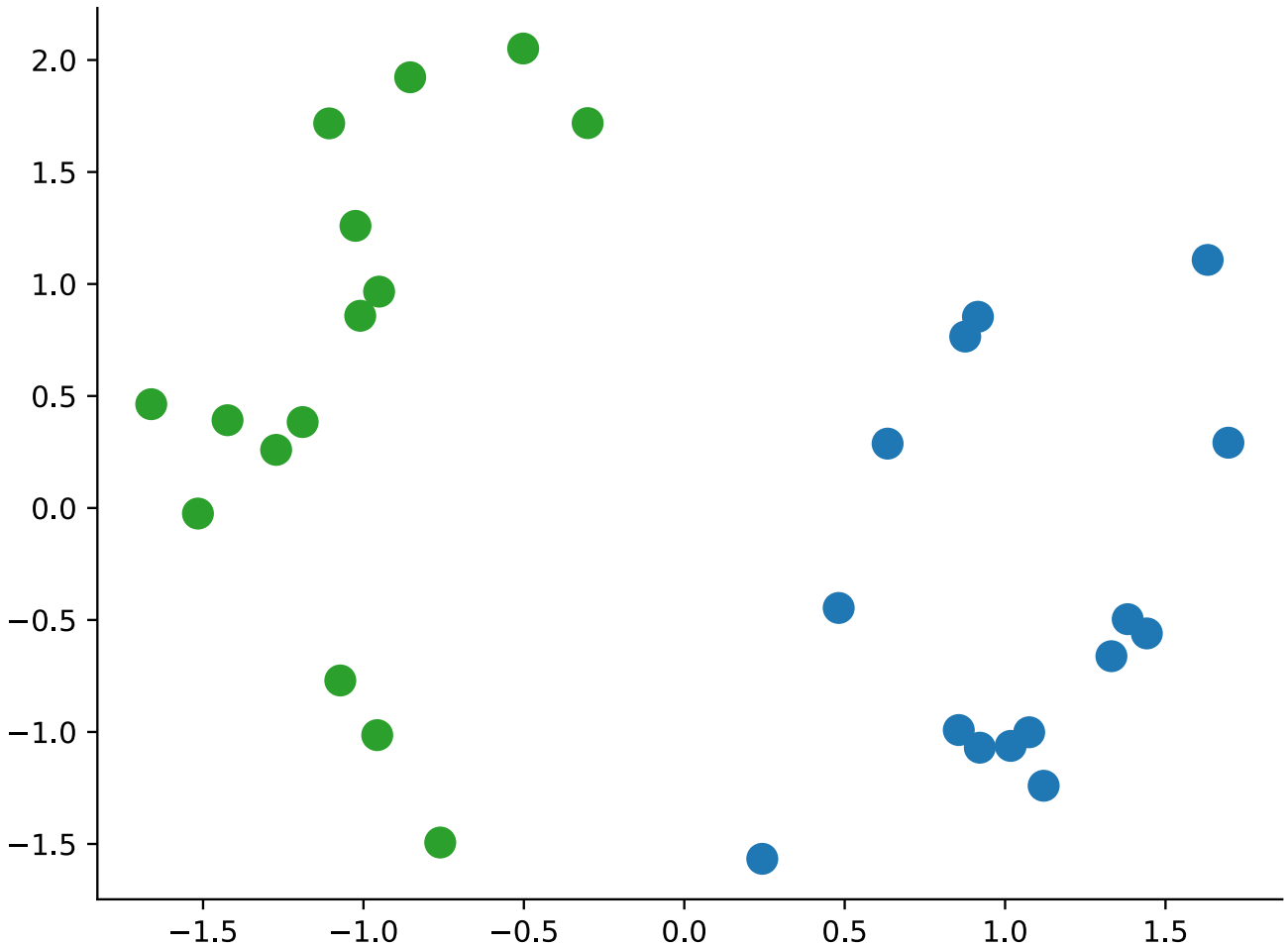
```python
from sklearn.ensemble import RandomForestClassifier
n_estimators = 20 # the number of trees in the forest
max_depth = None # expand as you can
max_features = "sqrt" # RTFM
clf = RandomForestClassifier(n_estimators=n_estimators,
                             max_depth=max_depth,
                             max_features=max_features)
clf.fit(X,y)
ypred = clf.predict(X)
```

- User guide for hyperparameters : link
- $\Rightarrow$ Notebook
- the documentation

Support Vector Machines

Principle

Find the best line which separates the data



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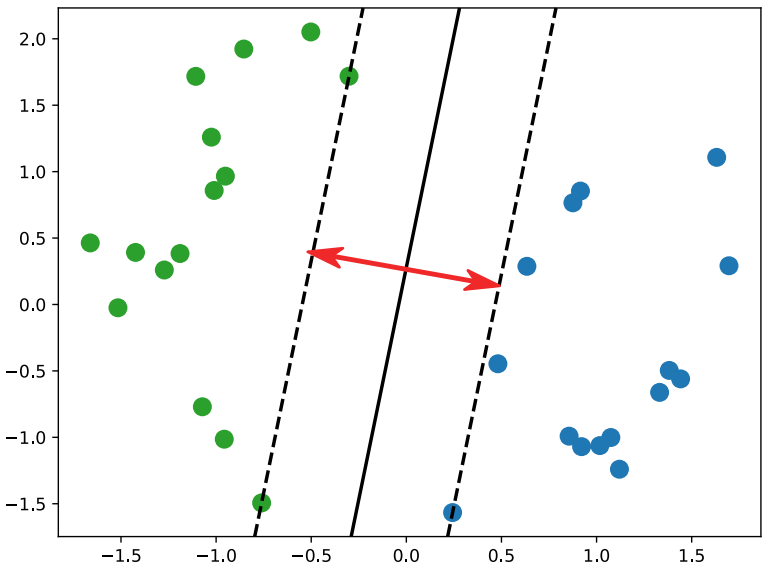
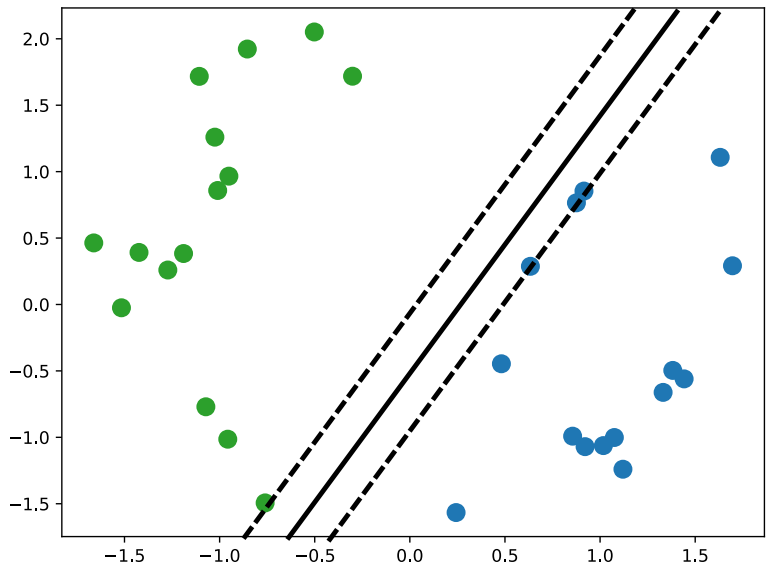


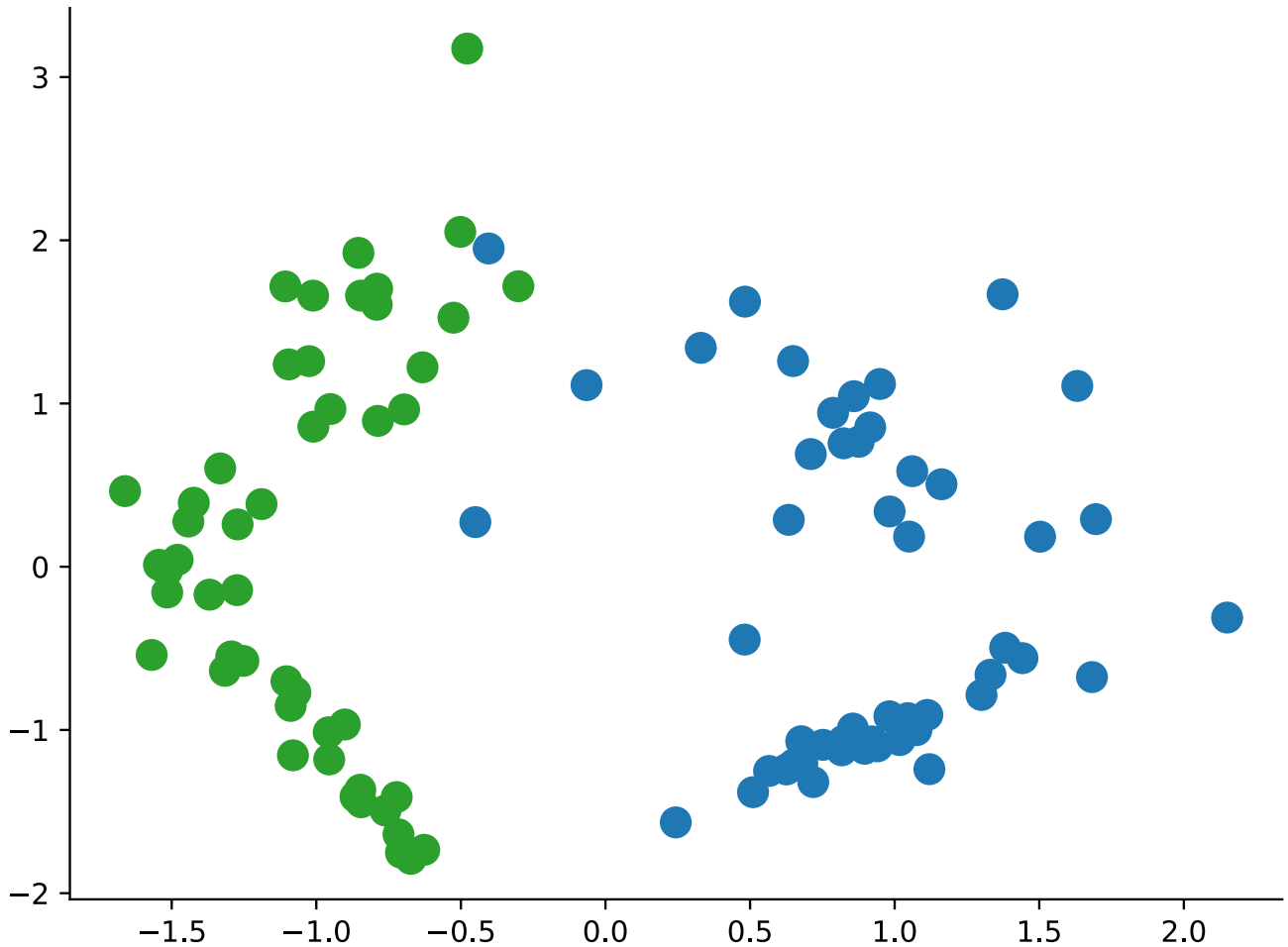


- Best separation $\Rightarrow$ points far away the separation
- Points on margin : support vectors

Support Vector Machines

General Principle

What happens when there is no separation line ?



Support Vector Machines

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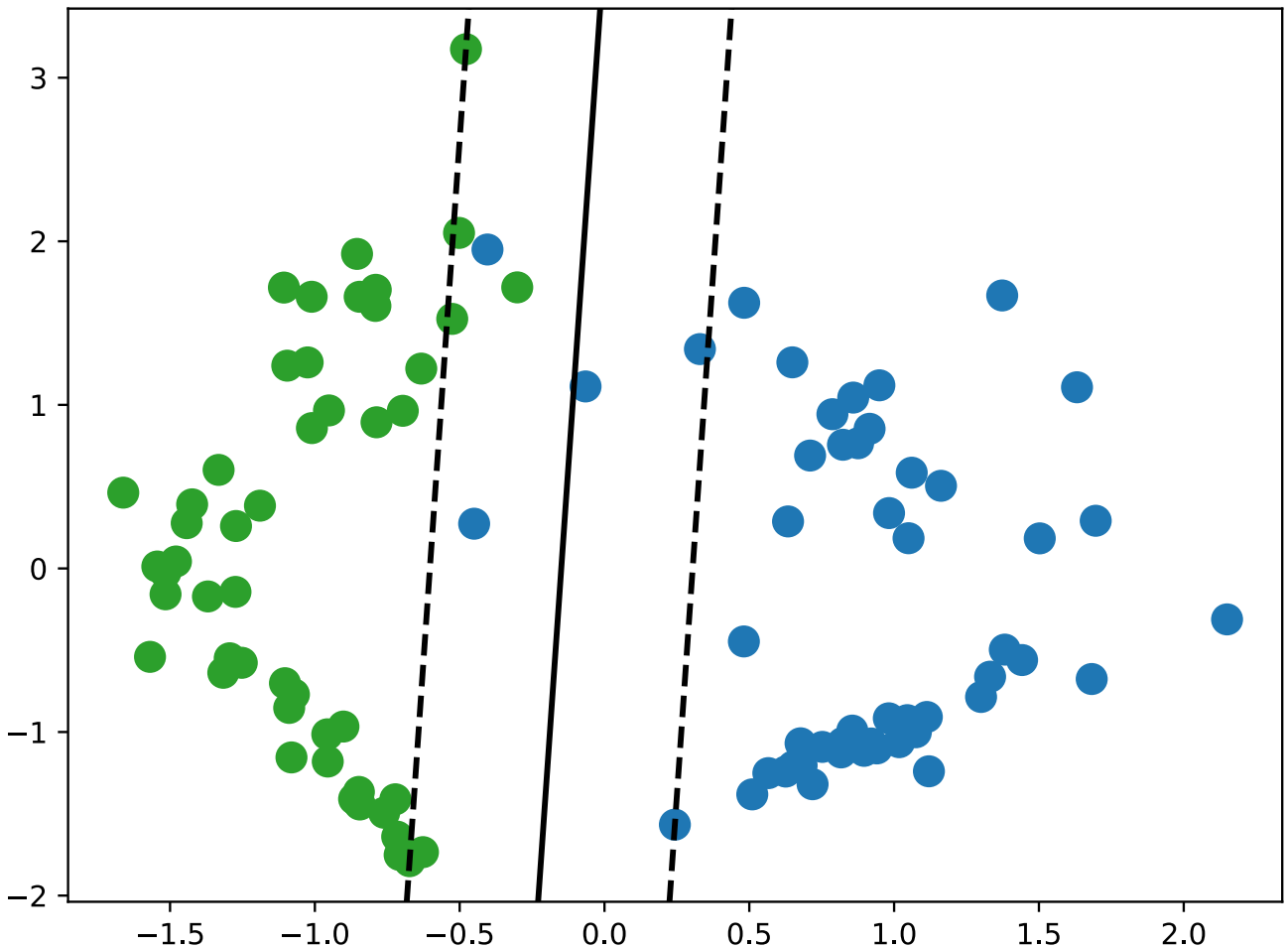
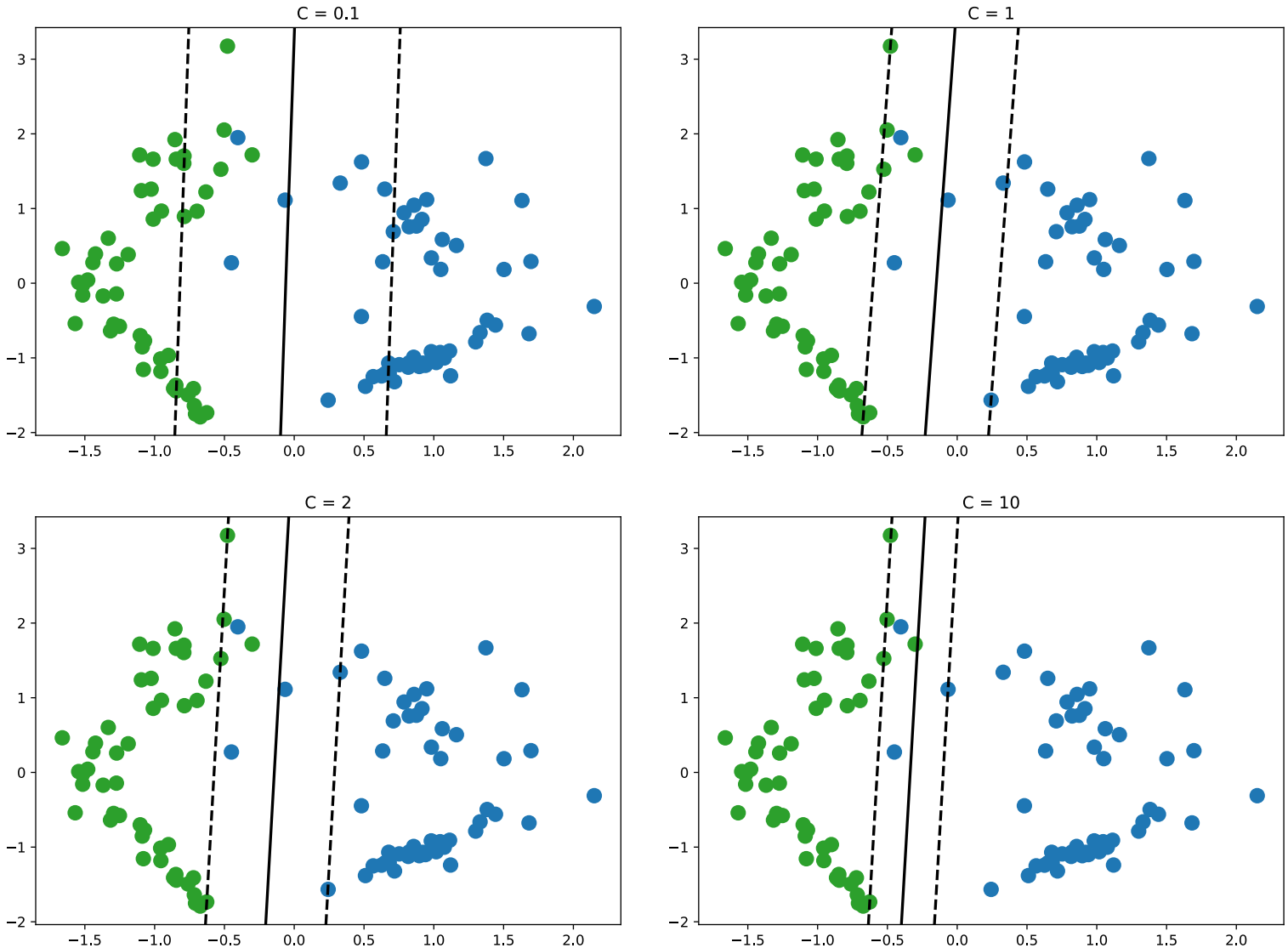


- $\Rightarrow$ We allow errors !

Support Vector Machines

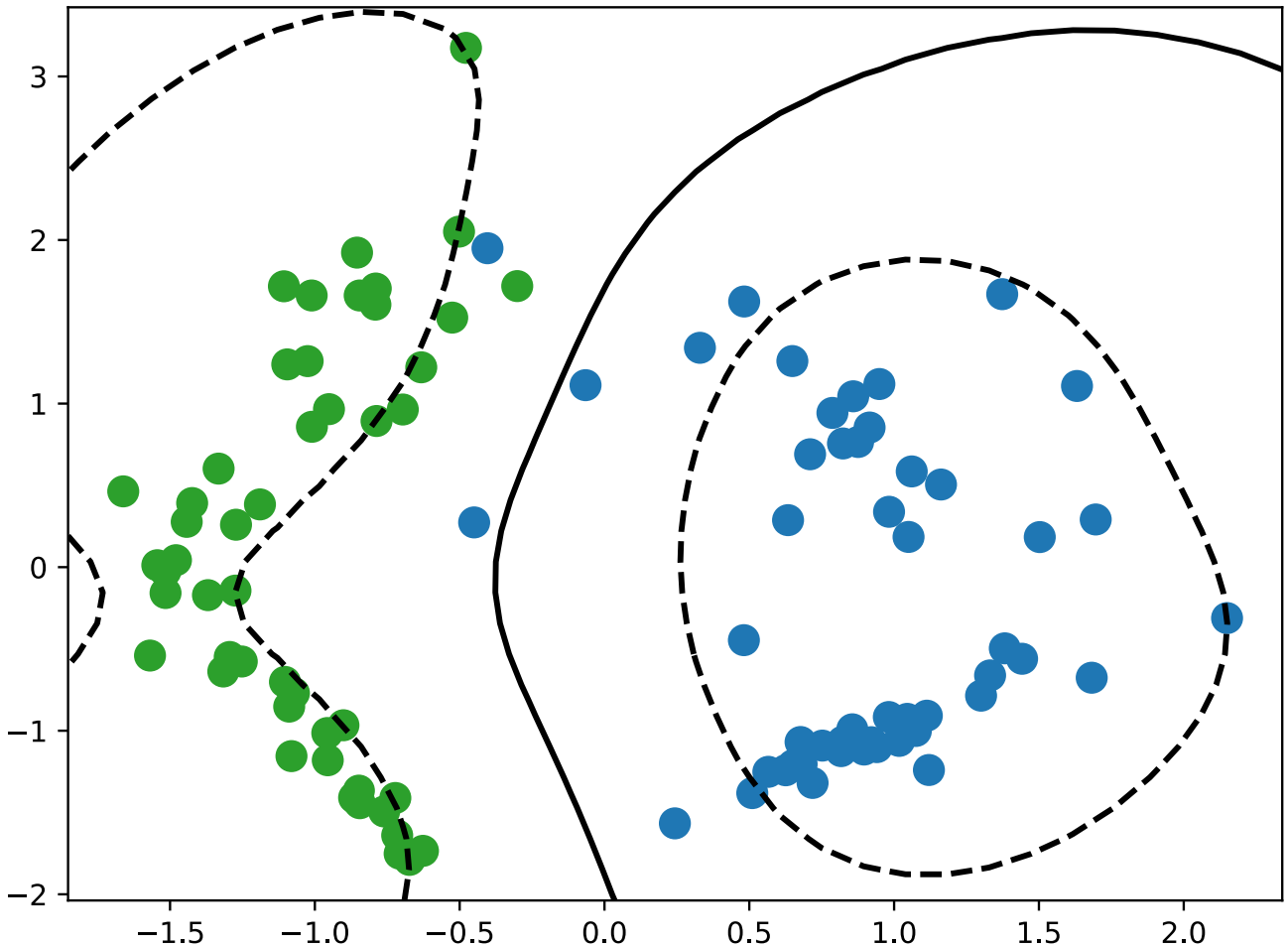
Error control

C controls the trade off between errors and separation



Extension to non linear separation

Thanks to kernel trick, SVM can compute any kind of separation line



- Depends on kernel

SVM Hyperparameters

C

Adjust the importance of errors

- low C : fast to compute, more simple separation, more errors
- high number : slower to compute, less errors, maybe too complex separation line

kernel

Determine how the separation line is build

- linear : straight line
- poly, rbf, sigmoid : complex lines, basic choice is rbf
- precomputed : provide a similarity matrix (more difficult)

SVM : the code !

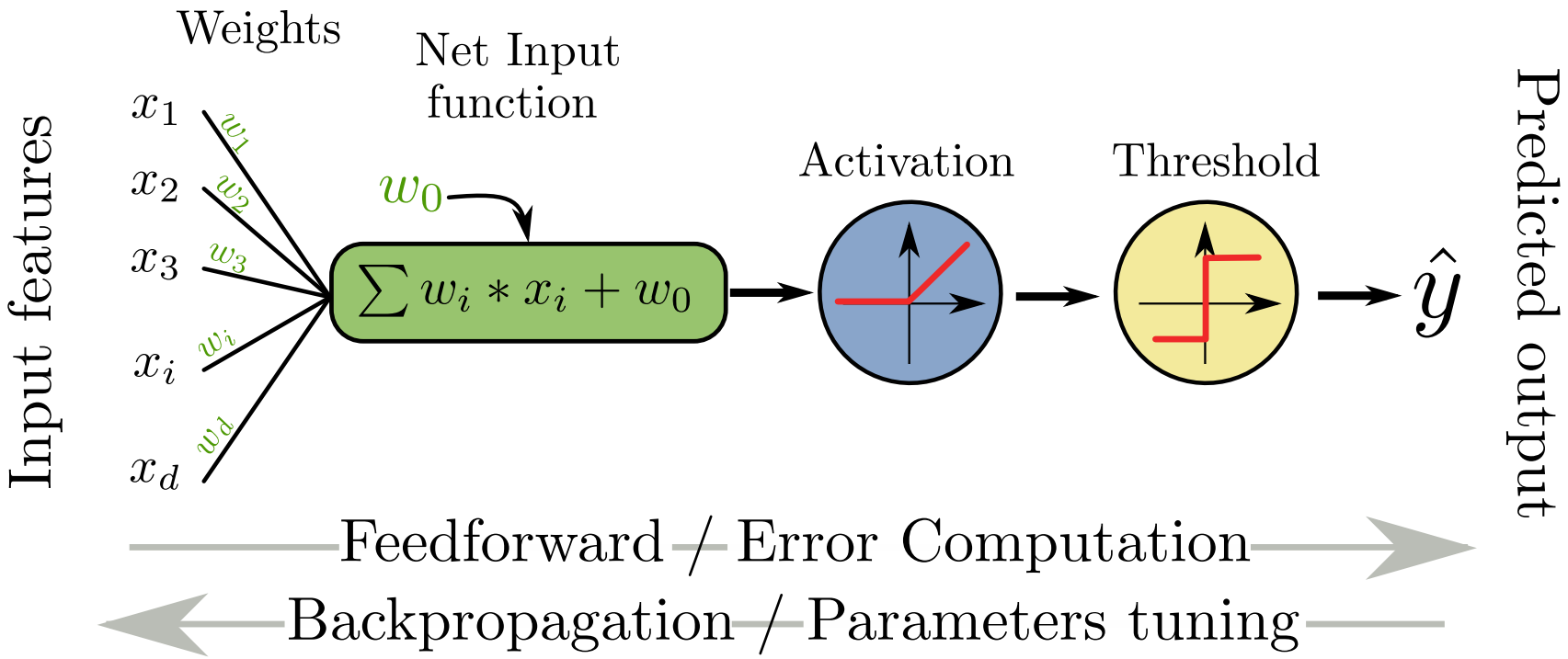
```
1  from sklearn import svm
2  C = 1
3  kernel = 'rbf'
4  clf = svm.SVC(C=C,kernel=kernel)
5  clf.fit(X,y)
6  ypred = clf.predict(X)
```

- User guide for hyperparameters : link
- $\Rightarrow$ Notebook
- the documentation

Multi Layer Perceptron

Principle

Learn the best representation of data



- Weights $\boldsymbol{w}$ are optimized by gradient descent
- Sequence of layers

MLP Hyperparameters

Hidden layers

Define the architecture of your MLP

- Number of layers : a high number tends to deep networks
- Number of neurons per layer : a high number tends to wide networks

The model will be more complex if more neurons are used

Activation function

Determine how the non linearity is brought to the model

- identity : linear model
- tanh, relu, logistic : non linears. ReLU is a very popular choice

MLP : the code !

```
1  from sklearn.neural_network import MLPClassifier
2  activation = 'relu' # default
3  layers = [32,64,128,64,32] #5 layers avec différentes tailles
4  clf = MLPClassifier(hidden_layer_sizes=layers,max_iter=500)
5  clf.fit(X,y)
6  ypred = clf.predict(X)
```

- User guide for tips and help : link
- $\Rightarrow$ Notebook
- the documentation

Pratical

How to learn a "good" model ?

- We want good performance
- Simple as possible
- Able to predict unseen data

Empirical Risk

Error on learning set

- Empirical risk:

$$R_{emp}(f) = \frac{1}{N} \sum_{i=1}^{N} \mathcal{L}(f(\mathbf{x}_i), y_i)$$

- $\mathcal{L}$ evaluates the performance of prediction $f(\mathbf{x}_i)$
- Error is computed on the training set
- The model can be too specialized on this particular dataset

Generalisation

Tentative of Definition

- Ability of the model to predict well unseen data
- Hard to evaluate
- Real objective of a model

Regularisation

- Regularization term control the model
- Balances between empirical risk and generalization ability
- Need to tune the balance (λ)

How to evaluate to ability to generalize ?

Evaluate on unseen data

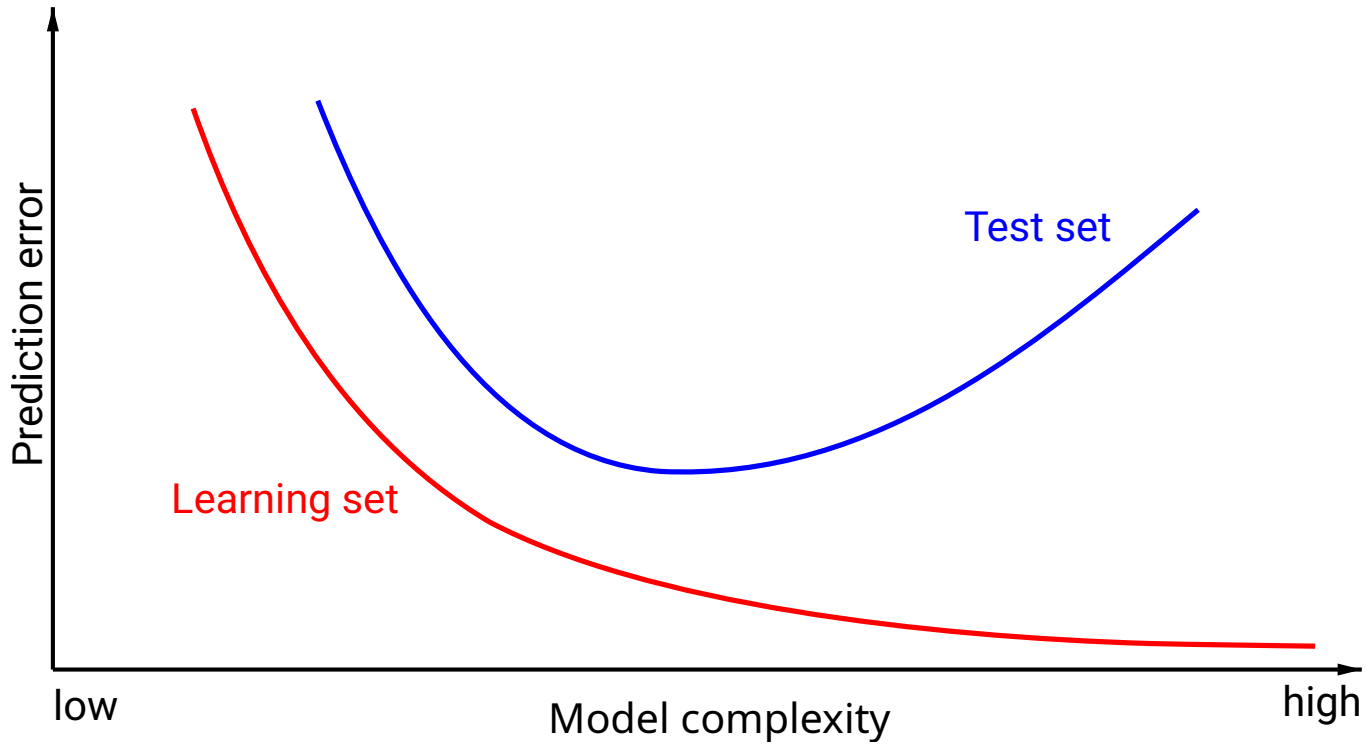
- Define and isolate a test set
- Evaluate on the test set

Bias

- Avoid to use same data in train and test
- Test set must be totally isolated

Overfitting vs Underfitting

- Overfitting: low R_{emp}, high generalization error
- Underfitting: high R_{emp}, medium generalization error



Hyperparameters

Parameters outside the model

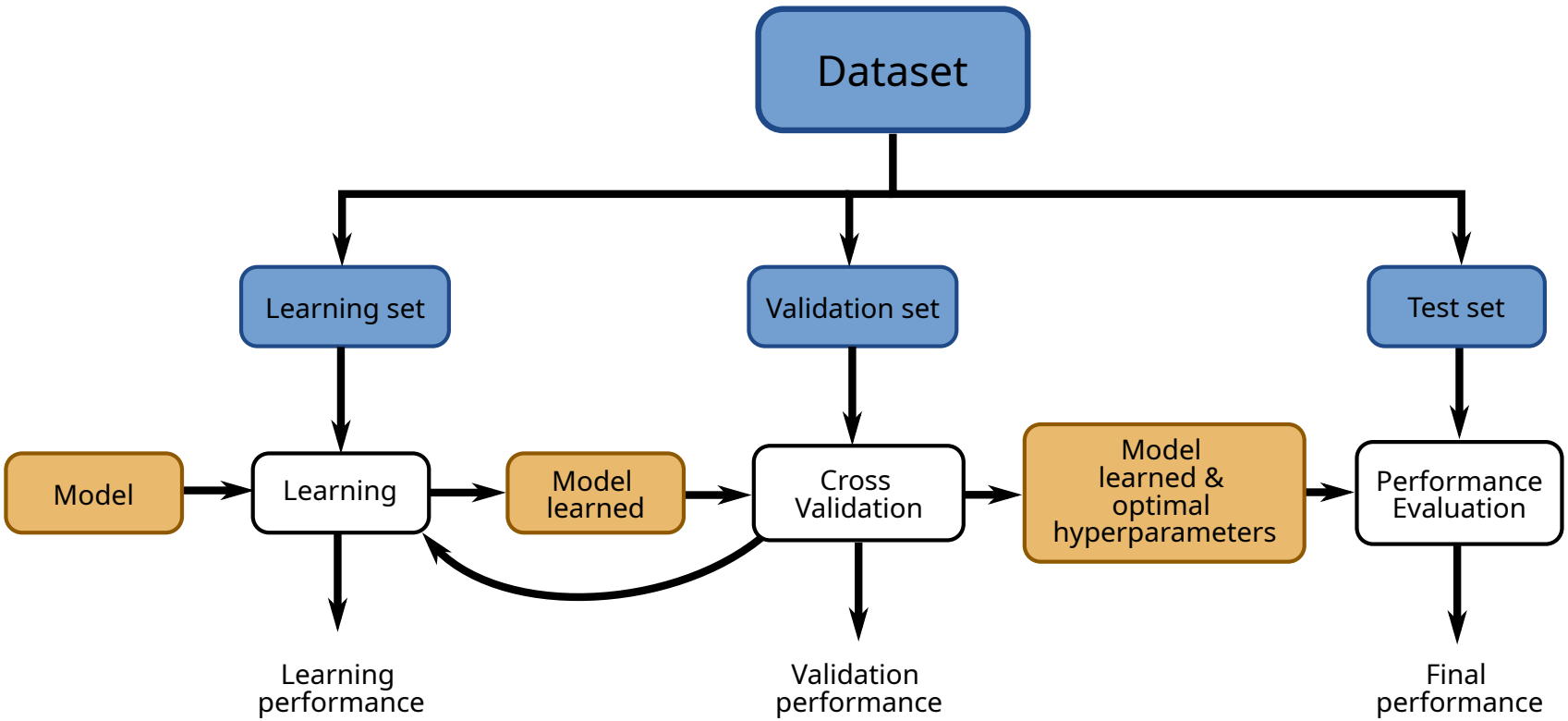
- Some parameters are not learned by the model
- They are "hyperparameters" and must be tuned
-  Tuned on data outside the test set
- Example: λ in Ridge Regression

How to tune the hyperparameters ?

Validation set

- Split train set into validation and learning set
- Learn model parameters using the learning set
- Evaluate the performance on validation set
- Validation set simulates the test set, aka unseen data

General framework



General CV pseudo code

1: **function** EVAL($X, y,$ model, h_params)
2: best_perf $\leftarrow 0$
3: $X_{train}, y_{train}, X_{test}, y_{test} \leftarrow$ split(X, y)
4: **for** h_param $\in$ h_params **do**
5: perf $\leftarrow 0$
6: **for** $i \in 1 \ldots 10$ **do**
7: $X_t, y_t, X_v, y_v \leftarrow$ cv_split$(X_{train}, y_{train}, i)$
8: fitted_model $\leftarrow$ train(model, $X_t, y_t,$ h_param)
9: $y_{pred} \leftarrow$ predict(fitted_model, X_v)
10: perf $\leftarrow$ perf + score(y_pred, y_v)
11: **end for**
12: **if** perf $<$ best_perf **then**
13: best_perf $\leftarrow$ perf
14: best_param $\leftarrow$ h_param
15: **end if**
16: **end for**
17: fitted_model $\leftarrow$ train(model, $X_{train}, y_{train},$ best_param)
18: $y_{pred} \leftarrow$ predict(fitted_model, X_{test})
19: **return** score(y_{pred}, y_{test})
20: **end function**

Still Learned at Top Conf

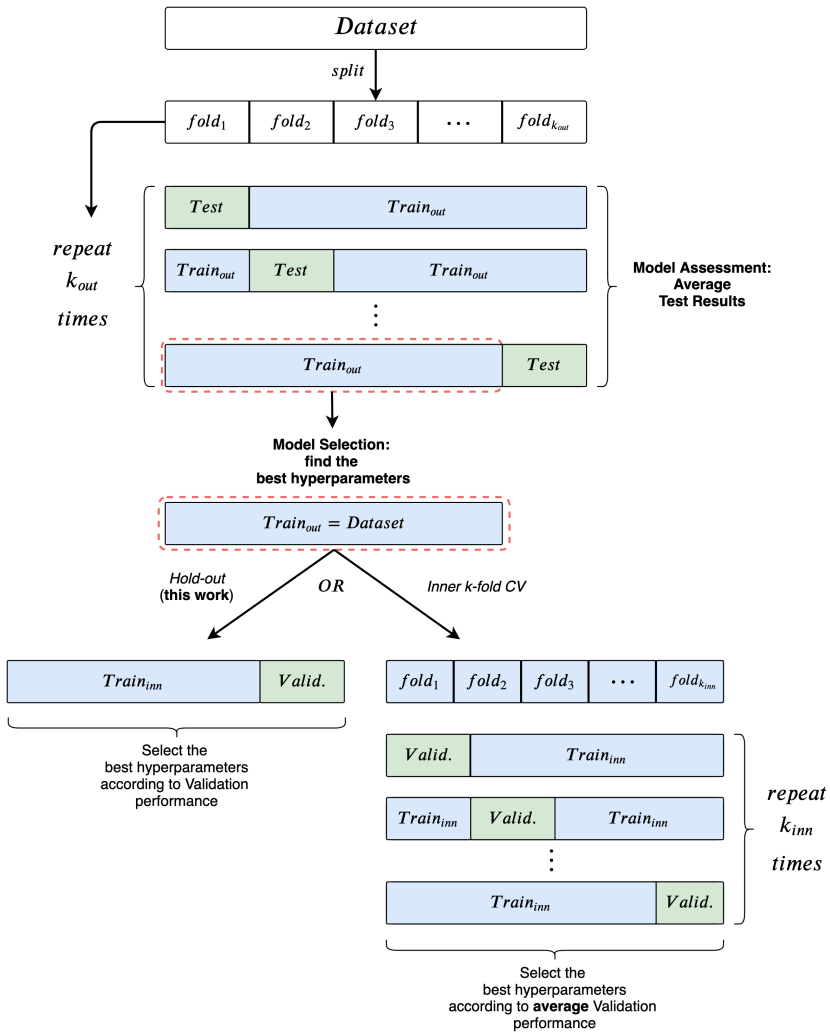
F. Errica, M. Podda, D. Bacciu, and A. Micheli, 'A Fair Comparison of Graph Neural Networks for Graph Classification'. ICLR 2020. http://arxiv.org/abs/1912.09893

Algorithm 1 Model Assessment (k-fold CV)

Input: Dataset $\mathcal{D}$, set of configurations Θ
Split $\mathcal{D}$ into k folds $F_1, \ldots, F_k$
for $i \leftarrow 1, \ldots, k$ **do**
    $\text{train}_k, \text{test}_k \leftarrow \left(\bigcup_{j \neq i} F_j\right), F_i$
    $\text{best}_k \leftarrow \text{Select}(\text{train}_k, \Theta)$
    for $r \leftarrow 1, \ldots, R$ **do**
        $\text{model}_r \leftarrow \text{Train}(\text{train}_k, \text{best}_k)$
        $\text{p}_r \leftarrow \text{Eval}(\text{model}_k, \text{test}_k)$
    end for
    $\text{perf}_k \leftarrow \sum_{r=1}^{R} \text{p}_r / R$
end for
return $\sum_{i=1}^{k} \text{perf}_i / k$

Algorithm 2 Model Selection

Input: train_k, Θ
Split train_k into *train* and *valid*
$\text{p}_\theta = \emptyset$
for each $\theta \in \Theta$ **do**
    $\text{model} \leftarrow \text{Train}(\text{train}_k, \theta)$
    $\text{p}_\theta \leftarrow \text{p}_\theta \cup \text{Eval}(\text{model}, \textit{valid})$
end for
$\text{best}_\theta \leftarrow \text{argmax}_\theta \, \text{p}_\theta$
return best_θ



Validation strategies

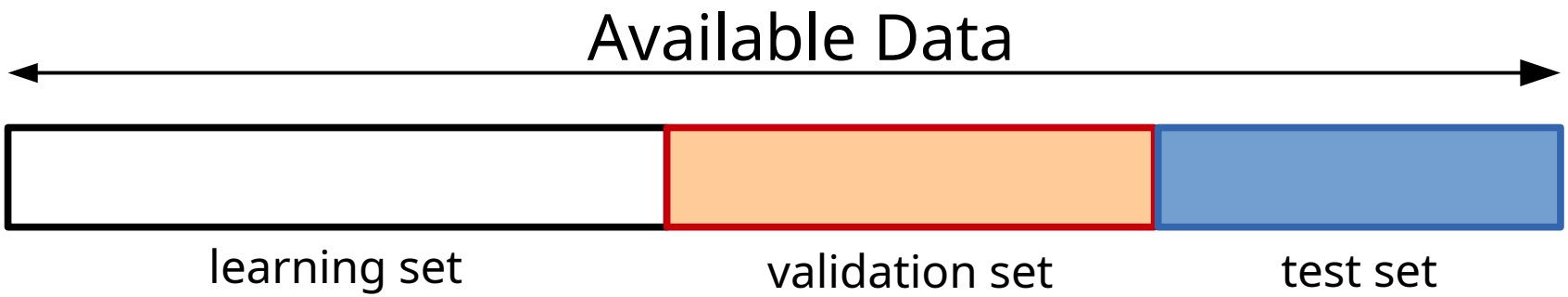
How to split validation/training set

- Need of a strategy to split between training and validation sets
- Training is used to tune the parameters of the model
- Validation is used to evaluate the model according to hyperparameters

Train/Validation/Test

Single split

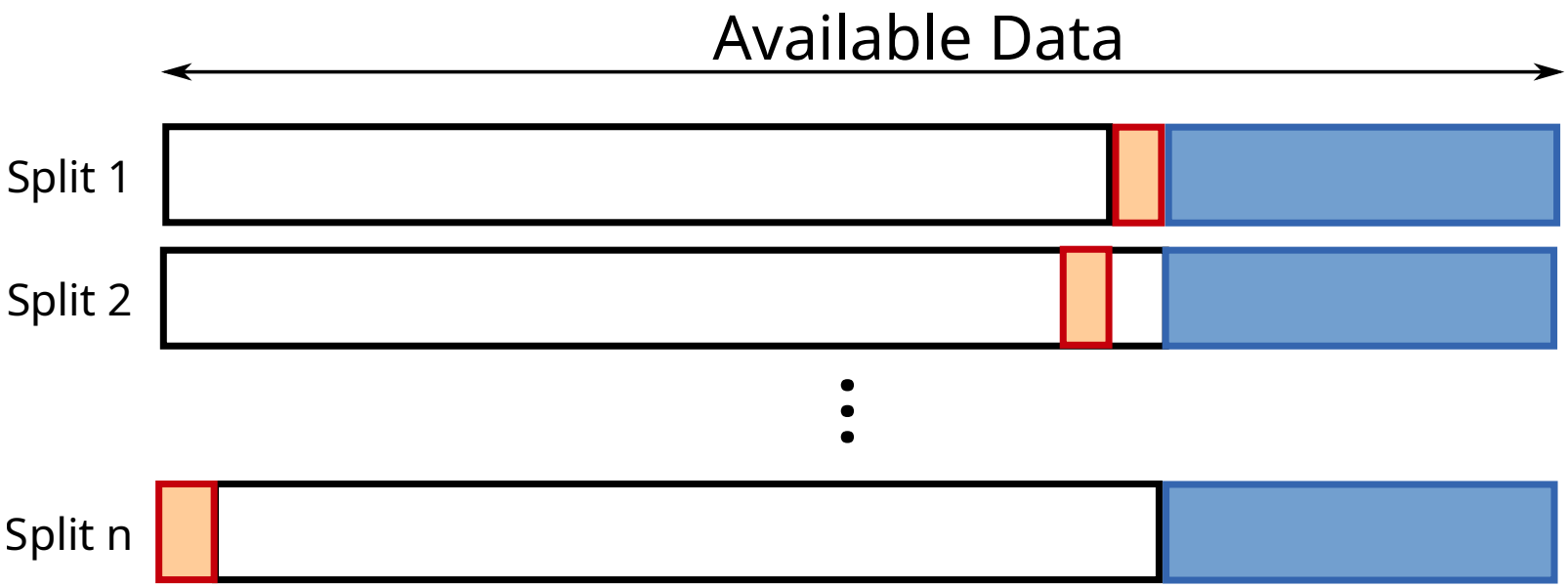
- ✚ An unique model to learn
- ▬ May be subject to split bias
- ▬ Only one evaluation of performance



Leave one out

N splits

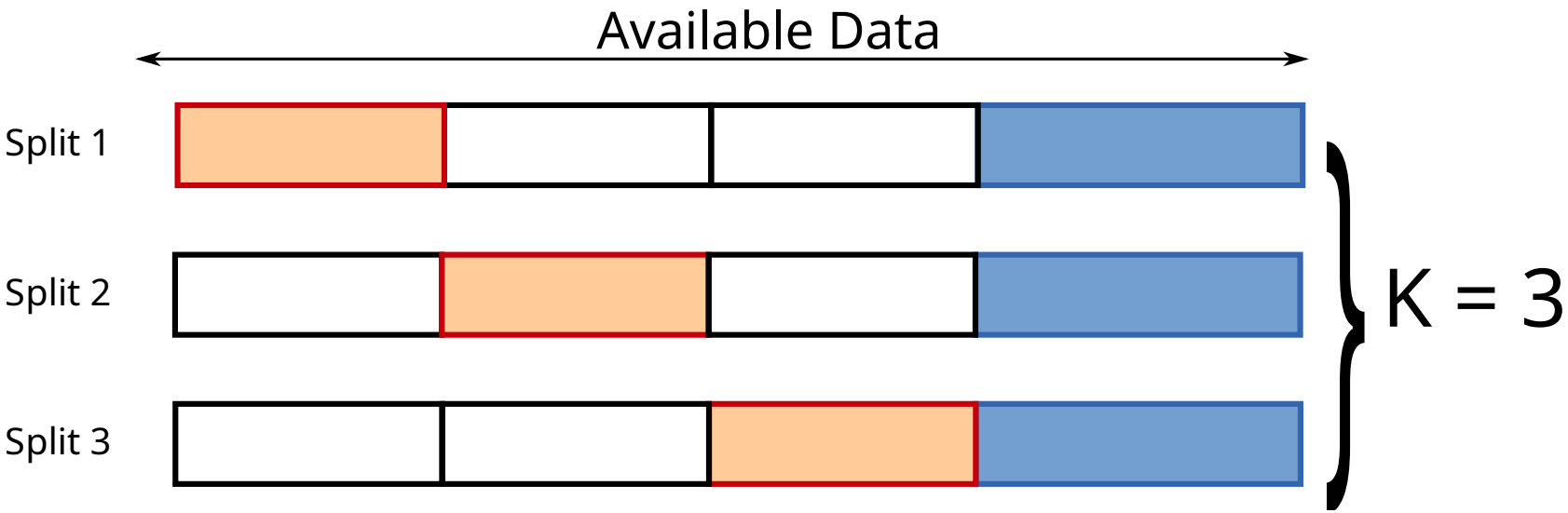
- N models to learn
- Validation error is evaluated on 1 data



KFold Cross validation

K splits

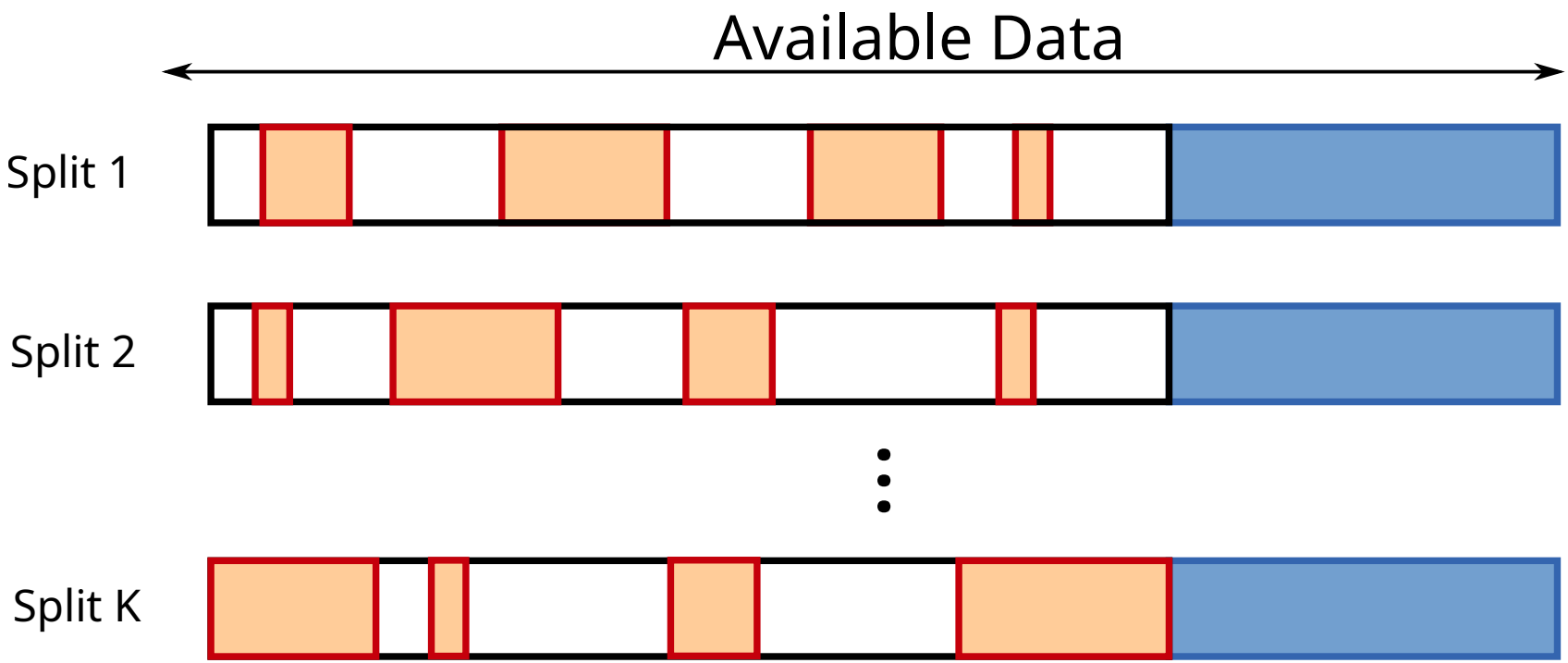
- K models to learn
- Validation error is evaluated on N/K data
- Some splits may be biased



Shuffle Split Cross validation

K splits

- Learn/Valid sets are randomly splited
- ✚ K models to learn
- ✚ Avoid bias
- ▬ Some data may not be evaluated



With scikit-learn

- sklearn.model_selection.train_test_split
- sklearn.model_selection.KFold
- sklearn.model_selection.ShuffleSplit
- sklearn.model_selection.GridSearchCV

Recommandation

Size of splits

- How many splits ?
- How many element by split ?
- Depends on the number of data
- Tradeoff between learning and generalization

Stratified splits

- Splitting may induce to imbalanced datasets
- Take care that the distribution of $\mathbf{y}$ is the same for all sets

Conclusion

- A good protocol avoid bias
- Test is never used during tuning of (hyper)parameters
- Perfect protocol doesn't exists