Operating Machine Learning

Introduction

How to learn a "good" model?

- We want good performance
- As 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 $\mathbf{x}_i$
- Error is computed on the training set
- The model can be too specialized on this particular dataset

Generalization

Tentative Definition

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

Regularization

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

How to Evaluate Generalization Ability?

Evaluate on Unseen Data

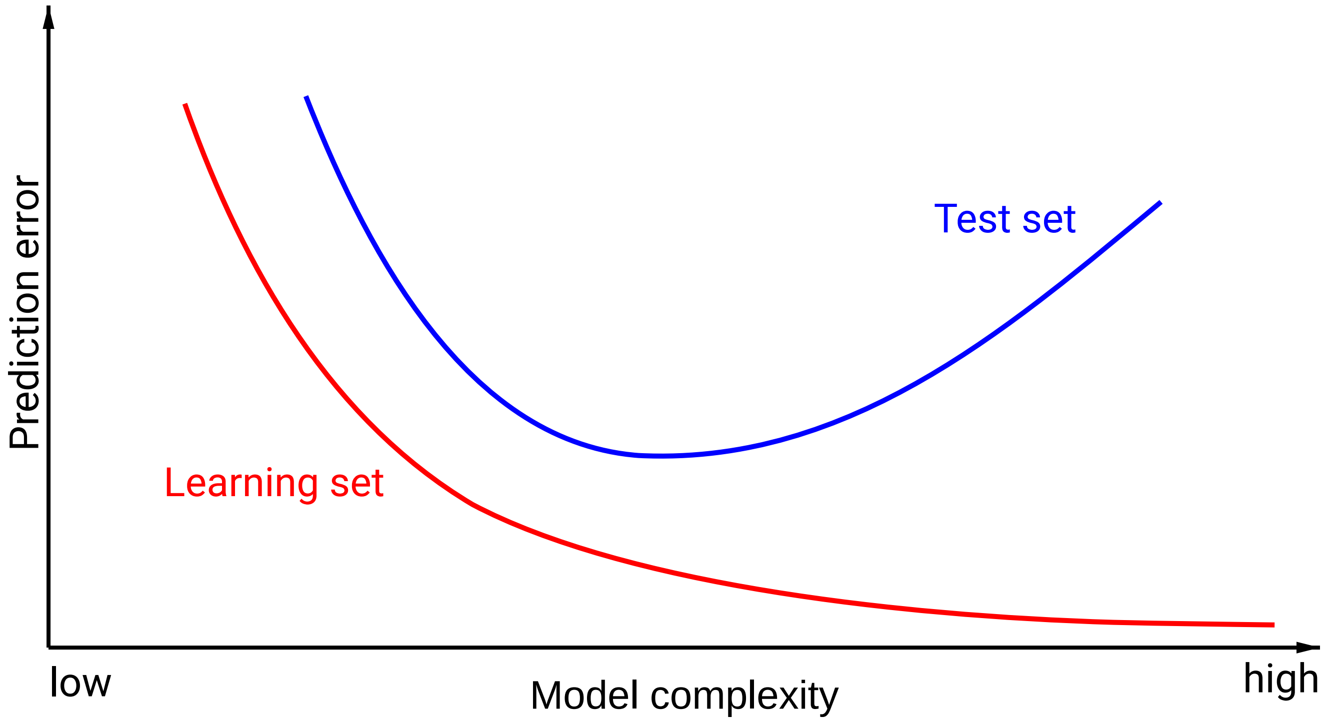
- Define and isolate a test set
- Evaluate on the test set

Bias

- Avoid using the same data for training and testing
- 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

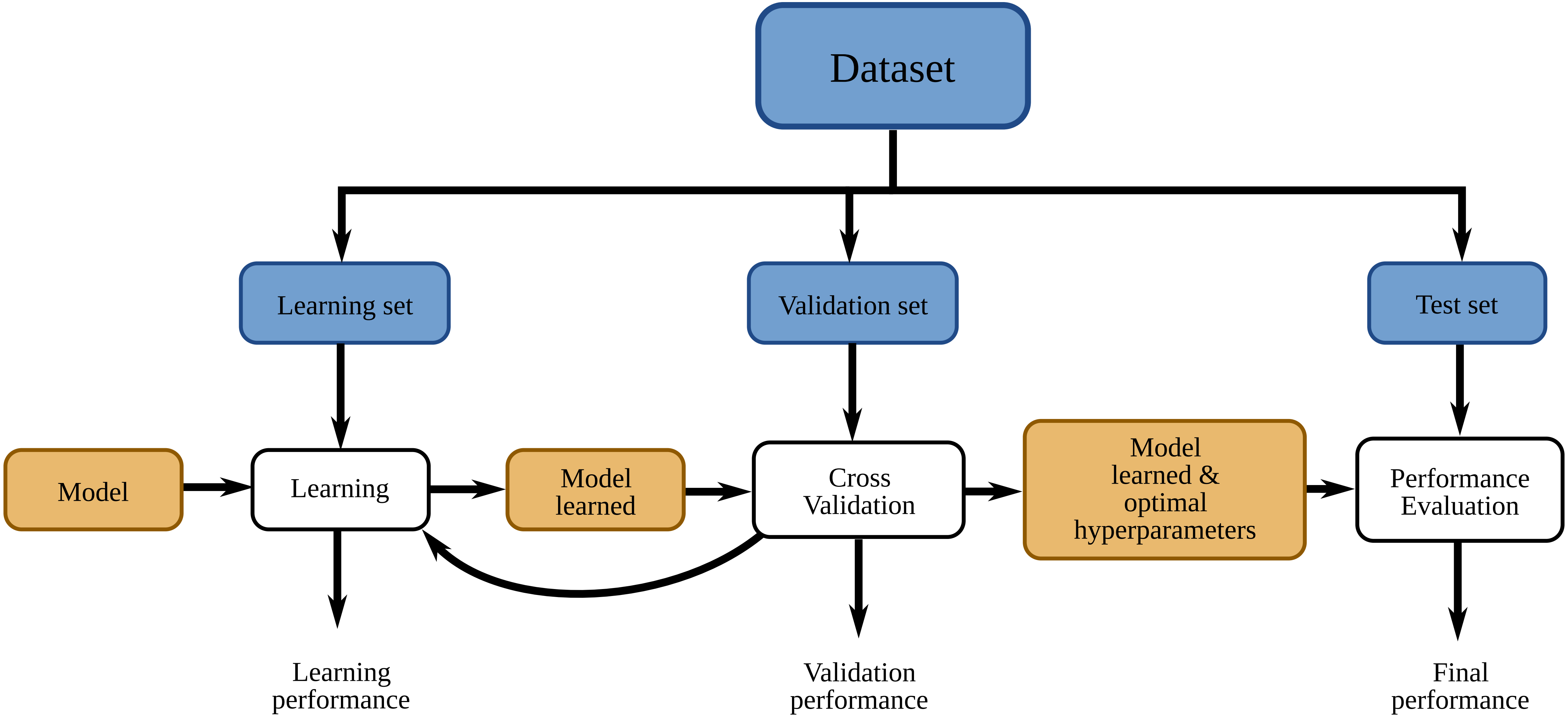
- Some parameters are not learned by the model
- They are **hyperparameters** and must be tuned
- ⚠️ Tuned on data outside the test set
- Example: λ in Ridge Regression, k in KNN.

How to Tune the Hyperparameters?

Validation Set

- Split training set into validation and learning set
- Learn model parameters using the learning set
- Evaluate performance on the validation set
- Validation set simulates the test set (unseen data)

General Framework



Validation Strategies

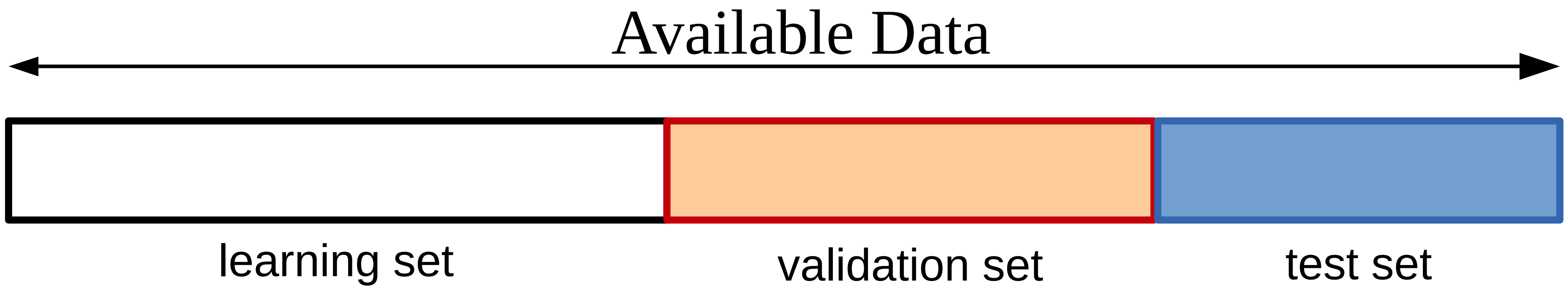
How to Split Validation/Training Set?

- Need a strategy to split between training and validation sets
- Training set is used to tune model parameters
- Validation set is used to evaluate model performance based on hyperparameters

Train/Validation/Test Split

Single Split

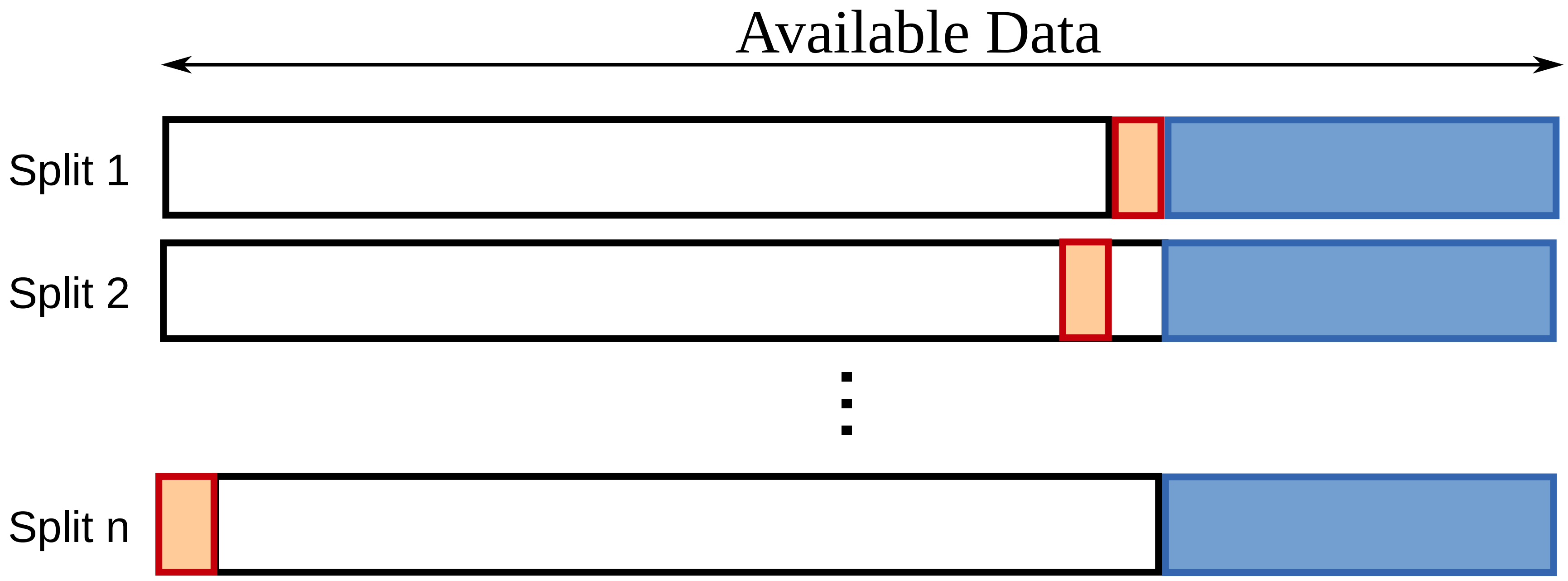
+ Only one model to learn
− May be subject to split bias
− Only one evaluation of performance



Leave-One-Out

N Splits

- N models to learn
- Validation error is evaluated on one data point



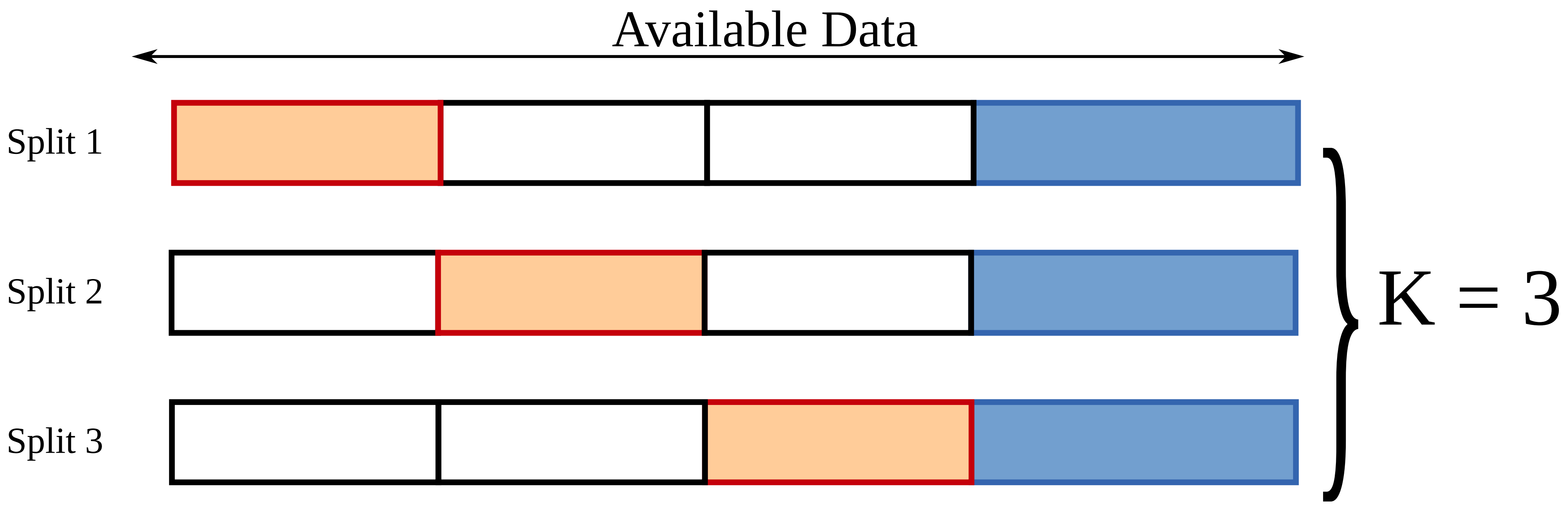
KFold Cross Validation

K Splits

+ K models to learn

Validation error is evaluated on (N/K) data points

Some splits may be biased

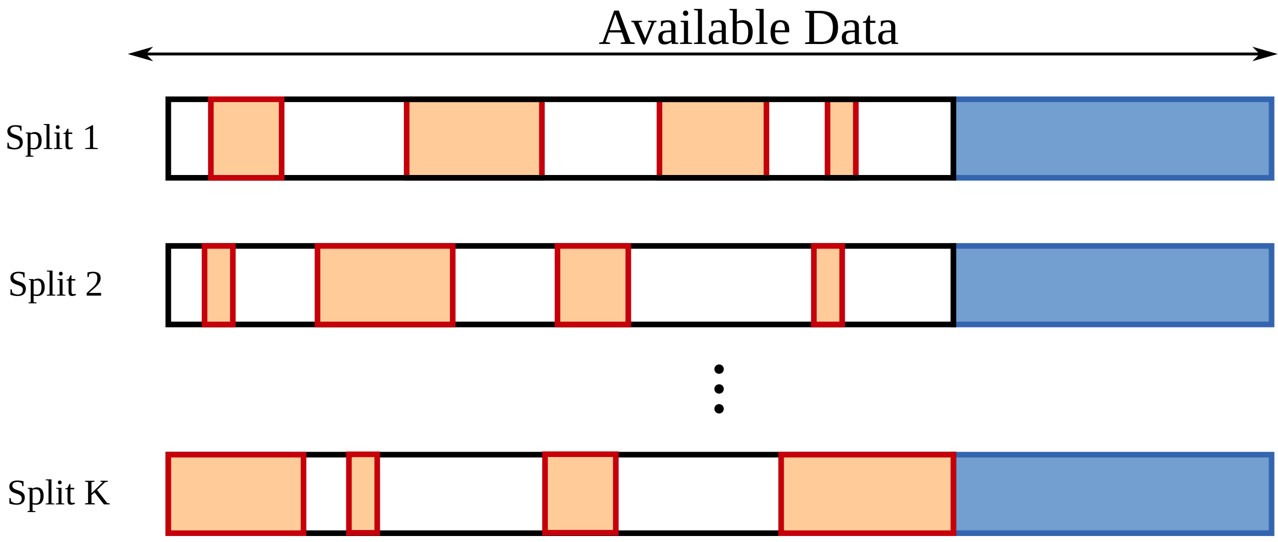


Shuffle Split Cross Validation

K Splits

Training/validation sets are randomly split

+ K models to learn
+ Avoids bias
− Some data may not be evaluated



Using Scikit-Learn

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

Recommendations

Size of Splits

- How many splits?
- How many elements per split?
- Depends on the number of data points
- Tradeoff between learning and generalization

Stratified Splits

- Splitting may induce imbalanced datasets
- Ensure the distribution of y is consistent across all sets

Conclusion

- A good protocol avoids bias
- Test set is **never** used during parameter tuning
- No perfect protocol exists

ML Methods

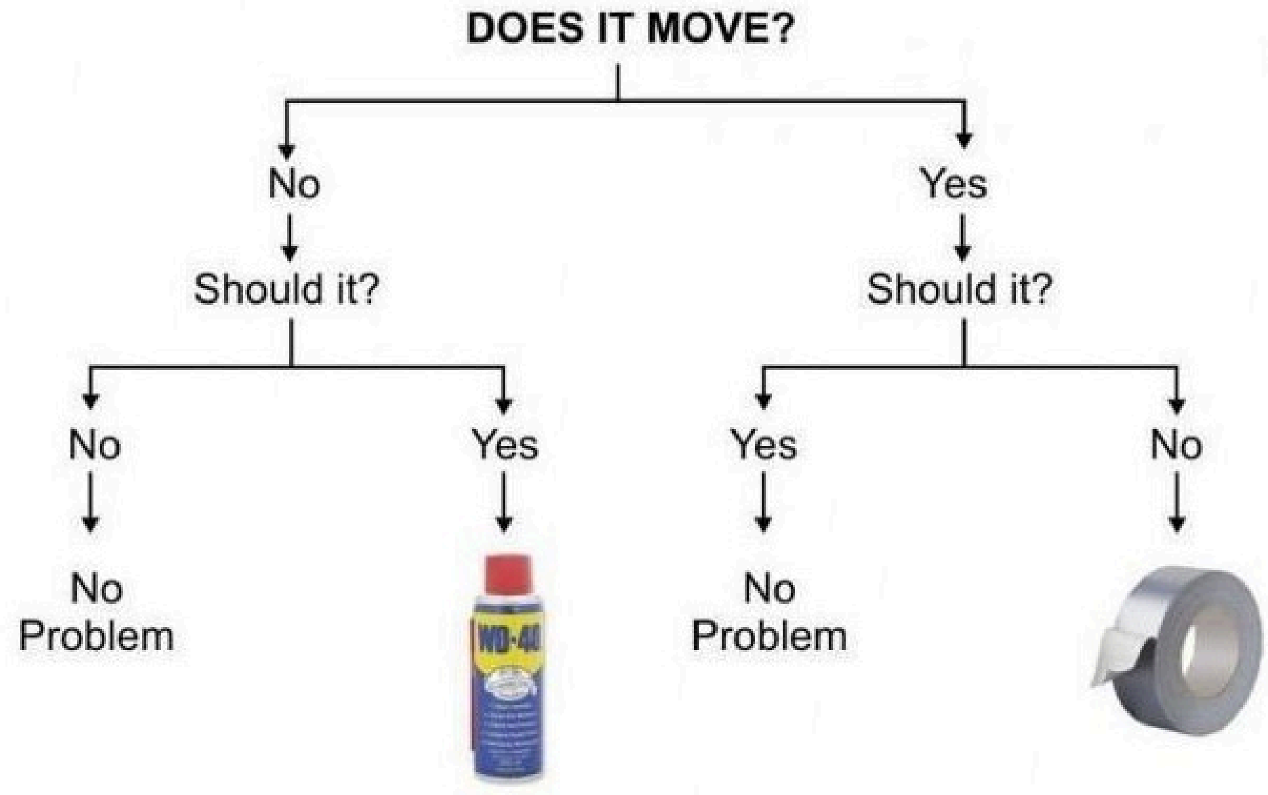
Most useful non-deep ML models

Decision Tree

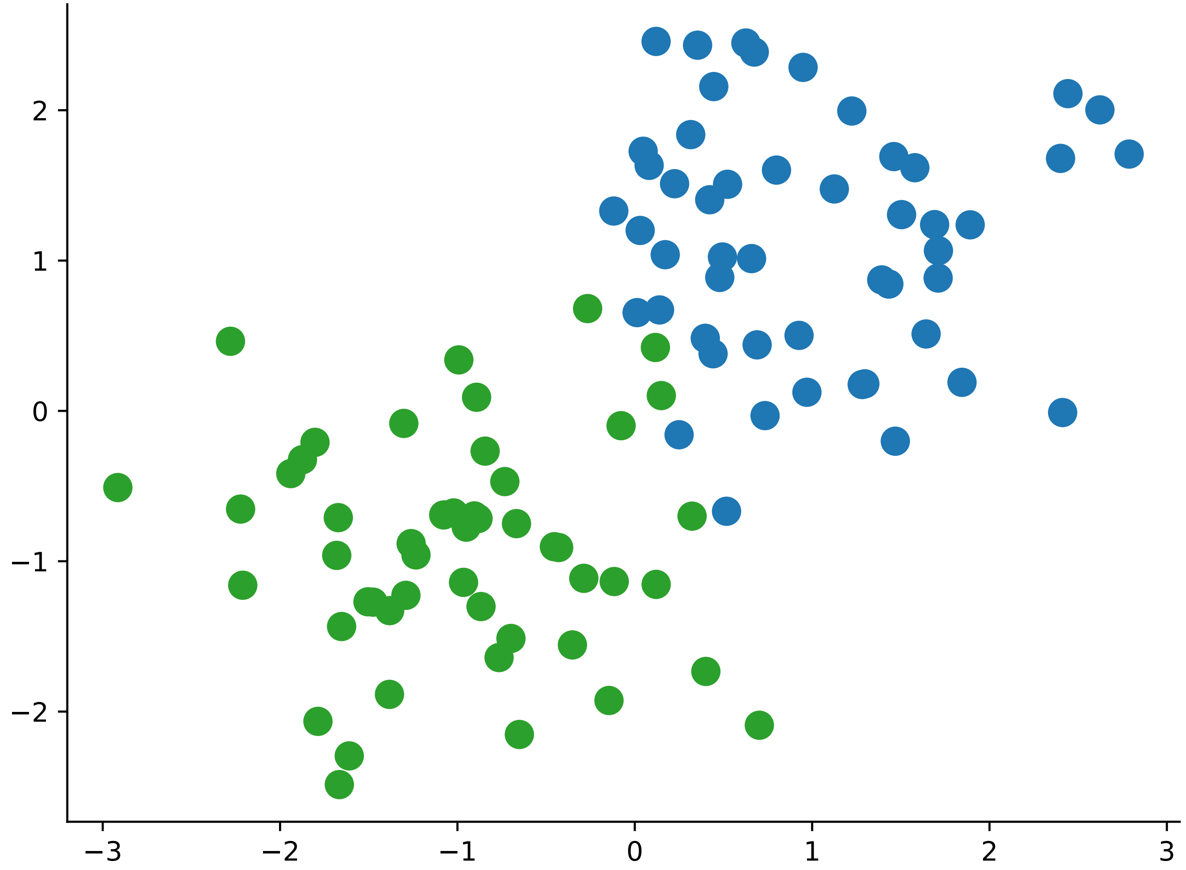
Principle

Learn decision rules to separate the data.

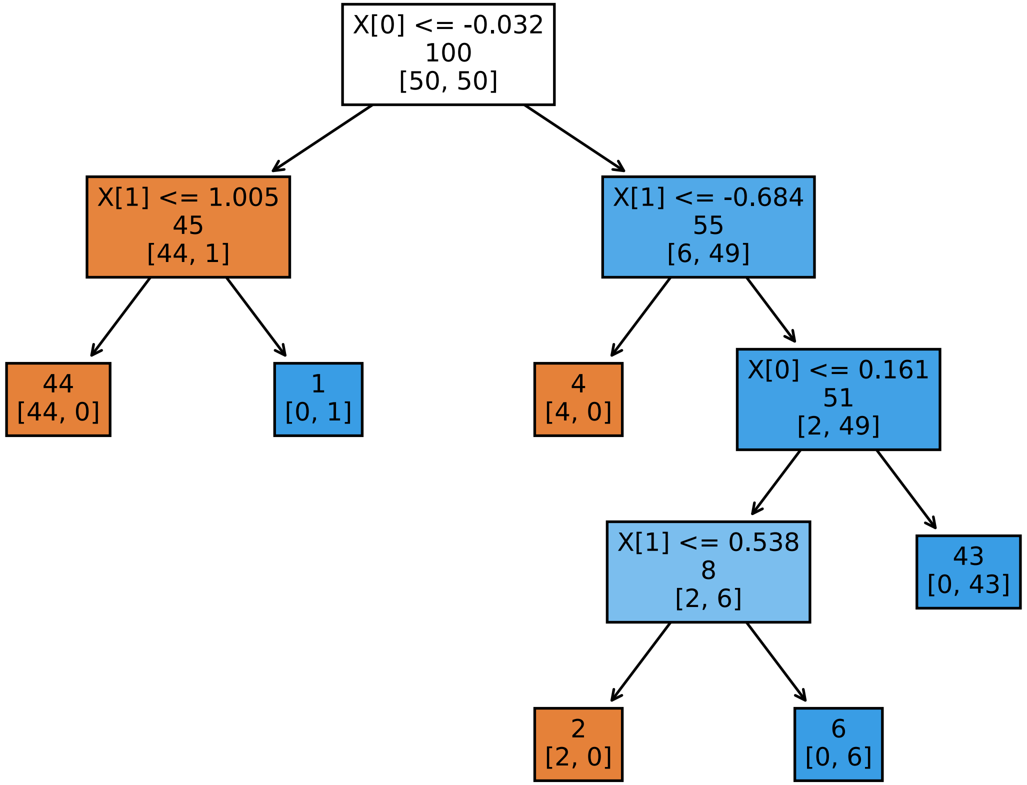
- Supervised learning for classification and regression.
- Simple to understand and interpret.
- Recursive algorithm to construct the decision trees



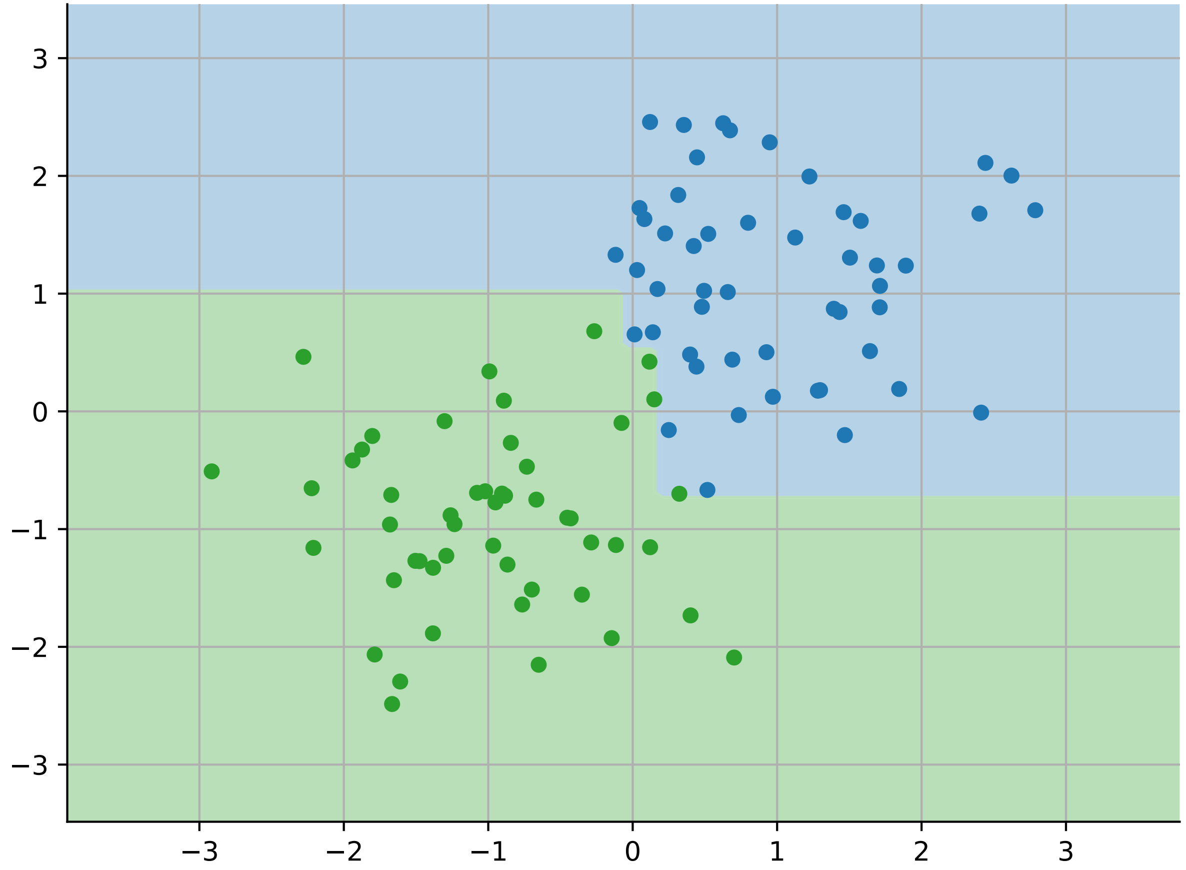
Decision Tree



Decision Tree



Decision Tree



Hyperparameters of Decision Tree

- Maximum depth

Specify the maximal depth of the tree. A higher depth will make dedicated categories, but prone to overfit.

- Min number of splits

Same action as previous one.

$\rightarrow$ Both are used to terminate the recursive operation

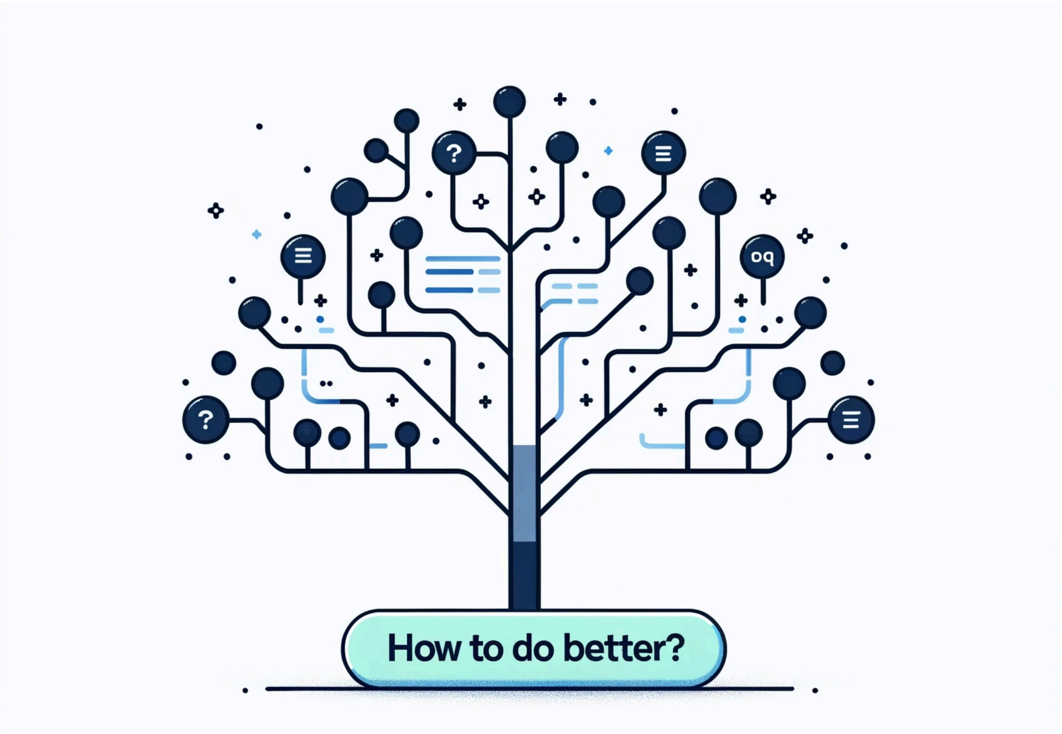
Building a decision tree - the code

```
from sklearn.tree import DecisionTreeClassifier
max_depth = 10
criterion = 'gini'
clf = DecisionTreeClassifier(max_depth=max_depth, criterion=criterion)
clf = clf.fit(X, y)
ypred = clf.predict(X)
```

- User guide for hyperparameters: link
- the documentation

Limitations

- Simple yet effective algorithm
- Prone to overfitting
  $\rightarrow$ one leaf $\Leftrightarrow$ one sample



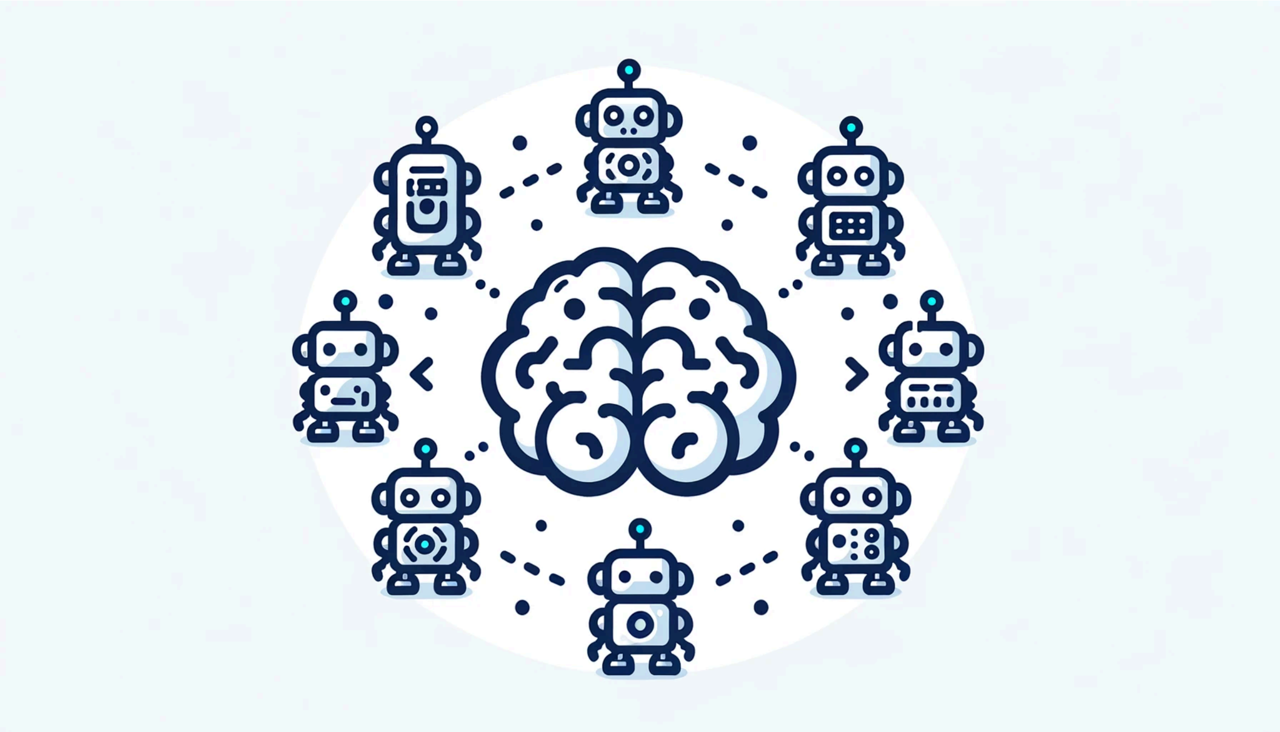
Ensemble Methods

Idea

United we stand

How to combine models ?

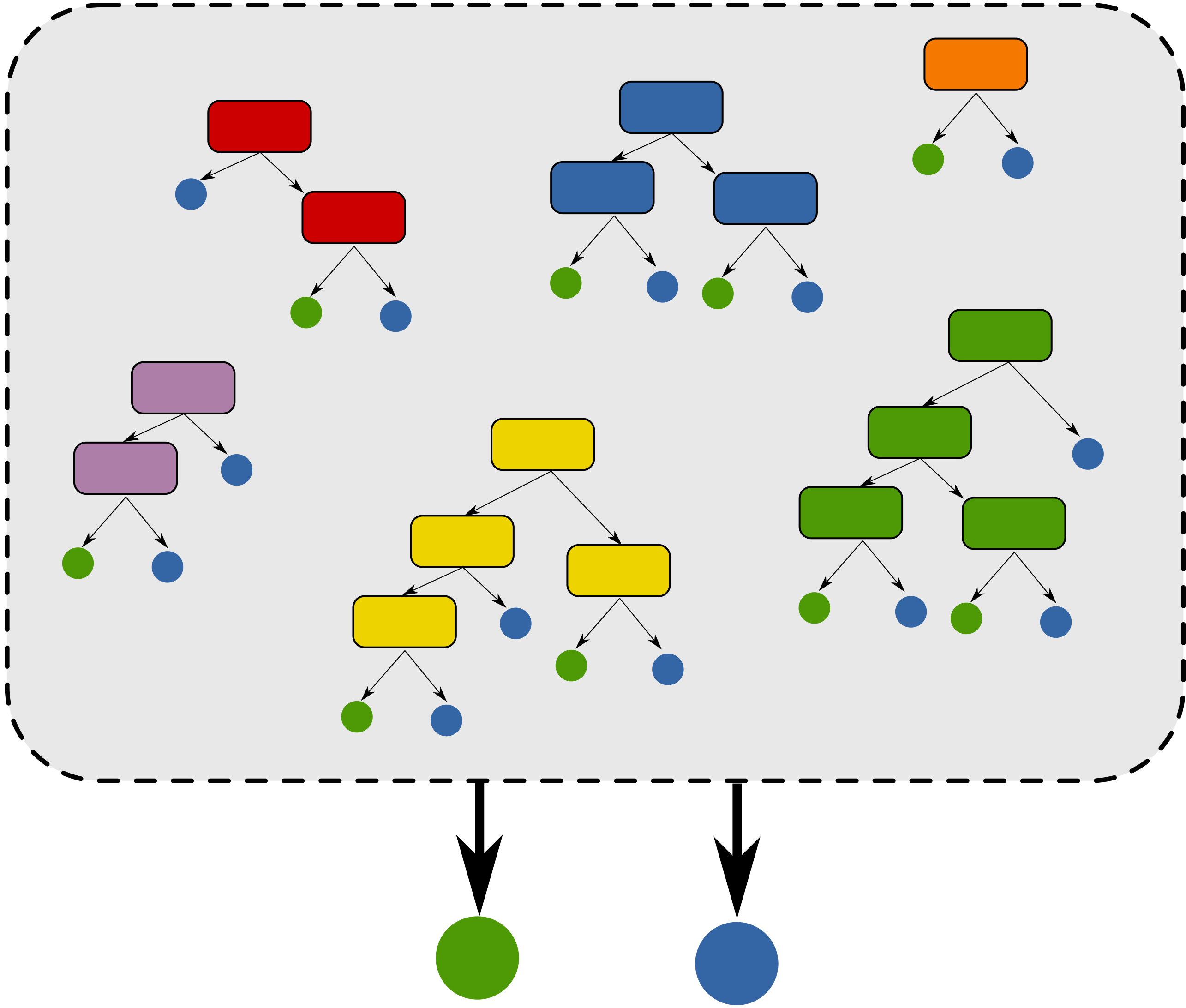
- Majority voting, Bagging, and Boosting



Random Forests

Principle

- Combine many decision trees to learn complex functions
- Ensemble methods, majority voting
- Bagging (Breiman, 1996)



Algorithm summarization

1. Randomly choose n examples (bootstrap)
2. Build a decision tree from the bootstrap
    - Randomly select d features
    - Split according to best pair feature/threshold
3. Repeat k times
4. Aggregate decision by majority vote or average probability

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. A higher depth will make dedicated categories, but less generalizable.

Random Forests: the code

```
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)
```

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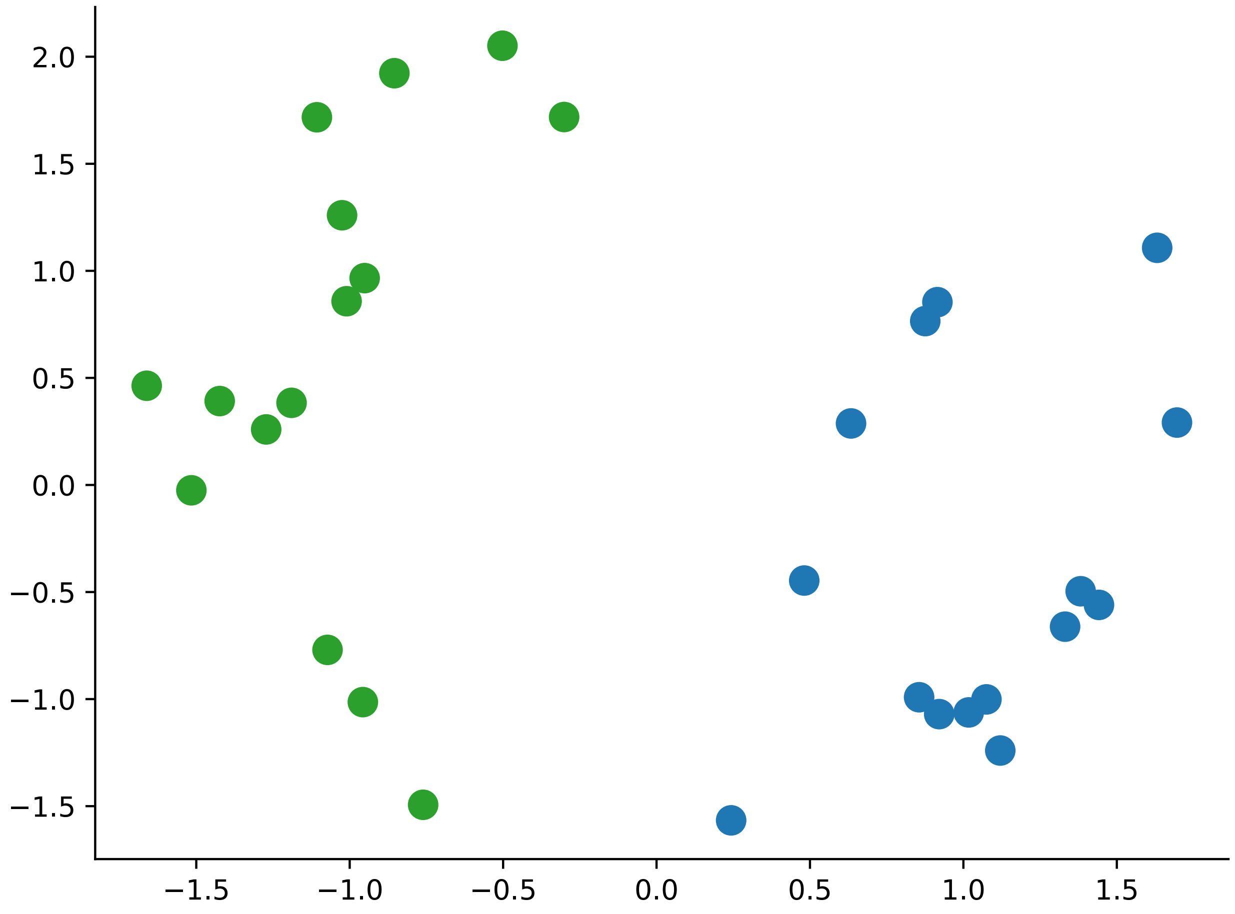
SVM & consorts

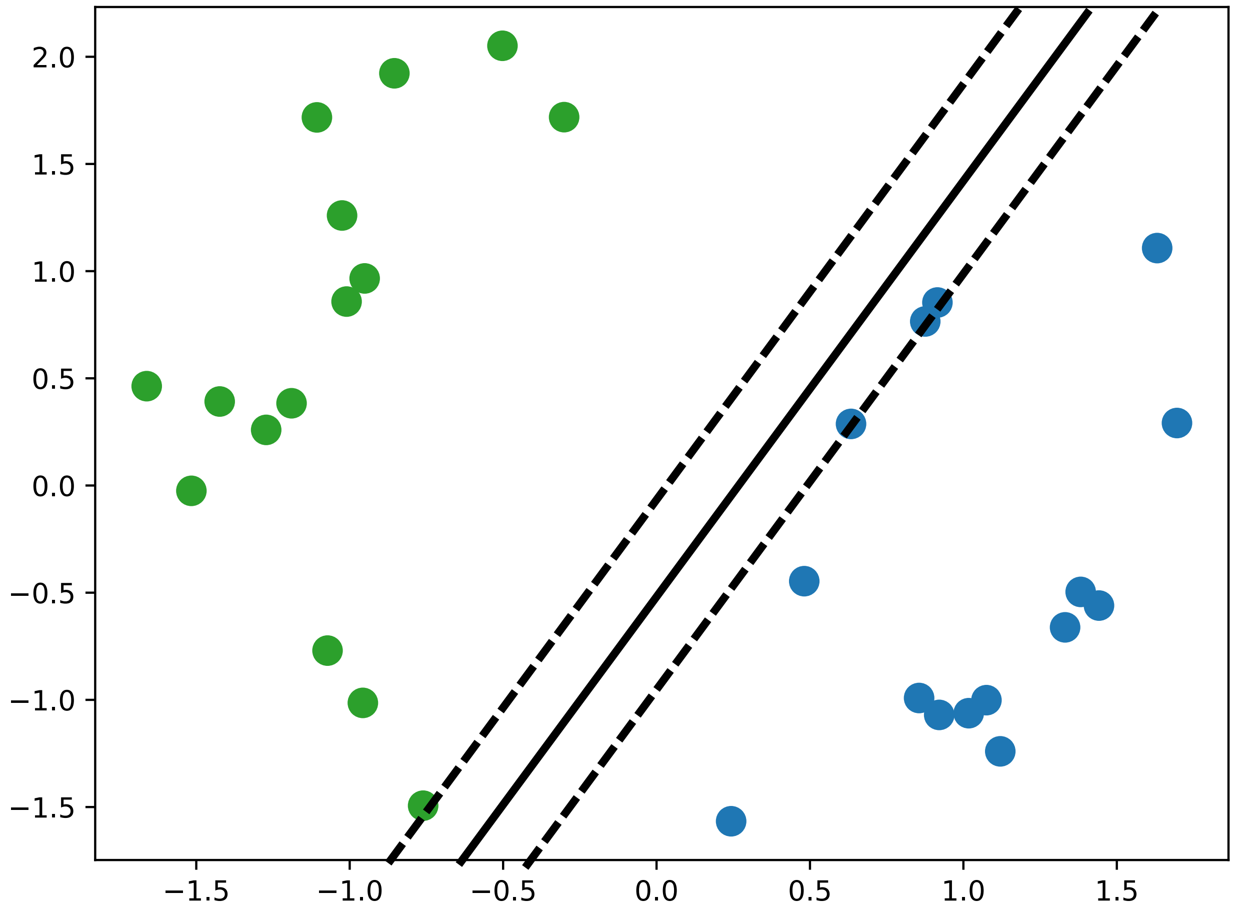
Support Vector Machines

Principle Find the best line which separates the data



Support Vector Machines

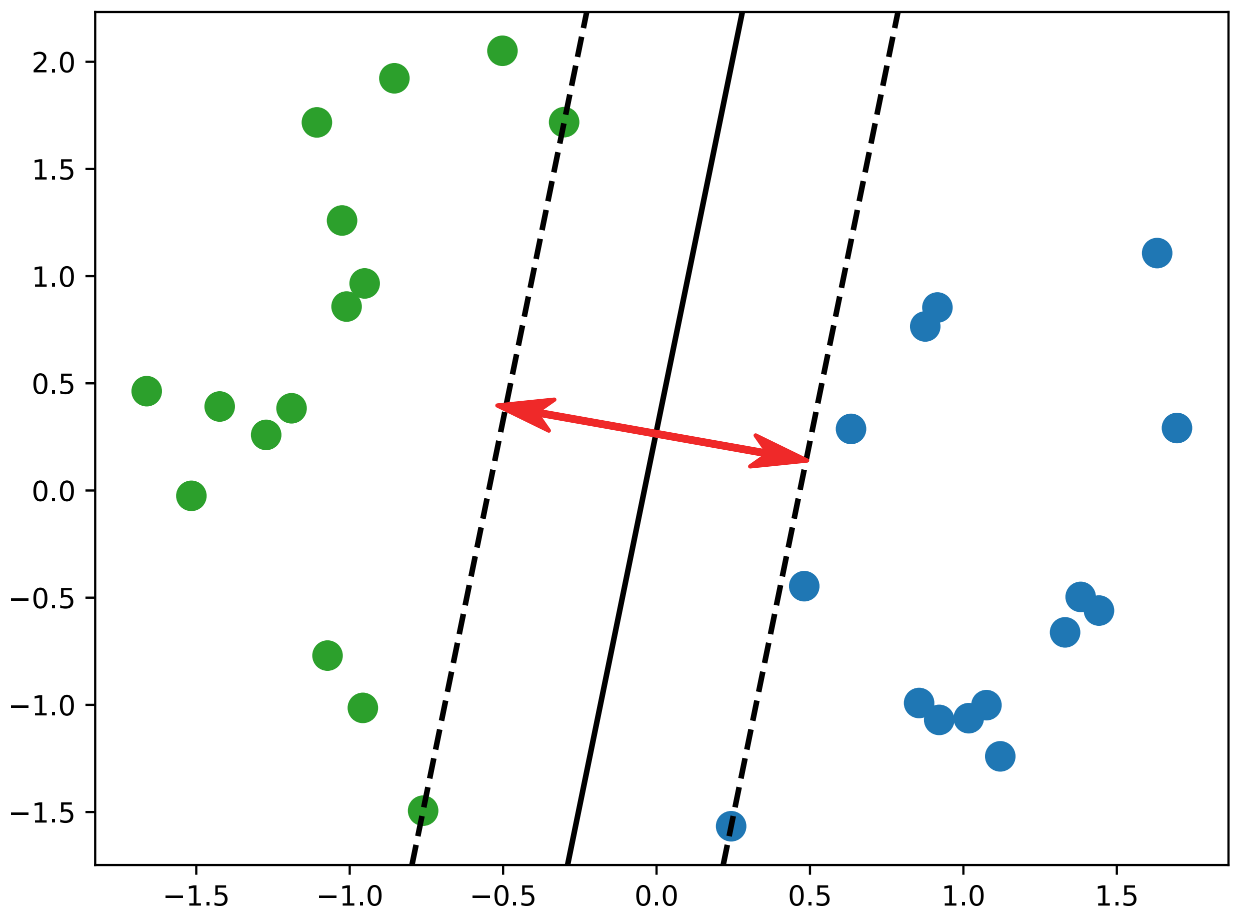
Principle Find the best line which separates the data



Support Vector Machines

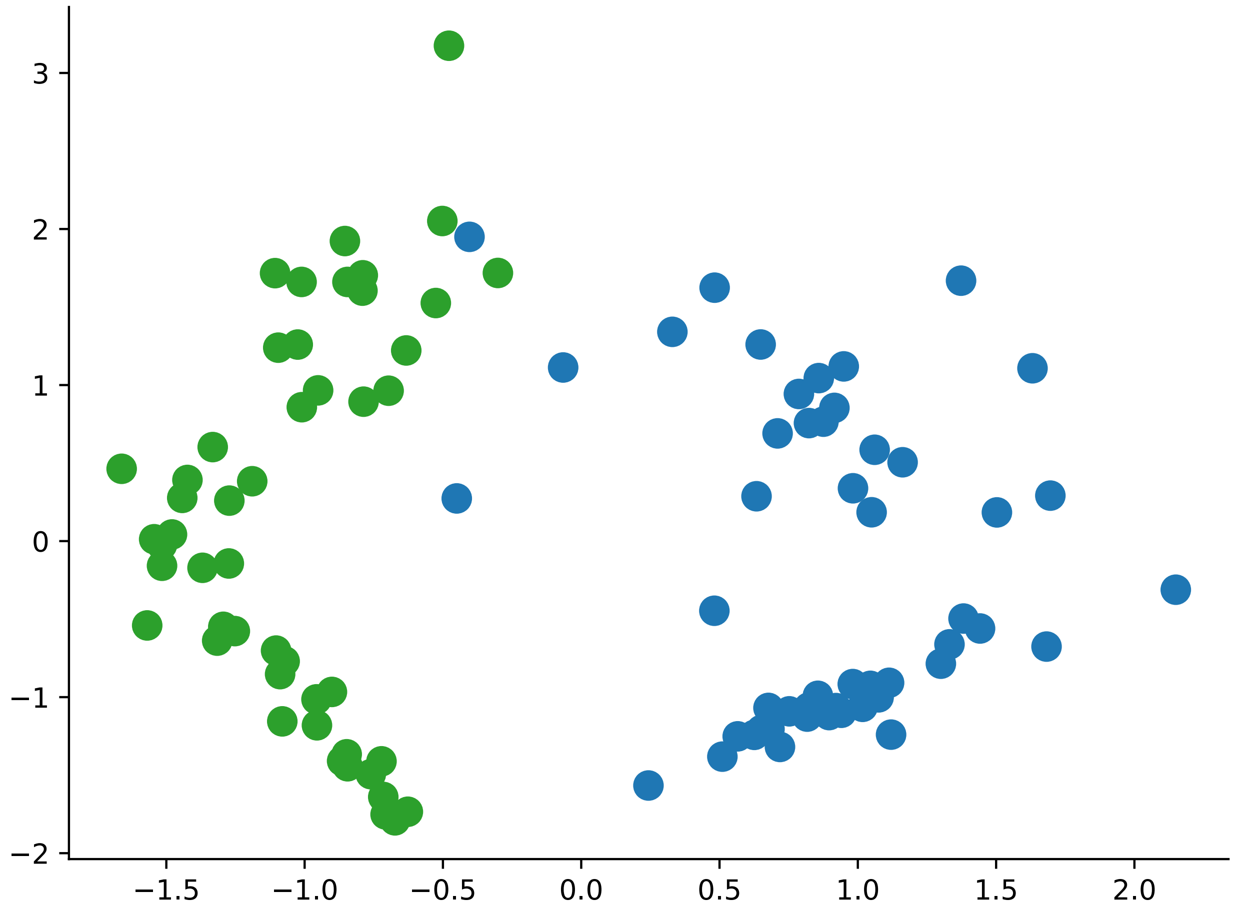
Principle Find the best line which separates the data

- Best separation $\Rightarrow$ points far away the separation
- support vectors



Support Vector Machines

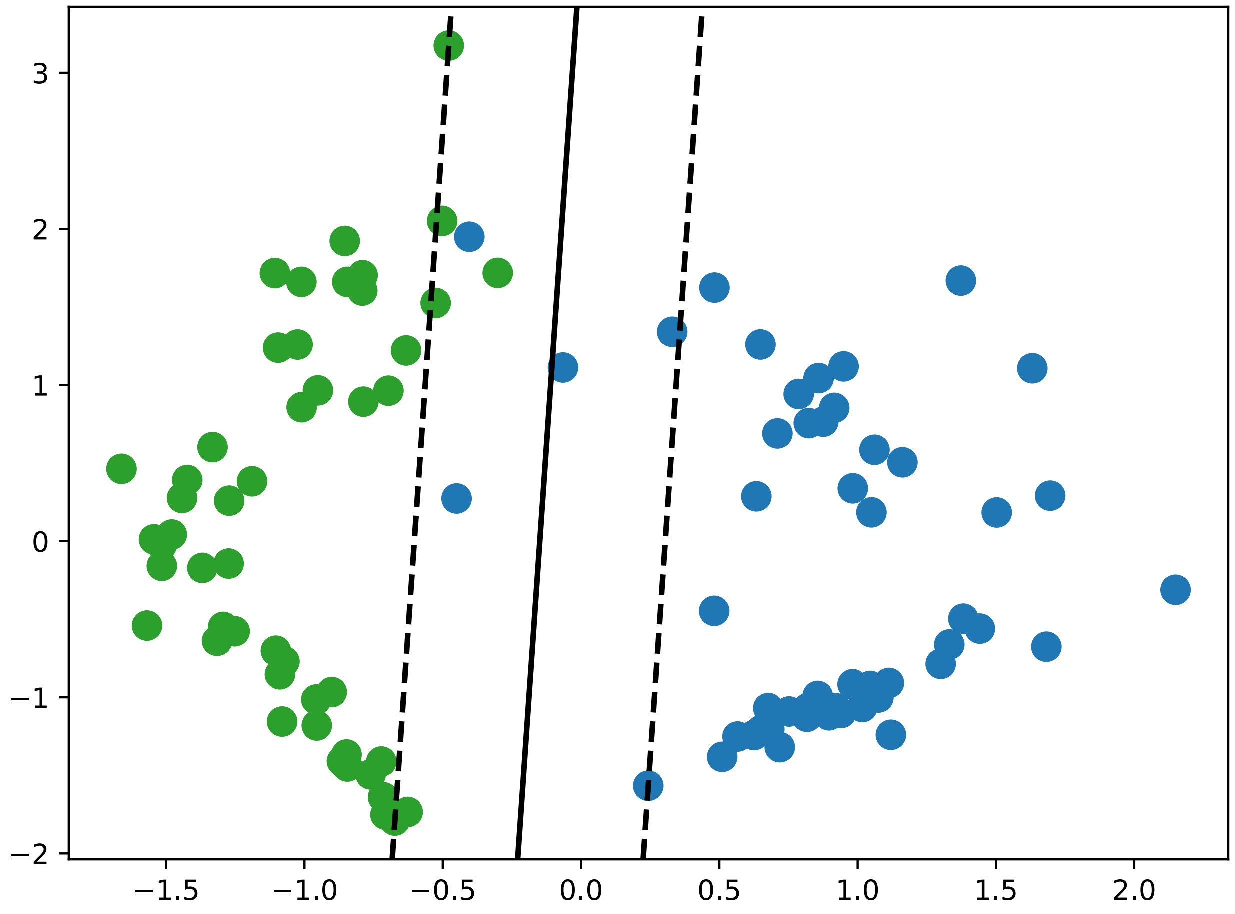
What happens when there is no separation line?



Support Vector Machines

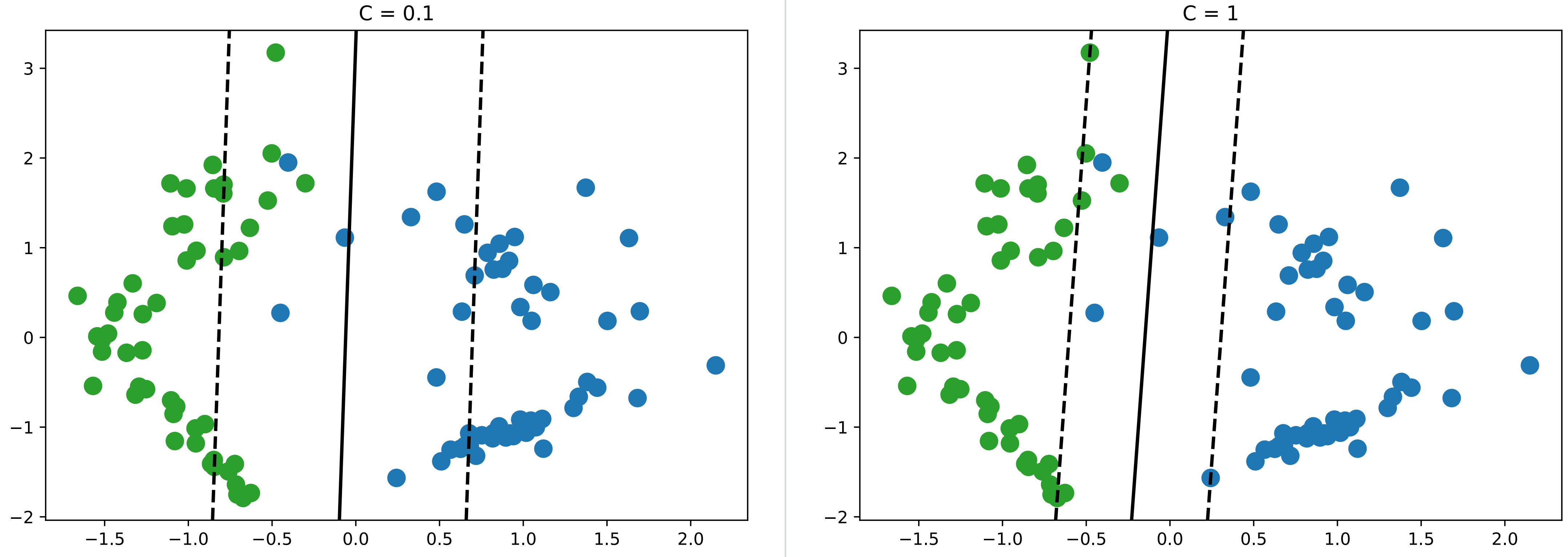
What happens when there is no separation line?

- $\Rightarrow$ We allow errors!

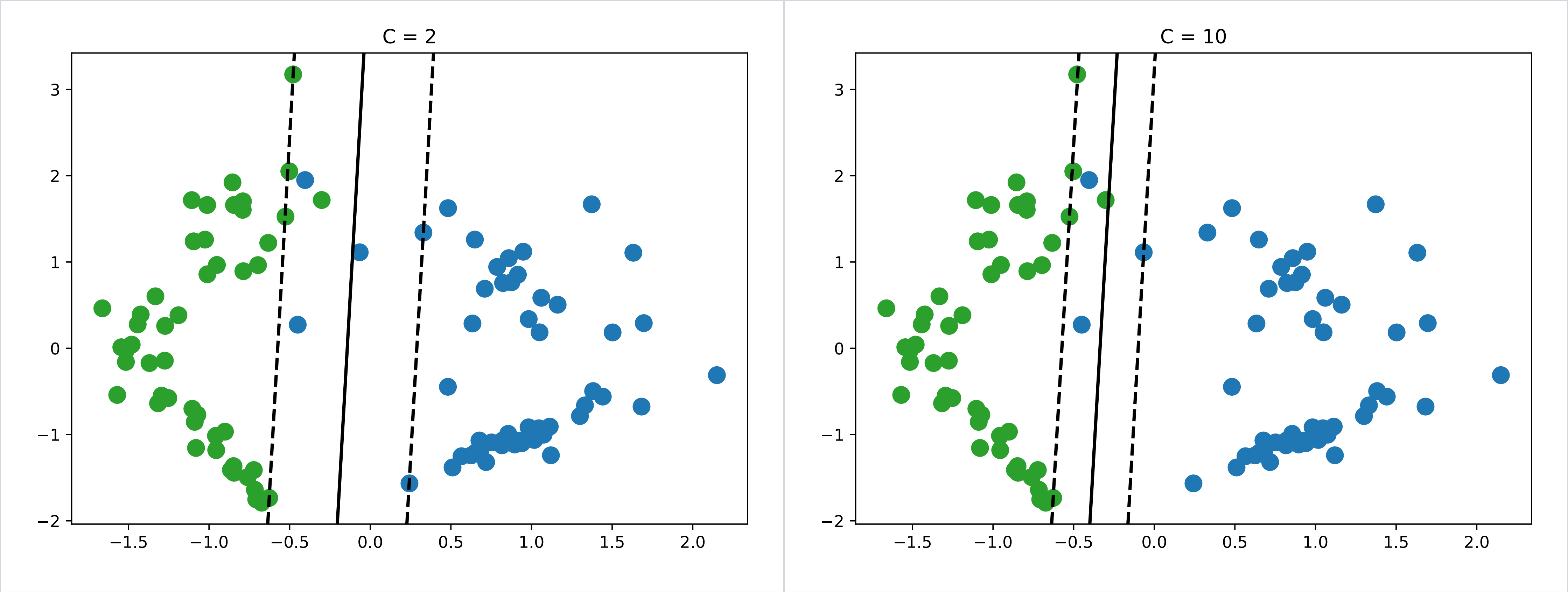


Support Vector Machines

Hyperparameter C controls the trade off between errors and separation



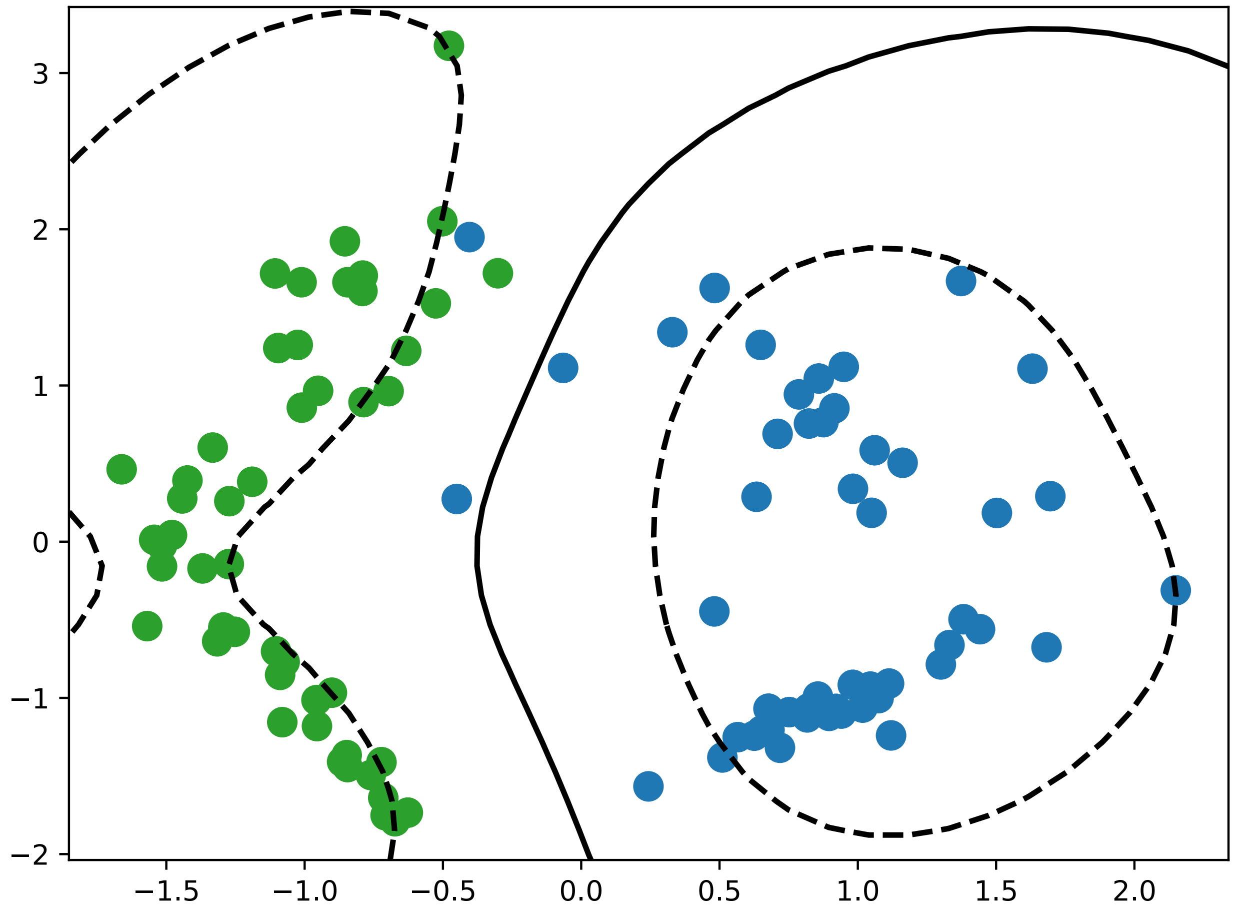
Support Vector Machines



Extension to non linear separation

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

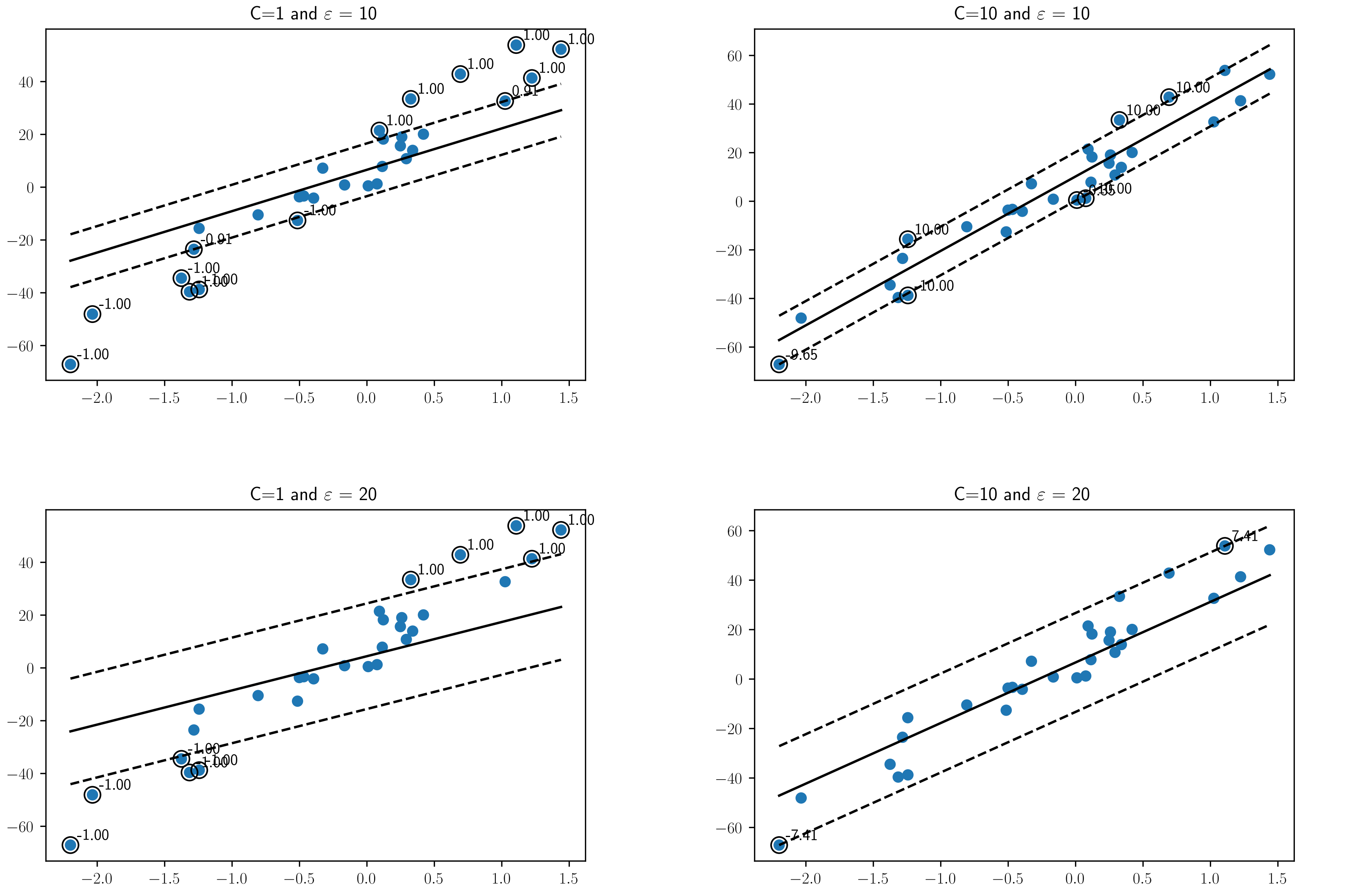
- Depends on kernel



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)

C and ε impact



SVM : the code !

```
python from sklearn import svm
C = 1
kernel = 'rbf'
clf = svm.SVC(C=C,kernel=kernel)
clf.fit(X,y)
ypred = clf.predict(X)
```

- User guide for hyperparameters : link
- the documentation

Conclusion

- **Understand key concepts**: cross-validation, unseen data evaluation.
- Use **proper validation strategies**: train/validation/test splits, leave-one-out, KFold, shuffle split.
- **Learn model specifics**: decision trees, random forests, SVMs, their principles, hyperparameters, and scikit-learn usage.
- **Avoid bias**: ensure proper validation and hyperparameter tuning for better performance and generalization.