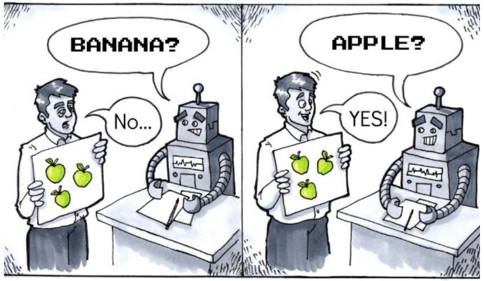
Supervised Learning

Let's use the first 20 minutes of the class to finish and review the last class exercises.

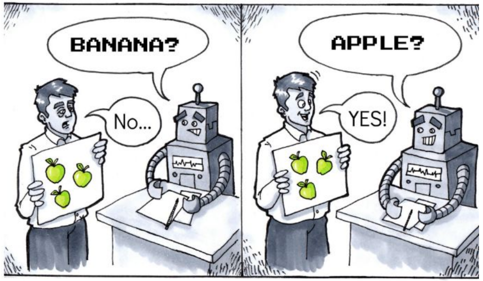
We will kick-off today’s topics at 17:50

Machines that Learn

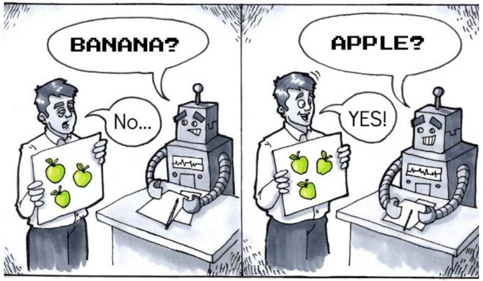
Today.



Supervised Learning



Supervised Learning



Supervised Learning

Cross-Validation
Hyperparameter Search

Supervised Learning

Some of the last class observations

- When I change the train and test split the results change, should I do this? There's not that much data, is my model robust?
- What K of KNN is the best? Do I try it out manually?

Supervised Learning

Robustness.

The ability of a model to **generalize** well to **unseen data** and perform **consistently** under **different conditions**.

Supervised Learning

It is not **generalizing** well.

Supervised Learning

It is not generalizing well.

Its either **underfitting** or **overfitting**

Supervised Learning

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Its either **underfitting** or **overfitting**

The model is too **simple** to capture the patterns in the data.

The model learns the **training data too well**, including noise, and fails to generalize to new data.

Supervised Learning

It is not generalizing well.

Its either **underfitting** or **overfitting**

The model is too simple to capture the patterns in the data - **underfitting**

The model learns the training data too well, including noise, and fails to generalize to new data - **overfitting**

Supervised Learning

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Note: if you increase test-size and the evaluation metrics improve, the model was *probably* overfitting.

Supervised Learning

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Note: if you increase test-size and the evaluation metrics improve, the model was *probably* overfitting.

Supervised Learning

When it is not generalizing well.

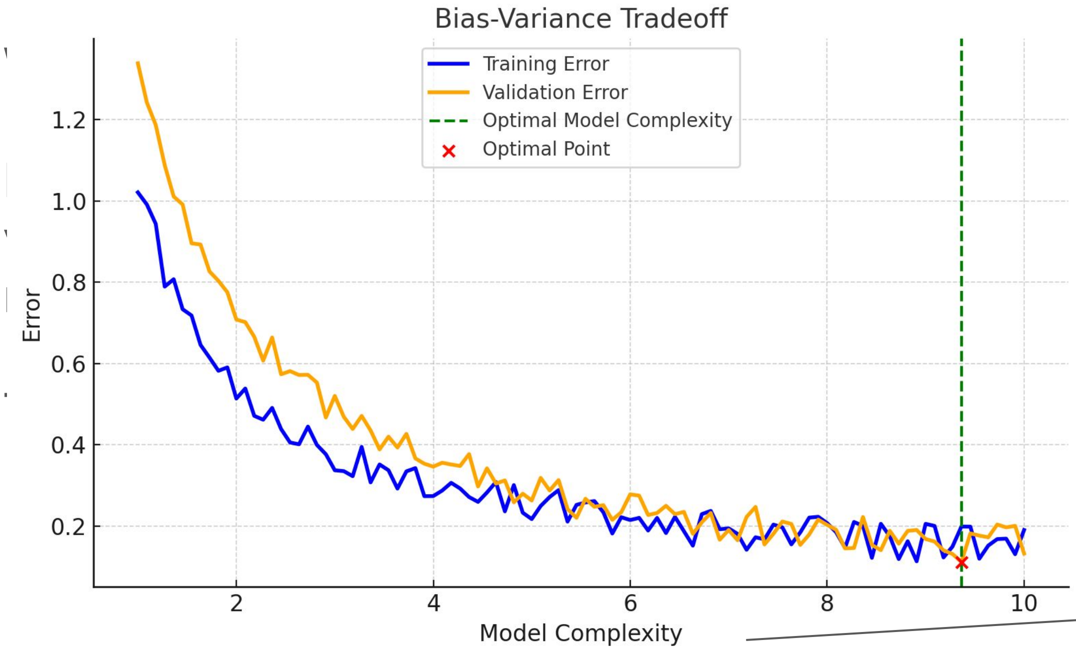
We also talk often about the Bias-Variance Trade-off.

Bias is the error from overly simplistic models that underfit the data, while variance is the error from overly complex models that overfit to training data noise.

The key to robustness is finding the balance between the two.

Supervised Learning

When it is not generalizing well.



ff.

underfit the data, while
at overfit to training data

en the two.

This can be number of iterations, as the model is trained, among other things, we will come back to this in a couple of minutes

Supervised Learning

Robustness.

The ability of a model to **generalize** well to **unseen data** and perform **consistently** under **different conditions**.

One of the best ways to assess this is with cross-**validation**.

Supervised Learning

Cross Validation

A technique to evaluate model performance by **splitting the data into multiple subsets (folds)** and **training/testing the model on different combinations of these subsets**

Supervised Learning

Cross Validation

A technique to evaluate model performance by **splitting the data into multiple subsets (folds)** and **training/testing the model on different combinations of these subsets**

using validation datasets*

Cross Validation

Cross-validation provides a **reliable** and **systematic approach to evaluate models**, especially when data is limited, **reducing the risk** of overfitting or underfitting

Supervised Learning

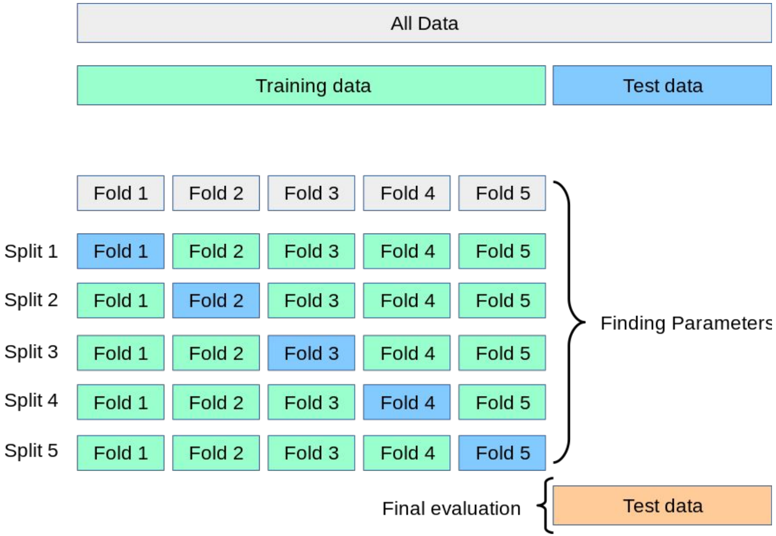
Cross Validation Schemes

- K-Fold Cross Validation
- Leave-One-Out Cross Validation
- Stratified Cross Validation
- Time-Series Cross Validation
- Repeated Cross-Validation

Supervised Learning

Cross Validation Schemes

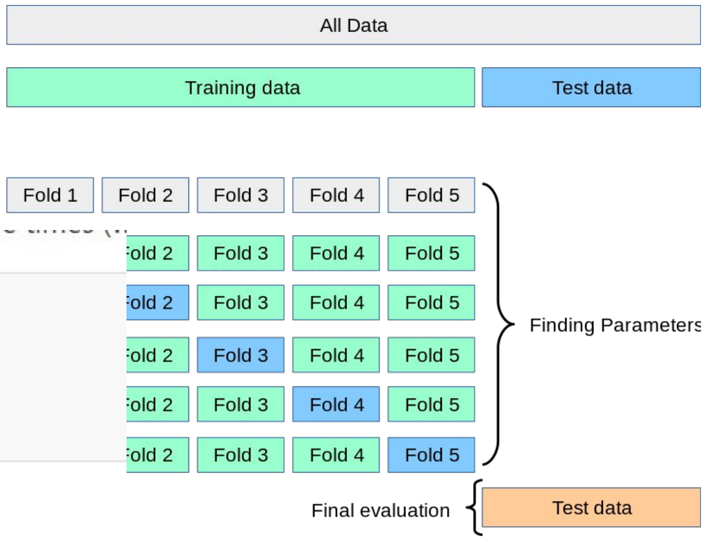
- K-Fold Cross Validation



Supervised Learning

Cross Validation Schemes

- K-Fold Cross Validation (sklearn.model_selection.cross_val_score)




```
>>> from sklearn.model_selection import cross_val_score
>>> clf = svm.SVC(kernel='linear', C=1, random_state=42)
>>> scores = cross_val_score(clf, X, y, cv=5)
>>> scores
array([0.96..., 1.  , 0.96..., 0.96..., 1.  ])
```

Cross Validation Schemes

- Leave-One-Out Cross Validation

Leave-One-Out

Supervised Learning

Cross Validation Schemes

- Leave-One-Out Cross Validation (sklearn.model_selection.LeaveOneOut)
  I.e leave one out and repeat process N times, where N is the time number of observations

Leave-One-Out

Supervised Learning

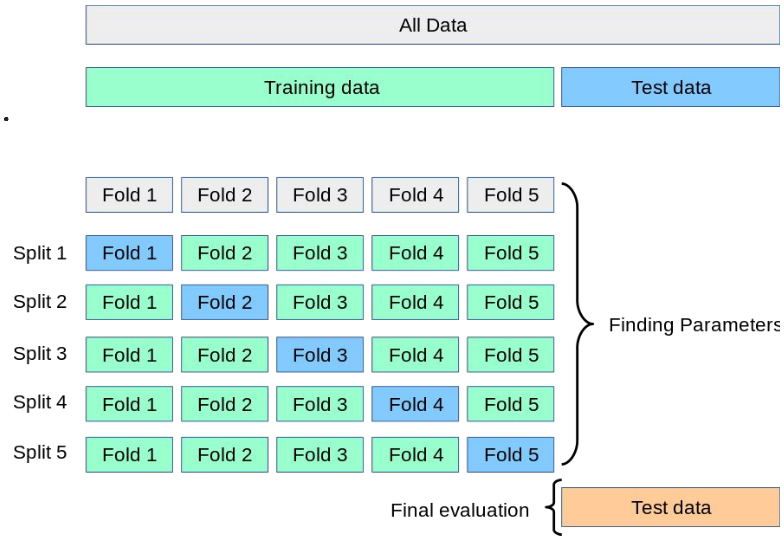
Cross Validation Schemes

- Stratified Cross Validation

Supervised Learning

Cross Validation Schemes

- Stratified Cross Validation (sklearn.model_selection.StratifiedKFold) is a variation of K-Fold that returns stratified folds. The folds are made by preserving the percentage of samples for each class.



Supervised Learning

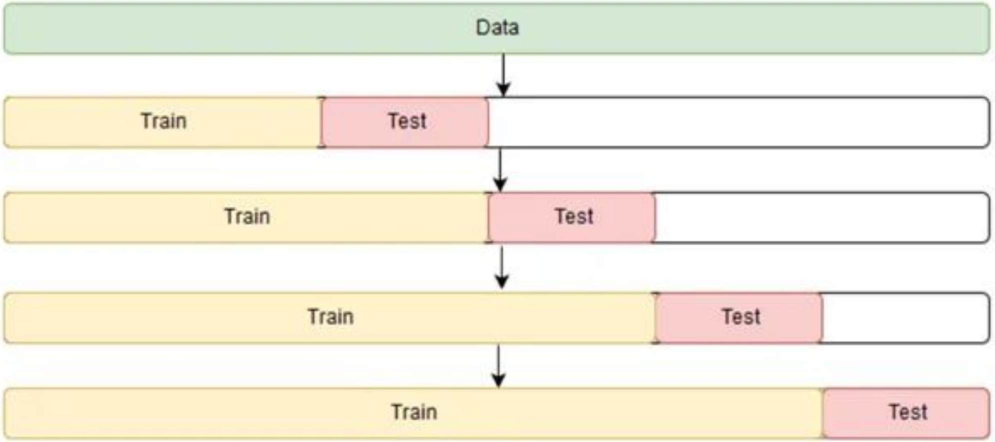
Cross Validation Schemes

- Time-Series Cross Validation

Supervised Learning

Cross Validation Schemes

- Time-Series Cross Validation
  (sklearn.model_selection.TimeSeriesSplit)
  i.e folds are sequential



Supervised Learning

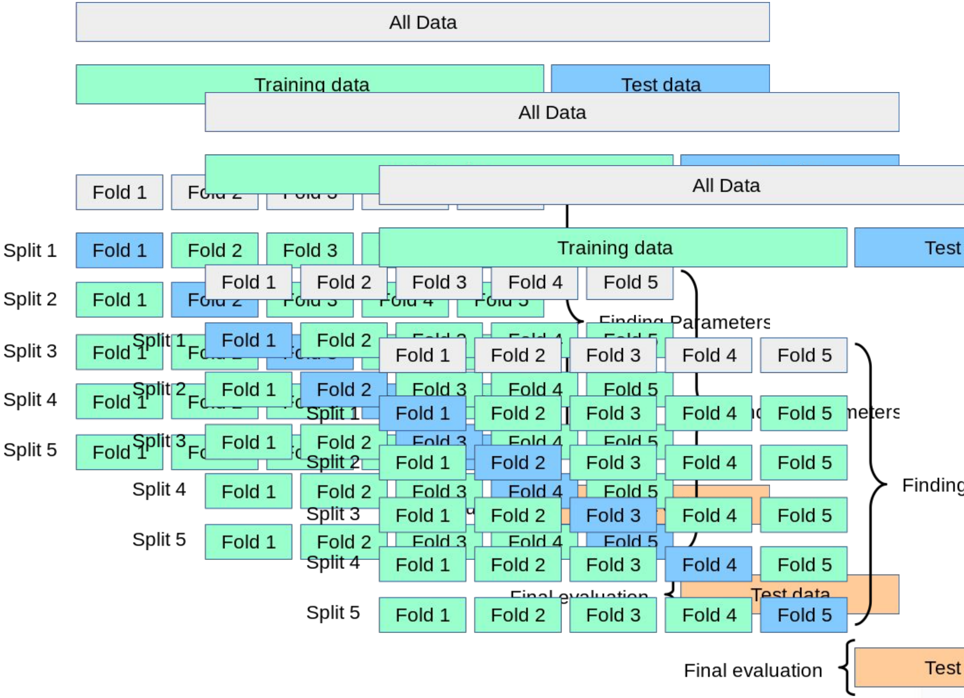
Cross Validation Schemes

- Repeated Cross Validation

Supervised Learning

Cross Validation Schemes

- Repeated Cross Validation
  i.e repeat k-fold validation multiple times (with different splits)



Supervised Learning

Last two things

Shuffle your dataset

P.s https://scikit-learn.org/stable/modules/cross_validation.html#a-note-on-shuffling

Supervised Learning

Last two things

Cross validation can be used during **feature engineering** to find the best set of features. For example, if you have features X_1, X_2, X_3, X_4, you might test subsets like $\{X_1, X_2\}, \{X_1, X_3, X_4\}$, etc.

P.s Ensure that feature selection or transformation is done **inside each fold** of the cross-validation process. Avoid data leakage.

Supervised Learning

Let's go back to our **classification** and **regression** notebooks and do some cross validation.

You can duplicate your notebook or use the same. You must adapt your code.

The questions that you need to be able to answer are:
Which of the algorithms is more robust ?

Supervised Learning

That was hard work.

Kudos.

Supervised Learning

Some of the last class observations

- When I change the train and test split the results change, should I do this? There's not that much data, is my model robust?
- **What K of KNN is the best? Do I try it out manually?**

Supervised Learning

Some of the last class observations

- When I change the train and test split the results change, should I do this? There’s not that much data, is my model robust?
- **What K of KNN is the best? Do I try it out manually?**
  Only if you want, but no. Not really.

Supervised Learning

Let’s take a step back.

Supervised Learning

What are we solving ?

Task

Supervised Learning

What are we solving ?

Task

Classification

Regression

Supervised Learning

How are we solving it?

Task → Classification → Models

Task → Regression → Models

Supervised Learning

How are we solving it?

Task

- Classification → Models → Hyperparameters
  (max_iter, k,...)
- Regression → Models → Hyperparameters

As data scientists we explicitly decide this, it can’t be automatically learned*

*or is it ?

Supervised Learning

Parameters vs Hyperparameters

Supervised Learning

Parameters vs Hyperparameters

Are learned by the model, i.e they change during training

Supervised Learning

Parameters	vs	Hyperparameters
Are learned by the model, i.e they change during training		Are decided before and fixed during training, i.e they are not learnt by the model and highly impact the model performance.

Supervised Learning

Hyperparameter Search

Find the best hyperparameters for the target task, model and existing data.

Supervised Learning

Hyperparameter Search

Find the best hyperparameters for the target task, model and existing data.

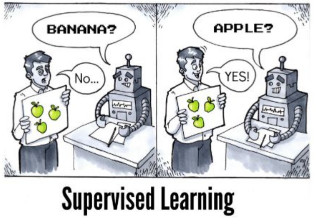
Search Space
 - given a model, all hyperparameters combinations possible

Supervised Learning

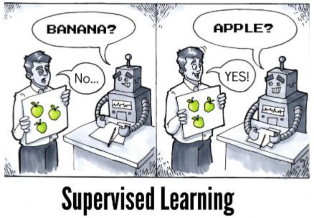
Hyperparameter search
Find the best hyperparameters for the target task, model and existing data.

DATA

TRAIN



TEST



Validation

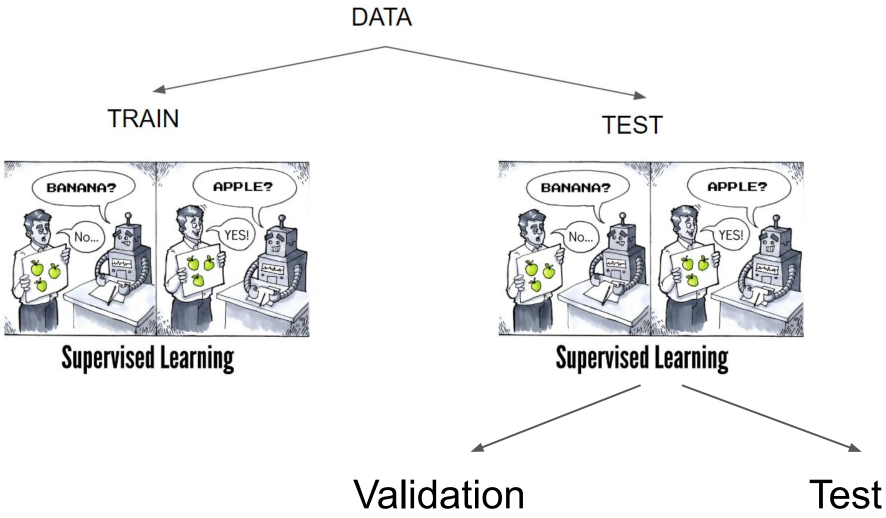
Test

Reminder

Supervised Learning

Hyperparameter search consists of:

- an estimator (regressor or classifier such as sklearn.svm.SVC()) - a model;
- a parameter space;
- a method for searching or sampling candidates;
- a cross-validation scheme
- a score function.



Reminder

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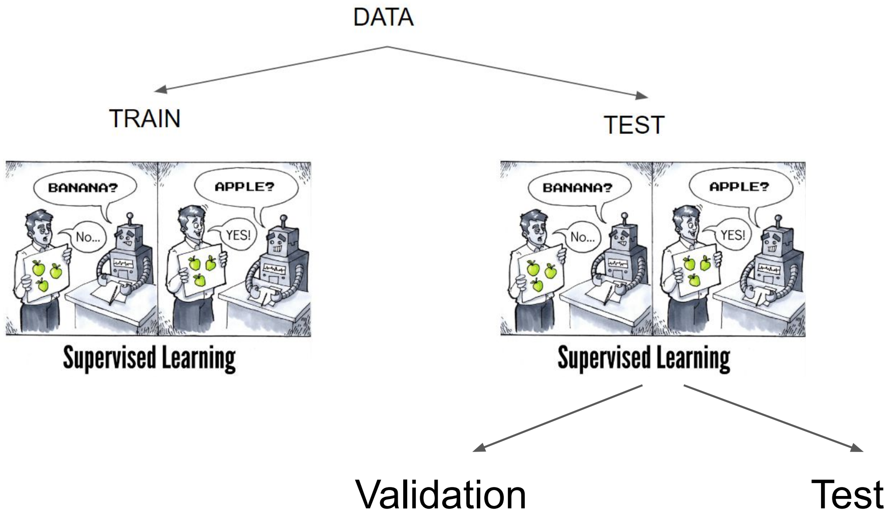


Reminder

Supervised Learning

Hyperparameter search

- Grid Search
- Random Search
- Bayesian Search

Supervised Learning

Hyperparameter search

- Grid Search
  (**systematically** evaluates a predefined set of hyperparameters combinations to find the best set of hyperparameter for a given model)
  (sklearn.model_selection.GridSearchCV)

Supervised Learning

Hyperparameter search

- Grid Search (sklearn.model_selection.GridSearchCV)

Supervised Learning

Hyperparameter search

- Grid Search
  (sklearn.model_selection.GridSearchCV)
- Random Search
  (randomly *samples* hyperparameter values from predefined distributions to efficiently explore the search space and find optimal hyperparameter configurations for machine learning models)
  (sklearn.model_selection.RandomizedSearchCV)

Supervised Learning

Hyperparameter search

- Grid Search (sklearn.model_selection.GridSearchCV)
- Random Search (sklearn.model_selection.RandomizedSearchCV)
- Bayesian Search

Supervised Learning

Hyperparameter search

- Grid Search
  (sklearn.model_selection.GridSearchCV)
- Random Search
  (sklearn.model_selection.RandomizedSearchCV)
- Bayesian Search
  (is a probabilistic optimization technique that uses surrogate models to efficiently explore and optimize complex hyperparameter spaces in machine learning by iteratively selecting hyperparameters to evaluate based on a balance of **exploration** and **exploitation**)
  (skopt.BayesSearchCV)

Supervised Learning

Hyperparameter search

- Grid Search - for smaller datasets and known limited search space
- Random Search - a good balance between simplicity and efficiency
- Bayesian Search - slightly more complicated to setup but smarter than random search

Supervised Learning

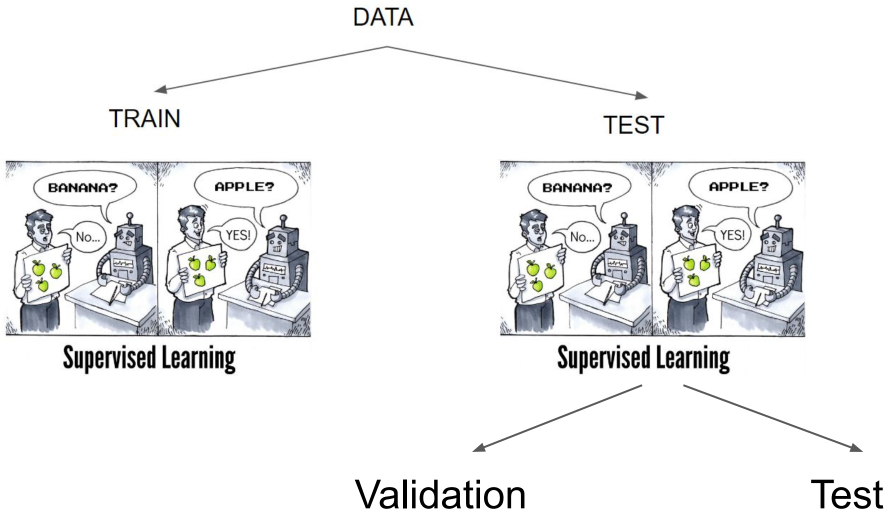
Which One Is Used the Most in Practice?

- **Random Search** is the most widely used in practice because:
  - It strikes a good balance between simplicity and efficiency.
  - It scales well for large hyperparameter spaces without requiring domain-specific expertise to define a probabilistic model.
  - Often, randomly sampling hyperparameters is surprisingly effective since only a few hyperparameters tend to dominate performance.
- **Bayesian Search** is gaining popularity, especially in resource-constrained scenarios or for complex pipelines, but it requires more setup and understanding of surrogate models.
- **Grid Search** is less commonly used in practical scenarios, except for small, well-defined spaces, due to its inefficiency in scaling.

Supervised Learning

Hyperparameter search consists of:

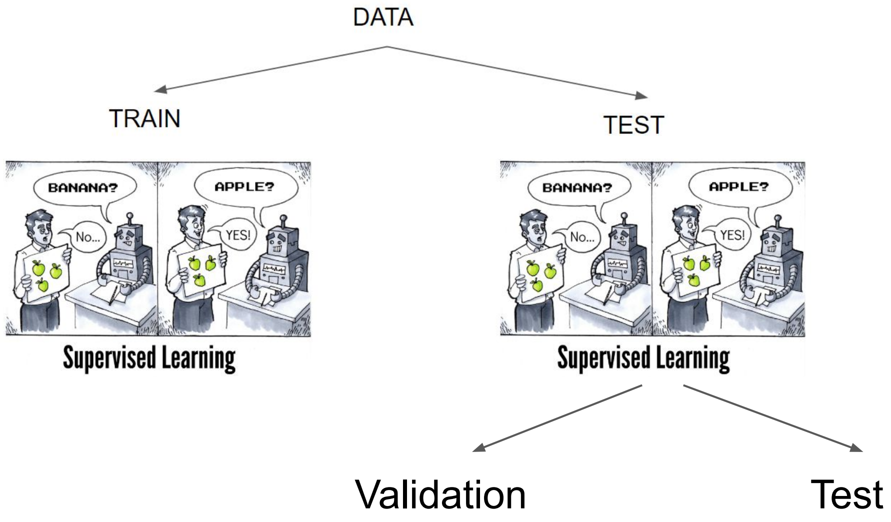
- an estimator (regressor or classifier such as sklearn.svm.SVC());
- a parameter space;
- a method for searching or sampling candidates;
- **a cross-validation scheme**
- a score function.



Supervised Learning

Dataset splits

- **Train** is used to train the selected model with the selected hyperparameters
- **Validation** is used to validate the trained models
- **Test** is used to test the validated model with the higher selected metric



Supervised Learning

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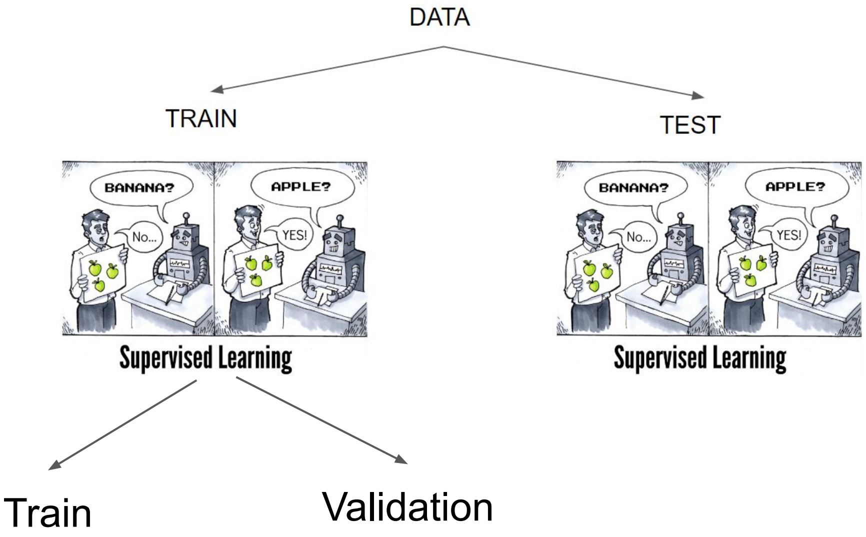

Supervised Learning

Hyperparameter search
consists of:

- an estimator (regressor or classifier such as sklearn.svm.SVC());
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- a cross-validation scheme
- **a score function**.

F1 Score
Precision
Recall
Accuracy

Supervised Learning

Hyperparameter search consists of:

- an estimator (regressor or classifier such as sklearn.svm.SVC());
- a parameter space;
- a method for searching or sampling candidates;
- a cross-validation scheme
- a score function.

In practice sklearn (and other libs) does most of it for us

Supervised Learning

Hyperparameter search consists of:

- an estimator (regressor or classifier such as sklearn.svm.SVC());
- a parameter space;
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- a cross-validation scheme
- a score function.

Supervised Learning

Let’s go **back to our classification notebooks** and do some hyperparameter search.
Try using Grid Search and Random Search.

- Which is faster?
- Does it make a difference?

You can duplicate your notebook or use the same. You must adapt your code.

The questions that you need to be able to answer are:
Which hyperparameters are the more suitable in all of the algorithms we’ve tried so far?

Supervised Learning

Submit.

Oops it's actually a regression problem.

Supervised Learning

Sidenote

If we have hyperparameter search to look for the best combination of hyperparameters, could we have model search ? To automatically look for the best model ? i.e "automate" a data scientist/machine learning engineer job ?

Supervised Learning

Demo ?

Supervised Learning

Let’s explore.

Supervised Learning

Packaging a model.

Supervised Learning

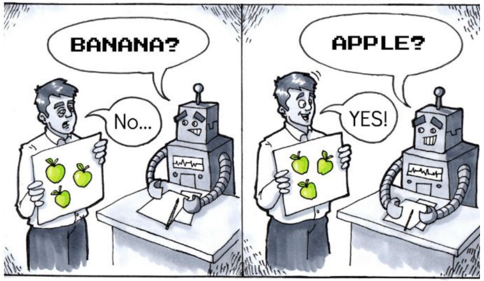
Packaging a model.

Use formats like `joblib`, `pickle`, or ONNX for portability.

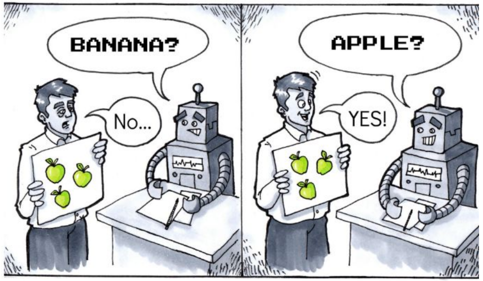
```
#after training and model is ready
import joblib
joblib.dump(model, 'model.pkl')



#on server
from fastapi import FastAPI
import joblib

app = FastAPI()
model = joblib.load('model.pkl')

@app.post("/predict")
def predict(features: dict):
    return {"prediction":
model.predict([features])}
```

Machines that Learn

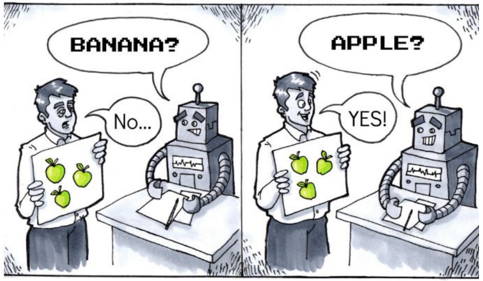
Next up



Supervised Learning



Supervised Learning



Supervised Learning

Multi-Class
Data Augmentation