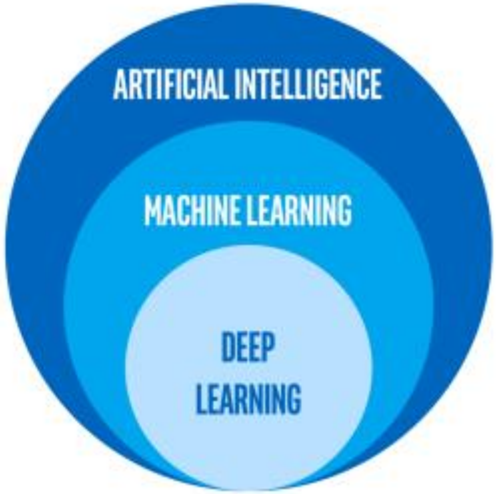
# Machine learning

## Hands on python and sklearn

# Machine learning

Machine Learning is the science (and art) of programming computers so they can learn from data

- Machine Learning is the field of study that gives computers the ability to learn without being explicitly programmed — Arthur Samuel, 1959
- A computer program is said to learn from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E — Tom Mitchell, 1997



# Machine learning

There are many types of Machine Learning algorithms

Classify them in broad categories, based on the following criteria:

- Whether they are trained with human supervision
  - supervised, unsupervised, semi-supervised, and reinforcement learning
- Whether they can learn incrementally
  - online, batch learning
- Whether they compare new to known data points, or detect patterns/models in the training
  - instance-based, model-based learning

In this session, the focus is not on the different models of ML

- We stick to "classical" ML algorithms

# Machine learning

## Supervised learning tasks

- The training set you feed to the algorithm includes the desired solutions, called labels
- Classification
  - Approximating a mapping function (f) from input variables (X) to discrete output variables (y)
  - The output variables are called labels or categories
  - The mapping function predicts the class or category for a given observation
  - E.g., a spam filter is trained with many example emails along with their class (spam or ham)
- Regression
  - Approximating a mapping function (f) from input variables (X) to a continuous output variable (y)
  - A continuous output variable is a real-value, such as an integer or floating-point value
  - E.g., predict the price of a car given a set of features (mileage, age, brand, etc.) called predictors

# Sklearn

**Scikit-learn (Sklearn)** is a well-known library for ML in Python

- This library, which is largely written in Python, is built upon NumPy, SciPy and Matplotlib
  - Open source and commercially usable
- Covers many algorithms
  - Supervised Learning algorithms: Linear Regression, Support Vector Machine, etc.
  - Unsupervised Learning algorithms: clustering, factor analysis, PCA, neural networks, etc.
  - Cross Validation: check the accuracy of supervised models on unseen data
  - Feature extraction: extract the features from data to define the attributes in image and text data

# scikit-learn

*Machine Learning in Python*

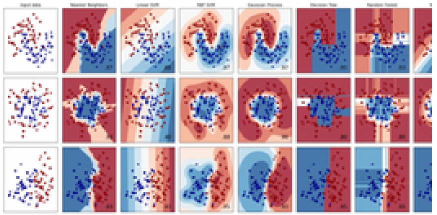
Getting Started | Release Highlights for 0.24 | GitHub

- Simple and efficient tools for predictive data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

## Classification

Identifying which category an object belongs to.

**Applications:** Spam detection, image recognition.
**Algorithms:** SVM, nearest neighbors, random forest, and more...

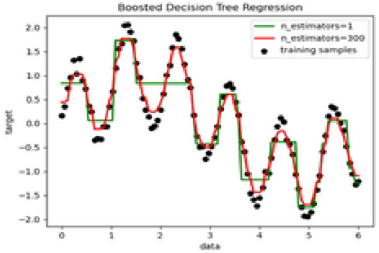


Examples

## Regression

Predicting a continuous-valued attribute associated with an object.

**Applications:** Drug response, Stock prices.
**Algorithms:** SVR, nearest neighbors, random forest, and more...

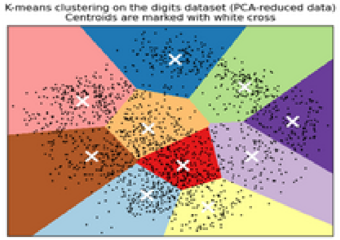



Examples

## Clustering

Automatic grouping of similar objects into sets.

**Applications:** Customer segmentation, Grouping experiment outcomes
**Algorithms:** k-Means, spectral clustering, mean-shift, and more...

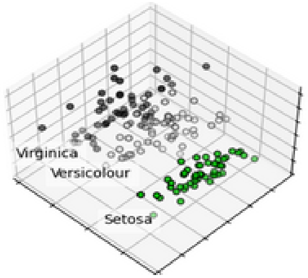



Examples

## Dimensionality reduction

Reducing the number of random variables to consider.

**Applications:** Visualization, Increased efficiency
**Algorithms:** k-Means, feature selection, non-negative matrix factorization, and more...

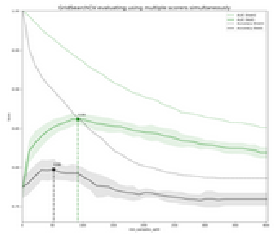



Examples

## Model selection

Comparing, validating and choosing parameters and models.

**Applications:** Improved accuracy via parameter tuning
**Algorithms:** grid search, cross validation, metrics, and more...

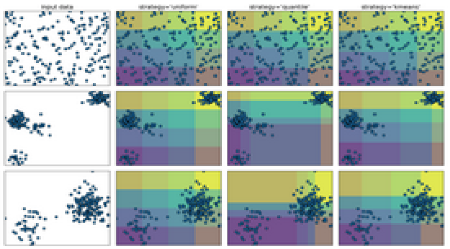


Examples

## Preprocessing

Feature extraction and normalization.

**Applications:** Transforming input data such as text for use with machine learning algorithms.
**Algorithms:** preprocessing, feature extraction, and more...



Examples

# Sklearn

Scikit-learn uses data in the form of N-dimensional matrix

- Data as a feature matrix (e.g., a Pandas DataFrame)
  - The samples represent the individual objects described by the dataset (e.g., a person)
  - The features describe each sample in a quantitative manner (e.g., age and height)
  - It is usually denoted by X
- Data as target array (e.g., a Pandas Series)
  - Along with features matrix, we also have the target array (e.g., or label)
  - It is usually denoted by y
- How do we distinguish target and feature columns?

# Estimator

Estimator

- A consistent interface for a wide range of ML applications
- The algorithm that learns from the data (fitting the data) is an estimator
- It can be used with any of the algorithms like classification, regression, and clustering

All the parameters can be set when creating the estimator

- >>> estimator = Estimator(param1=1, param2=2)
- >>> estimator.param1

All estimator objects expose a fit method that takes a dataset

- >>> estimator.fit(X)

Once data is fitted with an estimator, all the estimated parameters will be the attributes of the estimator object ending by an underscore

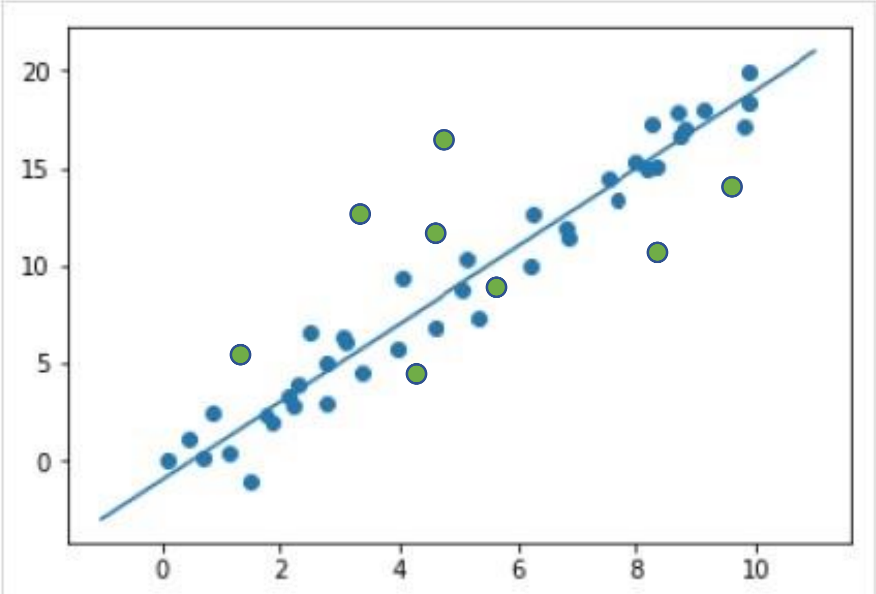
- >>> estimator.estimated_param_

# Estimator

1. Choose a class of model
   - Import the appropriate Estimator class from Scikit-learn (e.g., a decision tree)
2. Choose model hyperparameters
3. Arranging the data
   - Arrange the data into features matrix X and target vector y
4. Model Fitting
   - Fit the model by calling fit() method of the model instance
5. Applying the model to new data
   - For supervised learning, use predict() method to predict the labels for unknown data.
   - For unsupervised learning, use predict() or transform() to infer properties of the data.

# Estimator

1. Choose a class of model
   - >>> from sklearn.linear_model import LinearRegression
2. Choose model hyperparameters
   - >>> model = LinearRegression(fit_intercept = True)
3. Arranging the data
4. Model fitting
   - >>> model.fit(X, y)
   - >>> model.coef_
5. Applying the model to new data
   - >>> model.predict(new_X)



# Integrated analytics lab

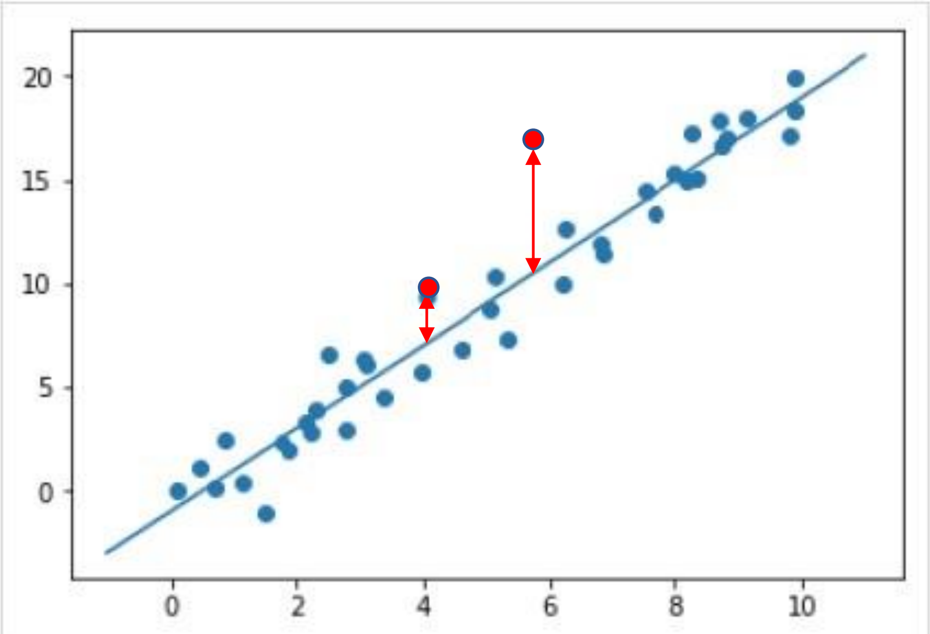
This checklist can help you while building your projects

- Frame the problem and look at the big picture
  - ✔ Define the objective in business terms
  - ✘ How should performance be measured? (let's do this!)

# Integrated analytics lab

We are facing a regression problem

- A typical performance measure for regression problems is the Root Mean Square Error (RMSE)
- RMSE is the standard deviation of the residuals (prediction errors)
- Residuals are a measure of how far from the regression line data points are; RMSE is a measure of how spread out these residuals are

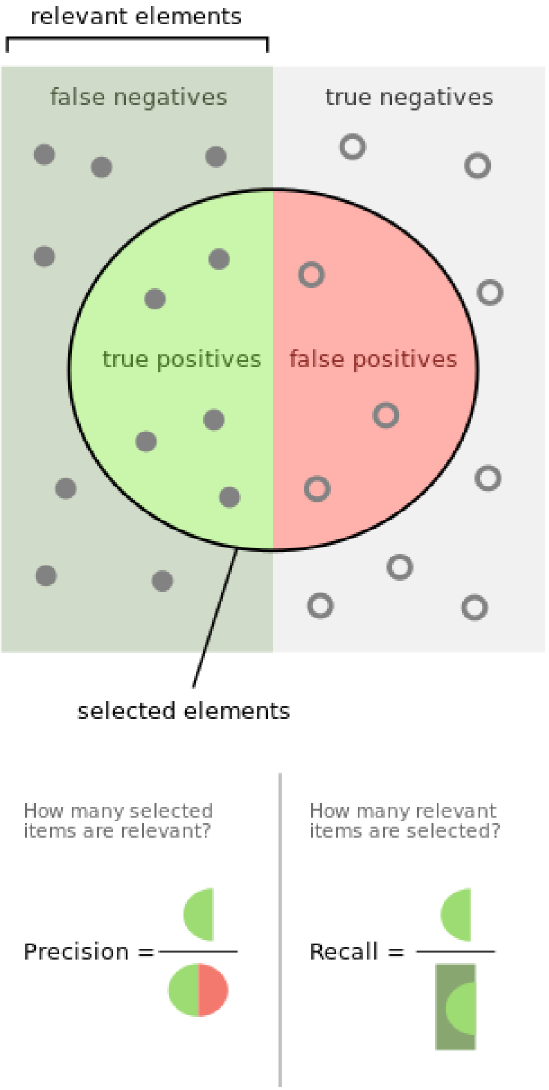



$$\mathrm{RMSE}(\mathbf{X}, h) = \sqrt{\frac{1}{m}\sum_{i=1}^{m}\left(h\left(\mathbf{x}^{(i)}\right) - y^{(i)}\right)^2}$$

# Integrated analytics lab

(If) We are facing a classification problem

| | | Predicted condition | |
|---|---|---|---|
| | Total population = P + N | Predicted condition **positive** (PP) | Predicted condition **negative** (PN) |
| **Actual condition** | Actual condition positive (P) | **True positive (TP), hit** | **False negative (FN), Type II error, miss, underestimation** |
| | Actual condition negative (N) | **False positive (FP), Type I error, false alarm, overestimation** | **True negative (TN), correct rejection** |
| | Prevalence = $\frac{P}{P + N}$ | Positive predictive value (PPV), $\boxed{\text{precision} = \frac{TP}{PP}}$ = 1−FDR | False omission rate (FOR) = $\frac{FN}{PN}$ = 1−NPV |
| | $\boxed{\text{Accuracy (ACC)} = \frac{TP + TN}{P + N}}$ | False discovery rate (FDR) = $\frac{FP}{PP}$ = 1−PPV | Negative predictive value (NPV) = $\frac{TN}{PN}$ = 1−FOR |
| | Balanced accuracy (BA) = $\frac{TPR + TNR}{2}$ | $F_1$ score = $\frac{2 \cdot PPV \cdot TPR}{PPV + TPR}$ = $\boxed{\frac{2TP}{2TP + FP + FN}}$ | Fowlkes–Mallows index (FM) = $\sqrt{PPV \cdot TPR}$ |



# Integrated analytics lab

## Precision

$$\text{Precision} = \frac{tp}{tp + fp}$$

## Recall

$$\text{Recall} = \frac{tp}{tp + fn}$$

## Accuracy

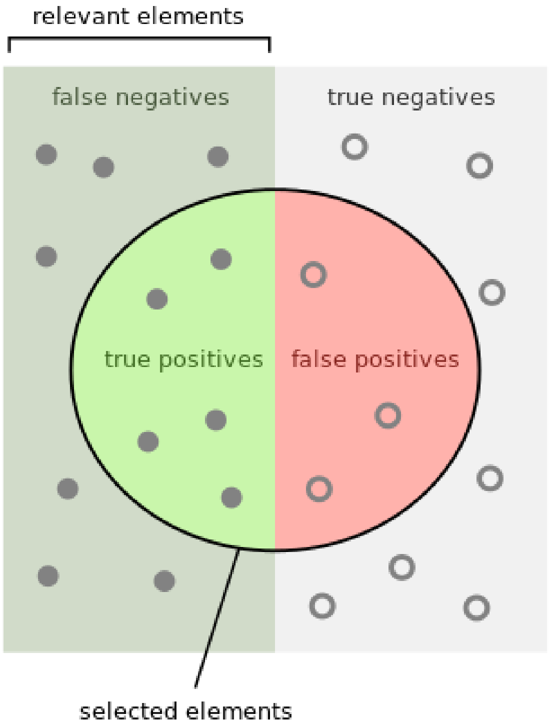
$$\text{Accuracy} = \frac{tp + tn}{tp + tn + fp + fn}$$

- Accuracy can be a misleading metric for imbalanced data sets

## F1-score

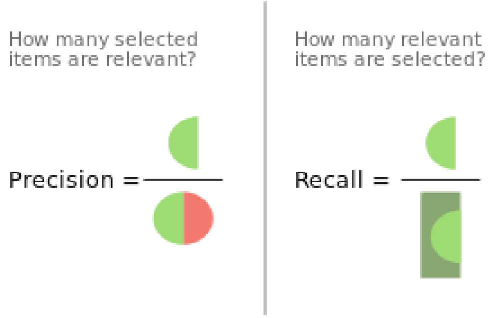
$$F = 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$

- Combines precision and recall




## Summing up

- Accuracy is used when TP and TN are more important while F1-score is used when FN and FP are
- Accuracy can be used when the class distribution is similar, while F1-score is a better when there are imbalanced classes



# Hyper-parameter tuning

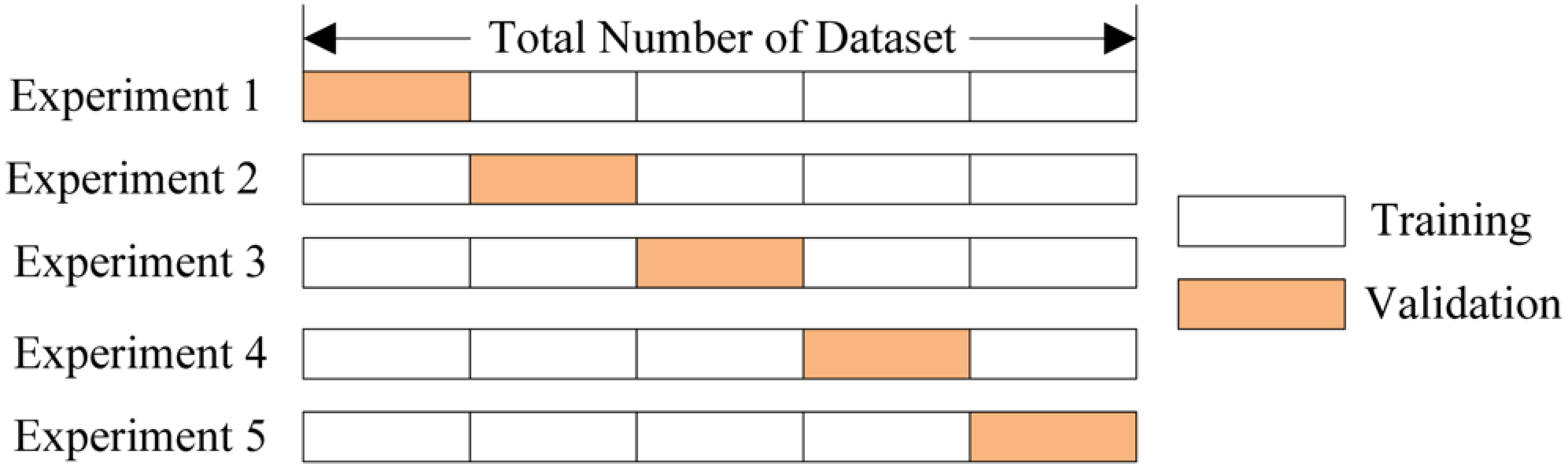
Hyper-parameters: parameters that are not directly learnt within estimators

- In scikit-learn they are passed as arguments to the constructor of the estimator classes
- Any parameter provided when constructing an estimator may be optimized
  - >>> estimator.get_params()

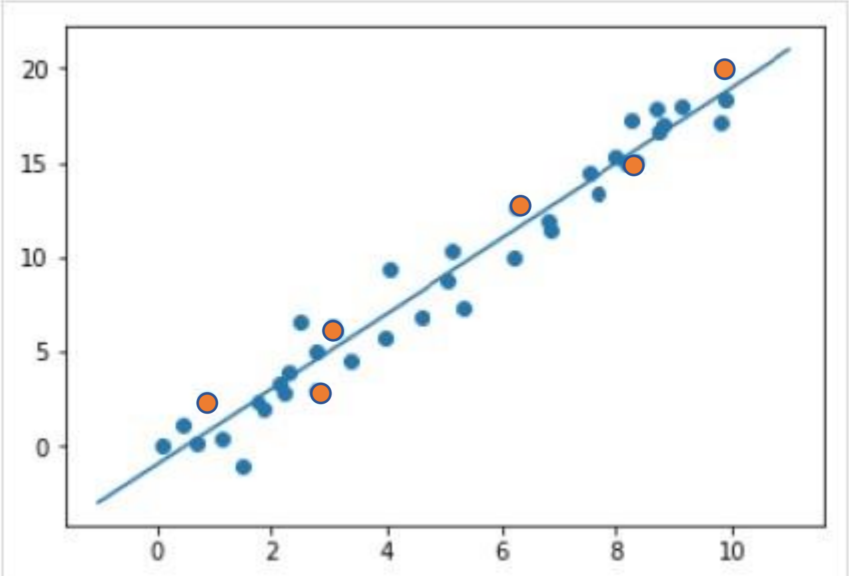
A search consists of:

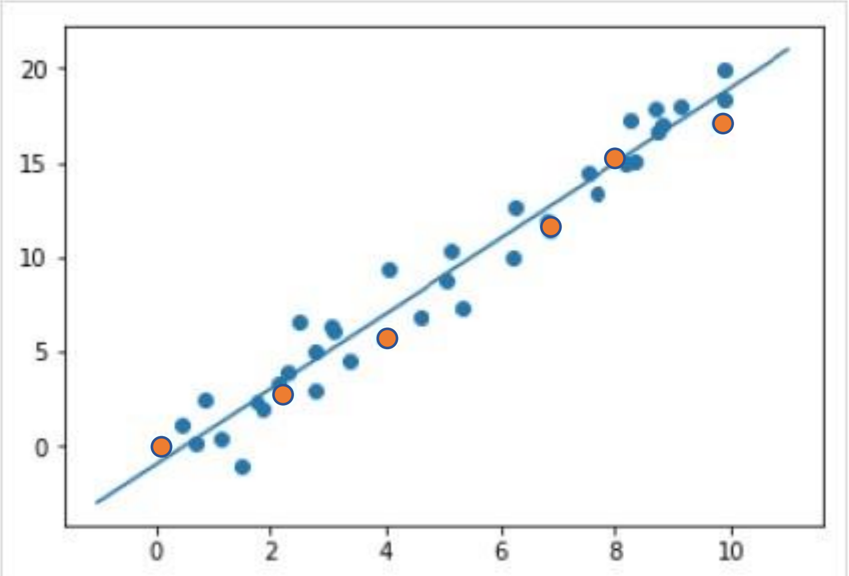
- an estimator
- a parameter space
- a method for searching or sampling candidates
- a cross-validation scheme
- a score function

# Cross validation



# Cross validation



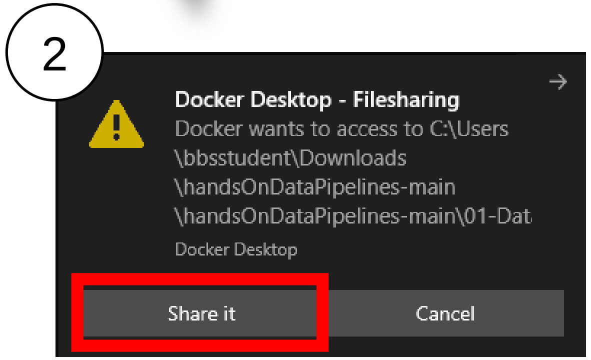
# Integrated analytics lab

## This checklist can help you while building your projects

- Frame the problem and look at the big picture
  - ✔ Define the objective in business terms
  - ✔ How should performance be measured?
- Get the data
  - ✔ List the data you need and how much you need
- Explore the data to gain insights
  - ✔ Create an environment to keep track of your data exploration
  - ✔ Study each attribute and its characteristics
- Prepare the data
  - ✔ Fix or remove outliers (optional)
  - ✔ Fill in missing values (e.g., with zero, mean, median…) or drop their rows (or columns)
  - ✔ Feature selection (optional): drop the attributes that provide no useful information for the task
  - ✔ Feature engineering, where appropriate: discretize continuous features
- Explore many different models and shortlist the best ones
  - ✔ Let's do this!

# In action!

- Enter the folder `02-MachineLearning`
- Double click on `run.bat`
- Open the browser
- Copy and paste the link to the notebook
- Enter the notebook `02-MachineLearning`



# Integrated analytics lab

This checklist can help you while building your projects

- ✔ Frame the problem and look at the big picture
- ✔ Get the data
- ✔ Explore the data to gain insights
- ✔ Prepare the data
- ✔ Explore many different models and shortlist the best ones
- ✔ Fine-tune your models and combine them into a great solution
- Present your solution
- Launch, monitor, and maintain your system