

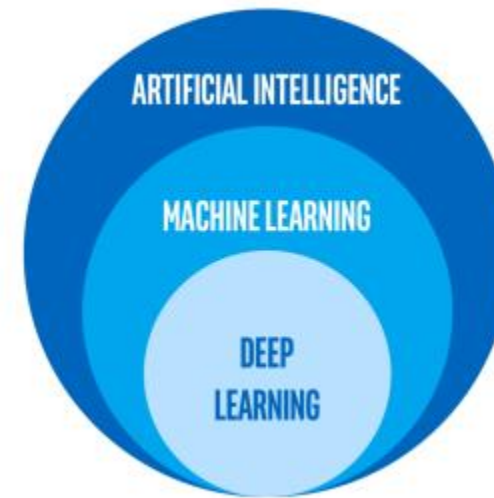
Machine learning

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

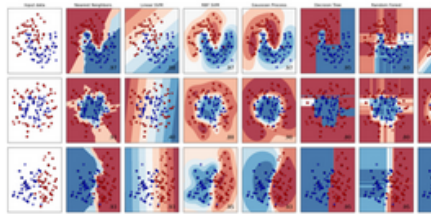
- Simple and efficient tools for predictive data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

Classification

Identifying which category an object belongs to.

Applications: Spam detection, image recognition.

Algorithms: SVM, nearest neighbors, random forest, and more...



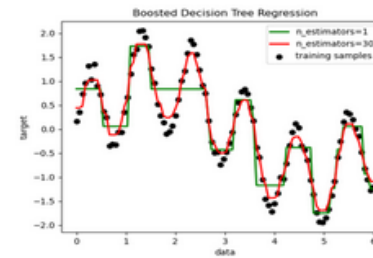
Examples

Regression

Predicting a continuous-valued attribute associated with an object.

Applications: Drug response, Stock prices.

Algorithms: SVR, nearest neighbors, random forest, and more...



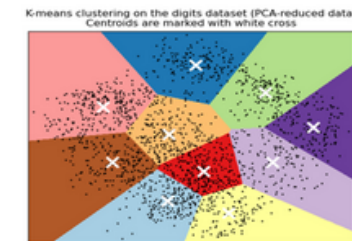
Examples

Clustering

Automatic grouping of similar objects into sets.

Applications: Customer segmentation, Grouping experiment outcomes

Algorithms: k-Means, spectral clustering, mean-shift, and more...



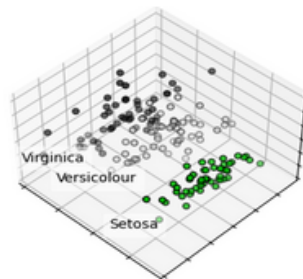
Examples

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...



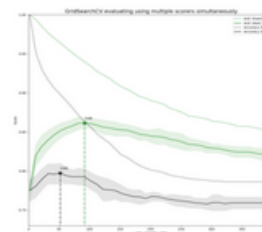
Examples

Model selection

Comparing, validating and choosing parameters and models.

Applications: Improved accuracy via parameter tuning

Algorithms: grid search, cross validation, metrics, and more...



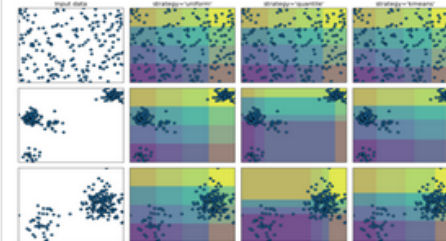
Examples

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)`

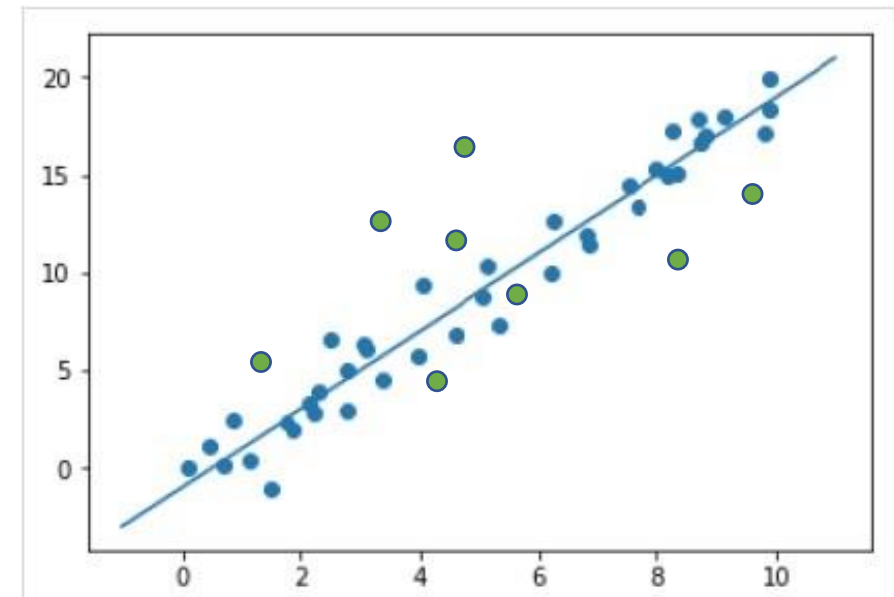
3. Arranging the data

4. Model fitting

- `>>> model.fit(X, y)`
- `>>> model.coef_`

5. Applying the model to new data

- `>>> model.predict(new_X)`



Integrated analytics lab

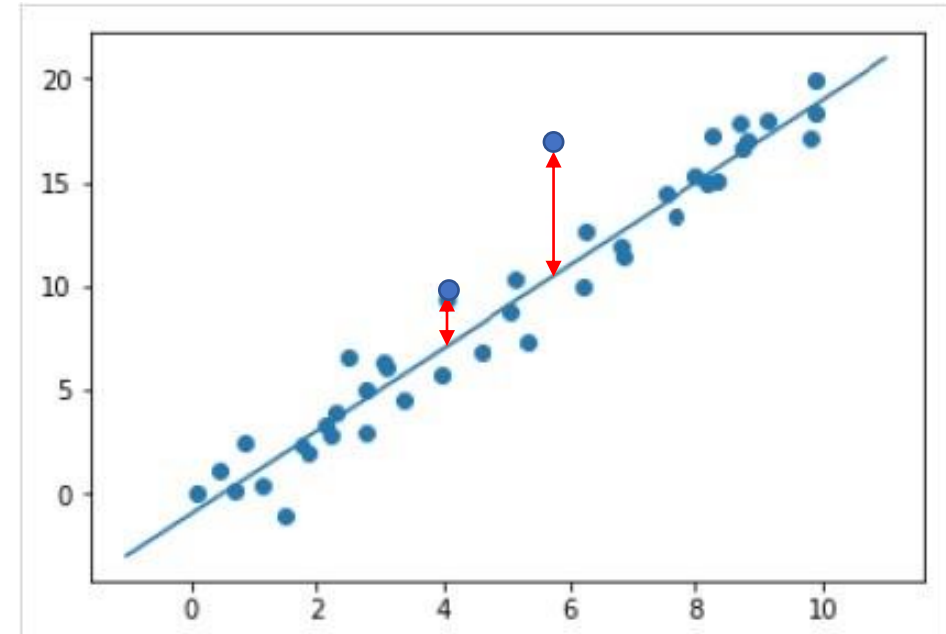
This checklist can help you while building your projects

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

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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

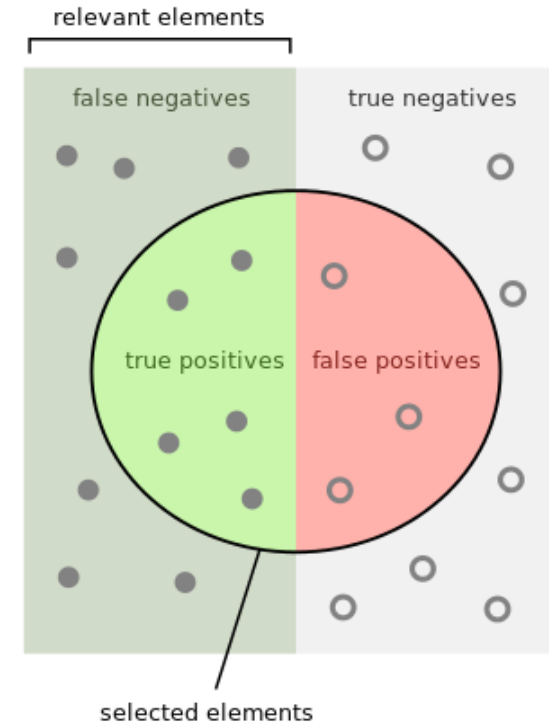


$$\text{RMSE}(\mathbf{X}, h) = \sqrt{\frac{1}{m} \sum_{i=1}^m \left(h(\mathbf{x}^{(i)}) - y^{(i)} \right)^2}$$

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(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) = $\frac{TP}{PP}$ precision = 1-FDR	False omission rate (FOR) = $\frac{FN}{PN}$ = 1-NPV
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) = $\frac{TPR+TNR}{2}$		F₁ score = $\frac{2 \cdot PPV \cdot TPR}{PPV + TPR} = \frac{2TP}{2TP + FP + FN}$	Fowlkes-Mallows index (FM) = $\sqrt{PPV \cdot TPR}$



How many selected items are relevant?

$$\text{Precision} = \frac{\text{true positives}}{\text{true positives} + \text{false positives}}$$

How many relevant items are selected?

$$\text{Recall} = \frac{\text{true positives}}{\text{true positives} + \text{false negatives}}$$

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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

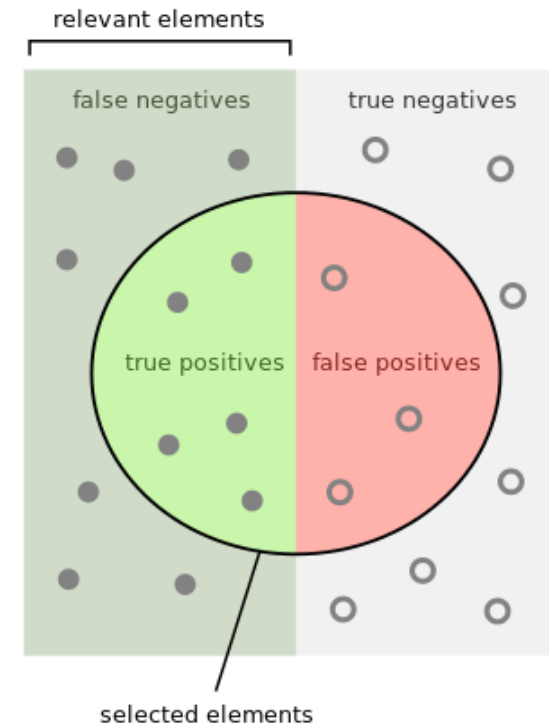
F1-score

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

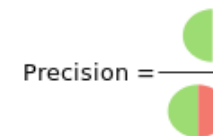
- Combines precision and recall

Summing up

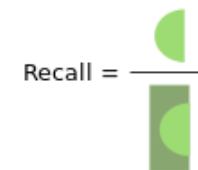
- Accuracy is used when TP and TN are more important while F1-score is used when FN and FP are
- Accuracy can be used when the class distribution is similar, while F1-score is a better when there are imbalanced classes



How many selected items are relevant?



How many relevant items are selected?



Hyper-parameter tuning

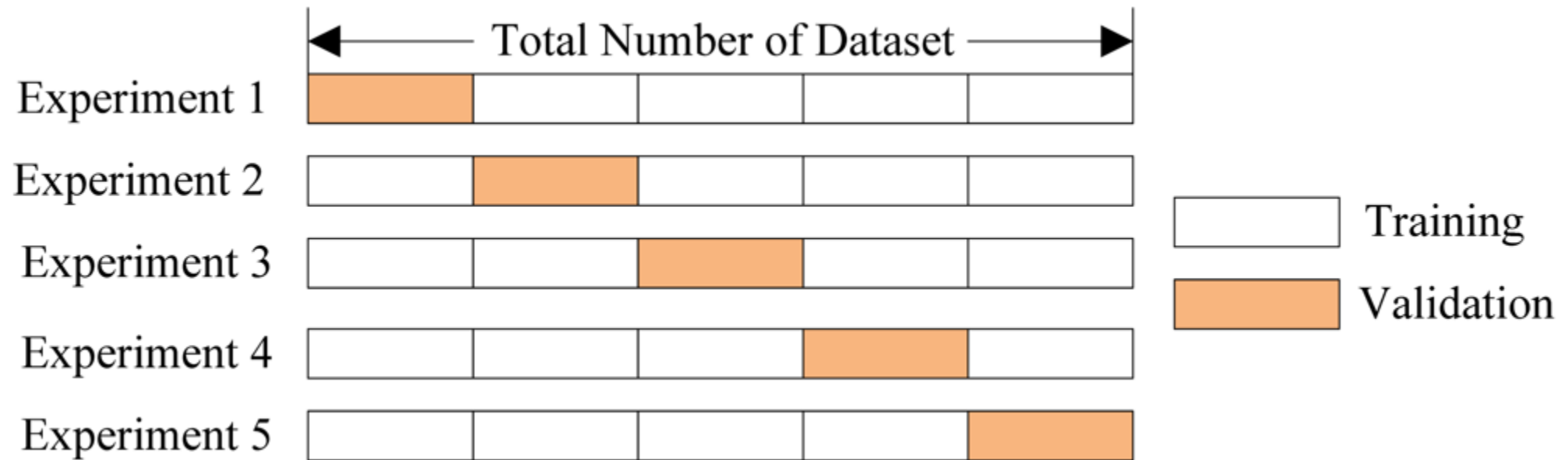
Hyper-parameters: parameters that are not directly learnt within estimators

- 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()`

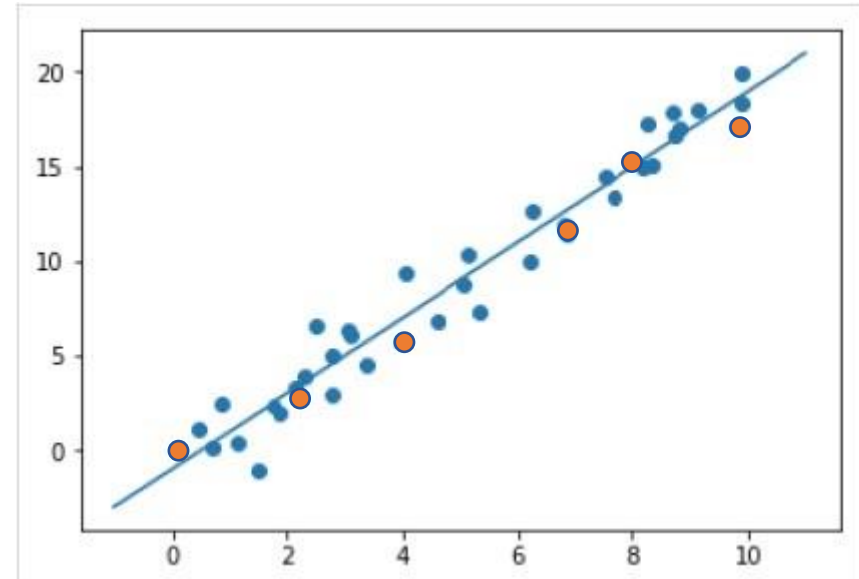
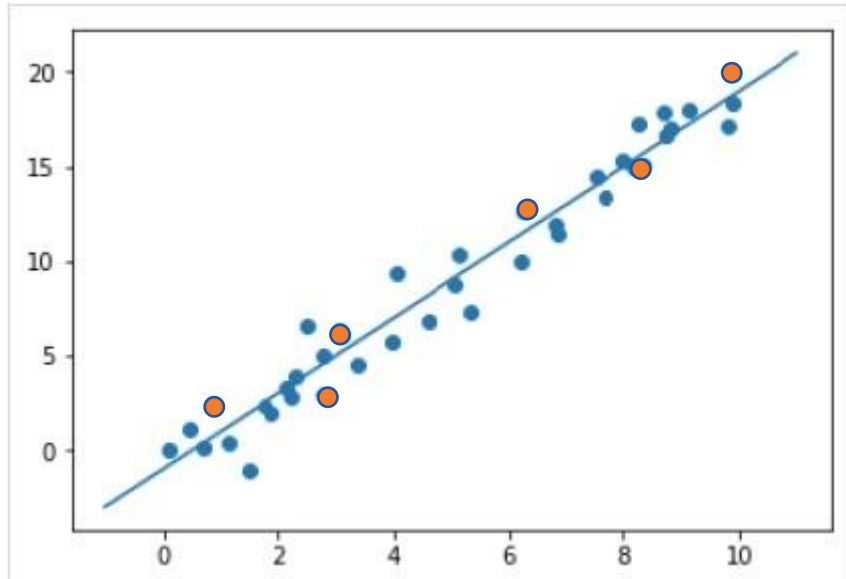
A search consists of:

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

Cross validation



Cross validation



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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



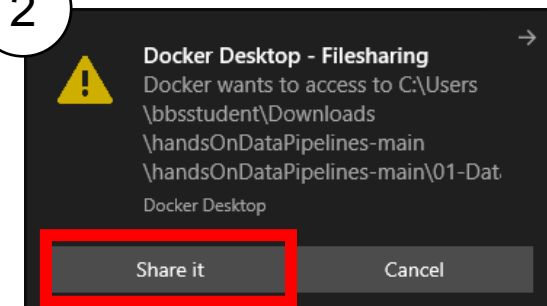
Copy and paste the link to the notebook



Enter the notebook `02-MachineLearning`



2



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