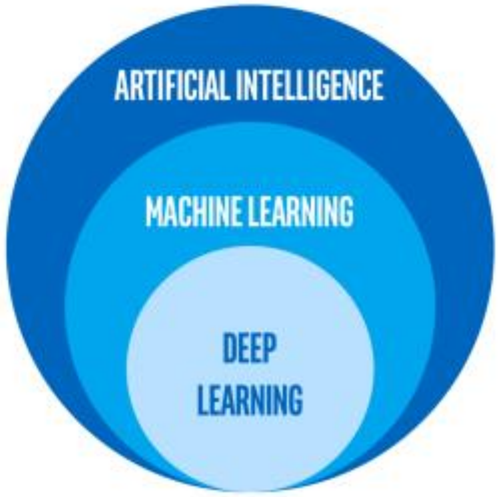
Machine learning

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

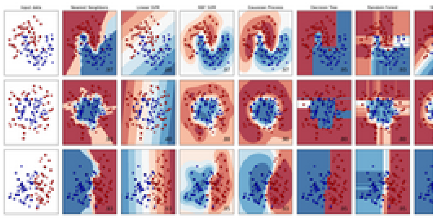
Getting Started | Release Highlights for 0.24 | GitHub

- 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...

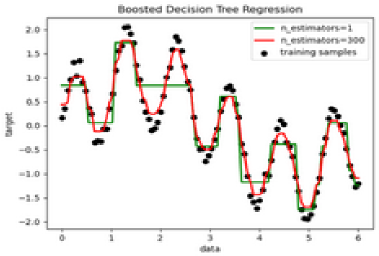


Examples

Regression

Predicting a continuous-valued attribute associated with an object.

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

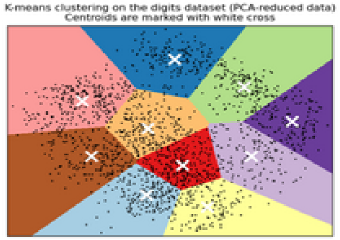


Examples

Clustering

Automatic grouping of similar objects into sets.

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

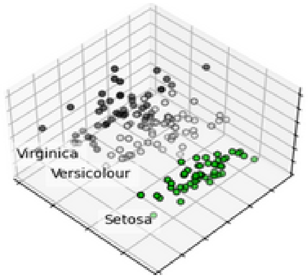


Examples

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...

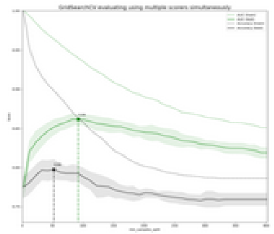


Examples

Model selection

Comparing, validating and choosing parameters and models.

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

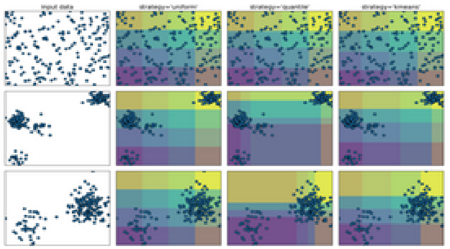


Examples

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

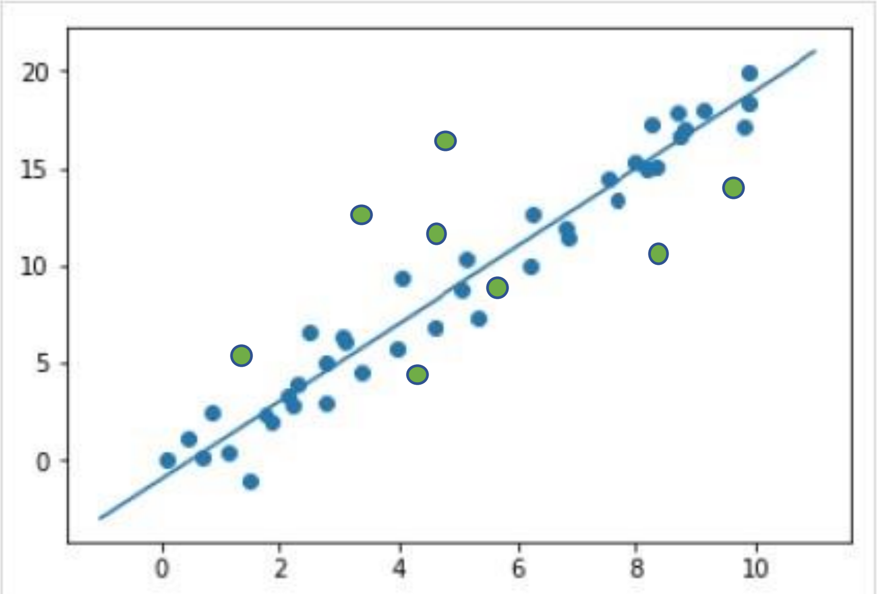
- >>> estimator.estimated_param_

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

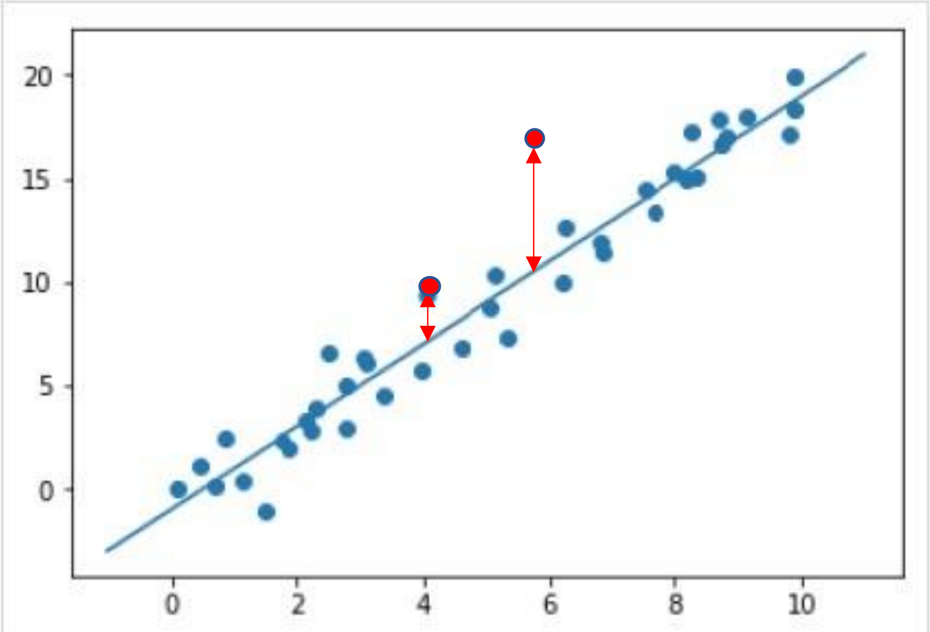
This checklist can help you while building your projects

- 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

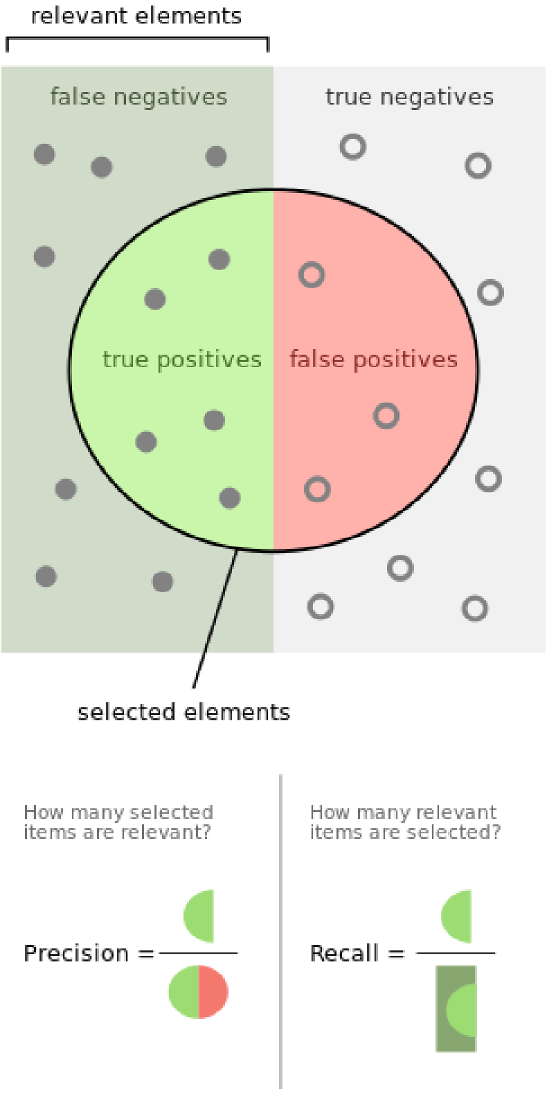


$$\mathrm{RMSE}(\mathbf{X}, h) = \sqrt{\frac{1}{m}\sum_{i=1}^{m}\left(h\left(\mathbf{x}^{(i)}\right) - y^{(i)}\right)^2}$$

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

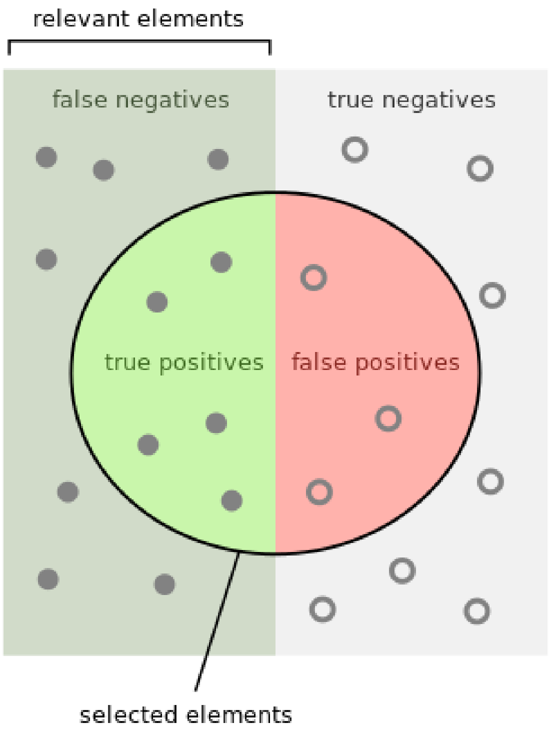
$$\text{Accuracy} = \frac{tp + tn}{tp + tn + fp + fn}$$

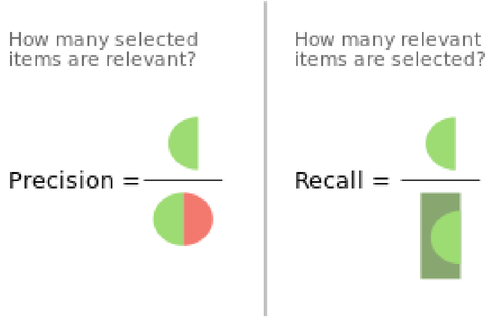
- Accuracy can be a misleading metric for imbalanced data sets

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

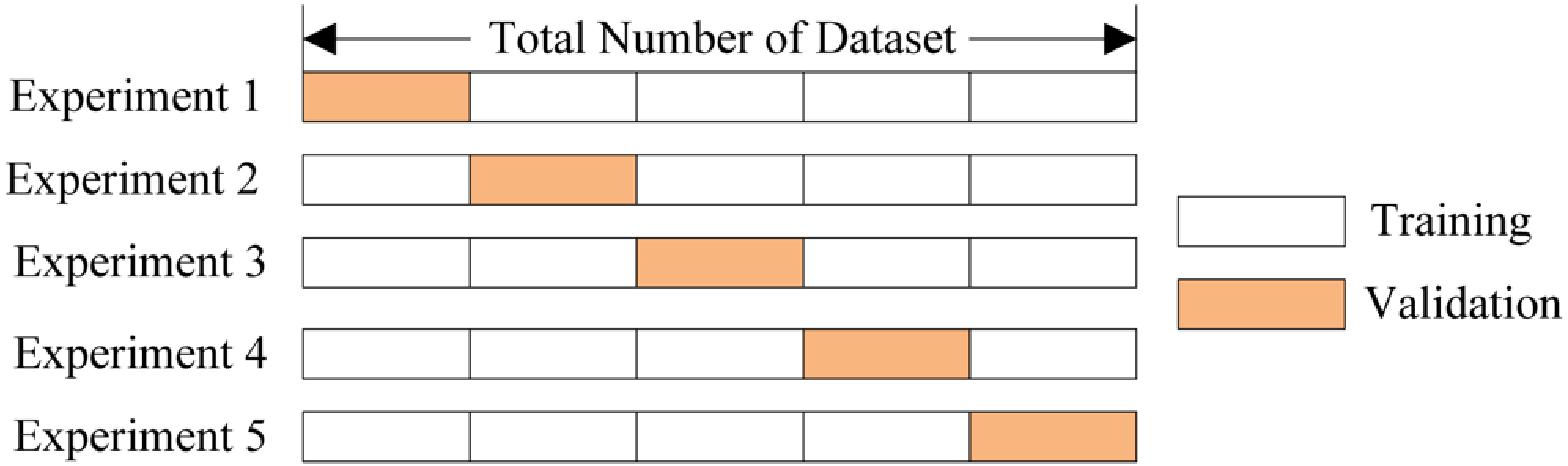
Hyper-parameters: parameters that are not directly learnt within estimators

- 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()

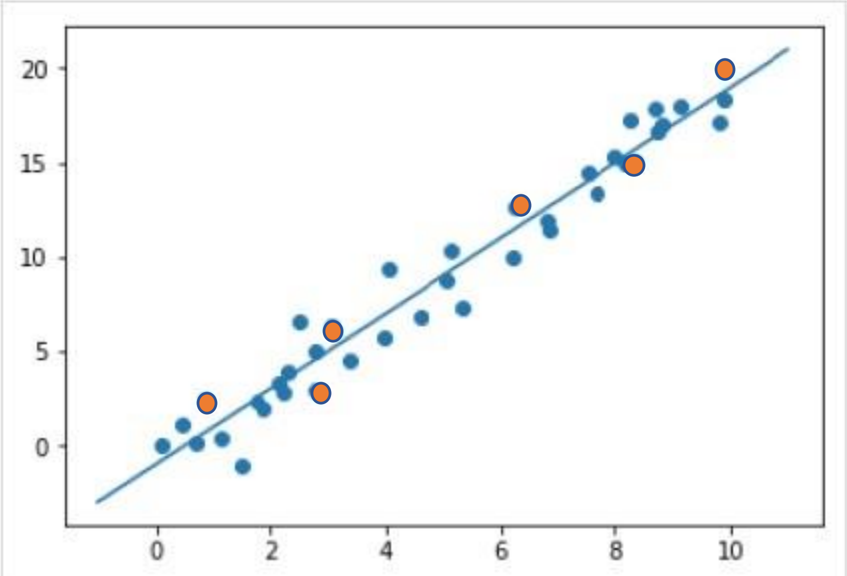
A search consists of:

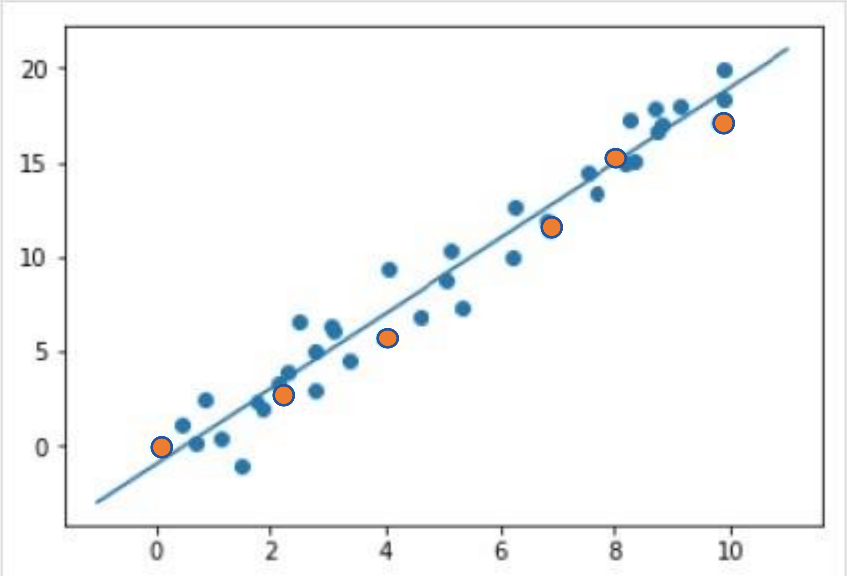
- an estimator
- a parameter space
- a method for searching or sampling candidates
- a cross-validation scheme
- a score function

Cross validation



Cross validation





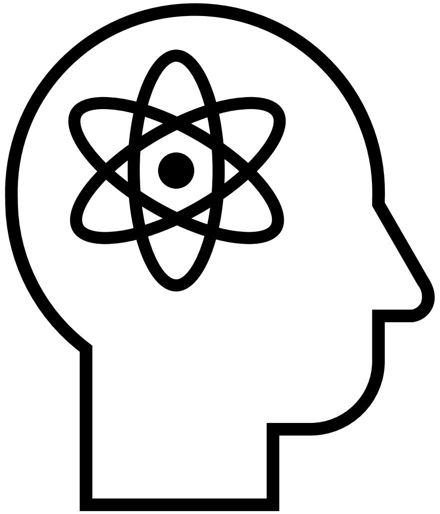
Integrated analytics lab

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 notebook `02-MachineLearning`



https://github.com/w4bo/2022-bbs-dsaa/blob/master/materials/02-MachineLearning.ipynb

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