IEMS 5780 / IERG 4080
Building and Deploying Scalable Machine Learning Services

Lecture 2 - Machine Learning

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Machine Learning

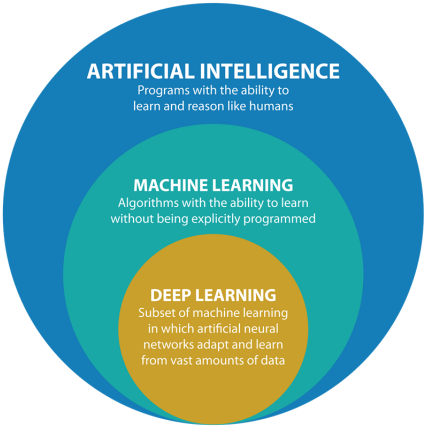
Agenda

- Introduction to Machine Learning
- Basic Concepts
- Common Algorithms
- Evaluation and Diagnosing
- Machine Learning in Python

Introduction to Machine Learning

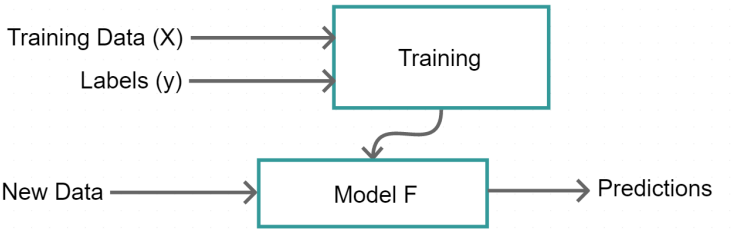
Machine Learning

- A computer program generates an input given and output, given some **pre-defined function(s)**
- ML aims at **learning** a function that maps the inputs to the outputs
- Instead of having a programmer writing down the **logic**, we let the computer **learn** from the data
- Given historical data, we train a **model** to generate predictions on **future or unseen** inputs



Machine Learning

- Given some input X and ouptut y, find a function $F(X)$ that maps X to y.
- Example: given (location, size) (X), predict the price of a house (y).
- Another example: give (previously watched movies) (X), predict the next movie(s) that will be watched (y).



Case Study: Spam Email Detection

- Let's consider the task of detecting **spam or junk emails**.
- Examples of spam emails:
  - scams
  - phishing
  - mass email marketing / advertisement
  - and many more
- How would you approach this problem?
- (It is a **classification** task: for each email, we want to label it as "spam" or "non-spam")

Case Study: Spam Email Detection

A non-ML approach

- To classify incoming emails, we need to find some **patterns** that are unique in each classes
- Example of useful patterns:
  - Name of the sender of the email
  - Key words/phrases in the subject (e.g. "You have won a lottery!")
  - A lot of words in capital letters in the content
  - ...
- You then write a program to look for these patterns in a email received
- **Done?**

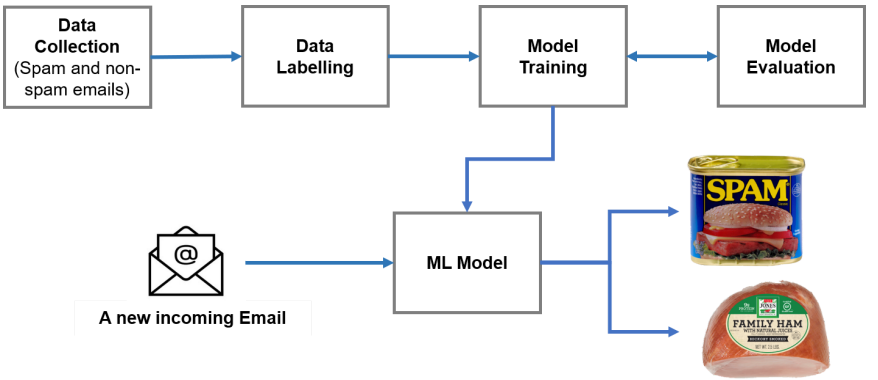
Case Study: Spam Email Detection

Limitation of a non-ML Approach

- You may need to have **a lot of** rules
- Rules too general may give you **false positives**
- Rules too specific will be useless if the spammers make slight changes
- How do you **weight** the importance of each rule?
- ...

Case Study: Spam Email Detection

A Machine Learning Approach



Case Study: Spam Email Detection

Advantages of using ML

- Learn the important patterns **automatically** from the training data
- An ML algorithm can go through **a large number of examples** to learn patterns
- Able to discover the **relative importance** of different patterns
- Model can be **re-trained** when the data has changed

- *Can you think of any weakness of ML?*

Basic Machine Learning Problems

- **Supervised Learning**

  You have **labelled data** for computer to learn from

  - Regression
  - Classification

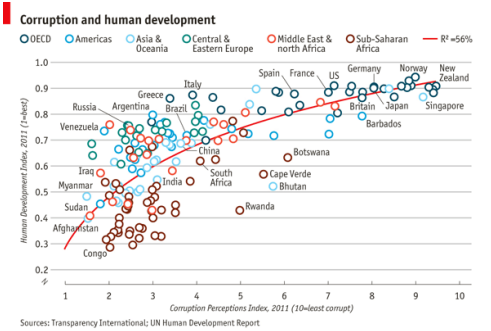
- **Unsupervised Learning**

  You don't have labelled data, but you want to find patterns in the data

  - Clustering / Dimensionality Reduction

Regression

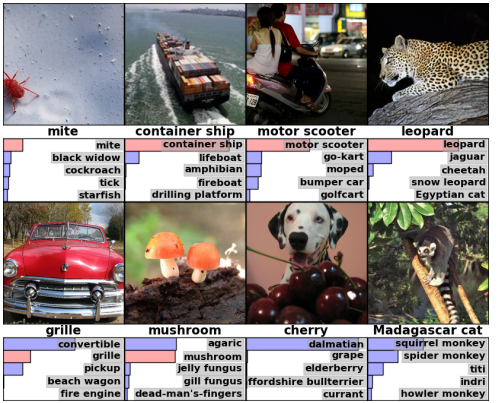
- In **regression**, we want to predict the value of a **continuous** variable based on some inputs
- **Examples**:
  - Predict the price of a house
  - Predict the number of products sold in a shop
  - Predict the number of users who will click an advertisement
  - Predict the price of a product given its descriptions



(From Economist: Corrosive corruption)

Classification

- Categorizing an input sample into one of the **pre-defined** classes
- **Examples**:
  - Predict whether a person will survive a shipwreck
  - Detect the sentiment of a movie review
  - Predict whether a driver will initiate an insurance claim
- In fact, a lot of problems can be defined as **classification problems**



ImageNet Classification with Deep Convolutional Neural Networks – Krizhevsky et al. 2012

Unsupervised Learning / Clustering

- To identify **hidden patterns** in a dataset without labels
- **Examples**:
  - Understand what products are usually bought together (Basket Analysis)
  - Understand major topics of news articles (e.g. News Clustering)
  - Identifying communities in social networks
- Clustering can be used to perform dimensionality reduction

Clusters of news articles about smog between May 2016 and May 2017 (Source)

Common ML Algorithms

In the following, we will introduce a few common ML algorithms:

- **Regression**
  - Linear regression
- **Classification**
  - Logistic regression
  - Decision trees

Regression: Linear Regression

- In regression, we want to predict the values of some targets given some **predictors** or **features**
- In the simplest case, we can assume that the relationship between the features and the target is **linear**:

$$y = a + bX$$

- In the equation above, y is the target, X is the feature, a is the intercept, and b is the weight of the feature
- **Learning** means estimating a suitable value for both a and b such that the resultant straight line best approximate the data we observed

Linear Regression

- Consider an example of predicting the **price of a house** given its **area**

- A few samples from a house price dataset

- Each row can be considered as a **training sample**

Linear Regression

- Using the ordinary least squares method, we can estimate the a and b in the equation
- The line with the estimated values of a and b is plotted on the right
- Note that **NOT** all points are lying on the line (Why?)
- How can we **predict** the price of other houses?
- How do we tell whether this is a **good** model?

Linear Regression

- In the above example, we have **one** feature, which is the area of the house
- Can you think of **other features** that are useful for predicting the price?
- If we have more features, the equation will become

$$y = b_0 + b_1 x_1 + b_2 x_2 + \ldots + b_n x_n$$

- This is still a **linear regression** model, sometimes called **multiple linear regression**
- b_0 is called the **bias term**, while b_1 to b_n are the weights of the features
- y is a **weighted linear combination** of the values of x_1 to x_n

Linear Regression

- If we consider $x_0 = 1$, then we can write the linear regression equation in terms of vectors
- Let $\boldsymbol{x}$ be the feature vector $(x_0, x_1, \ldots, x_n$ representing the input
- Let $\boldsymbol{b}$ as a vector of the weights $b_0, b_1, \ldots, b_n$

  (The b_i's are the parameters of this model, and in many cases are denoted by $\boldsymbol{\theta}$)

$$y = \theta^T x$$

- If we consider the **whole training dataset** with m samples, and each input has n features (and thus we will have $n + 1$ parameters):

Summary

What have we learnt?

- What is a **model**?
  - Your assumptions of how things work
  - A simplification of the world (or at least the problem you are trying to solve)
  - A model is usually characterized by some **parameters**
  - (Thus machine learning usually involves **parameter optimization**)
- The inputs are **represented** by **feature vectors**
  - **Representation** of input data is very important in ML
  - Very often we may even want to learn how to represent the raw data

Classification

- In classification, we are interested in putting each input sample into **two (or more) pre-defined classes**
- In other words, the target variable y is **discrete**
- Some **commong algorithms** for classification:
  - Logistic regression
  - Support vector machines
  - Decision Trees
  - K-nearest-neighbour (kNN)
- Some regression tasks can be **simplified** to classification tasks
  - E.g. predicting whether the price of a stock will go up, down or unchanged instead of predicting its absolute value

Classification

- For simplicity, we first consider the case in which we have **two classes** (binary classification)
- You can give the classes any names (e.g. cat vs. dog, rainy vs. sunny), but when doing the maths, we would simply label them as `0` and `1`
- Again, we consider that an input is represented as a **feature vector**
- Can we directly apply linear regression to a classification problem?

$$y = \theta^T x$$

Classification

- Consider an example of predicting whether a customer will **buy** a certain product given his/her demographic information
- We represent each person as a **feature vector**
- In our training data, we set $y = 1$ if the customer has bought the product, and $y = 0$ if the customer has not

Logistic Regression

- We can apply linear regression on this problem, but it is likely to perform badly
- For classification, we want to have a **decision rule**, linear regression's output lies on a straight line, and may not allow picking a threshold easily
- We don't really want the model to output some values too different from `0` or `1`
- However, we can apply a **transformation** to the output of linear regression:

- $g(z)$ is called the **logistic function** or **sigmoid function

Logistic Regression

- The logistic function has certain characteristics
  - Its value is always bounded by 0 and 1
  - Its value tends to 1 if z tends to $+\infty$, and tends to 0 if z tends to $-\infty$
  - It is more likely to output values close to 0 or 1

Decision Trees

- Another commonly used algorithm for classification: **decision trees**
- Consider the example on the right again
- Can we generate some **rules** from the data that can allow us to predict the outcome accurately?
- For example:

```
(gender = M) AND (age < 40) --> buy = 1
```

- **Decision trees** are constructed by finding these conditions to **split** the dataset into smaller subsets

Decision Trees

- A few algorithms have been proposed for **decision trees learning**, such as ID3 and C4.5
- The general idea is similar:
  - Identify a feature which is **best** for spliting a given subset of the data
  - What is best is determined by some metrics, such as the Gini coefficient or information gain
  - Create a **new node** using that feature
  - Continue the process on the subsets created by the split

An example decision tree learned from the Titanic survival dataset.

Decision Trees

- Decision trees can also be used to perform regression (thus the term **CART: Classification And Regression Trees**)
- Decision trees are usually vulnerable to **overfitting** (more on this later), thus we usually have to control the **depth** of a tree
- It is commonly used with **ensemble methods** to generate more accurate predictions, resulting in algorithms such as random forests or gradient boosted trees
- References:
  - Decision Trees and Ensemble Models
  - Decision Trees - scikit-learn

Choosing ML Algorithms

http://scikit-learn.org/stable/_static/ml_map.png

Basic Concepts in Machine Learning

Working on Machine Learning Projects

- Nowadays, it is easy to apply machine learning to a problem and obtain some results

```
from sklearn.datasets import load_iris
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import accuracy_score

iris = load_iris()
X = iris.data      # Training data inputs
y = iris.target    # Training data labels

model = LogisticRegression()   # Model initialization
model.fit(X, y)                # Training (fitting)

y_pred = model.predict(X)  # Generating predictions
accuracy_score(y, y_pred)  # Computing a metric (accuracy in this case)
```

- However, what would you do after this? Is it done *right*? Is it *good* enough? How to *improve* it?

Generalization

- (**Generalization theory** is a huge topic in statistical machine learning, let's discuss it conceptually here)
- When training a model, our hope is that what is learnt from **the past (training data)** can be applied to **predict the future (test data / unseen data)**
- In general, we are making some assumptions:
  - the past and the future are **similar**
  - **patterns** observed in the past will appear in the future
- Since our aim is to perform well in predicting the future:
  - Our model should **not only** achieve high accuracy on the training data
  - Our model needs to find out patterns that are likely to appear in **both the past and the future**, and ignore other **noise**

Model Complexity

- A **model** can be considered as a simplified view of a problem
  - Some features that are important and are related to the target
  - The relationship between the features and the target (e.g. linear vs. non-linear)
  - Random noise
- A **complex** model captures complex relationship between X and y, but it is also more likely to pick up noise --> **overfitting**
- A **simple** model is easy to interpret, but may not be able to capture the true relationship between X and y --> **underfitting**

Evaluation

Evaluation

- **Evaluation** is an important step in any machine learning project
- Purposes:
  - Understand the **quality of predictions** of a trained model
  - Understand when does a model perform well or badly
  - Understand the **limitation** of the model
- How:
  - Decide on a suitable **metric(s)** for your problem
  - Pick an algorithm and train a model
  - Compute the metric on the predictions on a test dataset

Evaluation

Splitting Your Dataset

- Let's assume that we have a dataset of 10,000 data points
- You should not **train** your model and **evaluate** your model on the same dataset
- **Why?**
  - We need to know whether the model can be generalized to **unseen** data (The model may only be **memorizing** the training data)
  - We need some test dataset to help us **fine tune** our model(s)
- **How?**
  - **Split** your dataset for different purposes

Splitting Your Dataset

- It is usually advised that we have **three splits** of the dataset:
  1. **training set**: for training your model(s)
  2. **validation/development set**: for tuning your model's **hyperparameters**
  3. **test/holdout set**: for testing the performance of your model
- For example:

Splitting Your Dataset

- There is no standard of the ratio of train/val/test data samples
- Generally:
  - You want to use **as much data as possible** to train your model
  - You want to have a **reasonable size** of validation and test data (so that your evaluation is meaningful)
- When you really don't have enough data
  - It is also acceptable to split only into two sets: **train** and **test**
    e.g. 70% for training and 30% for testing

Splitting Your Dataset

- Splitting your data is NOT a trivial task
- Normally, you **shuffle** your data and **randomly** splitting the data into different sets
- Consider an **imbalanced dataset** for classification: 90% `0`s and 10% `1`s
  - If you split randomly, there are chances that you don't have any `1`s in your training dataset!
  - In this case, you may want to use stratified sampling, to make sure that the ratio of `0`s and `1`s in all subsets are 9:1.

Splitting Your Dataset

- Consider another task of predicting **time-series** data (forecasting)
  - Should you split your data **randomly**?
- Your task is to train a model on **past** data to predict **future** targets
- You should respect the **chronological order** of the data

Cross Validation

- The train/test procedure can actually be repeated on **different splits**
- This usually reduces the **variance** of the estimated performance of a model
- A commonly used cross validation approach is **K-fold cross validation**
  - For example, when **k=4**, data is split into **4** subsets:
  - Each time, **3** subsets are used for training, the remaining **1** is for testing

Metrics

- When evaluating the performance of a model, we need to have:
  - **ground truths**: the correct answer / the true labels of the inputs
  - **metric**: a measure of how good the predictions are compared to the ground truths
- In the following, we focus on:
  - Metrics for **regression** tasks: usually a function that reflects how the **difference** between the predicted values and the true values
  - Metrics for **classification** tasks: usually a function that reflects how often the predicted values are the same as the true values
- Ref: Model evaluation: quantifying the quality of predictions

Metrics for Regression

- In regression tasks, for each test data point, we have a ground truth value y and a predicted value $\hat{y}$
- Intuitively, a model is good if all $\hat{y}$'s are close to their respective y's
- Hence, a straight forward metric would be the **Mean Absolute Error (MAE)**:
  - The mean of the absolute differences for all samples

$$MSE(\boldsymbol{y}, \hat{\boldsymbol{y}}) = \frac{1}{n} \sum_{i=0}^{n-1} |y_i - \hat{y}_i|$$

Metrics for Regression

- Another commonly used metric for regression is the **Root Mean Squared Error (RMSE)**
  - The square root of the mean of squared differences for all samples
  - Let $\boldsymbol{y}$ be the vector of ground truth, and $\hat{\boldsymbol{y}}$ be the vector of predicted values, root mean squared error is defined by:

$$RMSE(\boldsymbol{y}, \hat{\boldsymbol{y}}) = \sqrt{\frac{1}{n}\sum_{i=0}^{n-1}(y_i - \hat{y}_i)^2}$$

Metrics for Regression

- MSE will be **larger** if the model makes predictions that are **far** from the truth values (due to the square)

https://stats.stackexchange.com/questions/147001/is-minimizing-squared-error-equivalent-to-minimizing-absolute-error-why-squared

Metrics for Classification

- In classification, things are different:
  - The labels or classes do NOT lie on a continuous spectrum
  - Things are discrete: predictions are either **correct** or **incorrect**
  - We CANNOT measure **distance** between two labels
- In the following, we will discuss some important metrics for classification:
  - Accuracy
  - True/False positives/negatives
  - Precision and Recall
  - Area Under the ROC Curve

Accuracy

- A straight-forward metric for classification is **accruacy**
- Defined by **number of correct predictions / total number of predictions**
- For example:

$$y = (1, 0, 0, 0, 1, 1, 1, 0, 0)$$
$$\hat{y} = (1, 1, 1, 0, 0, 1, 1, 0, 0)$$

- Then, accuracy is **6/9 = 66.7%**
- This can also be applied to multi-class classification
- What is the limitation of the **accuracy score**?

True/False Positives/Negatives

- To have a better understanding of how well a model performs in predicting different classes
- Consider a binary classification task, where we have classes **0** (negative) and **1** (positive)
- We consider four different types of predictions:
  - **True Positives (TP)**: model predicted 1 correctly
  - **True Negatives (TN)**: model predicted 0 correctly
  - **False Positives (FP)**: it is 0, but model predicted 1
  - **False Negatives (FN)**: it is 1, but model predicted 0
- By using the number of these four types of predictions, we can come up with some useful metrics

The Confusion Matrix

		True condition				
	Total population	Condition positive	Condition negative	Prevalence = $\frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	Accuracy (ACC) = $\frac{\Sigma \text{ True positive} + \Sigma \text{ True negative}}{\Sigma \text{ Total population}}$	
Predicted condition	Predicted condition positive	**True positive**, Power	**False positive**, Type I error	Positive predictive value (PPV), Precision = $\frac{\Sigma \text{ True positive}}{\Sigma \text{ Predicted condition positive}}$	False discovery rate (FDR) = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Predicted condition positive}}$	
	Predicted condition negative	**False negative**, Type II error	**True negative**	False omission rate (FOR) = $\frac{\Sigma \text{ False negative}}{\Sigma \text{ Predicted condition negative}}$	Negative predictive value (NPV) = $\frac{\Sigma \text{ True negative}}{\Sigma \text{ Predicted condition negative}}$	
		True positive rate (TPR), Recall, Sensitivity, probability of detection = $\frac{\Sigma \text{ True positive}}{\Sigma \text{ Condition positive}}$	False positive rate (FPR), Fall-out, probability of false alarm = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Condition negative}}$	Positive likelihood ratio (LR+) = $\frac{\text{TPR}}{\text{FPR}}$	Diagnostic odds ratio (DOR) = $\frac{\text{LR+}}{\text{LR−}}$	F_1 score = $\frac{2}{\frac{1}{\text{Recall}} + \frac{1}{\text{Precision}}}$
		False negative rate (FNR), Miss rate = $\frac{\Sigma \text{ False negative}}{\Sigma \text{ Condition positive}}$	True negative rate (TNR), Specificity (SPC) = $\frac{\Sigma \text{ True negative}}{\Sigma \text{ Condition negative}}$	Negative likelihood ratio (LR−) = $\frac{\text{FNR}}{\text{TNR}}$		

- Reference: https://en.wikipedia.org/wiki/Confusion_matrix

Precision

- **Precision** aims at answering the following question:
  - **How often the model is correct when it predicts the target should be a certain class?**
- Precision is defined by:

$$Precision = \frac{TP}{TP + FP}$$

- For example:

$$y = (1, 0, 0, 0, 1, 1, 1, 0, 0)$$
$$\hat{y} = (1, 1, 1, 0, 0, 1, 1, 0, 0)$$

- We have **TP = 3**, **FP = 2**, so **precision = 3/5 = 60%**

Recall

- **Recall** aims at answering the following question:
  - **How many data of a certain class can the model correctly identifies?**
- Recall is defined by:

$$Recall = \frac{TP}{TP + FN}$$

- For example:

$$y = (1, 0, 0, 0, 1, 1, 1, 0, 0)$$
$$\hat{y} = (1, 1, 1, 0, 0, 1, 1, 0, 0)$$

- We have **TP = 3**, **FN = 1**, so **precision = 3/4 = 75%**

Task: Aeroplane Classifier

- If a model outputs **0** (not-an-aeroplane)

  for all images:

  - accuracy = 7/9 = 77.7%
  - precision = (undefined)
  - recall = 0%
- If a model outputs **1** (is-an-aeroplane)

  for all images:

  - accuracy = 2/9 = 22.2%
  - precision = 2/9 = 22.2%
  - recall = 2/2 = 100%

Trade-off Between Precision and Recall

- There is usually a **trade-off** between precision and recall
- For a classifier that outputs a score between 0 and 1, setting the **threshold** has a significant impact on precision and recall
- With a **high** threshold (e.g. 0.8)
  - Most predictions will be considered as **negatives**
  - Precision will tend to be **higher** (model is more **conservative**)
  - Recall will tend to be **lower** (likely to miss some positives)
- With a **lower** threshold (e.g. 0.3)
  - Most predictions will be considered as **positives**
  - Precision will tend to be **lower** (more false positives)
  - Recall will tend to be **higher** (more positives identified)

F1 Score

- **F1 Score** (or **F-Measure**) is a measure that takes both precision and recall into account
- In many cases, we would like to have a **balance** between precision and recall
- F1 Score allows us to choose a model that is reasonable good in terms of both precision and recall
- F1 is the **harmonic average** of precision and recall:

$$F_1 = \frac{2}{\frac{1}{Recall} + \frac{1}{Precision}}$$

Ranking Positives and Negatives

- In some tasks, we are interested in **accuracy**, ideally we want **every** prediction to be correct
- However, in some other tasks, it is sufficient that we can identify **one (or a few) positive cases** from a batch of inputs (Examples?)
- Or, in some cases, we are more concerned about the **ranking** of the inputs (Examples?)
- Ideally we want the positives to be always scored **higher** than the negatives

Area Under the ROC Curve

- **AUC** allows us to estimate the ability of a model to rank positives higher than negatives
- The **ROC Curve** (Receiver Operating Characteristic Curve) is plot by varying the **decision threshold** to obtain different **true positive rates (TPR)** and **false positive rages (FPR)**:

$$TPR = Recall = \frac{TP}{TP + FN}$$

$$FPR = \frac{FP}{FP + TN}$$

Area Under the ROC Curve

- Get a set of (FPR, TPR) points by varying the decision threshold
- Plotting the points will usually result in a graph that looks like the one on the right
- The larger the **area under the curve**, the better is your model (*Why?*)

Machine Learning in Python

Machine Learning in Python

- Many programming languages can be used to do machine learning, but mostly are done in **Python**
- Python has recently found to be the most popular programming language
- A lot of machine learning algorithms and tools are available in Python

  (Ref: Top 20 Python Libraries for Data Science)
- The Jupyter notebook has enabled interactive computing and fast prototyping with Python
  - Try it on Google's Colaboratory (You can even use GPU for free there!)

Machine Learning Libraries

Some commonly used libraries/packages in Python for machine learning

- **Numpy**, **Scipy** (numerical and scientific computation)
- **Pandas** (data preprocessing and analysis)
- **Scikit-learn** (machine learning)
- **Gensim**, **NLTK** (natural language processing)
- **Tensorflow**, **Keras**, **PyTorch** (deep learning)

Numpy and Scipy

- These are packages for doing numerical and scientific computation
- Numpy provides fast manipulation of **vectors** and **matrices**
- Scipy provides various functions for **scientific computation**

```
import numpy as np
a = np.random.rand(10)  # a vector of length 10 randomly initialized
b = np.random.rand(10)  # another vector
c = a.dot(b)            # compute dot product of two vectors
```

Scikit-learn

- A widely used open source machine learning library implementing a log of commonly used machine learning algorithms
- Most algorithms are well documented: (e.g. http://scikit-learn.org/stable/modules/tree.html)
- It has a common API for most machine learning algorithms

```
from sklearn.linear_model import LinearRegression

model = LinearRegression()    # Create an instance of a model
model.fit(X_train, y_train)   # Fit a model (i.e. training)

model.predict(X_new)          # Apply model on new data points
```

Scikit-learn

Check the examples:

- Linear regression:
  http://scikit-learn.org/stable/auto_examples/linear_model/plot_ols.html
- Logistic regression:
  http://scikit-learn.org/stable/auto_examples/linear_model/plot_iris_logistic.html
- Decision trees:
  http://scikit-learn.org/stable/modules/tree.html

Assignment 0

Assignment 0

- The first assignment: **Basic Python programming**
- Due date: **23:59, 21st September, 2018 (Friday)**
- A notebook template can be found at
  https://drive.google.com/open?id=1Fnp6R1YplvwhIfo1YgyMX2_5Zp9l8fav
- You should finish all problems in a **Jupyter notebook**
- Follow the instruction to submit a `.ipynb` file to Blackboard
- If you have any questions, ask on Slack

End of Lecture 2