Machine Learning in Python

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What is machine learning?

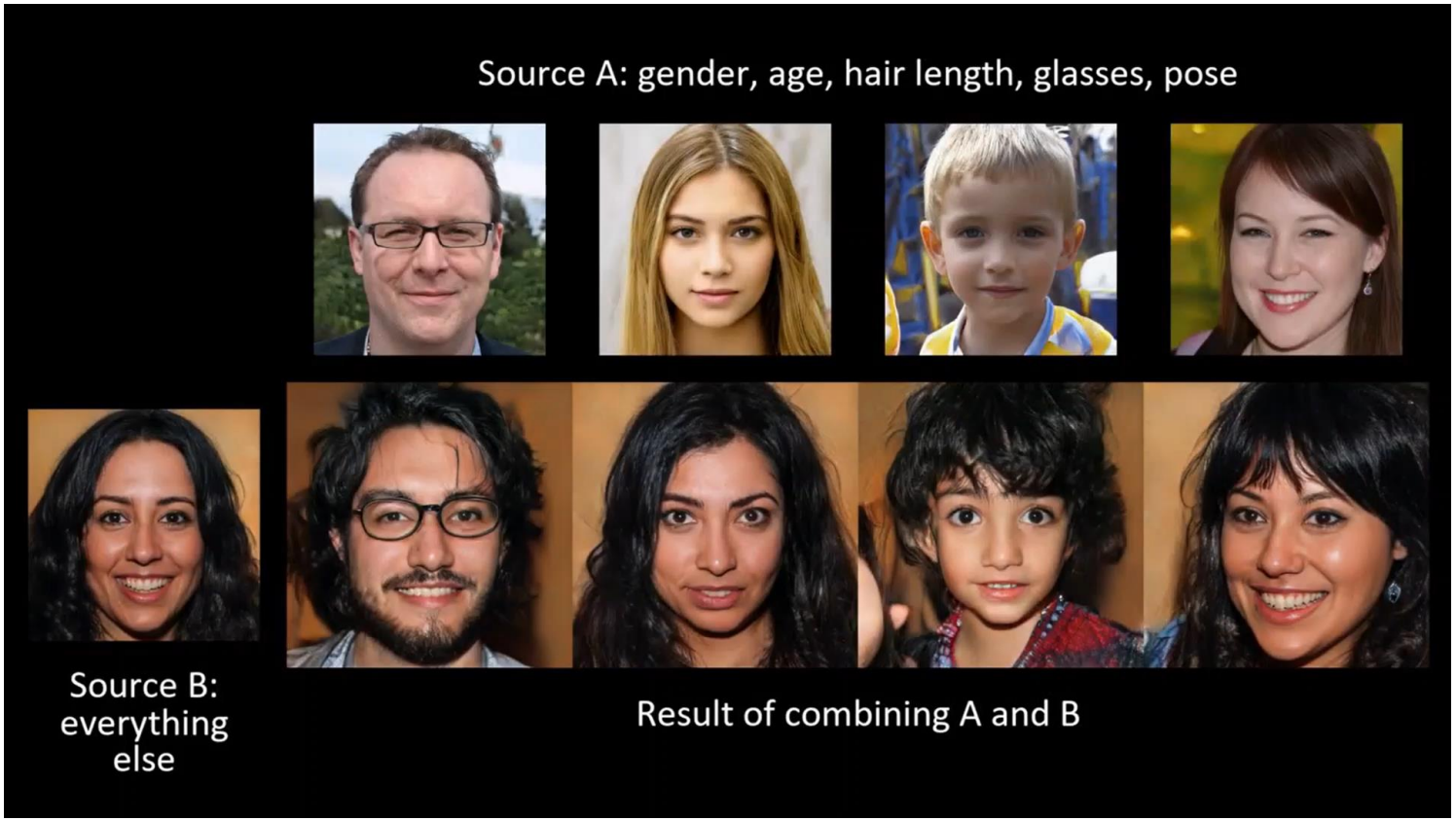
"Machine learning (ML) is the scientific study of algorithms and statistical models that computer systems use to effectively perform a specific task without using explicit instructions, relying on patterns and inference instead”

- https://en.wikipedia.org/wiki/Machine_learning

What is machine learning?

How it's branded

What is machine learning?



What you can do

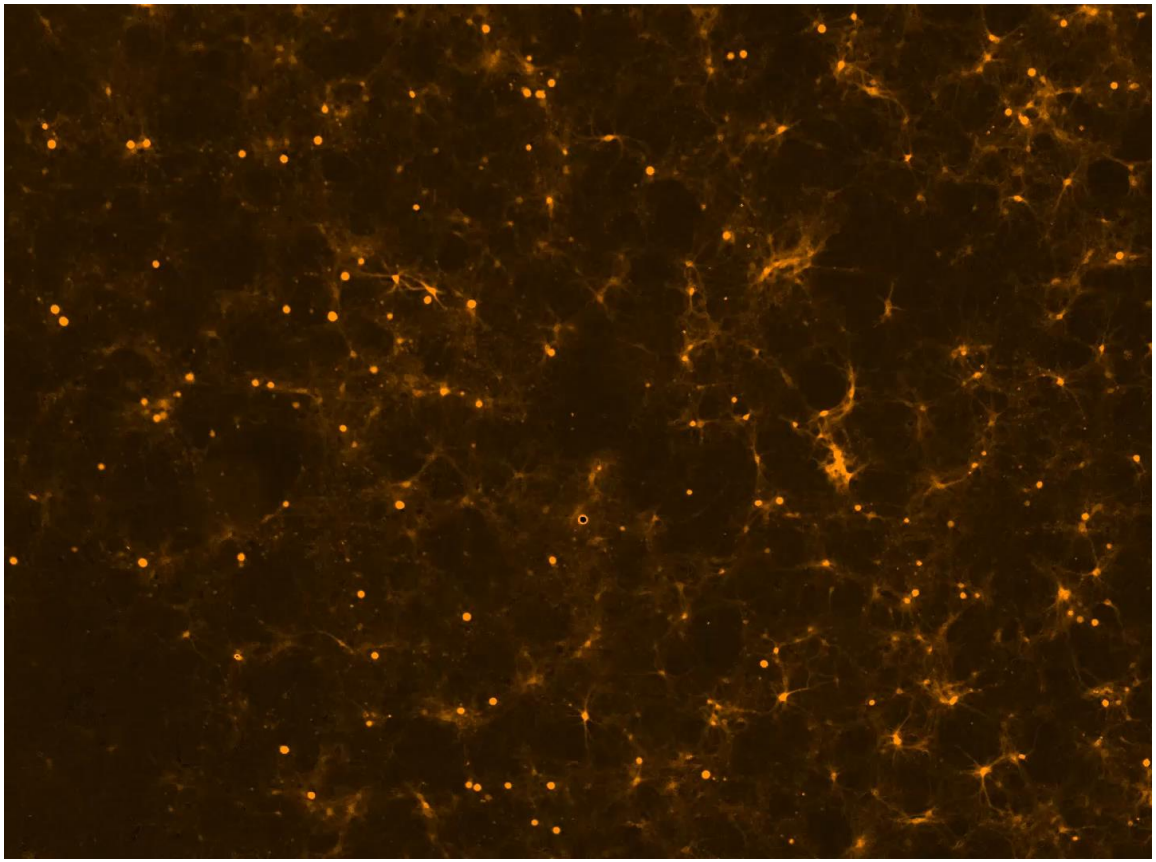
Karras, Tero, Samuli Laine, and Timo Aila. "A Style-Based Generator Architecture for Generative Adversarial Networks." *arXiv preprint arXiv:1812.04948* (2018).

What is machine learning?

What you can do

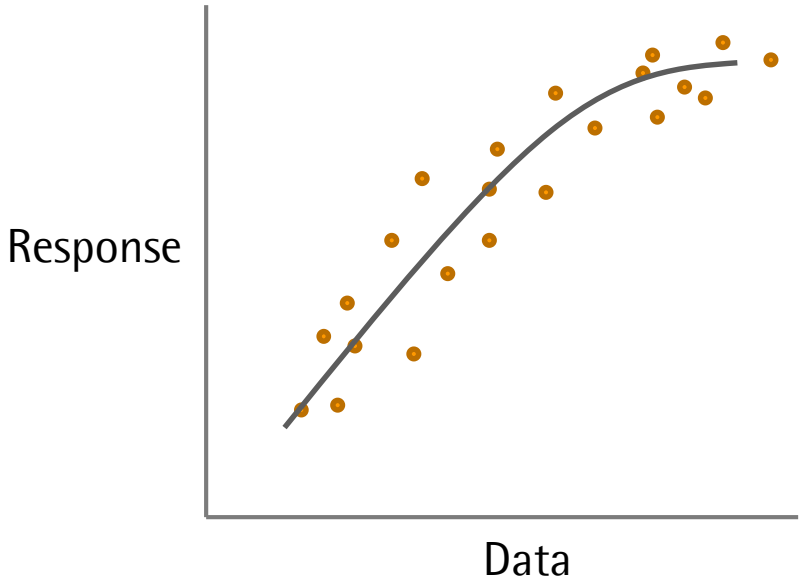
Peng, X. B., Kanazawa, A., Malik, J., Abbeel, P., & Levine, S. (2018, December). SFV: reinforcement learning of physical skills from videos. In *SIGGRAPH Asia 2018 Technical Papers* (p. 178). ACM.

What is machine learning?



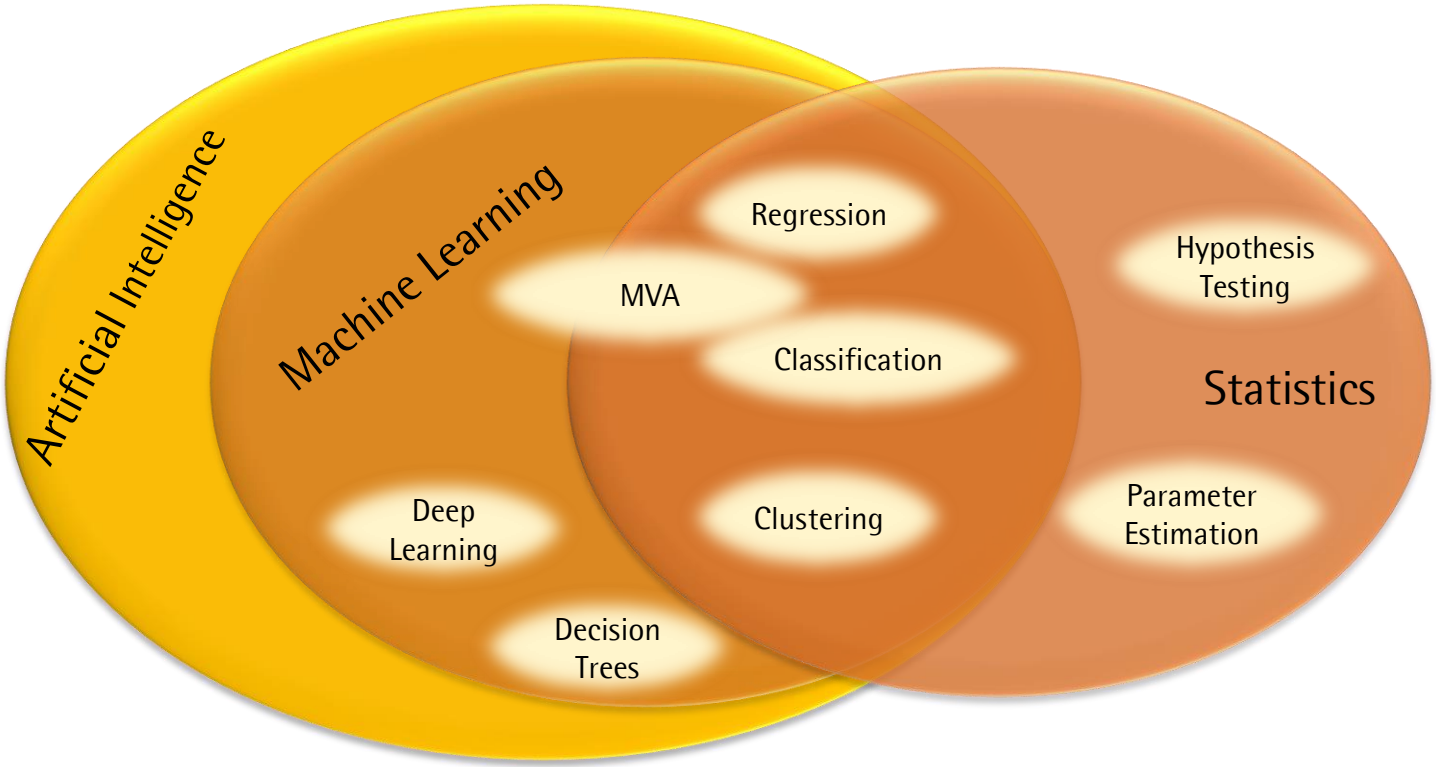
What you can do

What is machine learning?

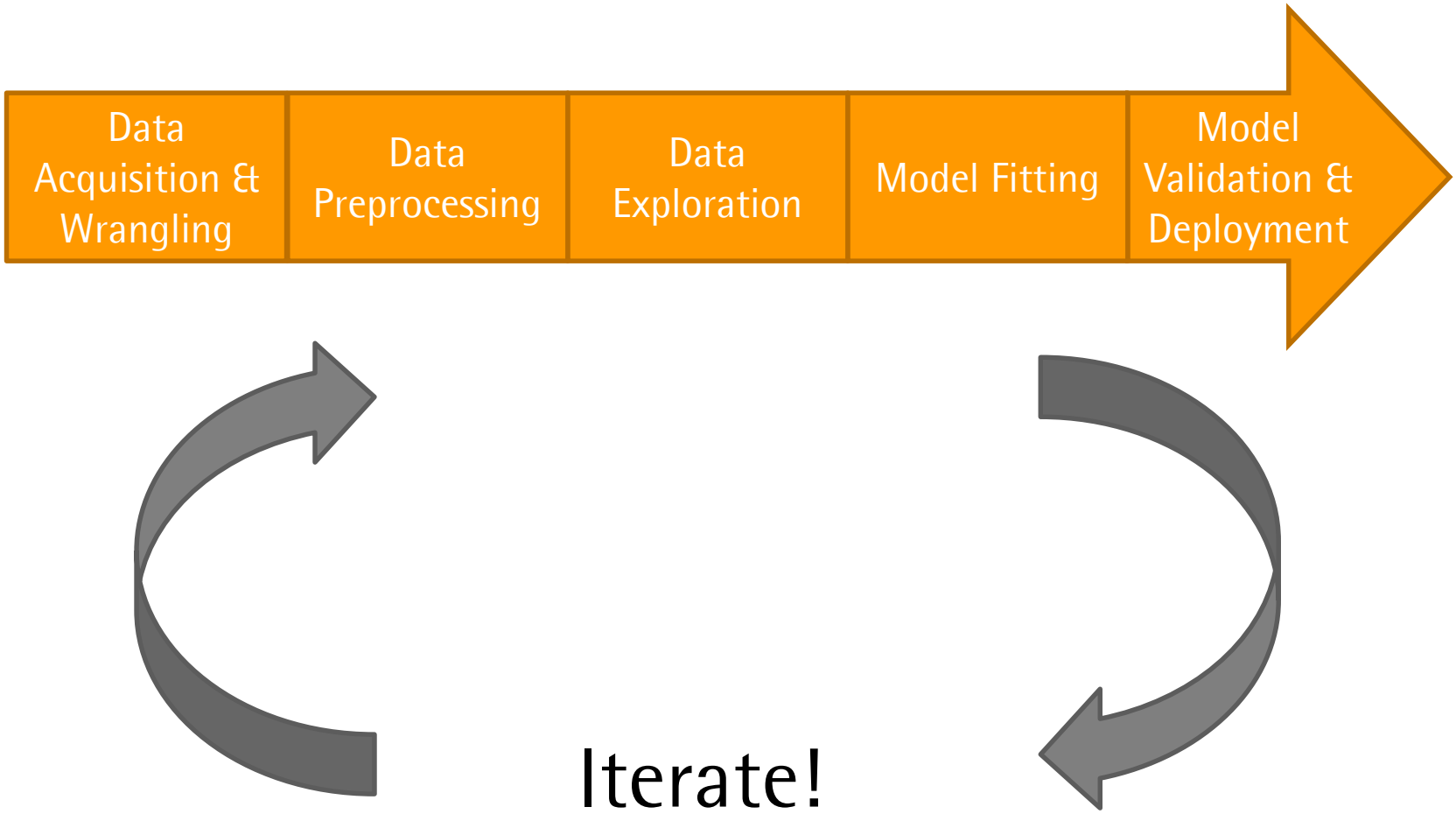


What you typically do

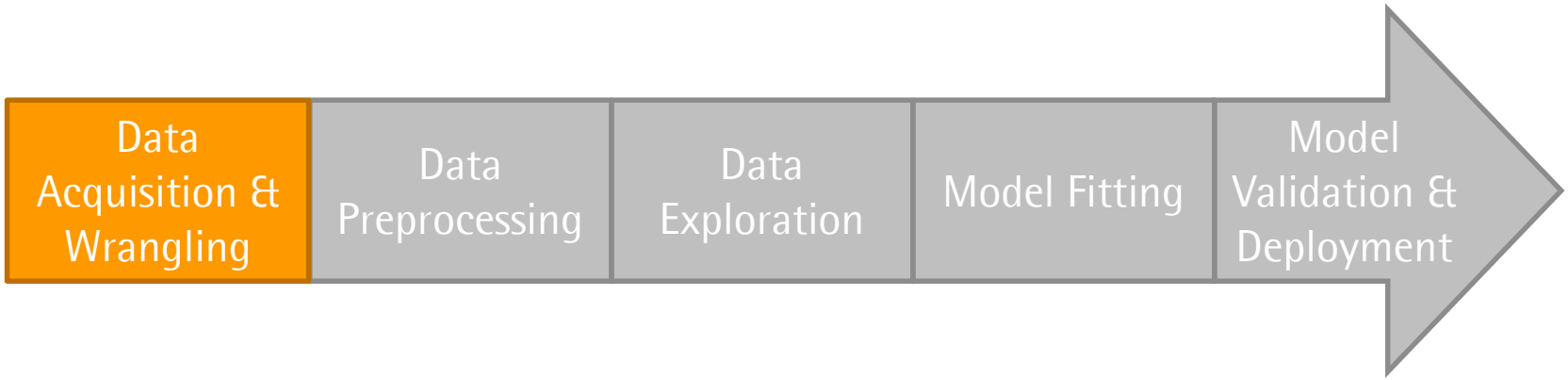
What is machine learning?



Machine Learning Process

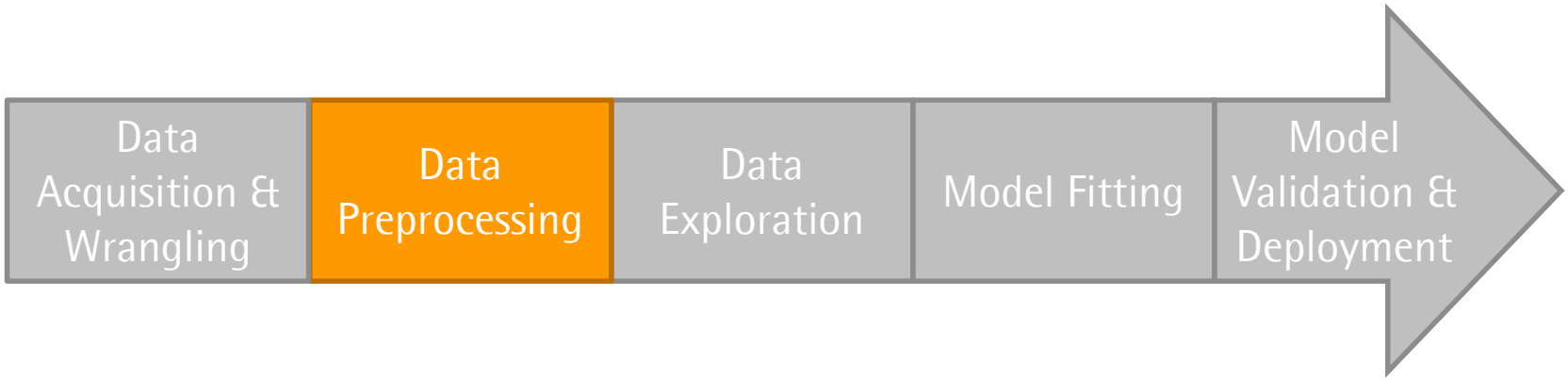


Machine Learning Process



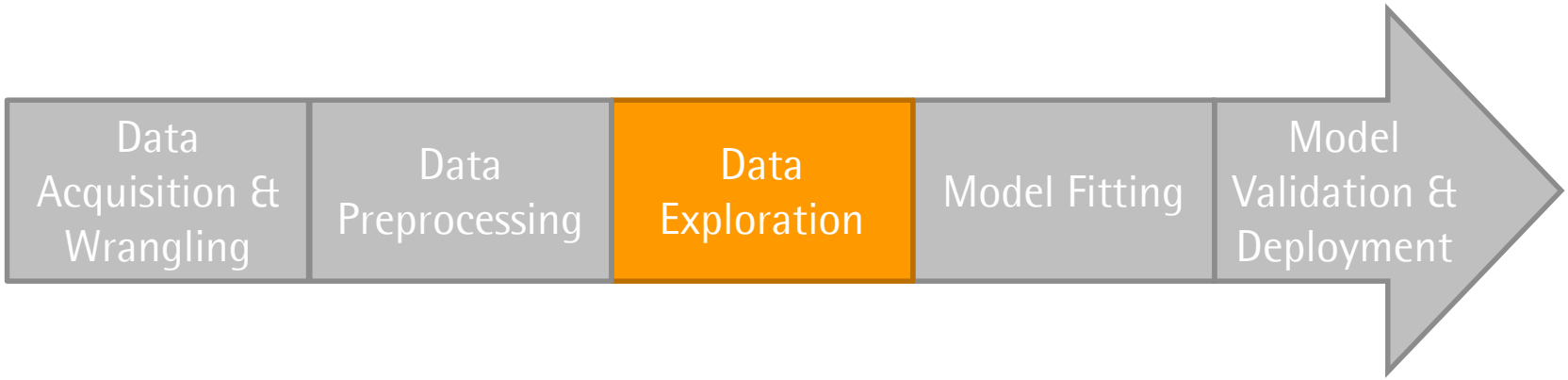
- Collect data and make it analyzable
  - Connect and query databases
  - Scrape and clean web-based text sources
- Time-consuming and often very manual
- Highly domain-specific

Machine Learning Process



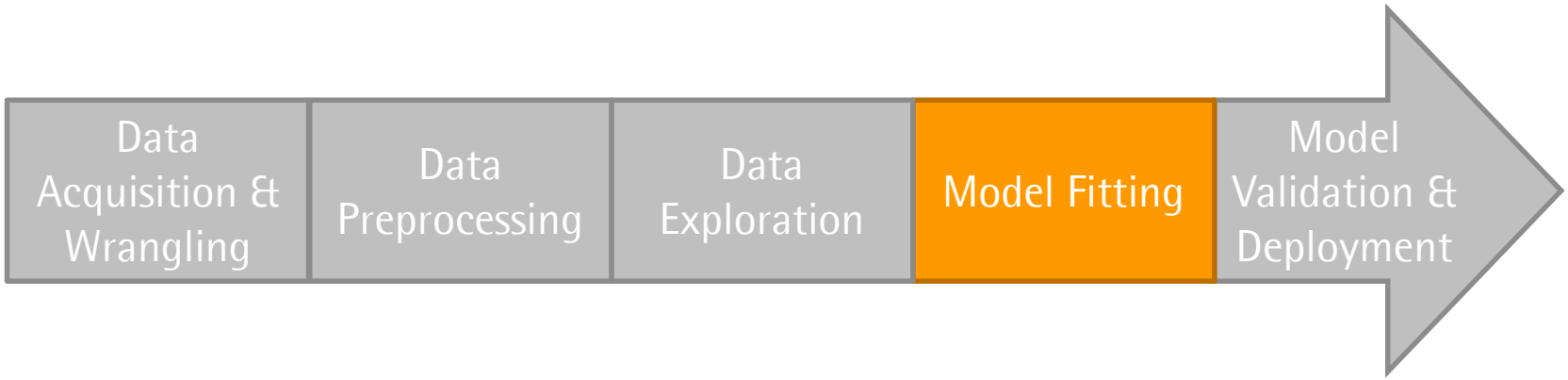
- "All you need is a table"
  - Transformation of unstructured data into structured
- Feature engineering
  - Find useful table representation

Machine Learning Process



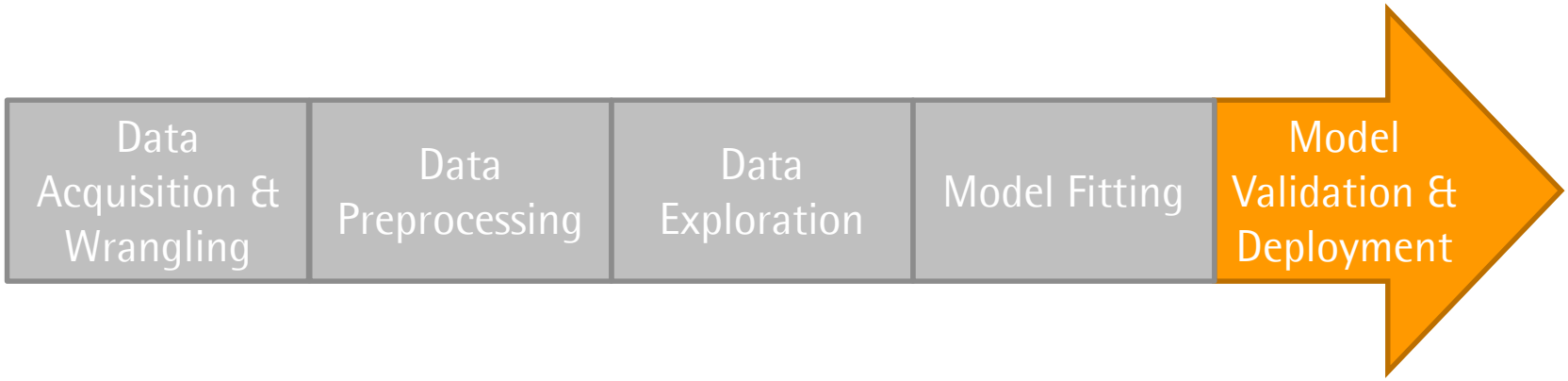
- Get to know your data
- Explore and visualize general trends
- Detect outliers and abnormal distributions

Machine Learning Process



- What most people think of as machine learning
- Algorithms that explain your relationship of interest
  - Support vector machines, Random Forests, Linear regression, Deep learning, Principal Component Analysis…

Machine Learning Process

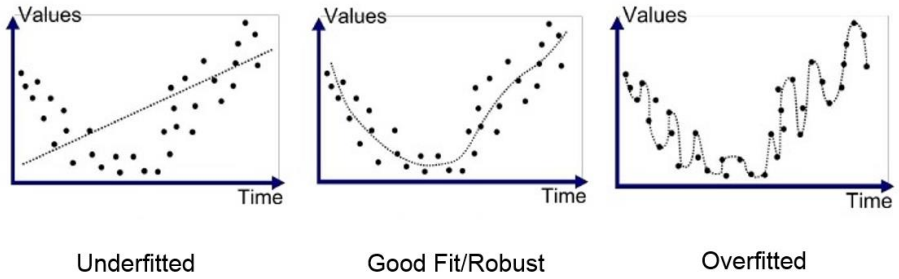


- Make sure that your model does what it's supposed to
- Cross-validation to find suitable model parameters
- Test-set evaluation to report performance to stakeholders

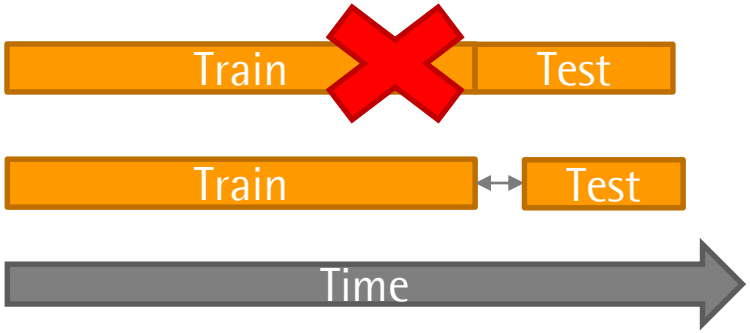
Why validation is so damn important

- You need an honest evaluation of what your model know
- A bit confusing nomenclature
  - Validation-set typically used to find good model parameters to balance over/under-fitting
  - Test-set used to asses real performance
- Beware of data leakage!
  - Preprocessing fitted for train- and test-data at the same time
  - Correlation between close time points in time series
  - Data from same person present in both training and test-set

https://en.wikipedia.org/wiki/Clever_Hans

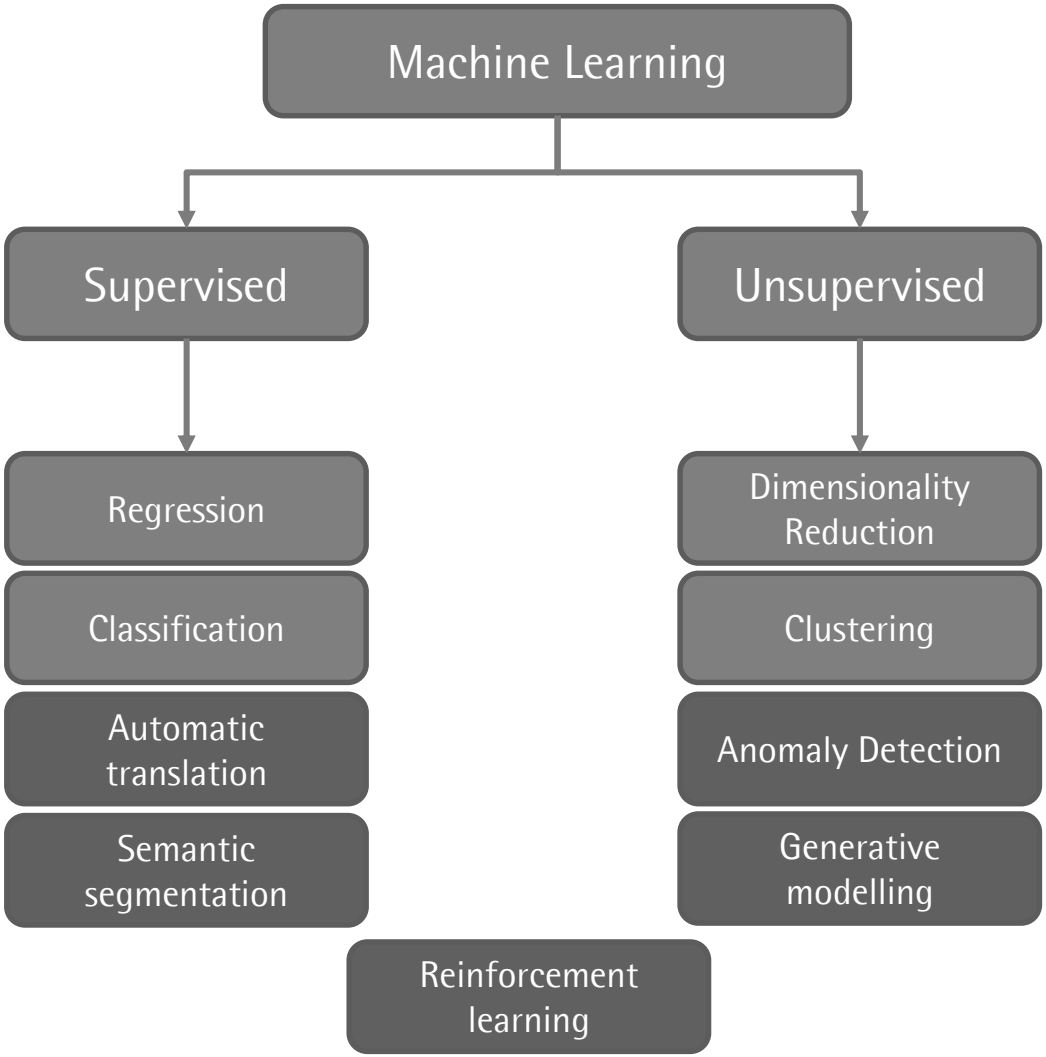


https://medium.com/greyatom/what-is-underfitting-and-overfitting-in-machine-learning-and-how-to-deal-with-it-6803a989c76

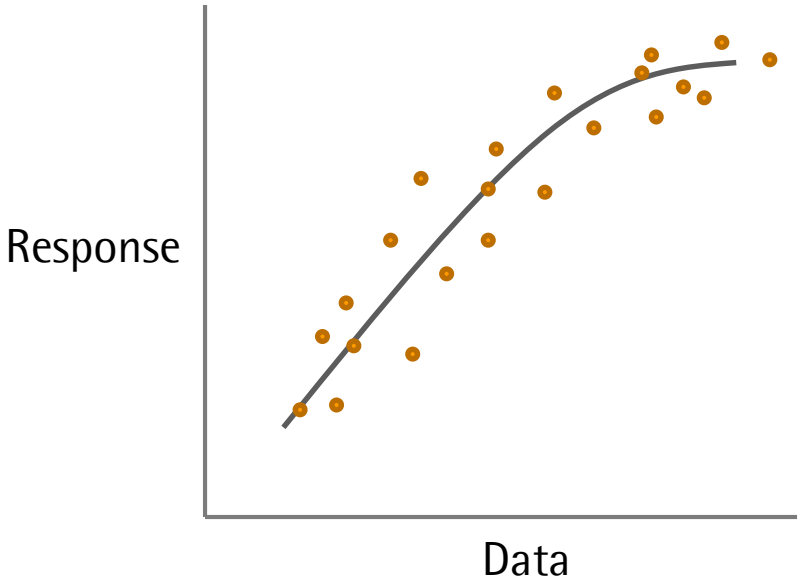


Machine Learning Methods

Machine Learning Models

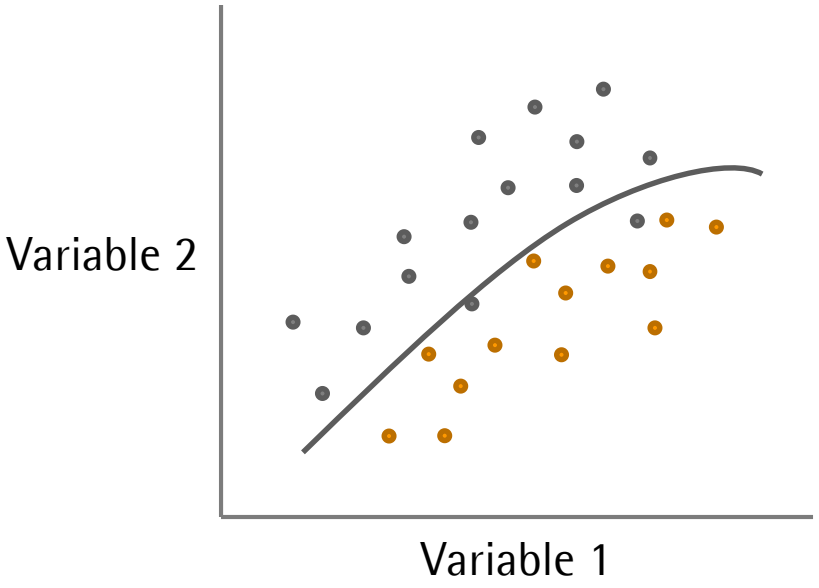


Supervised Machine Learning - Regression



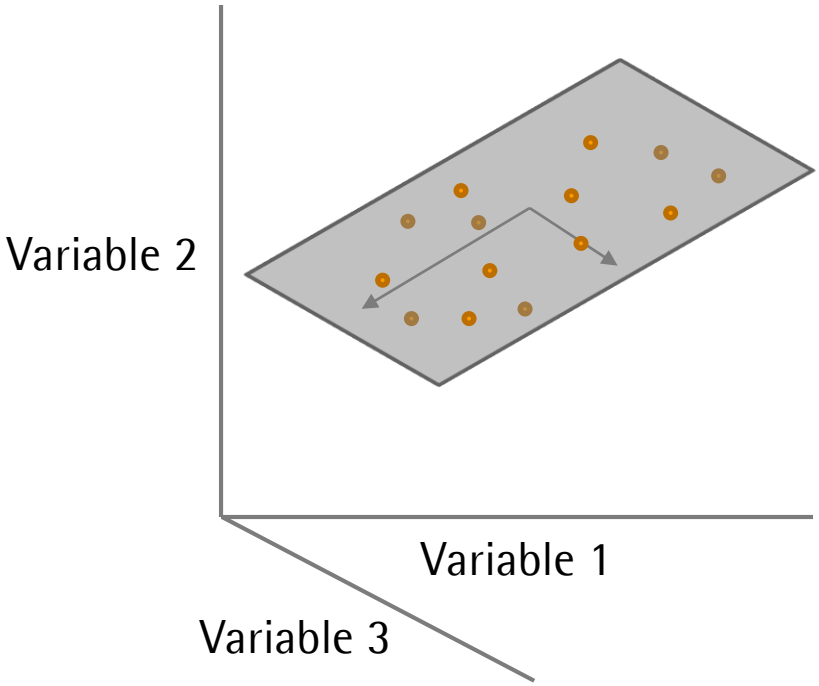
- Describe numerical relationship between variables
  - $Y \approx f(X, \beta)$
- Popular methods include
  - Linear regression
  - Partial Least Squares Regression (PLS)
  - Ridge or LASSO-regression
- Applications include
  - Business demand forecasting
  - Prediction of pharmaceutical binding affinity
  - Estimated future process yield

Supervised Machine Learning - Classification



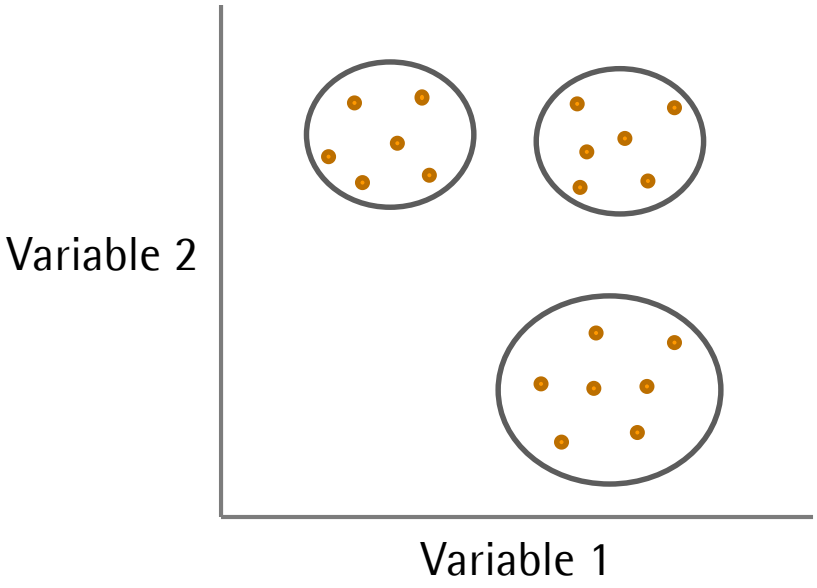
- Describe decision boundaries between classes
  - "Put data into buckets"
- Popular methods include
  - Support vector classifiers
  - Logistic regression
  - Random forests
- Applications include
  - Click stream analysis
  - Clinical case/control discrimination
  - Optical Character Recognition

Unsupervised Machine Learning – Dimensionality reduction



- Find descriptive representation of high-dimensional data
- Popular methods include
  - Principal Component Analysis (PCA)
  - Non-negative Matrix Factorization (NMF)
  - Uniform Manifold Approximation and Projection (UMAP)
- Applications include
  - Exploratory analysis of complex data
  - Data compression
  - Feature engineering

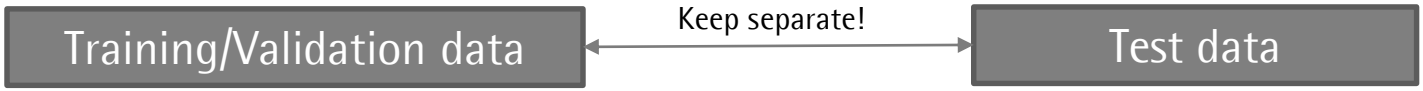
Unsupervised Machine Learning - Clustering

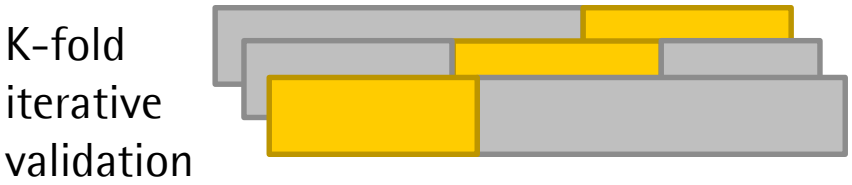


- Find groups in data
  - "Create buckets"
- Methods include
  - K-Means clustering
  - DBSCAN
  - Hierarchical /Agglomerative Clustering
- Applications include
  - Exploratory analysis
  - Customer segmentation
  - Cancer subtype detection

Model Validation

- How to choose train-val-test split?
  - If you don't know anything, randomize
  - Stratify based on prior knowledge to reduce risk of bias
  - Fixed or k-fold training/validation depends on size of data
- Double-check for dependencies between training- and test-data
- Use as much data in test set as you can afford

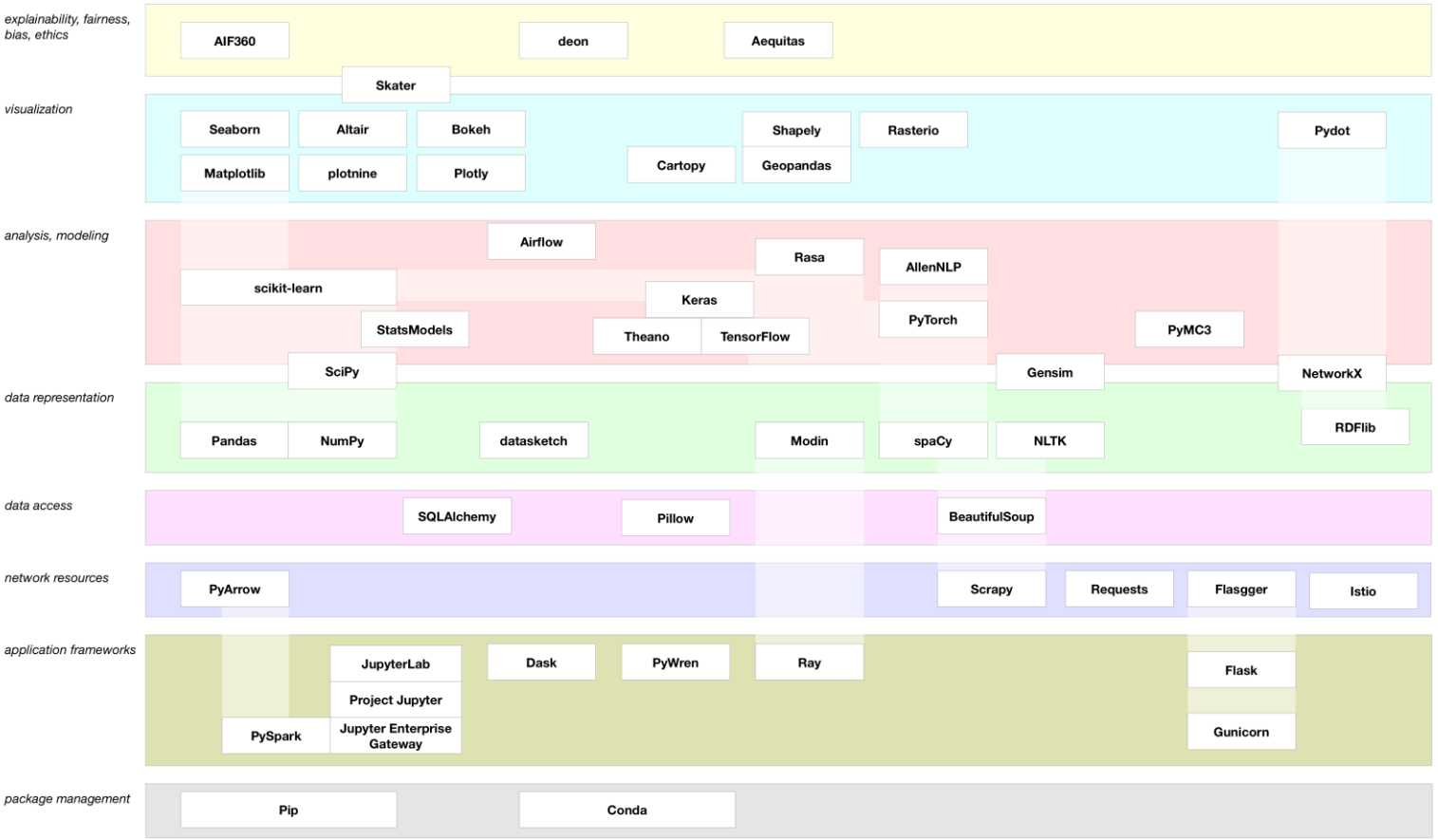




sartorius

Machine Learning in Python

Why Python?



https://community.ibm.com/community/user/datascience/blogs/paco-nathan/2019/03/12/a-landscape-diagram-for-python-data

NumPy

- Fundamental package for scientific computing.
  - N-dimensional array object
  - broadcasting functions
  - tools for integrating C/C++ and Fortran code
  - Linear algebra, Fourier transform, and random number functionality

- Most numerical Python libraries built are on top of NumPy

```
import numpy as np
```

http://www.numpy.org/

Pandas

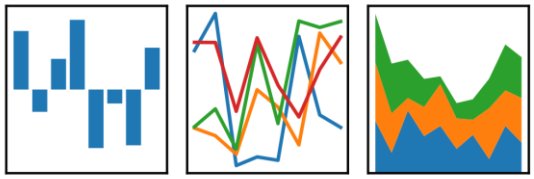
- Data structures for data analysis
  - DataFrame and Series
  - Semantic indexes
  - Groupby, resampling, joins
  - IO (csv, Excel, HDF5, parquet)

- NumPy N-dimensional array as backend

```
import pandas as pd
my_df = pd.DataFrame(my_array)
```

pandas

$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$



https://pandas.pydata.org/

Scikit-Learn

- Comprehensive library of machine learning methods
  - Models and algorithms
  - Preprocessing tools
  - Validation algorithms, model metrics, train-val-test splitting
  - Excellent documentation

- Also based on NumPy N-dimensional array

```
from sklearn.decomposition import PCA
my_pca_model = PCA(n_components=2).fit(my_array)
```

https://scikit-learn.org/

Some resources

- Scikit-Learn user guide
  - Comprehensive explanations of many algorithms
  - https://scikit-learn.org/stable/user_guide.html
- Machine Learning Mastery
  - Plenty of easy-to-follow tutorials
  - https://machinelearningmastery.com/
- Machine Learning on Coursera by Andrew Ng
  - Classic course, still very good
  - https://www.coursera.org/learn/machine-learning?

Today

https://github.com/Umetrics/machine-learning-workshop

Introduction to Pandas missing unfortunately

https://pandas.pydata.org/pandas-docs/stable/getting_started/10min.html