PROGRAMMING IN PYTHON II

Data Analysis and Preprocessing

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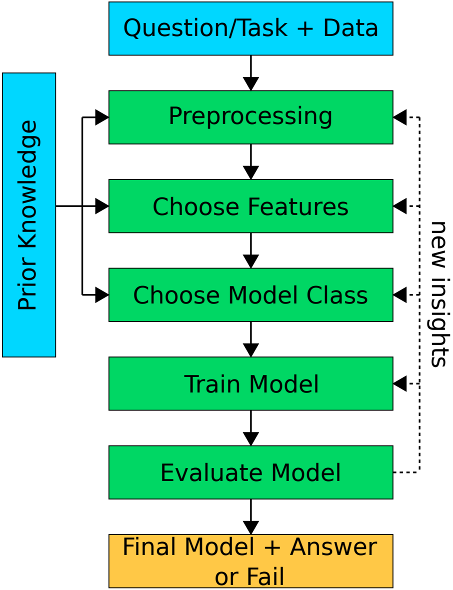
Terminology

- **Model**: parameterized function/method with specific parameter values (e.g., a trained neural network)
- **Model class**: the class of models in which we search for the model (e.g., neural networks, SVMs, ...)
- **Parameters**: what is adjusted during training (e.g., network weights)
- **Hyperparameters**: settings controlling model complexity or the training procedure (e.g., network learning rate)
- **Model selection/training**: process of finding a model (optimal parameters) from the model class

Basic Data Analysis Workflow



Motivation

- We want to train a machine learning (ML) model such that we get a “good” or even the “best” model
- How do we get the “best” model?
  1. How does our model perform on our data?
     $\rightarrow$ **Loss function**
  2. How will it perform on (unseen) future data?
     $\rightarrow$ **Generalization**

Generalization – Theory

- We train our model on a subset of data points (e.g., to predict labels)
  - We use **Empirical Risk Minimization (ERM)**
  - This subset of data points is called **training set**
- We want this trained model to also work on (e.g., correctly predict) unknown/future data
  - Problem: We might fit our parameters to noise specific to our training data set (=**overfitting**)
  - We can use a separate subset of samples to estimate the (true) risk on unknown data (=how well our model **generalizes**)
  - This separate subset of data points is called **test set**

Generalization – Assumptions

- Of course, there is a price to pay: The theory comes with assumptions:
  1. Strong law of large numbers: Our **subset of data points has to be large enough**
  2. Our data points have to be **independently and identically distributed (i.i.d.)**
- What does i.i.d. mean?
  - Each sample has the same probability distribution as the others and all are mutually independent.

i.i.d. With Respect to Our ML Project

- What we want:
  - We want our model to perform image depixelation on all kinds of pictures within certain restrictions (size, color)
  - The distribution our pictures are sampled from should be that of all possible pictures within these restrictions
  - The pictures should be sampled randomly from this distribution of all possible pictures
- What we have:
  - We collected 100 pictures per student
  - $\rightarrow$ The 100 pictures per student are probably not mutually independent
  - The pictures are not sampled from the distribution of all possible pictures but from another distribution (European setting, ML-students, $\ldots$)
  - $\rightarrow$ Pictures are not randomly drawn from the true distribution of all possible pictures!

Working With What We Have – Theory

- We need to consider the violations of i.i.d. properties in our data
- Training set and test set splitting must reflect this consideration
  - Test set must be drawn independently from training set (or as independently as possible) to get a good estimate of true risk
  - Preprocessing must not violate test and training set split
  - Data analysis done on complete set of data points cannot be used for training

Working With What We Have – Practice

- Example: our ML project
  - Random assignment of samples to training and test set will not be sufficient! (reason: not independently sampled!)
  - Better: Assign samples of one set of students to the training set and those of other students to the test set
  - In general: Assign samples of one set of clusters to the training set and those of other clusters to the test set if you want an estimate for generalization between clusters!
- Even then, we will not get rid of the problem that we did not sample correctly from the true distribution of all possible pictures
  - We do not know how well our model performs on this true distribution of all possible pictures
- Keeping that in mind, let's try our luck and get started!

Cleaning Up

- Never assume the data is valid or correctly formatted
- Typical problems:
  - Empty or corrupted files
  - Wrong filetypes
  - Duplicated datapoints
  - Missing datapoints
  - Outlier values
  - Inconsistent filenames/sample names
  - Inconsistent label names
  - Incorrect labeling
  - ...

First Analysis

- Check mean/standard deviation of data points
- Check number of valid samples
- Check number of classes and valid labels
- If applicable, visualize (parts of) the data set

Data Preprocessing

- What violates the training and test split?
  - Do not compute global values for the whole data set for normalization!
  - Do not perform feature-selection on the whole data set!
- What preprocessing should be done once and saved and what should be done on-the-fly?

Normalization

- Many ML methods profit from normalized data
  - Make data more homogeneous
  - Reduce chances to overfit
  - Some methods require a specific normalization
- Different normalization schemes for different settings/tasks
  - Typical for NN: Mean=0, Variance=1 (often referred to as standardization)
- Clustering and down-projection methods also benefit from normalized data

Normalization – Common Approaches

- Normalization per sample
  - Mean and variance computed and normalized per sample
  - Does not violate data set splits
  - Removes offsets of samples (e.g., brightness in images)
- Normalization per data set
  - Mean and variance computed over all samples in data set and then used for normalization
  - Violates data set splits! $\rightarrow$ Mean and variance need to be computed on training set and these values should be used for other sets too!
  - Keeps offsets of samples

Normalization – Other Approaches

- Other approaches for normalization or scaling
  - Scaling values to range $[0, 1]$ for each sample or complete data set
  - Scaling values to range $[-1, 1]$ for each sample or complete data set
- Best normalization/scaling depends on the data set, method and task

Normalization – Tips and Tricks

- Check the publication of the method you are applying for theory/recommendations
- You can evaluate different normalization schemes on another separated set (=**validation set**)
- Using pretrained models? If your data is similar, you can often keep the normalization constants from the pretraining

Optimization

- Prepare data such that we do not need to convert it before feeding it to our models
- Load data set in RAM if possible to decrease loading time
- Compress data set to save disk space
  - Max. number of files per directory, max. size per file, max. length of file paths depend on file system/OS

Clustering and Down-Projection (1)

- After normalization, look into clustering and down-projection methods
  - They often give us valuable insights in the data
  - If you use such clusters to create test and training splits, verify them manually! (Do not trust clustering methods.)
- Popular clustering methods: k-means, DBSCAN, ...
- Popular down-projection methods: PCA, t-SNE, ...
- Our raw data might be incompatible with these methods
  - Too many feature values
  - Datapoints in odd feature space
  - $\rightarrow$ We need to be creative

Clustering and Down-Projection (2)

- For our ML project, for instance, we would like to inspect whether there are certain clusters/patterns in our data
- What we want:
  - Small suitable feature space
  - Constant number of features
- What we have:
  - Huge feature space (number of pixels)
  - Odd feature space (pixel space)
  - Images of different size (different number of features)
- Possible solution:
  - Down-project images into better feature space before clustering and/or visualization (e.g, using pretrained CNN features)

  $\rightarrow$ Fewer features, constant number of features, better feature-space (hopefully)