Machine Learning I

Chapter 2 - Data Preprocessing

Prof. Dr. Sandra Eisenreich

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Hochschule Landshut

Agenda

 I. Data Preprocessing: Collect and clean up data.

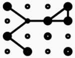
 II. Choosing/Training Model(s): see below.

 III. Evaluating the Model(s): Check the performance on new, unseen data.

... Back to II., if III. is not good enough. If only some hyperparameters are changed, this is called finetuning the model.

II. The choice of ML model depends on the kind of

TASK, DATA, COMPLEXITY, FOCUS,

Challenges in ML

Insufficient quantity of data
solutions: get more data, create more data (simulations, generative AI), use unsupervised or semi-supervised machine learning (ML models which doesn't need labels; see soon)

Poor quality data: e.g. due to sensor malfunction, human error, poor calibration, false data...
solutions:

- Find outliers and errors and remove them from the dataset.
- Find missing values and drop these data or replace the missing values.

Irrelevant or insufficient features: Irrelevant information in the data can "confuse"the model, insufficient information can make good prediciton impossible.
solutions:

- Feature selection is the process of selecting the most useful features.
- Feature extraction is the process of combining features to produce more useful ones.
- Gather more data.

Challenges in ML

Nonrepresentative Data:

- Too few data: If you only flip a coin twice and the result is always head, your model will predict 100% head results. This effect is called sampling noise.
- Biased data from only a fraction of cases:
  - e.g.: If you conduct a poll before a vote and only question people who play golf, you will not get a result representative of the entire population. This effect is called sampling bias.
  - e.g.: If you conduct a poll about your product by email, you will probably mainly get responses from those who care strongly about the matter (five stars or no stars), you won't get the opinion of the average customer. This is called nonresponse bias.

Steps of data preprocessing

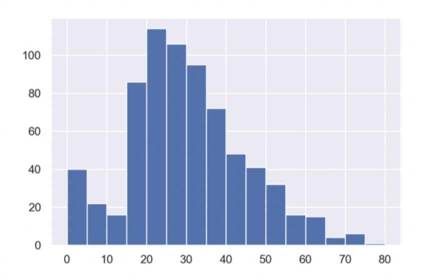
- Getting to know the data; visualizations (Data Science 2)
- Feature engineering
- Creating a train-test split (see later)
- Data Cleaning
- Handling Categorical Attributes
- Feature Scaling

You often combine the last three in a Transformation Pipeline. See the jupyter Notebook on Data Preprocessing for details.

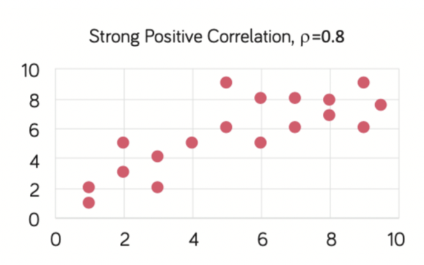
Step 1: Visualizations

Histograms:

- divide the data into discrete bins;
- height of each bar = number of instances in the bar/width of the bar (theory); in pandas/matplotlib: number of instances



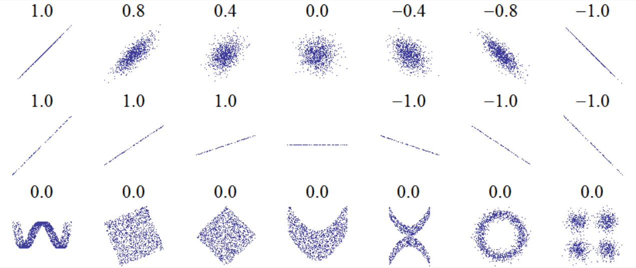
Scatterplots:
to visualize relationship between features.
To compute how linearly correlated features are use Pearson's correlation value.



Step 1: Understanding feature correlations

Correlation = a **linear** relationship between two features. **Pearson's correlation coefficient** describes the strength of the correlation.

- close to 1/-1: strong correlation with positive/negative slope
- close to 0: weak/no correlation (there still can be a relationship, just not a linear one)



Quelle: Wikimedia Commons

Example of a correlation matrix (correlation coefficients for each pair of features):

	a	b	c
a	1	0.7	-0.1
b	0.7	1	-1
c	-0.1	-1	1

2nd and 3rd Step

2nd step: Feature Engineering

- Feature selection: Drop irrelevant features, if there are any.
- Feature extraction: combine existing features to produce a more useful one. Experiment with attribute combinations and find out if they are useful by repeating step 1 (Data Visualizations, correlation matrix).

3rd step: Train-Test Split

- Divide data into training and test set BEFORE cleaning or transforming data in a way that might mix information from the train and test set (like computing the mean or median or most frequent category), to keep the model unbiased towards the test data.
- Always permute data before the split (to mix classes)
- Use a stratified split to make sure classes are evenly distributedïnto test and train set (i.e. the data distribution is the same as in the overall data set).

4th Step: Data Cleaning, 5th step: Handling Categorical Features

4th step: Data Cleaning

- drop irrelevant features,
- clean missing values by either dropping instances/features or imputing "good" values like
  - for numerical features: mean or median or a constant value
  - for categorical features: most frequent category or a constant value

  Alternatively, one could train an additional model predicting missing values.

5th step: Handling Categorical Features like (Green, red, . . . , yellow...). Two possibilities:

- Ordinal encoding: Convert the categories to numbers (Green $= 1$, Red $= 2$, $\ldots$ Yellow $=$ C). Disadvantage: only makes sense for ordinal data (with a natural ordering)
- One-hot encoding: Convert the C categories to C-dimensional one-hot vectors (Green $= e_1$, Red $= e_2$, $\ldots$)

6th step: Feature Scaling

Most ML algorithms perform badly when the numerical attributes have different scales.

Solutions:

- Min-max scaling: values are shifted and rescaled so that they end up in the range of 0 to 1, by substracting the min value and dividing by the max minus the min:

$$x \mapsto \frac{x - \min}{\max - \min}$$

- Standardization: substract the mean value μ and divide by standard deviation σ so values have mean 0 and 1 variance.

$$x \mapsto \frac{x - \mu}{\sigma}$$

Important: If you preprocess training data one way, it's important to do exactly the same to the test data, i.e. don't compute mean and deviation or min/max of the test data for standardization, but those of the *training data*!

Transformation Pipelines, Column Transformer

To keep it simple, combine 4-6 into a pipeline which deals with numerical and categorical data separately:

- divide features into numerical and categorical features
- define a transformation pipeline for numerical features (impute e.g. mean or median for missing data, scale data)
- define a transformation pipeline for categorical features (impute e.g. most frequent category, encode categories)
- combine the two pipelines in a single Transformer.

Chapter II Summary

Steps of Data Preprocessing for ML:

- Getting to know the data and visualizations: look at data and summary statistics, plot histograms and scatterplots, compute correlation matrix.
- Feature engineering: feature selection, feature extraction (create new features from old)
- Create a train-test split (after a random permutation of the dataset): simple split or stratified split (equal distribution of categories).
- Data Cleaning: drop columns/instances with missing values, or insert "good"values for missing values:
    - for numerical features: mean or median or constant
    - for categorical features: most frequent category or constant
    - alternative: prediction model to insert missing data
- Handling Categorical Attributes: ordinal or one-hot encoding.
- Feature Scaling to make all features have similar size and variance: MinMaxScaling or Standardization.
- Important: use the transformation parameters from the training set (mean, standard deviation, most-frequent-categories...) for the transformation of the test set.