General Q&A

No questions.

Theory Tasks

Chapter 1: Introduction

Explain the difference between over- and underfitting!

- overfitting:
 - model is too complex for dataset
 - model also captures outliers/noise that are not generalizable
- underfitting:
 - model is too simple for dataset
 - model not able to capture general trend in data properly

How can we use training data and validation/test data to avoid overfitting?

- can observe overfitting as difference in prediction performance between training data and validation/test data
- in particular, models might be better on data they are trained on than on separate data
- thus, should split data into training part and validation/test part
- train models on training data only
- make predictions and observe prediction performance mainly on validation/test data
- split methods like holdout split, cross-validation, etc. will be discussed in a later lecture

How can we avoid overfitting when trying to decide which order of regression model to fit to our data?

- split data into training part and validation part
- train models of different order on training data
- compare models on validation data; pick the one with highest prediction performance
- this should result in best compromise between underfitting and overfitting
- in contrast, on training data, prediction performance probably just gets better the more complex the model gets

Explain the One-Rule algorithm! Why is it used for small/noisy datasets?

- rough explanation:
 - check for each value of each feature which class is most frequent
 - count all data objects with deviating class labels as classification errors
 - count number of errors per feature
 - pick feature with lowest error
 - for numeric features, discretization necessary
- benefits: very simple model, less prone to overfitting than more complex models
 - makes it suitable for small/noisy datasets
 - main danger causing overfitting: features with many values
 - * can also happen for categorical features, not only numeric ones

Chapter 2: Fundamentals

Data & Descriptive Statistics

How can you categorize data?

- basic categorization from lecture:
 - categorical
 - * nominal
 - * ordinal
 - numerical
 - * discrete
 - * continuous
- other categorizations possible, e.g., by dimensionality (part of lecture as well):
 - one-dimensional (univariate)
 - multi-dimensional (multivariate); special cases:
 - * two-dimensional (bivariate)
 - * high-dimensional (definition of 'high' depends on use case)
 - dimensionless

Compare the three types of aggregates!

- distributive: store only the desired aggregate for each partition of data
- algebraic: store multiple (but fixed number of) aggregates for each partition of data
- holistic: number of aggregates to be stored for each partition is potentially unlimited
 i.e., in worst case, need to store all data objects, so no aggregation at all

Why are distributive aggregates efficient?

- need only to store one aggregate for each (arbitrarily large) partition of data
- from partition aggregates, can directly compute value of aggregate for full dataset
 - i.e., without needing to look into (individual data objects of) partitions again
- can also be easily updated if new data arrives:
 - i.e., self-maintainable regarding insertion
 - first, compute aggregate on new data
 - second, combine with aggregate on old data to get overall value of aggregate

What is the difference between variance and covariance?

- variance
 - univariate statistic
 - describes how much a random variable varies around its expected value (i.e., mean)
 - $Var(x) = \frac{1}{n} \sum_{i=1}^{n} (x_i \overline{x})^2$ (population variance)
- covariance
 - bivariate statistic
 - describes how much two random variables vary in same direction
 - $Cov(x,y) = \frac{1}{n} \sum_{i=1}^{n} (x_i \overline{x})(y_i \overline{y})$
 - unnormalized (gets larger if you scale variables larger, e.g., multiply with factor)
 - * Pearson correlation is a normalized version of this statistic

Statistical Tests

What is the null hypothesis of the χ^2 test?

- in lecture: two random variables are independent
- more general: check frequencies of one random variable against some distribution

How can one conduct feature selection with the χ^2 test?

- see subtask f) of first programming-exercise sheet
- χ^2 test statistic collects evidence against independence of random variables
- i.e., it can be used as a measure of dependency
 - if you want a normalized measure, can use 1 p-value as well
- use case 1: only select features that show highest dependency to target variable
 - i.e., keep most relevant features
 - can be absolute number (select top k features)
 - can be threshold-based (select all features with a p-value lower than some threshold)
- use case 2: if two features show a strong dependency to each other, remove one of them
 i.e., reduce redundancy in data

Does the χ^2 test also work if random variables have a non-normal distribution?

- yes
- non-parametric test, i.e., does not assume any distribution
- also, works with categorical data (which are not normally distributed anyway)

Assume two samples are given. Is the following statement correct? "If a Kolmogorov-Smirnov test concludes that both samples were not drawn from the same distribution, then a Wilcoxon-Mann-Whitney test is redundant."

- Wilcoxon-Mann-Whitney test compares distributions based on median
- KS test compares distributions based on whole cumulative distribution function
- thus, KS test seems more general and Wilcoxon-Mann-Whitney test seems redundant
- if it comes to actual statistical power, situation is more complicated, as paper Comparison of the Powers of the Kolmogorov-Smirnov Two-Sample Test and the Mann-Whitney Test for Different Kurtosis and Skewness Coefficients Using the Monte Carlo Simulation Method shows
- decision also depends on what you actually want to compare
 - in some situations, you are only interested in central tendency of distribution
 - i.e., spread of distribution, long tails, etc. might be irrelevant for you

Data Reduction

Name three different ways to reduce data!

- numerosity reduction: reduce number of data objects
- dimensionality reduction: reduce number of features
- discretization: reduce number of values per feature

How can you automatically select important features? What do you need to consider to perform feature selection?

- features should be relevant for prediction target
- features should not be redundant to each other
- search strategy for feature sets should be efficient
 - since there are 2^n feature sets for n features
 - some approaches evaluate each feature individually
 - * e.g., how strongly is each feature correlated to target variable
 - some approaches iterate over space of potential feature sets
 - * e.g., greedy forward/backward selection, genetic algorithms, etc.
 - some prediction models implicitly select features
 - * e.g., decision trees

How does PCA work?

- is a dimensionality-reduction technique
- rotation: does not select (original) features, but transforms dataset to new basis
- projection: under new basis, first few features should capture most variance of dataset
- mathematical details:
 - principal components are eigenvectors of covariance matrix of original dataset
 - * computation based on covariance matrix is called eigendecomposition
 - * also other ways of computation, e.g., via singular value decomposition (SVD)
 - principle components constitute columns of rotation matrix
 - * form an orthonormal basis of feature space
 - * transformation (rotation) is a simple matrix multiplication
 - * features under new basis are linear combinations of features from original dataset
 - * transformation from new basis back to old one is possible as well
 - eigenvalues associated with principal components (eigenvectors) help to project data
 - * are proportional to amount of variance captured in principal component
 - * components in rotation matrix should be ordered by decreasing eigenvalues
 - * to reduce dimensions, only keep first few columns of rotation matrix
 - * if you keep all components, transformation is lossless
 - features under new basis are uncorrelated
 - to conduct PCA, features should be standardized
 - * mean of zero (if PCA computed via covariance matrix, this happens automatically)
 - * variance of one (else, feature with higher variance dominate result)