Exercise Set 3

- Answer anonymously, i.e., do not write your name to the answer sheet.
- Submit the answer via Moodle at latest on 6 December 2020 (Moodle submission will open during the week starting on 30 November).
- Your answer will be peer-reviewed by other students and you will review your answer and answers of 2 random peers during the week starting on 7 December.
- The assignment should be completed by one person, but discussions with others are encouraged. Your final solution must be your own.
- The language of the assignments is English.
- The submitted report should be in a single Portable Document Format (pdf) file.
- Answer to the problems in the correct order.
- Read the general instructions in Moodle before starting with the problems.
- Notice that you can submit your answer to the Moodle well before deadline and revise it until the deadline. Therefore: please submit your answer well in advance, alraedy after you have solved some problems!

These are the last exercises. Problems 16-18 are about clustering, which will be covered in the 25 November lecture, and problem 19 about PCA, which will be covered in the 27 November lecture. Problems 18-19 deal directly with the term project data sets: hopefully doing the problems helps you to solve the term project more efficiently. The final problem 20 is the learning diary for the whole course.

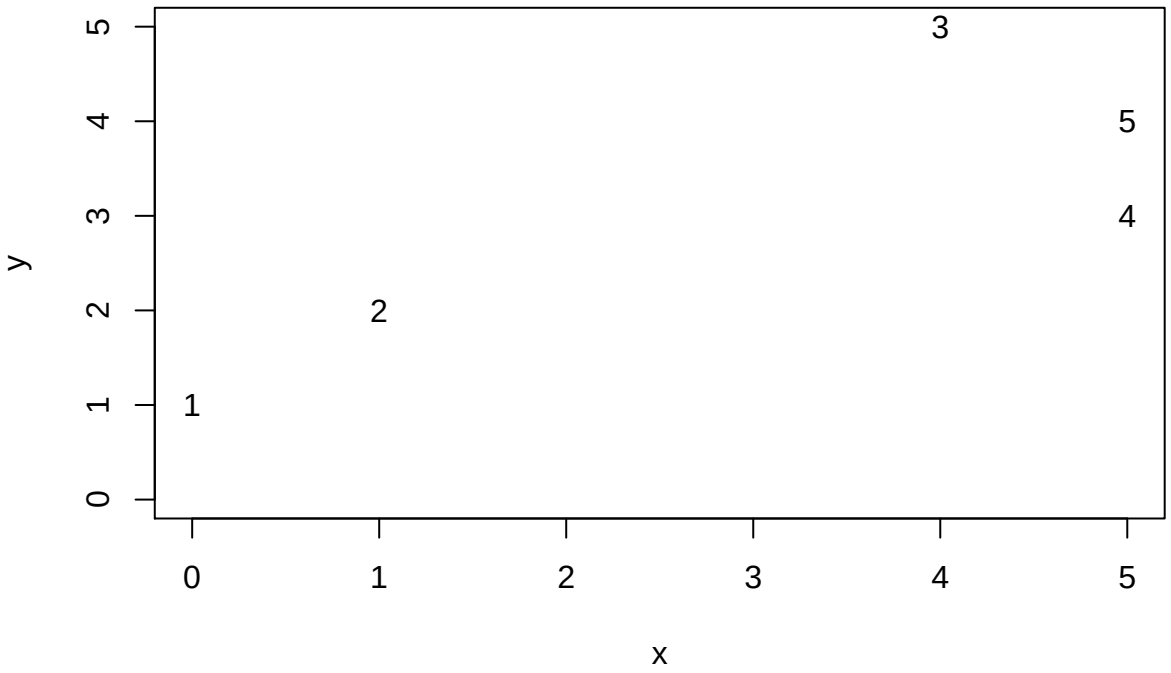
2 December lecture will include recap of the course topics and on 4 December we will have machine learning guest lectures (see the last page!).

Problem 16

[20% points]

Objectives: k-means loss and Lloyd's algorithm

```
data <- data.frame(x=c(0,1,4,5,5),y=c(1,2,5,3,4))
```



You should be able to do this problem with a pen and paper.

Task a

What kind of tasks can we use the Lloyd's (k-means) algorithm for? Explain what the *inputs* and *outputs* of the algorithm are. How to interpret the results?

Task b

Define the objective (or cost) function that the Lloyd's algorithm tries to minimize. What can be said about the value of the objective function during the two stages of each iteration of Lloyd's algorithm?

Task c

Consider the following set of data points in $\mathbb{R}^2$: $x_1 = (0, 1)$, $x_2 = (1, 2)$, $x_3 = (4, 5)$, $x_4 = (5, 3)$, $x_5 = (5, 4)$. Sketch the run of the Lloyd's algorithm using $K = 2$ and initial prototype (mean) vectors $\mu_1 = (0, 2)$ and $\mu_2 = (2, 0)$. Draw the data points, cluster prototype vectors, and cluster boundary after each iteration until convergence.

Also, write down calculation procedure and the cluster memberships as well as prototype vectors after each iteration.

Problem 17

[20% points]

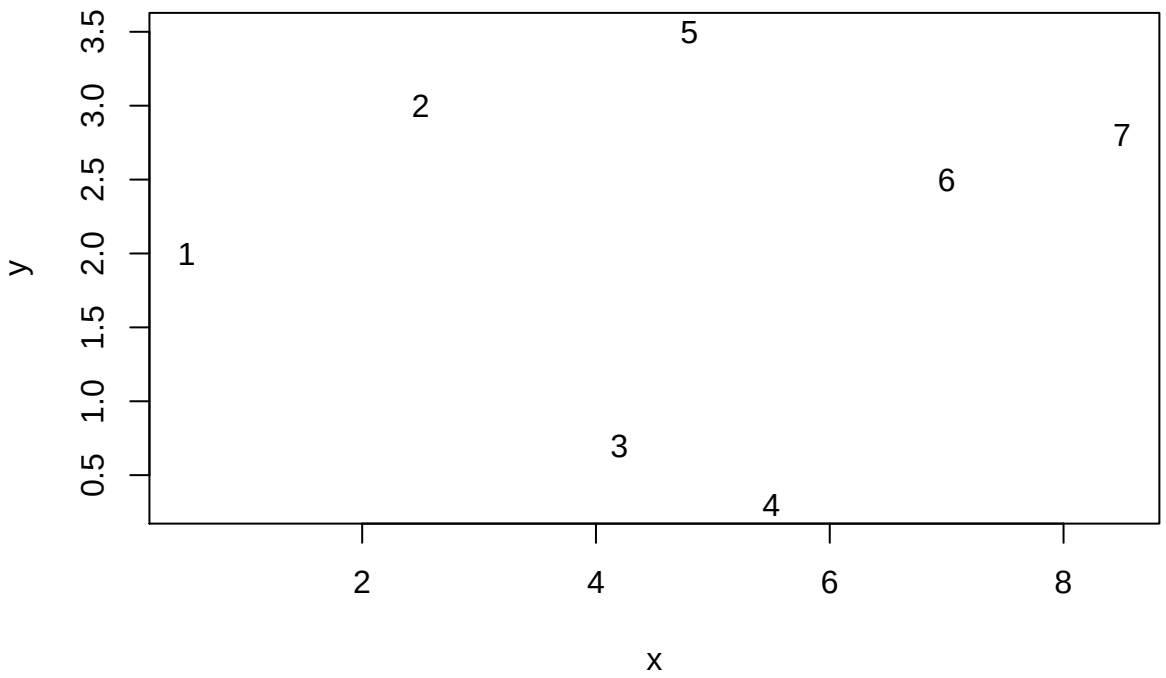
Objectives: understanding hierarchical clustering algorithms

We consider *hierarchical clustering* on a toy data set $D = \{(x_i, y_i)\}_{i=1}^{7}$, where $(x_i, y_i) \in \mathbb{R}^2$. You should be able to do this problem with a pen and paper.

The data points are shown in the table and figure below.

```
data <- data.frame(x=c(0.5,2.5,4.2,5.5,4.8,7.0,8.5),
                   y=c(2.0,3.0,0.7,0.3,3.5,2.5,2.8))
```

	x	y
1	0.5	2.0
2	2.5	3.0
3	4.2	0.7
4	5.5	0.3
5	4.8	3.5
6	7.0	2.5
7	8.5	2.8



The matrix of Euclidean distances between the data points is given below.

	1	2	3	4	5	6	7
1	0.00	2.24	3.92	5.28	4.55	6.52	8.04
2	2.24	0.00	2.86	4.04	2.35	4.53	6.00
3	3.92	2.86	0.00	1.36	2.86	3.33	4.79
4	5.28	4.04	1.36	0.00	3.28	2.66	3.91
5	4.55	2.35	2.86	3.28	0.00	2.42	3.77
6	6.52	4.53	3.33	2.66	2.42	0.00	1.53
7	8.04	6.00	4.79	3.91	3.77	1.53	0.00

Task a

Sketch a run of the basic agglomerative hierarchical clustering algorithm to this data using the single link (min) notion of dissimilarity between clusters. Visualise the result as a dendrogram. Draw a sketch of the above figure in your answer sheet and indicate in this how the algorithm forms clusters step-by-step. It is not necessary to show detailed calculations, but indicate the cost of the join that you select.

Task b

Repeat the task a, but using complete link (max) dissimilarity. Compare the results.

Problem 18

[25% points]

Objectives: practical application of k-means and hierarchical clustering

For this problem you can use the term project dataset in file `npf_train.csv`. Your task is to cluster the data matrix, where the rows are given by the days and columns by various observations during that day. In this task you need only the class variable (`class4`) and the real valued mean measurements (variable names ending with `.mean`). You should end up with a dataset of 430 rows and 50 real valued variables and one class variable as columns. The R code to produce the data is given below for reference (in the last line we strip out the redundant `.mean` from the variable names!).

```
npf <- read.csv("npf_train.csv")
## choose variables whose names end with ".mean" together with "class4"
vars <- colnames(npf)[sapply(colnames(npf),
                             function(s) nchar(s)>5 && substr(s,nchar(s)-4,nchar(s))==".mean")]
npf <- npf[,c(vars,"class4")]
## strip the trailing ".mean" to make the variable names prettier
colnames(npf)[1:length(vars)] <- sapply(colnames(npf)[1:length(vars)],
                                        function(s) substr(s,1,nchar(s)-5))
vars <- colnames(npf)[1:length(vars)]
```

Unless otherwise instructed, please scale the variables to zero mean and unit variance.

Task a

Cluster the rows of the data matrix and plot the k-means loss as a function of the number of clusters from 1 to 20. Should you normalise the columns and what effect does the normalization of the columns have? You can use a library function such as `kmeans` in R.

Task b

By using the Lloyd's algorithm and scaled variables, cluster the rows into four clusters and make a confusion matrix (contingency table where the rows are the true classes, columns the cluster indices, and entries the counts of rows). Order the rows and columns so that the sum of diagonal entries in your contingency table is maximized. Where are most "errors" made, if you would use your clusters as a rudimentary classifier (i.e., you would associate each of the clusters with a class)? (See the hint below!)

Task c

Repeat the clustering of task b above with 1000 different random initialisations (for example, picking in random 4 data vectors for your initial centroids in the Lloyd's algorithm). Make histogram of the losses. What is the minimum and maximum k-means losses for your 1000 random initialisations? How many initialisations would you expect to need to have to obtain one reasonably good loss (say, a solution with a loss within 1% of the best loss out of your 1000 losses), for this dataset and number of clusters?

Then try how using some smart initialisation such as kmeans++ affects your results.

Task d

Try clustering the same data with agglomerative hierarchical clustering with at least 2 different linkage functions. Produce a dendrogram and corresponding flat clustering (e.g., by splitting the dendrogram with `cutree`) and compare their properties (e.g., comparing sizes of clusters, by looking at confusion matrices). Find and report at least one interesting feature or reproduce some of the properties of hierarchical clustering (e.g., differences between the linkage functions) discussed in the lecture. (Hint: See Sections 10.5.2 and 10.6.2 of James et al. for examples in R.)

Instructions and hints

You can use, e.g., `kmeans` to run the Lloyd's algorithm. Please use the Lloyd's algorithm, e.g., as follows (the code below uses Lloyd's algorithm with one random initialisation on scaled dataset).

```
cl <- kmeans(scale(npf[,vars]),
             centers=4,algorithm="Lloyd",nstart=1,iter.max=100)
```

In task b you are asked to combine the class variables and the cluster indices and in task d you are asked to compare clusterings. Because all permutations of cluster indices are equally good it is useful to be able to, e.g., find the best match between the know classes (`class4`) and the cluster indices. One way to do this is the Hungarian algorithm which you can use to find a permutation of cluster indices such that sum of entries in the diagonal of the confusion matrix is maximised. An example in R is given below, where the implementation `solve_LSAP` of Hungarian algorithm in the `clue` library is used. In Scipy, the Hungarian algorithm is provided, e.g., by `linear_sum_assignment` from `scipy.optimize`.

```
library(clue)
## Create confusion matrix between the known classes (class 4) and
## cluster indices.
tt <- table(npf$class4,cl$cluster)
## Find a permutation of cluster indices such that they
## best match the classes in class4.
tt <- tt[,solve_LSAP(tt,maximum=TRUE)]
```

If you use R, you can use the following function to use the kmeans++ algorithm find the initial cluster centroids. You can give the resulting centroids directly as a parameter to `kmeans` function (parameter `centers`). If you use SciPy, `KMeans` from `sklearn.cluster` kmeans++ is the default initialisation.

```
# kmeansppcenters - Finds initial kmeans++ centroids
# Arguments:
# x        numeric matrix, rows correspond to data items
# k        integer, number of clusters
# Value:
# centers  a matrix of cluster centroids, can be fed to kmeans
#
# Reference: Arthur & Vassilivitskii (2007) k-means++: the
# advantages of careful seeding. In Proc SODA '07, 1027-1035.
kmeansppcenters <- function(x,k) {
  x <- as.matrix(x)
  n <- nrow(x)
  centers <- matrix(NA,k,ncol(x))
  p <- rep(1/n,n)
  for(i in 1:k) {
    centers[i,] <- x[sample.int(n,size=1,prob=p),]
    dd <- rowSums((x-(rep(1,n) %o% centers[i,]))^2)
    d <- if(i>1) pmin(d,dd) else dd
    if(max(d)>0) { p <- d/sum(d) }
  }
  centers
}

cl <- kmeans(scale(npf[,vars]),centers=kmeansppcenters(scale(npf[,vars]),4),
             algorithm="Lloyd",iter.max=100)
```

Problem 19

[25% points]

Objectives: uses of PCA

Continue with the same dataset as in Problem 18 above.

Task a

Make a PCA projection of the data into two dimensions. Indicate the class index (`class4`), e.g., by color and/or the shape of the glyph. Be sure to indicate which color/shape corresponds to which class, e.g., by `legend`.

Task b

Compute and plot the proportion of variance explained and the cumulative variances explained for the principal components. Study the effects of different normalisations - at least compare difference if you do not scale the data at all vs. you normalize each variable to zero mean and unit variance! Why for unnormalized data it seems that fewer components explain a large proportion of the variance, as compared to the normalized data? (Hint: See Sec. 10.4 Fig 10.4 of James et al.)

Task c

Pick one classification algorithm that is implemented in R or SciPy or in your other favourite environment that would work with this data and choose one of the challenge performance measures (binary accuracy, multiclass accuracy, or perplexity). Split the data in random into training and validation sets of equal sizes. Train your classification algorithm first without the dimensionality reduction on the training set and report the performance (=your chosen performance measure) on the validation set. Do the same on the data where the dimensionality has been reduced by the PCA (see task b above). How does the performance of your classifier vary with the (reduced) dimensionality and is there an "optimal" dimensionality which gives you the best performance on the validation set?

Hint: Notice that you can do the PCA on the combined training and validation sets. This is a simple form of semi-supervised learning: this way you can utilise the structure of the validation/test set even if you don't know the class labels on the validation/test set!

Task d (optional)

This is a bonus tasks for which no points are awarded.

Repeat task a above, but this time with isometric multidimensional scaling (MDS) and t-distributed stochastic neighbor embedding (t-SNE).

If you use R, you can use `isoMDS` from library `MASS` and `tsne` from library `tsne`. Notice that neither MDS nor t-SNE algorithms are guaranteed to converge to a local optimum. Therefore, a good initial position - one good choice is the PCA solution - is essential.

```
library(MASS)
library(tsne)
d <- dist(scale(npf[,vars]))
## cmdscale essentially does PCA. Both MDS and t-SNE are sensitive to initial
## configuration and the PCA initialisation generally leads to reasonable convergence.
## (Even though R isoMDS and tsne can handle bad initial config fine, we are being explicit here.)
y <- cmdscale(d,2)
## isometric MDS embedding coordinates
x.mds <- isoMDS(d,y=y)$points
## t-SNE embedding coordinates
x.tsne <- tsne(d,initial_config=y,k=2)
```

Problem 20

[10% points]

Objectives: self-reflection, giving feedback of the course

Task a

Write a learning diary of the topics of lectures 1-12 and exercise sets 1-3.

Instructions

The length of your reply should be 3-6 paragraphs of text. Guiding questions: What did I learn? What did I not understand? Was there something relevant for other studies or (future) work? Notice that this entry should typically be longer than your earlier learning diary entries in E1 and E2.

Machine Learning Guest Lectures

We will have two machine learning guest lectures on Friday **4 December 2020 at 10:15–12**. The tentative programme includes two 15–20 minute presentations, followed by a discussion where you can ask questions from the speakers.

The lectures will take place via the usual Zoom link at https://helsinki.zoom.us/j/68680705433?pwd=RTVTdWFSdS96S3h0NkU5S1lFRkdnZz09 (Meeting ID: 686 8070 5433, Password: 014569).

The speakers and the topics are:

Andreas Henelius: Data Science in Finance - Machine learning for overdue invoice prediction

Abstract: Invoice financing is a concept in banking enabling short-term borrowing by the bank's customers against the amounts due from the invoices held by the customer. Such borrowing can help the customer, e.g., with cash flow management. For this process to be feasible, it must be automated, and the bank needs to estimate the net present value of invoices, which depends on the expected payback time. In this presentation I talk about how to leverage machine learning to predict if invoices will be overdue.

About the speaker: D.Sc. (Tech.) Andreas Henelius is a data scientist at the OP Financial Group. Previously he worked at the University of Helsinki, Aalto University and the Finnish Institute of Occupational Health.

Antti Ukkonen: From voice to meaning: Machine learning for spoken language understanding

Abstract: I will discuss some of the many technical challenges we face at Speechly (www.speechly.com) when building a SaaS -solution using which developers with no prior ML or speech recognition experience can integrate voice functionality to their mobile or web applications. I will talk about deep learning, transfer learning, neural language models, perhaps a bit about reinforcement learning, and how to put these together in an autonomous cloud-based model training infrastructure.

About the speaker: Antti works currently as the Head of Natural Language Understanding at Speechly. In this role he is mainly in charge of developing and maintaining machine learning models that extract meaning from spoken language. Prior to joining Speechly in summer 2019, Antti spent almost 15 years in industry and academia as a data mining researcher. He has held positions at Yahoo! Research, Helsinki Institute for Information Technology HIIT, Finnish Institute for Occupational Health. Most recently, until December 2019, he was an Academy Research Fellow at University of Helsinki. Antti got his doctoral degree from Aalto University in 2008.

Welcome!

The lectures are part of the course DATA11002 Introduction to Machine Learning (access to the web site requires registration). Please see the course web site for possible updates.

Kai Puolamäki