Machine Learning Exercise Sheet 2

k-Nearest Neighbors and Decision Trees

Exercise sheets consist of two parts: Homework and in-class exercises. The homework is for you to solve at home and upload to Moodle for a possible grade bonus. The in-class exercises will be solved and discussed during the tutorial along with some difficult and/or important homework exercises. You do not have to upload any solutions of the in-class exercises.

Homework

kNN Classification

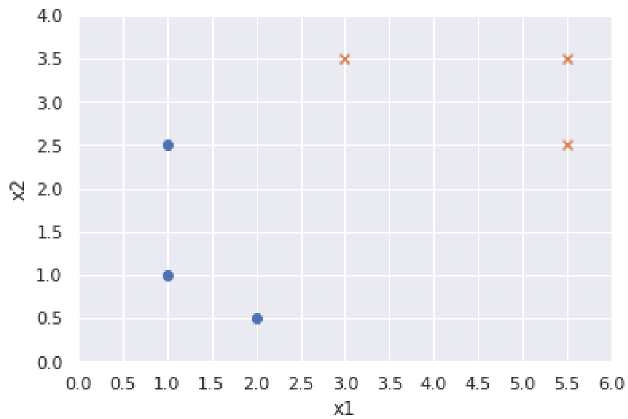
Problem 1: You are given the following dataset, with points of two different classes:

Name	x_1	x_2	class
A	1.0	1.0	1
B	2.0	0.5	1
C	1.0	2.5	1
D	3.0	3.5	2
E	5.5	3.5	2
F	5.5	2.5	2

We perform 1-NN classification with leave-one-out cross validation on the data in the plot.

a) Compute the distance between each point and its nearest neighbor using L_1-norm as distance measure.

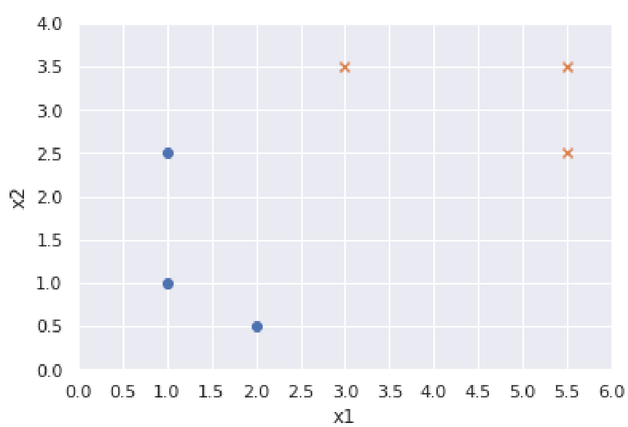
If you draw the points, you can identify the nearest neighbor without computing all distances:



$$d_1(X,Y) = \sum_i |X_i - Y_i|$$

L_1-norm	A	B	C	D	E	F	nn	class
A	0.00	**1.50**	**1.50**	4.50	7.00	6.00	B/C	1 ✓
B	**1.50**	0.00	3.00	4.00	6.50	5.50	A	1 ✓
C	**1.50**	3.00	0.00	3.00	5.50	4.50	A	1 ✓
D	4.50	4.00	3.00	0.00	**2.50**	3.50	E	2 ✓
E	7.00	6.50	5.50	2.50	0.00	**1.00**	F	2 ✓
F	6.00	5.50	4.50	3.50	**1.00**	0.00	E	2 ✓

b) Compute the distance between each point and its nearest neighbor using L_2-norm as distance measure.



$$d_2(X,Y) = \left(\sum_i (X_i - Y_i)^2\right)^{\frac{1}{2}}$$

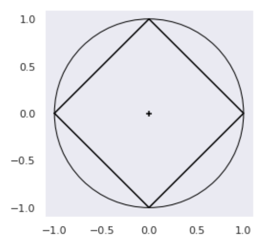
Upload a single PDF file with your homework solution to Moodle by 27.10.2019, 23:59 CET. We recommend to typeset your solution (using LaTeX or Word), but handwritten solutions are also accepted. If your handwritten solution is illegible, it won't be graded and you waive your right to dispute that.

L_2-norm	A	B	C	D	E	F	nn	class
A	0.00	**1.12**	1.50	3.20	5.15	4.74	B	1 ✓
B	**1.12**	0.00	2.24	3.16	4.61	4.03	A	1 ✓
C	**1.50**	2.24	0.00	2.24	4.61	4.50	A	1 ✓
D	3.20	3.16	**2.24**	0.00	2.50	2.69	C	2 ×
E	5.15	4.61	4.61	2.50	0.00	**1.00**	F	2 ✓
F	4.74	4.03	4.50	2.69	**1.00**	0.00	E	2 ✓

c) What can you say about classification if you compare the two distance measures?

Different distance measures can result in a different nearest neighbor and change the class a point is assigned to. Point D (orange cross) is closest to E (orange cross) regarding L_1-norm but closest to B (blue dot) regarding L_2-norm.

Regarding the distance measures it always holds that $L_2 \leq L_1$ (see unit circles of the two norms).



Problem 2: Consider a dataset with 3 classes $\mathcal{C} = \{A, B, C\}$, with the following class distribution $N_A = 16, N_B = 32, N_C = 64$. We use unweighted k-NN classifier, and set k to be equal to the number of data points, i.e. $k = N_A + N_B + N_C =: N$.

a) What can we say about the prediction for a new point x_{new}?

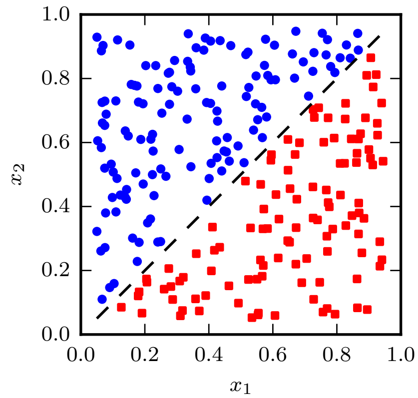
It will be classified as class C. When k is equal to the number of data points, the neighborhood of a new point contains all points in the training set regardless of their distance. The majority class in the neighborhood is thus equal to the majority class in the dataset.

b) How about if we use the weighted (by distance) version of k-Nearest Neighbors?

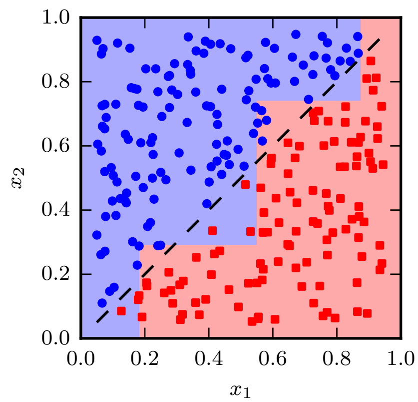
For the distance weighted variant we don't have enough information to answer the question, since the *weighted* distribution depends on the distances.

Decision Trees

Problem 3: The plot below shows data of two classes that can easily be separated by a single (diagonal) line. Does there exist a decision tree of depth 1 that classifies this dataset with 100% accuracy? Justify your answer.



No, there does not exist a decision tree of depth 1 that classifies this dataset with 100% accuracy. The feature test in a node can only use a single feature to split the training data. This leads to axis-parallel decision boundaries. Below you see the decision boundaries for a tree of depth 3. It classifies the dataset with 92.8% accuracy.



Problem 4: You are developing a model to classify games at which machine learning will beat the world champion within five years. The following table contains the data you have collected.

a) Calculate the entropy $i_H(y)$ of the class labels y.

$$p(y = W) = \frac{4}{10}$$
$$p(y = L) = \frac{6}{10}$$

No.	x_1 (Team or Individual)	x_2 (Mental or Physical)	x_3 (Skill or Chance)	y (Win or Lose)
1	T	M	S	W
2	I	M	S	W
3	T	P	S	W
4	I	P	C	W
5	T	P	C	L
6	I	M	C	L
7	T	M	S	L
8	I	P	S	L
9	T	P	C	L
10	I	P	C	L

$$\begin{aligned} i_H(y) &= -p(y=W)\log p(y=W) - p(y=L)\log p(y=L) \\ &= -\frac{4}{10}\log(\frac{4}{10}) - \frac{6}{10}\log(\frac{6}{10}) \\ &\approx 0.97 \end{aligned}$$

b) Build the optimal decision tree of depth 1 using entropy as the impurity measure.

Split 1, test x_1:

$$\begin{aligned} p(x_1 = T) &= \frac{1}{2} \qquad p(x_1 = I) = \frac{1}{2} \\ p(y=W|x_1=T) &= \frac{2}{5} \qquad p(y=L|x_1=T) = \frac{3}{5} \\ p(y=W|x_1=I) &= \frac{2}{5} \qquad p(y=L|x_1=I) = \frac{3}{5} \\ i_H(x_1=T) &= -\frac{2}{5}\log\frac{2}{5} - \frac{3}{5}\log\frac{3}{5} \approx 0.97 \\ i_H(x_1=I) &= -\frac{2}{5}\log\frac{2}{5} - \frac{3}{5}\log\frac{3}{5} \approx 0.97 \\ \Delta(x_1) &= i_H(y) - p(x_1=T)i_H(x_1=T) - p(x_1=I)i_H(x_1=I) \\ &= 0.97 - \frac{1}{2}\cdot 0.97 - \frac{1}{2}\cdot 0.97 \\ &= 0 \end{aligned}$$

Split 1, test x_2:

$$
\begin{aligned}
p(x_2 = M) &= \frac{4}{10} \qquad p(x_2 = P) = \frac{6}{10} \\
p(y = W|x_2 = M) &= \frac{2}{4} \qquad p(y = L|x_2 = M) = \frac{2}{4} \\
p(y = W|x_2 = P) &= \frac{2}{6} \qquad p(y = L|x_2 = P) = \frac{4}{6} \\
i_H(x_2 = T) &= -\frac{2}{4}\log\frac{2}{4} - \frac{2}{4}\log\frac{2}{4} = 1.0 \\
i_H(x_2 = I) &= -\frac{2}{6}\log\frac{2}{6} - \frac{4}{6}\log\frac{4}{6} \approx 0.92 \\
\Delta(x_2) &= i_H(y) - p(x_2 = M)i_H(x_2 = M) - p(x_2 = P)i_H(x_2 = P) \\
&= 0.97 - \frac{4}{10}\cdot 1.0 - \frac{6}{10}\cdot 0.92 \\
&= 0.018
\end{aligned}
$$

Split 1, test x_3:

$$
\begin{aligned}
p(x_3 = S) &= \frac{5}{10} \qquad p(x_3 = C) = \frac{5}{10} \\
p(y = W|x_3 = S) &= \frac{3}{5} \qquad p(y = L|x_3 = S) = \frac{2}{5} \\
p(y = W|x_3 = C) &= \frac{1}{5} \qquad p(y = L|x_3 = C) = \frac{4}{5} \\
i_H(x_3 = S) &= -\frac{3}{5}\log\frac{3}{5} - \frac{2}{5}\log\frac{2}{5} \approx 0.97 \\
i_H(x_3 = C) &= -\frac{1}{5}\log\frac{1}{5} - \frac{4}{5}\log\frac{4}{5} \approx 0.72 \\
\Delta(x_3) &= i_H(y) - p(x_3 = S)i_H(x_3 = S) - p(x_3 = C)i_H(x_3 = C) \\
&= 0.97 - \frac{5}{10}\cdot 0.97 - \frac{5}{10}\cdot 0.72 \\
&= 0.125
\end{aligned}
$$

Split 1: We would split on x_3 since it yields the highest information gain.

$$
\begin{tikzcd}
& x_3 \arrow[dl, dash, "S"'] \arrow[dr, dash, "C"] & \\
(3,2) & & (1,4)
\end{tikzcd}
$$

Programming Task

Problem 5: Load the notebook `exercise_02_notebook.ipynb` from Piazza. Fill in the missing code and run the notebook. Export (download) the evaluated notebook as PDF and add it to your submission.

Upload a single PDF file with your homework solution to Moodle by 27.10.2019, 23:59 CET. We recommend to typeset your solution (using LaTeX or Word), but handwritten solutions are also accepted. If your handwritten solution is illegible, it won't be graded and you waive your right to dispute that.

Note: We suggest that you use Anaconda for installing Python and Jupyter, as well as for managing packages. We recommend that you use Python 3.

For more information on Jupyter notebooks, consult the Jupyter documentation. Instructions for converting the Jupyter notebooks to PDF are provided within the notebook.

See the solution notebook `exercise_solution_02_notebook.html`.

In-class Exercises

There are no additional in-class exercises this week.