Machine Learning Exercise Sheet 2

k-Nearest Neighbors and Decision Trees

Exercise sheets consist of two parts: In-class exercises and homework. The in-class exercises will be solved and discussed during the tutorial. The homework is for you to solve at home and further engage with the lecture content. There is no grade bonus and you do not have to upload any solutions. Note that the order of some exercises might have changed compared to last year's recordings.

In-class Exercises

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.

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

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

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}?

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

P1

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

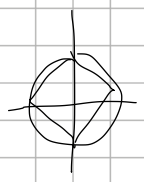
L_1 Norm: $\sum |u_i - v_i|$

L_2 Norm: $\sqrt{\sum (u_i - v_i)^2}$

	A	B	C	D	E	F	nn
A	0	1.5	1.5	4.5	7	6	B/C
B	1.5	0	3	4	6.5	5.5	A
C	1.5	3	0	3	5.5	4.5	C
D	4.5	4	3	0	2.5	3.5	E
E	7	6.5	5.5	2.5	0	1	F
F	6	5.5	4.5	3.5	1	0	E

c) different result

$L_2 < L_1$



	A	B	C	D	E	F	nn
A	0	1.12	1.5	3.20	5.15	4.74	A/B
B	1.12	0	2.24	3.16	4.61	4.03	A
C	1.5	2.24	0	2.24	4.61	4.5	A
D	3.2	3.16	2.24	0	2.5	2.69	C ✗
E	5.15	4.61	4.61	2.5	0	1	F
F	4.74	4.03	4.5	2.69	1	0	E

P2 $C = \{A, B, C\}$ $N_A = 16$ $N_B = 32$ $N_C = 64$ kNN $k = 112$

a) All new data will be classified as class C

b) —

P3 Scaling problem, data are not on the same scaling ← normalization data standardization $x = \frac{x - \mu}{\sigma}$

Too much features → high dim → space is empty ← dimensionality reduce

bad hyperparameter ← optimize hyperparameters

Mix-data ← data split

Data set different distribution ← reshuffle data

too less training set ← collect more data / data augmentation

① NO, DT can handle different scaling problem

②

③ NO, DT has no parameters

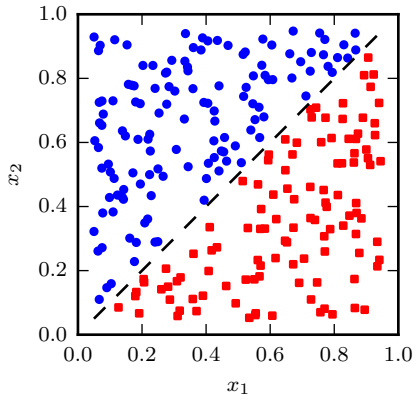
Problem 3: Assume you use a KNN-classifier on the following training data, that contains at least 100 samples of each class.

Acceleration	max. velocity [km/h]	PS	cylinder capacity [cm^3]	weight [kg]	class
3.6	250	600	3996	2150	car
12.5	178	150	1968	2001	van
3.5	200	113	937	227	motorcycle
...	...	...	...	...	...

You observe that the obtained model performs poorly on the test set. What might be the problem? Name at least two possible problems and explain how you would solve them. Would a decision tree have the same problems? Justify your answer.

Decision Trees

Problem 4: 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.



Problem 5: 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.

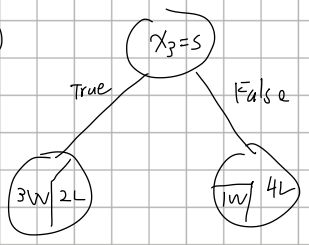
No.	x_1 (Team or Individual)	x_2 (Mental or Physical)	x_3 (Skill or Chance)	y (Win or Lose)
1	T	M	S	W
2	I	M	S	W
3	T	P	S	W
4	I	P	C	W
5	T	P	C	L
6	I	M	C	L
7	T	M	S	L
8	I	P	S	L
9	T	P	C	L
10	I	P	C	L

P4. No, DT can only create vertical and horizontal linear boundary
can maximally approximate 100% but can't reach it

P5. $i_H(y) = -\sum \pi_{Ci} \cdot \log_2(\pi_{Ci})$

$= -\left(\frac{4}{10} \cdot \log_2\left(\frac{4}{10}\right) + \frac{6}{10} \log_2\left(\frac{6}{10}\right) \right) = 0.97$

b)



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

$\Delta i = i - p_L\, i(t_L) - p_R i(t_R)$

① x_1

$\Delta i = 0.97 - \frac{1}{2} \cdot 0.97 - \frac{1}{2} 0.97 = 0$

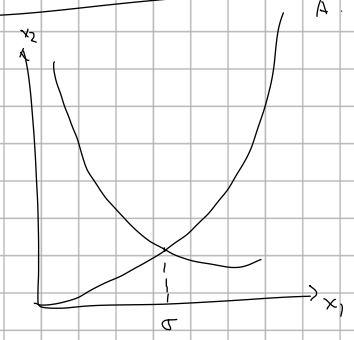
② x_2

$\Delta i = 0.97 - \frac{2}{5} \cdot 1 - \frac{3}{5} \cdot 0.92 = 0.018$

③ x_3

$\Delta i = 0.97 - \frac{1}{5} \cdot 0.97 - \frac{1}{2} \cdot 0.72 = 0.125$

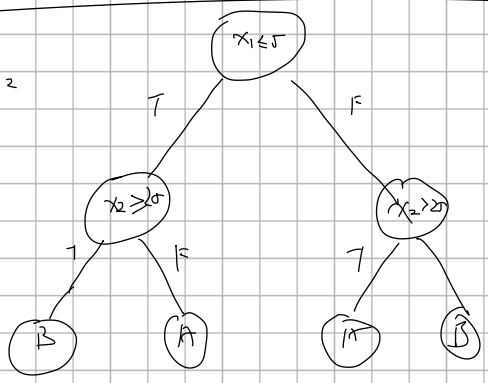
P6



A.

$\frac{125}{i} = i^2$

$i = 5$



Only 1 point are misclassified

$i = 5$

P7

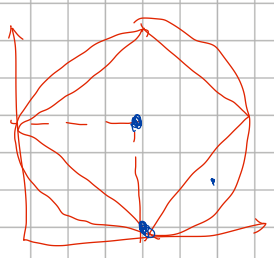
$d_2^2 = \sum (x_i - y_i)^2$

$= \sum |x_i - y_i||x_i - y_i| \le \sum |x_i - y_i||x_i - y_i| + \sum_i \sum_{i \neq j} |x_i - y_i||x_j - y_j|$

$= \left| \sum (x_i - y_i) \right|^2$

$d_2^2(x,y) \le = d_1^2(x_1, y_1)$

P8 Because ~~$d_2(x,y) \le d_1(x,y)$~~



$y = (0,0)$

$x_1 = (0,-1)$

$x_2 = (0.5, -0.65)$

x_1 是 L1 的 NN，在 L_1

x_2 是 L2 的 NN，在 L_2

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

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

Problem 6: Assume you have a dataset with two-dimensional points from two different classes C_1 and C_2. The points from class C_1 are given by $A = \{(i, i^2) \mid i \in \{1...100\}\} \subseteq \mathbb{R}^2$, while the points from class C_2 are $B = \{(i, \frac{125}{i}) \mid i \in \{1...100\}\} \subseteq \mathbb{R}^2$.

Construct a decision tree of minimal depth that assigns as many data points as possible to the correct class. Provide for each split the feature and corresponding thresholds. How many and which datapoints are missclassified?

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1 Homework

Problem 7: You want to perform 1-kNN-classification based on

i) L_1-norm

ii) L_2-norm

Prove or disprove: The L_2-distance $d_2(\boldsymbol{x}, \boldsymbol{y}) = \left(\sum_{i=1}^{d}(x_i - y_i)^2\right)^{\frac{1}{2}}$ between two points $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$ is always smaller or equal than the L_1-distance $d_1(\boldsymbol{x}, \boldsymbol{y}) = \sum_{i=1}^{d} |x_i - y_i|$.

Problem 8: Prove or disprove: Consider two arbitrary points $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^2$. If $\boldsymbol{x}$ is the nearest neighbor of $\boldsymbol{y}$ regarding the L_2-norm then $\boldsymbol{x}$ is the nearest neighbor of $\boldsymbol{y}$ regarding the L_1-norm.

Programming Task

Problem 9: Load the notebook `exercise_02_notebook.ipynb` from Moodle. Fill in the missing code and run the notebook.

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.