Machine Learning Homework Sheet 1

k-Nearest Neighbors and Decision Trees

1 Dataset

You are free to do the following exercises completely by hand or use a computer to help speed things up (e.g., using Python). You should, however, show the basic steps of your work and implement your own "helpers" instead of blindly using existing implementations. Using a machine learning toolbox and copying the result will not help you understand the material.

The table below gives you a feature matrix $\boldsymbol{X}$ together with the targets $\boldsymbol{y}$, where each row i represents one sample. This data is also available on Piazza as `homework_01_dataset.csv`. The column with names for each datapoint i can help you reference specific data points.

i	$x_{i,1}$	$x_{i,2}$	$x_{i,3}$	y_i
A	5.5	0.5	4.5	2
B	7.4	1.1	3.6	0
C	5.9	0.2	3.4	2
D	9.9	0.1	0.8	0
E	6.9	-0.1	0.6	2
F	6.8	-0.3	5.1	2
G	4.1	0.3	5.1	1
H	1.3	-0.2	1.8	1
I	4.5	0.4	2.0	0
J	0.5	0.0	2.3	1
K	5.9	-0.1	4.4	0
L	9.3	-0.2	3.2	0
M	1.0	0.1	2.8	1
N	0.4	0.1	4.3	1
O	2.7	-0.5	4.2	1

2 Decision Trees

Problem 1: Build a decision tree T for your data $\{\boldsymbol{X}, \boldsymbol{y}\}$. Consider all possible splits for all features and use the Gini index to build your tree. Build the tree only to a depth of two! Provide at least the value of the final Gini index at each node and the distribution of classes at each leaf.

Let $T^1, T^2, \ldots$ denote the "versions" of the whole tree generated by iteratively adding nodes and T_i denote the subtree of T that has node i as root node. Furthermore, let $i(T_i)$ be the Gini index of the distribution $\boldsymbol{n_i}$ at a node i. We write $\text{Gini}(n_0, n_1, n_2)$ as a shorthand for individual class occurrences.

Upload a single PDF file with your solution to Moodle by 29.10.2018, 9:59am CET. We recommend to typeset your solution (using LaTeX or Word), but handwritten solutions are also accepted.
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$$i(T_i) = \text{Gini}(\boldsymbol{n_{i0}}, \boldsymbol{n_{i1}}, \boldsymbol{n_{i2}}) = 1 - \left(\frac{\boldsymbol{n_{i0}}}{\boldsymbol{n_{i0}} + \boldsymbol{n_{i1}} + \boldsymbol{n_{i2}}}\right)^2 - \left(\frac{\boldsymbol{n_{i1}}}{\boldsymbol{n_{i0}} + \boldsymbol{n_{i1}} + \boldsymbol{n_{i2}}}\right)^2 - \left(\frac{\boldsymbol{n_{i2}}}{\boldsymbol{n_{i0}} + \boldsymbol{n_{i1}} + \boldsymbol{n_{i2}}}\right)^2$$

For each feature, we use the values that occur in the data, but exclude the maximum as a potential splitting value e.g. x_1 can be split on $0.4, 0.5, \ldots, 7.4, 9.3$.

Before splitting: $\boldsymbol{n}_0 = (5, 6, 4)$ $i(T_0) = \text{Gini}(5, 6, 4) \approx .658$

After splitting at $x_1 \leq 4.1$:

Left $\boldsymbol{n}_L = (0, 6, 0)$ $i(T_L) = \text{Gini}(0, 6, 0) \approx .000$ $p_L = \frac{6}{15}$

Right $\boldsymbol{n}_R = (5, 0, 4)$ $i(T_R) = \text{Gini}(5, 0, 4) \approx .494$ $p_R = \frac{9}{15}$

$$\Rightarrow \Delta i(x_1 \leq 4.1, T^1) = i(T_0) - p_L i(T_L) - p_R i(T_R) \approx .296$$

Node L is pure. $i(T_L) = .00$

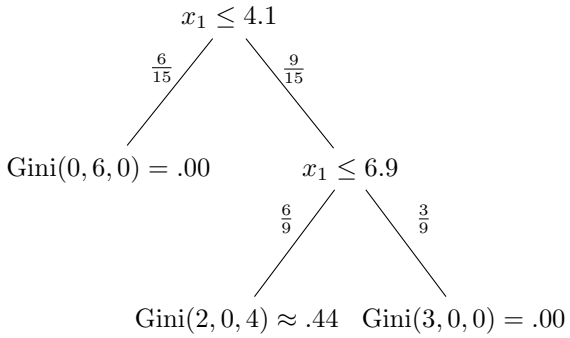
Split node R at $x_1 \leq 6.9$:

Left $\boldsymbol{n}_{RL} = (2, 0, 4)$ $i(T_{RL}) = \text{Gini}(2, 0, 4) \approx .444$ $p_{RL} = \frac{6}{9}$

Right $\boldsymbol{n}_{RR} = (3, 0, 0)$ $i(T_{RR}) = \text{Gini}(3, 0, 0) = .000$ $p_{RR} = \frac{3}{9}$

$$\Rightarrow \Delta i(x_1 \leq 6.9, T^2) = i(T_R) - p_{RL} i(T_{RL}) - p_{RR} i(T_{RR}) \approx .198$$

This leads to the final tree T^3 or T:



Problem 2: Use the final tree T from the previous problem to classify the vectors $\boldsymbol{x}_a = (4.1, -0.1, 2.2)^T$ and $\boldsymbol{x}_b = (6.1, 0.4, 1.3)^T$. Provide both your classification $\hat{y}_a$ and $\hat{y}_b$ and their respective probabilities $p(c = \hat{y}_a \mid \boldsymbol{x}_a, T)$ and $p(c = \hat{y}_b \mid \boldsymbol{x}_b, T)$

To classify $\boldsymbol{x}_a$ we use the path $0 - R$ to reach leaf R, similarly we reach leaf node LR by following $0 - L - LR$ for $\boldsymbol{x}_b$.

$$p(c = 1 \mid \boldsymbol{x}_a, T) = 1 \Rightarrow y_a = 1$$

$$p(c = 2 \mid \boldsymbol{x}_b, T) = \frac{2}{3} \Rightarrow y_b = 2$$

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3 k-Nearest Neighbors

Problem 3: Load the notebook `homework_01_notebook.ipynb` from Piazza. Fill in the missing code and run the notebook. Convert the evaluated notebook to PDF and add it to the printout of your homework.

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 `homework_solution_01_notebook.html`.

Problem 4: Classify the two vectors $\boldsymbol{x}_a$ and $\boldsymbol{x}_b$ given in Problem 2 with the k-nearest neighbors algorithm. Use $k = 3$ and Euclidean distance.

Let $\boldsymbol{x}_A \dots \boldsymbol{x}_O$ denote the training sample points in the order given. (The index is given in the table as well.)

We compute the distances of all training points to the given vectors with

$$d(\boldsymbol{u}, \boldsymbol{v}) = \textstyle\sum_i |u_i - v_i|$$

Nearest neighbors of $\boldsymbol{x}_a = (4.1, -0.1, 2.2)^T$:

I	0.671	0
C	2.184	2
O	2.474	1
A	2.759	2
...		

$\Rightarrow \mathcal{N}_3(\boldsymbol{x}_a) = \{C, I, O\}$

$\mathcal{N}_3(\boldsymbol{x}_a)$ produces a tie.
Tie-breaking: randomly assign a class, use the next neighbor as a tie-breaker, ... With the latter: $y_a = 2$.
Note: In tasks where you prefer not to make a prediction if the certainty of your prediction is low, you could also return "unassigned" if $p(y \mid \boldsymbol{x}, \mathcal{M}) < t$ (the probability of your prediction given your model $\mathcal{M}$ is below a certain threshold.)

Nearest neighbors of $\boldsymbol{x}_b = (6.1, 0.4, 1.3)^T$:

E	1.175	2
I	1.746	0
C	2.119	2
B	2.733	0
...		

$\Rightarrow \mathcal{N}_3(\boldsymbol{x}_b) = \{C, E, I\}$

$$y_b = 2,\ p(y_b \mid \boldsymbol{X}, k = 3) = \frac{2}{3}$$

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Problem 5: Now, consider y_i to be real-valued targets rather than classes. Perform 3-NN regression to label the vectors from Problem 2.

$$y_a = \frac{1}{\mathcal{C}} \sum_{i \in \mathcal{N}_3(\boldsymbol{x}_a)} \frac{y_i}{\mathrm{d}(\boldsymbol{x}_a, \boldsymbol{x}_i)} = \frac{1}{\frac{1}{0.671} + \frac{1}{2.184} + \frac{1}{2.474}} \times \left(\frac{0}{0.671} + \frac{2}{2.184} + \frac{1}{2.474} \right) \approx 0.561$$

$$y_b \approx 1.396$$

Problem 6: Look at the data. Which problem do you see w.r.t. building a Euclidean distance-based k-NN model on $\boldsymbol{X}$? How can you compensate for this problem? Does this problem also arise when training a decision tree?

The standard deviations of features are $\sigma_1 \approx 2.99, \sigma_2 \approx .37, \sigma_3 \approx 1.41$. The scale of the second feature is very low and has little influence on the overall result. When using k-NN, useful class-specific information in this feature will be lost.
This can be compensated by rescaling all features with their respective scale either by standardizing the features or using Mahalanobis distance.
Decision trees are scale-invariant.