Homework 3: *k*-Nearest Neighbours and Naïve Bayes

Part 1

Question 1.b.

The output_knn.txt file contains the accuracy, precision and recall metrics for the different values of k, after predictions are made on the test set. However, the value of k should be chosen based only on the training set as this would cause overfitting. One way to choose k in this case is by performing bootstrapping on the training data set. It will be split into two data subsets; one will act as the internal training dataset and the other as an internal testing dataset. Accuracy will be computed on the internal test set using the internal training dataset for different values of k. The splitting and accuracy calculations will be performed multiple time. The k with obtaining the highest accuracy on average from the different steps will be chosen.

Question 1.c.

Assuming data have been loaded and considering the *k*-NN algorithm is an instance based learning algorithm, all computation happens in the prediction phase, therefore both the time complexity is O(1). If storage of the data is done during this step the space complexity would be O(n), where n is the number of samples in the training dataset. If this is done only during the prediction step, the space complexity would also be O(1).

Question 1.d.

In the case of a problem with *c* classes, where c>2, the time or the space complexity of the prediction step does not change noticeably compared to the case in which the problem has two classes. The only difference consists in the use of a larger vector (or more than two variables) to store the number of neighbours in the *c* classes when predicting the label of a sample from the test set. This difference in complexity is very small when compared to the one for two classes.

Question 1.e.

Yes, *k*-NN works with other metrics and with semi-metrics as well. The choice of distance measurement affects which are the k-nearest neighbours. The goal of the algorithm is to find the entries in the training set that are most similar to the one for which you are trying to predict the label. This can be attained using other metrics like Manhattan distance or similarity measures such as DTW, so *k*-NN would work using these. In the case a more efficient running time would want to be achieved by exploiting the triangle inequality, this would not be accessible for k-NNs using semimetrics.

Question 1.f.

Yes, it is possible to use *k*-NN for regression as well. Instead of having a class as the output, a value for the measurement will now by computed: y’. These would be done by averaging the measurements of the k nearest neighbours to the new data point x’.

Part 2

Question 2.a.

As shown in the submitted script, the label predicted for the given sample is 2.

Question 2.b.

The missing data can affect the computation of the probabilities in different ways depending on the value of the missing entry. If it was different from the one for which the probability is being calculated than the resulting probability in Figure 4 is higher than expected (it would be divided by a higher number => lower probability). In the case the missing entry would have taken the value for which the probability is calculated than the result in Figure 4 is lower than expected.

Question 2.c.

To avoid the ‘zero-frequency’ problem for attributes that do not occur with every class, the constant 1 can be added to all attribute value-class combination. Alternatively, another non-negative constant different than one can be used depending on what best suits the problem. In this way, $P(Xj = xj|Y = yi)$ will never be 0 for a given i and j.

Part 3

Question 3.a.

To calculate the probability the bowl 1 was selected given a vanilla brownie was drawn, we apply Bayes theorem. We denote P(B=1|F=V) as the posterior probability to be determined, where B is the bowl (takes value 1 or 2) and F is the flavour of the brownie (takes value V – vanilla or C - chocolate). According to Bayes theorem, P(B=1|F=V) = P(F=V|B=1) * P(B=1)/P(F=V), where the first term is the likelihood, the second one is the prior probability and the last one is the evidence. The likelihood can be calculated using the given data, 30 of the 40 brownies in the first bowl are vanilla flavoured so it is equal to 30/40. The prior probability, namely the probability of choosing bowl 1 is ½ as there are a total of two bowls with equal probability of them being chosen. The evidence, the probability of drawing a vanilla flavoured brownie regardless of the bowl is equal to the total number of vanilla brownies (30+20=50) divided by the total number of brownies (40+40=80), which is equal to 50/80. Now the posterior probability can be calculated: P(B=1|F=V) = P(F=V|B=1) * P(B=1)/P(F=V) = (30/40)*(1/2) / (50/80)= (15/40)/(50/80)= 3/5.

Question 3.b.

As detailed in the script attached (*nbayes_uber.py*), calculating the posterior probability requires the calculation of the likelihood, of the prior probability and of the evidence. The prior probability and the evidence do not change when N changes and they can be calculated using the formulas provided in the homework description: prior probability = 1/Nmax, evidence = the sum over all joint probabilities P(D,N) for all N in [D, Nmax]. Then, the likelihood is calculated separately for every N: 1/N. For all N higher than or equal to D, the posterior probability is calculated din the script. The maximum is attained for N=60, when the probability is 0.0059. All posterior probabilities can be seen in the appendix as well.

Appendix

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