

Assignment 3

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1 KNN

1.1 Methodology and notation

I randomly select 20% of data as test (TtD) and considered the rest as training data (TD). I select subsets of $p\%$ ($p \in P = \{20, 50, 80, 100\}$) from TD and generate 5 training sets for each of these subsets. The set of training sets is $TSS = \{TS_1, TS_2, TS_3, TS_4, TS_5\}$. It is these TS_i 's that I do n -fold cross validation on ($n \in N = \{2, 5, 10, |TS_i|\}$). Note that $|TS_i|$ stands for the cardinality of TS_i and that $|TS_i|$ -fold cross validation corresponds to leave one out cross validation.

Notationally, I carry out several cross validation runs. Each run uses a value of k ($k \in K$) for the KNN (the set K used is mentioned for each dataset in the following sections) and carries out n -fold cross validation on a particular TS generated using a particular percent subset of the TD. $R[p_a, t_b, n_c, k_d]$ refers to the run using the a^{th} indexed element of P , the b^{th} indexed element of TSS , the c^{th} indexed element of N and the d^{th} indexed element of K . For conciseness, in the remainder of the writeup, I often used the term “cross validation batch” to refer to sets of cross validation runs as determined by conditions on elements of P, T, N, K . For example, the n -fold cross validation batch is the set $B = \{R[p_a, t_b, n_c, k_d] \mid n_c = n, p_a \in P, t_b \in T, k_d \in K\}$. Cross validation batches are also often expressed by abusing Python's splicing notation for indexing. Thus, $B = R[:, :, n_c == n, :]$ or even more shorthand, $B = R[:, :, n, :]$.

Metric Learning: I use the metric-learn module (<https://github.com/all-umass/metric-learn>) as mentioned by a TA on piazza. I use the LMNN algorithm to learn a Mahalanobis distance metric.

Stability: Each run in the cross validation batch $R[p, :, n, k]$ has an average cross validation error. This is different for each cross validation run, even with the same p due to differing TS_i . Looking at the average cross validation error for each run as samples of a random variable, the stability (here tacitly assumed as the inverse of the variance) of the cross validation error gives some insight on the homogeneity of the dataset and I comment on this stability for each of the datasets. Intuitively, one would also expect the variance to decrease with increasing values of p , and thus, the stability to increase with increasing subset sizes used for cross validation runs. I see if this holds.

Selecting k : The training errors of each batch for a fixed k ($R[:, :, :, k]$) cannot simply be computed by averaging the training error of each run in the batch, as the runs are heterogeneous (are obtained from different values of p and n). Instead, I use the box-and-whisker's plot as suggested by a TA to eyeball a good k for the data-set.

Testing: Now, I train my KNN model using the “optimal” value of k using the entire TD, learning the suitable distance metric and use the trained model for computing the error on TtD. I compare this with the cross validated errors, determining which cross validation split (value of $n \in N$) had given an error that is most correlated with the error on the test data. The most correlated n also gives some subtle insight into the distribution of data for the dataset. Note that for Wine, I use the 20% split of the data (TtD) for testing, but for MNIST and office datasets, I use the separate testing data. In these two cases, I don't split the training data into test and train as the separate testing data implies no need for hold out testing from the training set itself (thus TD = all of training data, TtD = $\{\}$ for MNIST and office datasets).

1.2 Wine dataset

1.3 MNIST dataset

For MNIST, I used PCA to reduce dimensionality, retaining enough principal component vectors that explain 80% of the variance in the data. I feel this gives me a good balance between a performant algorithm and execution time. The plots for the errors for the two iterations are shown in Fig. ??.

1.4 Discussion

Notes to combine: For small dataset such as wine, especially when using a smaller subsampled dataset, k-fold cross validation is expected to be extremely noisy, more so for smaller k. In some extreme cases, it may be possible that a k-fold training set does not contain any data for one class, and thus, no testing data would be classified to that class. Alternatively, there could be lesser samples in training for a class than the value of 'k' and, in this case, the LMNN algorithms of metric-learn errors out — in this case, I've capped the range of k's tried to the minimum number of training data-points for any class.