02450 Project 2

Report

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Introduction to Machine Learning and Data Mining
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Abstract

The objective of this second report is to apply the methods you have learned in the second section of the course on „Supervised learning: Classification and regression” in order to solve both a relevant classification and regression problem for your data.

Clustering

We clustered our data containing letters with a set of their attributes using Gaussian Mixture Model as well as with Hierarchical clustering. We used cross-validation to estimate the optimal parameters for both algorithms. At the end we estimated the quality of both algorithms in terms of our true labels which are letters.

0.1 Gaussian Mixture Model (GMM)

For GMM algorithm we used double cross-validation to estimate the best number of components in internal loop and calculating quality score in external loop as an average of scores. We also applied Principal Component Analysis to visualize the results in more human friendly way. We used only a subset of our dataset for performance reasons, using random sampling. We can see the results in the figure 0.1 In an average the most optimal number of components choosed in internal cross-validation loop was 30. Which is a close to the number of actual classes. We can see how the quality of GMM clustering in terms of actual labels depends on the number of components in the figure 0.2 Cluster centers should be in ideal case (especially if we consider number of components equal to the number of actual classes - 26) an average vector

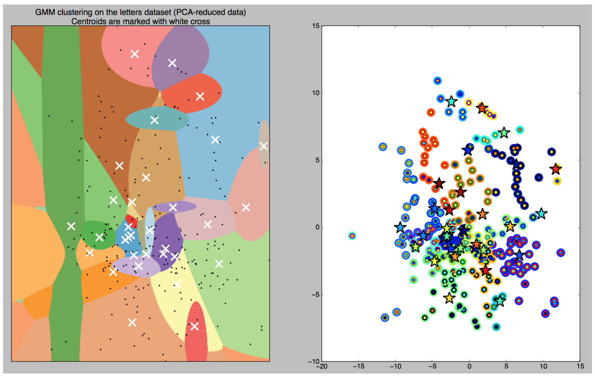


Figure 0.1: GMM - clustered (data reduced using PCA)

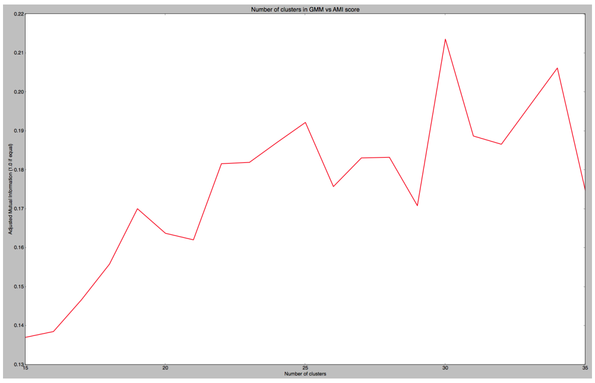


Figure 0.2: GMM - quality vs components count

from the attribute vectors corresponding to particular letters. So the centroids should correspond to some „unified" letters.

0.2 Hierarchical Clustering

We also used single cross-validation technique in Hierarchical Clustering and choose the best metric and linkage function from all available options. Score results are mesured for best performing option sets. We also used PCA to help visualize results (Figure 0.3 and Figure 0.4). Even using first two principal

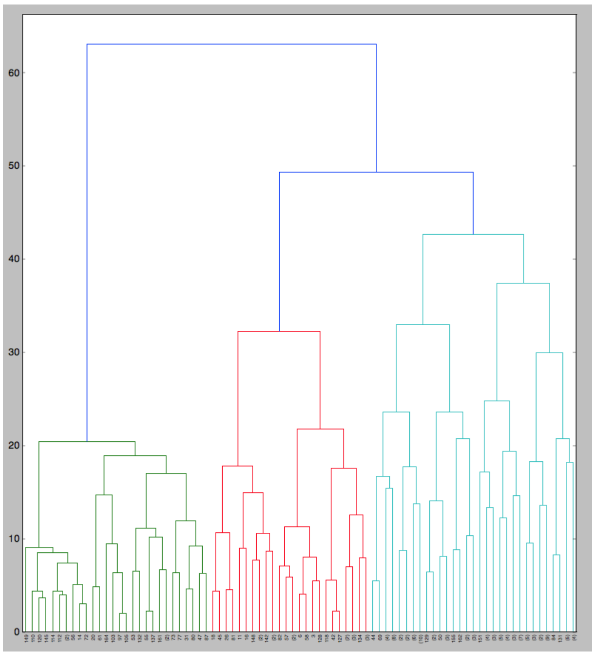


Figure 0.3: Hierarchical clustering (without PCA reduction)

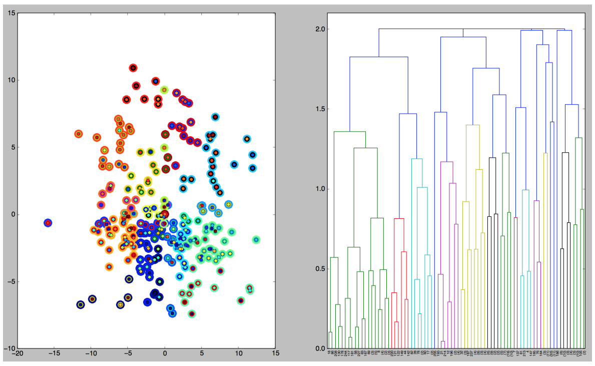


Figure 0.4: Hierarchical clustering (data reduced using PCA)

components explaining the most variance, results are dyrastically worse than when we use all data dimensions. The most commonly choosed options by the program were ('ward', 'euclidean') which means that the ward linkage function and euclidean metric were most suitable for our data.

0.3 Evaluation

We choosed an adjusted mutual info score metric as our quality messure for clustering methods. For two clusterings U and V, the AMI is given as:

$$AMI(U,V) = [MI(U,V) - E(MI(U,V))]/[max(H(U),H(V)) - E(MI(U,V))]$$

And has following properties:

1. Perfect labeling is scored 1.0
2. Independent labelings have non-positive scores
3. No assumption is made on the cluster structure
4. It is symmetric
5. It is independent of the absolute values of the labels: a permutation of the class or cluster label values won't change the score value in any way
6. It accounts for the fact that the MI is generally higher for two clusterings with a larger number of clusters, regardless of whether there is actually more information shared

Reaserch has shown that Hierarchical clustering performs better for our data than GMM and also that both methods have better scores while having more data. However it was impossible for performance reasons to run this methods on more than 3000 records of our data, where results would be even better. It is visualized in the figure 0.5

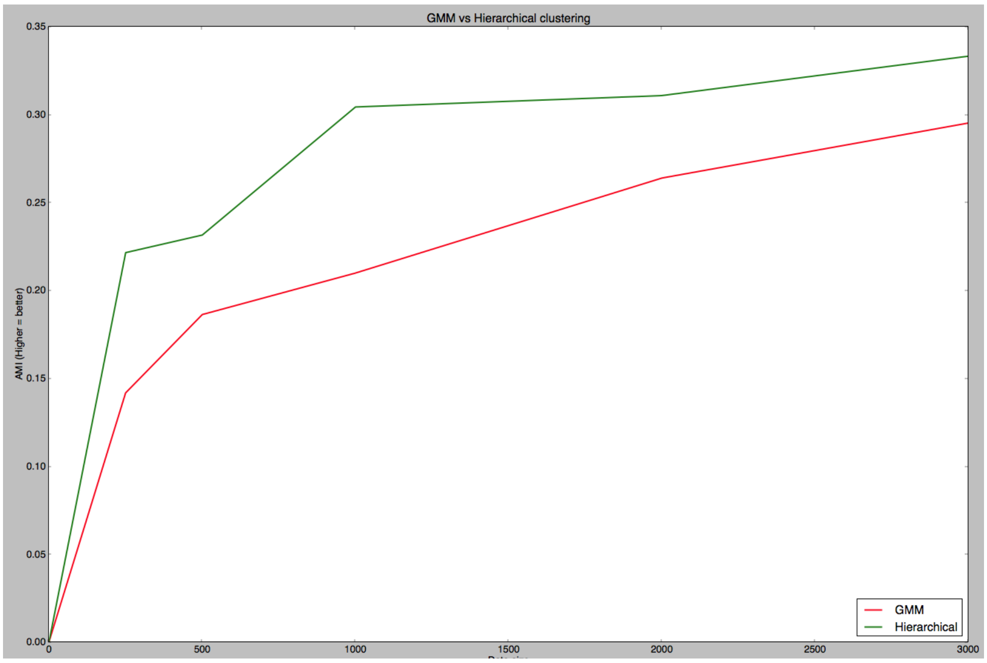


Figure 0.5: GMM vs Hierarchical clustering quality

Association Mining

Association rule learning is a popular and well researched method for discovering interesting relations between variables in large databases. We divide values of features into three categories: small values, medium values and high values and than we are going to do association mining for this three categories separately. So we have three different dataset and attributes are in set when they belong to that category. For instance if we consider the item set of smal values (from 1 to 4) we binarize our data by transforming the value of each attribute to 1 if it belong to the interval [1-4], and 0 otherwise. The medium values are defined from 5 to 7 while high values are defined from 8 to 16 and we binarized the data in the same way described above. For each item set we apply Apriori algorithm in order to find possible associations among the attributes.

The table below shows the best association rules found by the algorithm including its confidence percentage.

RULE	CONFIDENCE
Assiociations for HIGH values of attributes (from 8 to 16)	
xegvy → xy2br	62.96 %
xy2br → xegvy	74.62 %
yegvx → xy2br	72.00 %
xy2br → yegvx	72.64 %
yegvx → xegvy	76.39 %
xegvy → yegvx	65.03 %
Assiociations for MEDIUM values of attributes (from 4 to 7)	
x2ybr → width	67.53 %
width → x2ybr	60.37 %
width → x-box	63.67 %
x-box → width	82.51 %
high → width	80.93 %
width → high	69.55%
Assiociations for SMALL values of attributes (from 1 to 4)	
x-ege → onpix	76.01 %
onpix → x-ege	72.54 %
y-ege → onpix	78.07 %
onpix → y-ege	60.95 %
onpix → x-box	76.15 %
x-box → onpix	81.39 %
x-ege → x-box	68.88 %
x-box → x-ege	70.25 %

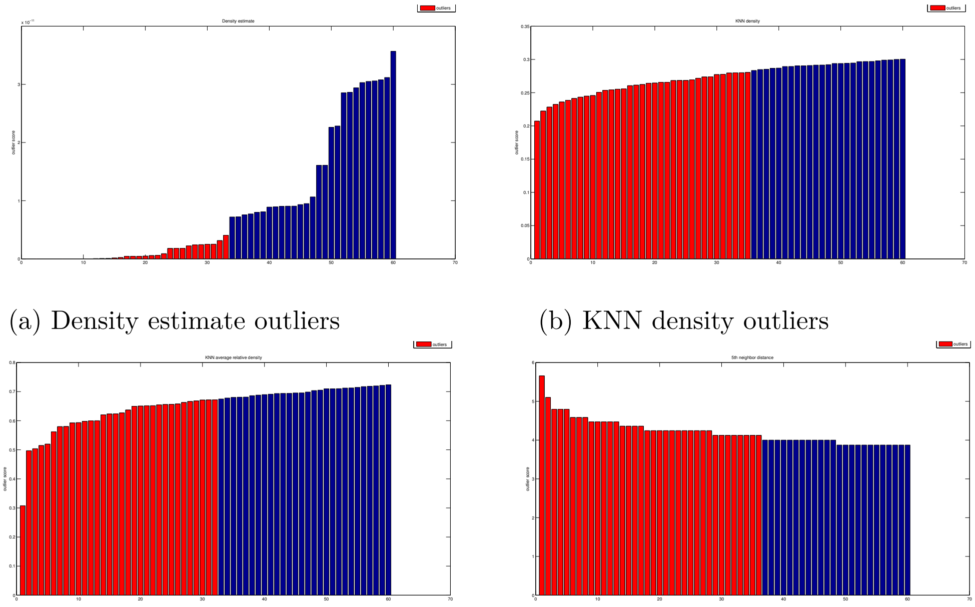
In the first report we computed correlation between attributes and we found out that the strongest correlation was between x-box and width (corr=0.85). Thus the results of Apriori confirms the findings from the our previous analysis ,in fact, the association for medium values of attributes x-box → width has the highest confidece.

Outlier / Anomaly detection

In statistics, an outlier is an observation point that is distant from other observations. For this reason we apply outlier / anomaly detection for each class of our dataset in order to consider which data for each class could be excluded from the data set. Below is shown an example of outlier detection applied to the subset that correspond to the letter 'A'. We calculate for all the samples the leave-one-out Gaussian Kernel density, KNN density, KNN average relative density and distance to K-th nearest neighbor for with K=5.
For each of the metrics, we sort the outlier scores and inspect their distribution. We set an outlier threshold where there is a significant "jump" in the scores, in order to have around 35 outliers (about 5% of the total samples). We consider only the outliers which are detected by all four methods, and in this way we obtain 4 outliers (about 0.5% of the samples). In the bottom table are specified our results:

Method	**Selected outliers (indices)**
Gaussian Kernel density	[495 741 311 133 159 51 18 399 86 739 136 566 515 423 2 227 760 285 489 152 149 572 655 688 469 114 124 762 130 638 327 645 307]
KNN density	[18 311 495 741 133 159 515 86 399 51 739 136 489 566 285 116 688 760 227 152 423 500 469 114 655 2 149 657 504 696 238 604 572 439 124]
KNN average relative density	[197 156 102 215 356 31 399 217 127 573 701 617 124 355 530 86 36 304 450 184 133 452 321 183 746 728 714 724 638 627 285 149]
Distance to 5th nearest neighbor	[18 311 116 515 741 399 439 500 86 133 230 495 739 159 292 489 657 51 132 136 152 238 284 285 390 438 604 688 57 114 212 227 504 566 655 696]
Common to all method	[51 86 739 688]

In figure 0.6 we represent one bar plot for each metrics. Each column is a pattern and the y-axis is the outlier score density (or distance for for 5th nearest neighbor). Red columns are patterns with lower outlier score (or highest for 5th nearest neighbor) that we decided to set as otliers.



(a) Density estimate outliers

(b) KNN density outliers

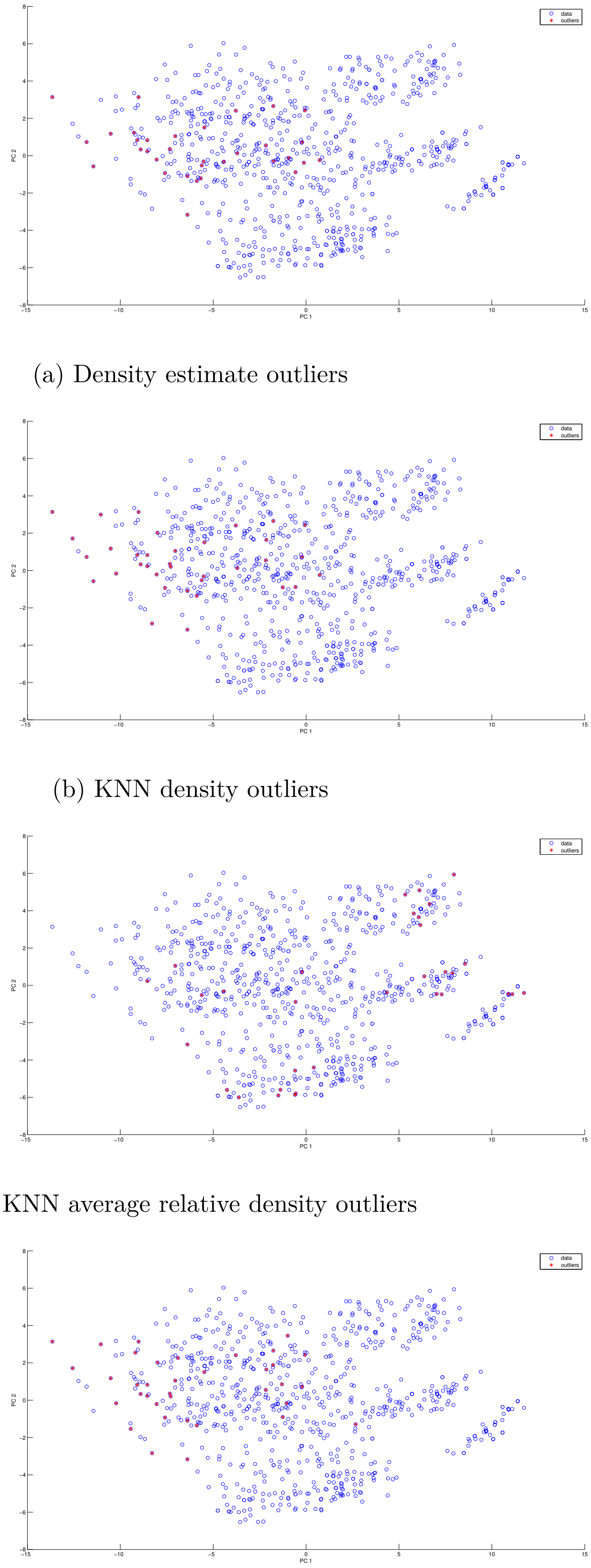
(c) KNN avg rel. density outliers

(d) 5th neighbor distance outliers

Figure 0.6: bar graph outliers

To further understand the outliers distribution, for each scoring method we plot the outliers in the PCA space. Figures 0.7 shows that is not really possible to see a pattern for outliers in the PC1/PC2 space (maybe it could be possible find only few of them). In figure 0.8 you can see the outliers detected by all four methods.

We applied outlier detection using different metrics, and by setting an appropriate threshold we identified some outliers, constituting about 0.5% of our dataset. Anyway we are never sure whether a certain pattern is an outlier but we can just suppose it especially because we have a wide dataset so is probable that some patterns are distant from other observations.



(a) Density estimate outliers

(b) KNN density outliers

(c) KNN average relative density outliers

(d) 5th neighbor distance outliers

Figure 0.7: Principal component plot with outliers

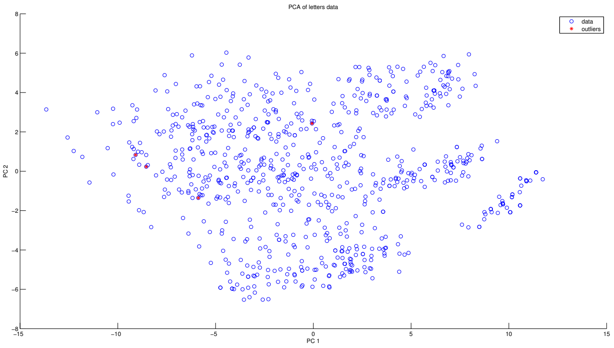


Figure 0.8: outliers detected by all four methods