

Comparison of Four Multi-Label Classification Methods

Abstract

Multi-label classification methods are closely related to modern real-world applications, including diseases diagnostics and genre classifications. Extending from the single-label classification techniques we learned in class, this project looks into four different methods (*Binary Relevance One-vs-all*, *Binary Relevance One-vs-one*, *Label Powerset*, *ML-kNN*) for multi-label classification by comparing the different methods theoretically as well as applying the methods to a real dataset on music and emotions. Through analyzing the results from real data analysis using four evaluation metrics (Accuracy, Precision, Hamming Loss, and Recall), we conclude that Binary Relevance One-vs-All method outperforms the other three methods whereas the ML-kNN method yields the worst performance.

Background and Significance

Traditional single-label classification methods associate each observation with only one class. In our statistics class, we focused on various techniques for single-label classification, including logistic regression, multivariate discriminant analysis, tree-based method, and support vector machines, etc. In real-world applications, however, an observation may be associated with more than one classes. For example, a patient may be diagnosed with multiple diseases at the same time; a song may belong to more than one genre; and a newspaper article may be classified into multiple categories. Thus, in this project, we focus on explaining and comparing four fundamental methods in multi-label classification through reading existing literatures and applying the methods in real data analysis.

Concept and Methodology

Multi-label classification techniques fall into two major categories -- *problem transformation* and *algorithm adaptation*. *Problem transformation* methods transform a multi-label classification dataset into one or more single-label classification datasets so that the classification problem will be further solved by single-label classifiers. *Algorithm adaptation* methods are extended from specific learning algorithms in order to handle multi-label data directly. Here, we introduce three problem transformation methods (*Binary Relevance One-vs-all*, *Binary Relevance One-vs-one*, and *Label Powerset*) and one algorithm adaptation method (*Multi-label k-Nearest Neighbor*).

Example	x_1	...	x_7	Adventure	Drama	Comedy
Game of Thrones	x_{11}	...	x_{17}	1	1	0
The Big Bang Theory	x_{21}	...	x_{27}	0	0	1
Rick and Morty	x_{31}	...	x_{37}	1	0	1
College Romance	x_{41}	...	x_{47}	0	1	1

Table 1

To exemplify these methods we will use the data set of Table 1. It consists of four TV shows that belong to one or more of the three classes: *adventure*, *drama*, and *comedy*. Having value 1 means the TV show is labeled with that class, having 0 means the TV is not labeled with that class. In addition, associated with each TV show are 7 variables (X_1 to X_7) that are used as predictor variables for fitting classification models.

1 Binary Relevance

Binary relevance methods convert a multi-label dataset into multiple single-label binary datasets. One technique under binary relevance is called One-vs-All (*BR-OvA*). The *BR-OvA* method transforms the dataset with k labels into k single-label datasets and fits a binary classifier for each label. In our example, *BR-OvA* method transforms the original dataset in Table 1 to what is shown in Table 2. Solution for each of the three dataset in Table 2 will be created according to single-label binary classification.

Another technique under binary relevance is called One-vs-One (*BR-OvO*). *BR-OvO* converts a multi-label dataset into several binary datasets, where each dataset contains two different labels. In our example, dataset transformation is shown in Table 3. Note that in a dataset, instances with both labels or none of the

Example	x_1	...	x_7	Adventure
Game of Thrones	x_{11}	...	x_{17}	1
The Big Bang Theory	x_{21}	...	x_{27}	0
Rick and Morty	x_{31}	...	x_{37}	1
College Romance	x_{41}	...	x_{47}	0

Example	x_1	...	x_7	Drama
Game of Thrones	x_{11}	...	x_{17}	1
The Big Bang Theory	x_{21}	...	x_{27}	0
Rick and Morty	x_{31}	...	x_{37}	0
College Romance	x_{41}	...	x_{47}	1

Example	x_1	...	x_7	Comedy
Game of Thrones	x_{11}	...	x_{17}	0
The Big Bang Theory	x_{21}	...	x_{27}	1
Rick and Morty	x_{31}	...	x_{37}	1
College Romance	x_{41}	...	x_{47}	1

Table 2

labels are removed, and the binary classifier solution is obtained from the rest of the dataset. When making prediction for a new instance, we use each binary classifier to choose one out of the two labels in a transformed dataset. Then we rank all the labels assigned to the instance according to the votes from the individual binary classifiers. Finally, we achieve multi-label classification through choosing the labels with higher ranking given a threshold.

Example	x_1	...	x_7	Adventure vs. Drama
Game of Thrones	x_{11}	...	x_{17}	
The Big Bang Theory	x_{21}	...	x_{27}	
Rick and Morty	x_{31}	...	x_{37}	Adventure
College Romance	x_{41}	...	x_{47}	Drama

Example	x_1	...	x_7	Drama vs. Comedy
Game of Thrones	x_{11}	...	x_{17}	Drama
The Big Bang Theory	x_{21}	...	x_{27}	Comedy
Rick and Morty	x_{31}	...	x_{37}	Comedy
College Romance	x_{41}	...	x_{47}	

Table 3

Example	x_1	...	x_7	Comedy vs. Adventure
Game of Thrones	x_{11}	...	x_{17}	Adventure
The Big Bang Theory	x_{21}	...	x_{27}	Comedy
Rick and Morty	x_{31}	...	x_{37}	
College Romance	x_{41}	...	x_{47}	Comedy

2 Label Powerset

The label powerset method converts a multi-label dataset to a single multi-class dataset by considering each label combination as a unique class. It achieves multi-label classification by assigning an instance to a class that consists of a set of labels. In our example, we give each unique label set a class ($C110$, $C001$, $C101$, $C011$). Then a multi-class classifier is trained to assign an instance to one of the above classes.

Example	x_1	...	x_7	Adventure	Drama	Comedy	Class
Game of Thrones	x_{11}	...	x_{17}	1	1	0	$C110$
The Big Bang Theory	x_{21}	...	x_{27}	0	0	1	$C001$
Rick and Morty	x_{31}	...	x_{37}	1	0	1	$C101$
College Romance	x_{41}	...	x_{47}	0	1	1	$C011$

Table 4

3 Multi-Label k-Nearest Neighbor (ML-kNN)

ML-kNN is an algorithm adaptation method that predicts if an instance should be labeled with label y_k based on whether a sufficient number of its k nearest neighbors are labeled with y_k . In particular, for an unknown instance x_t , the method predicts whether x_t has label y_k by comparing which of the following probabilities is higher: $P(x_t \text{ has label } y_k \mid \text{the number of } k\text{-nearest neighbors labeled } y_k)$ and $P(x_t \text{ does not have label } y_k \mid \text{the number of its } k\text{-nearest neighbors labeled } y_k)$. By applying Bayes' Theorem, the objective turns into a comparison between $P(x_t \text{ has label } y_k) * P(\text{the number of } k\text{-nearest neighbors labeled } y_k \mid x_t \text{ has label } y_k)$ and $P(x_t \text{ does not have label } y_k) * P(\text{the number of } k\text{-nearest neighbors labeled } y_k \mid x_t \text{ does not label } y_k)$, both of which could be easily calculated from the given data.

Real Data Analysis and Result

We used the dataset *emotions* that contains 593 instances, 72 independent variables and 6 labels. Each instance is a song clip, with 72 quantitative variables describing various music features, labeled with either one or more of the 6 labels indicating emotions evoked by the music, such as "amazed-surprised" and "happy-pleased". Initial data exploration suggests that there exists a high level of correlation among the 6 labels, as can be seen from the large number of label co-concurrences in Figure 2. We divided the original dataset into a train set containing 475 instances, and a test set containing 118 instances. Using the train set, we fit the four multi-label classifiers One-vs-All, One-vs-One, Label Powerset, and ML-kNN, and then compare the performance of these four models when applied on the test set. For the problem transformation methods, we used the default SVM classifier after the dataset is transformed into

single-label data, so the comparison across methods is fair. At the prediction stage, we used two different threshold methods: SCut threshold (Yang, 2001), which adjusts the threshold for each label to minimize MSE for the train set, and MCut threshold (Largeron, Moulin, & Gery, 2012), which determines a unique threshold for each instance based on the largest difference in ranked probabilities of the labels.

Here we define the four evaluation metrics for multi-label classification that we used when comparing the performance of the four models. Let D be a multi-label data set with $|D|$ instances, each having a set of labels Y_i ; let H be a classifier, and Z_i be the set of predicted labels for an instance x_i . Then

$$\text{Accuracy}(H, D) = \frac{1}{|D|} \sum_{i=1}^{|D|} \frac{|Y_i \cap Z_i|}{|Y_i \cup Z_i|}, \quad \text{Precision}(H, D) = \frac{1}{|D|} \sum_{i=1}^{|D|} \frac{|Y_i \cap Z_i|}{|Z_i|}, \quad \text{HammingLoss}(H, D) = \frac{1}{|D|} \sum_{i=1}^{|D|} \frac{|Y_i \Delta Z_i|}{|L|}, \quad \text{Recall}(H, D) = \frac{1}{|D|} \sum_{i=1}^{|D|} \frac{|Y_i \cap Z_i|}{|Y_i|}.$$

The Δ in hamming loss stands for XOR operation in boolean logic (Tsoumakas, 2007).

The results are summarized in the following table:

	Using Scut Threshold				Using Mcut Threshold			
	One vs All	One vs One	Label Powerset	ML-KNN	One vs All	One vs One	Label Powerset	ML-KNN
Accuracy	0.707	0.640	0.666	0.424	0.649	0.453	0.662	0.433
Precision	0.785	0.732	0.739	0.638	0.768	0.824	0.718	0.598
Recall	0.771	0.763	0.717	0.486	0.731	0.456	0.740	0.547
Hamming Loss	0.122	0.163	0.149	0.265	0.146	0.201	0.160	0.285

When SCut threshold is used, the One-vs-All classifier consistently performs the best in accuracy, precision, recall and hamming loss. One-vs-One classifier and Label Powerset yield similar results, with Label Powerset slightly outperforming in terms of accuracy, precision and hamming loss. ML-kNN method yields the worst result among the four classifiers, with the lowest accuracy, precision, recall and the highest hamming loss. When MCut threshold is used, the One-vs-All classifier still performs well with respect to all four metrics, yielding the highest precision and the lowest hamming loss. Label Powerset performs the best in accuracy and recall. ML-kNN method still yields the worst result compared to the other classifiers. However, it is noteworthy that the above comparison may be data dependent. If we use other multi-label datasets or other threshold criteria then the results may differ.

Conclusions and Future Work

In this paper we summarized four methods for multi-label classification (*Binary Relevance One-vs-all*, *Binary Relevance One-vs-one*, *Label Powerset*, *ML-kNN*) and compared their performance on a multi-label data set on emotions evoked by music. Binary Relevance method, specifically One-vs-all, yields the best result in the real data analysis, but has the drawback of neglecting correlation among labels. Label Powerset considers correlation between labels indirectly, but has the drawback of not including all possible label combinations in the model-fitting process, which leads to overfitting of the train set. ML-kNN performs the worst for the given dataset, but it has the advantage of producing a ranking of the labels. In the future we intend to fit the classifiers on more multi-label data sets and investigate how the classifiers perform differently on data sets with different features.

References

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Appendix

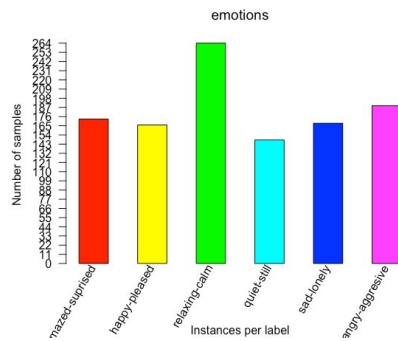


Figure 1: Number of instances for each label

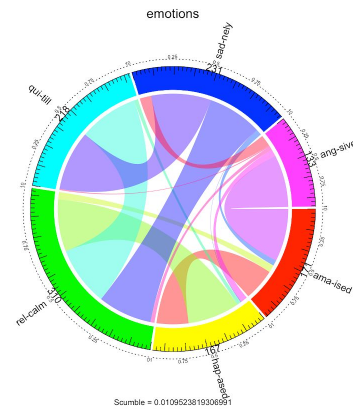


Figure 2: Label Co-Concurrence

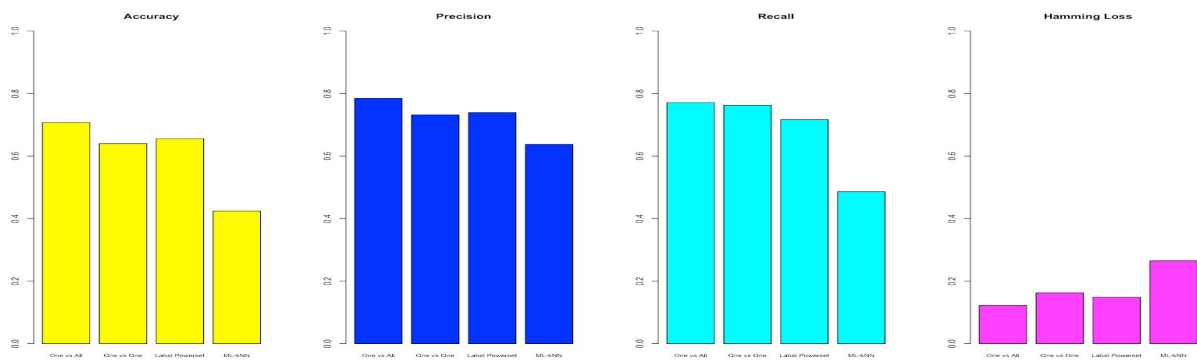


Figure 3: Performance of the four classifiers using Scut threshold

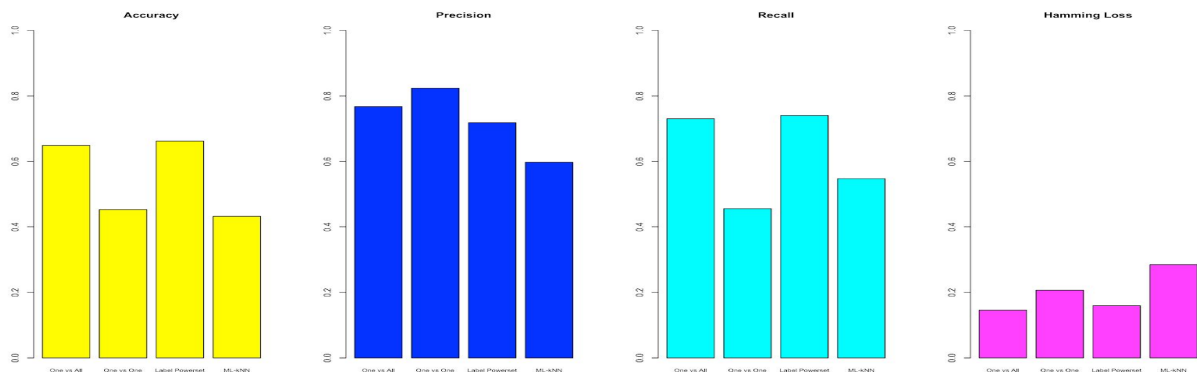


Figure 4: Performance of the four classifiers using Mcut threshold