

Extreme Multi-label Classification

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1. Introduction

Extreme classification is a multi-label classification problem that annotates a data point with the most relevant subset of labels from an extremely large label set. It has wide applications in diverse areas such as dynamic search advertising, text classification, and recommender systems. The main technical challenges include improving the prediction accuracy and reducing the training time, prediction time and model size. In this project, we perform extreme multi-label classification on EURLex-4K dataset [26], a collection of documents about European Union Law with 3993 categories. We first applied traditional multi-label algorithms as baseline. We further implemented embedding based models Principal Label Space Transformation (PLST) [34] and Sparse Local Embeddings for Extreme Multi-label Classification (SLEEC) [3], and innovatively modify existed algorithms for desired property. We finally focus on one of the leading one-vs-all based extreme classifiers Partitioned Label Trees (Parabel) [30]. We use label ranking average precision (LRAP) as our evaluation metric to assess label ranking performance. We also record training times to evaluate model efficiency. The result shows that the Parabel [30] model achieves the highest LRAP score with the fastest training time among all algorithms we experimented.

2. Related Works

2.1. Traditional Multi-label Classifiers

Traditional algorithms for solving multi-label classification are mainly categorized into Problem Transformation and Algorithm Adaption [39].

Problem Transformation Methods This category of algorithms tackles multi-label learning problem by transforming it into well-established single-label problems (binary-class or multi-class) [39]. Representative transformations include (1) transforming to binary classification, such as Binary Relevance [4] and Classifier Chains [32], (2) transforming to label ranking, such as Calibrated Label Ranking [10], (3) transform to multi-class classification, such as

Random k-labelsets [15] (See further details in 3.2.1).

Algorithm Adaption Methods Opposite to Problem Transformation methods, the key idea of Algorithm Adaption methods is to adapt well-established popular machine learning algorithms, usually by changing the cost functions, so that the adapted algorithms can fit the multi-label data [39]. Representative methods include Multilabel-KNN [40], Multilabel-Decision Tree [8], Rank-SVM [9], and Collective Multi-Label Classifier [11].

2.2. Extreme Multi-label Classifiers

However, when it comes to extreme multi-label classification, there emerge problems of data scalability and sparsity [25]. Data scalability problem comes from the rapidly increasing training examples, dimensionality and the number of class labels, whereas sparsity raises challenges to extract correlations among labels.

Over the years, researchers have developed more carefully designed algorithms to deal with such extremeness, most of which are based on trees [1, 17, 20, 29, 31], embeddings [3, 6, 7, 24, 33, 3, 36] and One-vs-All approaches [2, 25, 27, 37, 30]. For this project, we focus on embedding-based and One-vs-All extreme classifiers, and interpret how they successfully deal with scalability and sparsity.

Embedding Based Embedding based extreme multi-label classifiers are based on Label Space Dimension Reduction (LSDR), which assumes that the training label matrix is low-rank, and reduces the effective number of labels by projecting the high dimensional label vectors into a low dimensional linear subspace [3]. LSDR has been an effective and efficient paradigm in extreme multi-label classification [34, 14]. Popular LSDR algorithms include Singular Value Decomposition [12], Locality Preserving Projections [13], Multi-label informed Latent Semantic Indexing [38] etc. Due to different objective functions and optimizing routines, these compression algorithms differ in performances and scalability.

One-vs-All (OvA) OvA method learns weights corresponding to each individual label, and distinguishes the label from the rest. The OvA framework is empirically one of the best solutions for extreme multi-label classification

due to its high accuracy. However, the framework greatly suffers from training and prediction inefficiency, since the great amount of labels yields extremely large model size and training complexity. Recent works have been trying to improve efficiency through various methods. Distributed Sparse Machines (DiSMEC) [2] adds a step on top of model training to predict sparsity for each weight parameter and keeps only non-trivial parameters. This solution successfully controls model size without sacrificing prediction accuracy, and its parallel training system reduces the training time. Partitioned Label Trees (Parebel) [30] adopts a tree-structure for model training steps instead of linear loops, which significantly improves the training and predicting efficiency. Scalable Linear Extreme Classifiers (SLICE) [16] solves extreme classification problems with low dimensional dense feature space. It reduces training sample size by negative sampling, approximates a conditional distribution from generative models, and learns linear classifiers for each label using MAP. All these works have been proved successful on the EURLex-4K dataset [26] and has been applied to constructing industry solutions.

3. Problem Definition and Algorithm

3.1. Task

In this project, we performed extreme multi-label classification on the EURLex-4K dataset. We formularized this task as follows¹. Define $\mathcal{X} = \mathbb{R}^d$ as the d -dimensional input space, $\mathcal{Y} = \{y_1, y_2, \dots, y_{|L|}\}$ as the output space with $|L|$ possible class labels, and hypothesis space as \mathcal{H} . Our task of multi-label learning is to learn a function $h \in \mathcal{H}$, $h : \mathcal{X} \rightarrow 2^{\mathcal{Y}}$ from the multi-label training set $\mathcal{D} = (X, Y) = \{(x_i, y_i) \mid 1 \leq i \leq N\}$. For each multi-label example (x_i, y_i) , $x_i \in \mathcal{X}$ is a d -dimensional feature vector, and $y_i \subseteq \mathcal{Y}$ is the set of labels associated with x_i . For a test point $x \in \mathcal{X}$, the multi-label classifier $h(\cdot)$ predicts $h(x) \subseteq \mathcal{Y}$ as the set of proper labels for x .

3.2. Algorithms

3.2.1 Problem Transformation Models

Binary Relevance (BR) Binary Relevance [4] decomposes the multi-label problem into $|L|$ independent binary classification problem, where every binary classifier corresponds to one label. However, this approach doesn't take correlations between labels into consideration.

Classifier Chains (CC) Classifier Chains [32] transforms multi-label learning problem into a chain of binary classification problems, where subsequent binary classifiers are built upon the predictions of preceding ones. CC has the advantage of exploiting label correlation, while losing parallelization ability due to its chain property.

¹The definition is adopted from reference paper [39]

Label Powerset (LP) LP [15, 35] transforms a multi-label problem into a multi-class problem with one multi-class classifier trained on all unique label combinations found in the training data. This approach suffers from inefficiency and incompleteness, as the number of label sets could be exponentially large, and all random label sets comes from the training set and leads to poor generalization performance.

We combine these problem transformation techniques with Logistic Regression, Decision Tree, Random Forest, SVM and XGBoost [5]. Altogether, we have 15 models.

We also apply inherent multiclass classifiers like multi-layer perceptron (MLP), K Neighbors Classifier (KNN), and Random Forest Classifier (RF) to the dataset.

3.2.2 Principal Label Space Transformation (PLST)

Compared with traditional problem transformation methods in Section 3.2.1, PLST is faster and more effective as it captures key correlations among labels and reduces the number of needed classifiers significantly. During training, PLST projects standardized label vectors from high-dimensional label space into lower-dimensional space using Singular Value Decomposition (SVD) [12]. It then trains M linear ridge regressors $r(x)$ on each principal component. During prediction, it utilizes the projection matrix V_M to project predictions back to the original label space.

To capture complicated relations and further improve PLST performance, we **innovatively** replaced the linear Ridge Regression models by non-linear Decision Tree regressors to trade performance with computation efficiency.

Algorithm 1 Modified PLST algorithm

Input: Data $[(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)]$, Embedding Dimension M

Output: Predictions $[h(x_1), h(x_2), \dots, h(x_N)]$

/* **Training stage** */

Let $Z = [z_1 \dots z_N]^T$ with $z_i = y_i - \bar{y}$

Preform SVD on Z to obtain $Z = A\Sigma B$ with $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_N$. Let V_M contain the top rows of A .

for $i = 1$ **to** N **do**

 └ Encode (x_i, y_i) to (x_i, t_i) , where $t_i = V_M z_i$

Learn a **decision tree regressor** $r(x)$ from $\{(x_i, t_i)\}_{i=1}^N$

/* **Prediction stage** */

for $i = 1$ **to** N **do**

 └ Predict the label-set of an instance x by $h(x_i) = \text{round}(V_M^T r(x_i) + \bar{y})$

3.2.3 Sparse Local Embeddings for Extreme Multi-label Classification (SLEEC)

Unlike PLST which globally projects onto a linear low-rank subspace, SLEEC learns an embedding which captures

non-linear label relationships by preserving the pair-wise distance between only the closest rather than all label vectors [3]. SLEEC first partitions all the training points X into Q_1, Q_2, \dots, Q_C clusters by K-means [22]. Then for each cluster, SLEEC constructs a KNearestNeighbor graph Ω to capture pairwise distances. During training, it maps the label vectors y_i to M -dimensional vectors $t_i \in R^M$ and learns a set of regressors $V \in R^{M \times d}$ s.t. $t_i \approx Vx_i, \forall i$. During prediction, for an unseen point x , it first computes an embedding Vx and then performs kNN [21] over the set $[Vx_1, Vx_2, \dots, Vx_N]$.

We **innotatively** modified the SLEEC [3] algorithm to improve its performance and efficiency by: **1.** using KD-tree [28] to search for nearest neighbors to fight against curse of dimensionality; **2.** solving matrix completion problem with Alternating Least Square [19] instead of the Singular Value Projection [18] to learn low-rank embedding, which trades performance for computation efficiency; **3.** using Elastic Net [41] instead of L1 norm as regularization term for our multi-linear regressor to gain more robustness while controlling model complexity.

Algorithm 2 Modified SLEEC: Training algorithm

Input: Train Data (X, Y) , $X \in R^{N \times d}$, $Y \in R^{N \times L}$, Embedding Dimension M , Number of Neighbors \bar{n} , Number of Clusters C , Regularization Parameter for Elastic Net Regressor λ ,

Output: $[(Q_1, r_1, Z_1), (Q_2, r_2, Z_2), \dots, (Q_N, r_N, Z_N)]$
Partition (X, Y) into Q_1, Q_2, \dots, Q_C using K-means

for each partition Q_j do

```

/* Construct Nearest Neighbor Graph
*/
Form index set  $\Omega$  containing  $\bar{n}$  nearest neighbors using
KD-tree for each label vector  $y_i \in Q_j$ 
/* Label Space Dimension Reduction
*/
 $[UV] \leftarrow \mathbf{ALS}(P_\Omega(Y_j Y_j^T), M)$ 
 $Z_j \leftarrow UV$ 
Elastic-net Regressor  $r_j \leftarrow \mathbf{TRAIN}(X_j, Z_j, \lambda)$ 
 $Z_j = r_j(X_j)$ 
```

Algorithm 3 SLEEC: Testing algorithm

Input: Test point x , Number of Neighbors \bar{n} , Number of Desired labels p ,

Output: Predictions $h(x)$

$Q_c \leftarrow$ partition closest to x

$z \leftarrow r_c(x)$ where r_c is the regressor

$N_z \leftarrow \bar{n}$ nearest neighbors of $z \in Z^c$

$P_x \leftarrow$ empirical label distribution for points $\in N_z$

$h(x) \leftarrow \mathbf{TOP}_p(P_x)$

3.2.4 Partitioned Label Trees (Parabel)

While leading One-vs-All extreme classifiers achieve high prediction accuracies, their training and prediction costs are linear in the number of labels times instances. Parabel [30] is a logarithmic-time One-vs-All algorithm that efficiently learns a balanced label hierarchy using tree structure, where labels in the same leaf are most similar, and negative examples used for training One-vs-All label classifiers are drawn from those examples having labels in the same leaf. It is still one of the fastest algorithms among all leading extreme classifiers.

The algorithm of Parabel can be summarized as follows. It learns a small ensemble of 3 label trees, where each label tree is grown by recursively partitioning the labels into two balanced groups using constrained spherical k=2-means. Nodes become leaves when a minimum leaf size is reached. The leaf nodes contain linear One-vs-All classifiers, one for each label in the leaf, trained on only those examples having at least one leaf node label. At prediction time, a test point will traverse the label tree and reach multiple leaves, as each node learns two linear classifiers indicating whether the test point should be passed down to the left, right, or both children. The One-vs-All classifiers in these leaves are evaluated to determine the probability that the corresponding labels are relevant to the test point, and predictions are made by averaging these probabilities across trees.

4. Experiments

4.1. Data

The EUR-LEX website contains a collection of documents about European Union Law with categorization provided by the EUROVOC descriptors, which is a topic hierarchy with 3993 categories regarding different aspects of European laws. The data [26] we use in this project has already been preprocessed. The input features are TF-IDF representation of the documents with the first 5000 most frequent features after tokenization, stopwords removal, and stemming. The outputs are a set of labels encoded with value between 0 and 3992. There are 15511 examples in training set, and each example contains 5.32 labels on average.

4.2. Methodology

Preprocessed training, validation, and test set are given for this project. For all algorithms mentioned in Section 3.2, we perform grid search on multiple parameters on the training set, and choose the best model based on the prediction accuracy on validation set. For model selection and evaluation, we use Label Ranking Average Precision (LRAP) as the evaluation criteria, which measures the percentage of the true labels among the higher-ranked labels for each of the given samples. We also adopt a popular ranking evaluation metric precision@k, which describes the proportion of

recommended items in the top-k set that are relevant. Precision@k focuses more on the accuracy of the top k labels instead of averaged performance. As for the final model submitted on Gradescope, we choose the optimal model with best hyperparameter settings, train the model on both training and validation set together, and make predictions on the test set.

4.3. Results

We list models that give best LRAP scores from section 3.2.1 in Table 1. We compare original PLST results with our modified version in Table 2, and display comparison results between original SLEEC and modified version in Table 3.

Model	LRAP	Training time (s)
Parabel	0.6337	285.55
MLP	0.6041	4813.29
CC + RF	0.5647	17285.29
BR + RF	0.5593	19268.47
PLST	0.5028	20633.94
KNN	0.3936	466.44 ²
RF	0.2887	1244.80
LP+RF	-	Out of RAM

Table 1. Best validation model performance

Embedding Dimension	Original LRAP	Modified LRAP	Original Runtime (s)	Modified Runtime (s)
10	0.1512	0.1586	655.1667	472.3658
50	0.2640	0.2748	467.6908	2304.2881
100	0.3208	0.3391	874.6648	5381.154
500	0.4564	-	3995.0264	Out of time
2000	0.5028	-	20633.9433	Out of time

Table 2. PLST performance on full data

Model	Original SLEEC	Modified SLEEC
LRAP	0.3529	0.2584
Precision@1	0.5050	0.4200
Precision@3	0.4227	0.3467
Precision@5	0.3576	0.2752
Training time(s)	3267.44	2145.55

Table 3. SLEEC performance on 10% data

4.4. Discussion

In general, our experiment outcomes are in accordance with our expectations for each category of algorithms.

Parabel Parabel has the highest LRAP and least training time, which proves the effectiveness of OvA methodology class as well as the effectiveness of tree structure training. We adopt Parabel as the best solution for our problem for its outstanding performance in both accuracy and efficiency.

MLP After extensive hyperparameter tuning on hidden dimension, we used a MLP with a single 4300-dimensional

²KNN is a lazy learner, using training set in test phase rather than model generation.

hidden layer. It yields a decent LRAP score due to its complicated model structure compared to traditional methods, but it does take longer training time due to the wide network. This result is consistent with Leshno and Schocken’s theorem that a neural network with one huge hidden layer can uniformly approximate any continuous function on a compact set with a non-polynomial activation function [23].

Problem Transformation Methods Among the 15 combinations of problem transformation techniques and conventional classifiers, transformed Random Forest models stand out. "CC + RF" and "BR + RF" gives decent LRAP scores whereas "LP + RF" runs out of RAM. Compared with BR, CC gives higher score, which is consistent with the summary [39] that chain property would capture label dependence. However, these algorithms takes extremely long time to run, and has problem of scalability.

PLST From 2, higher label space embedding dimension tend to give better overall model performance. To further improve PLST performance, we innovatively replace the linear Ridge Regression models by non-linear Decision Tree regressors. It is able to improve Label Ranking Average Precision score by 0.6% to 1% under different parameter settings of our choice. However, this non-linearity trades performance with computation efficiency, increasing running time by approximately 5 times.

SLEEC Due to lack of necessary RAM and computing resources, we haven’t been able to run our python implementation of modified SLEEC on full data. Instead, performance results on 10% data are compared with original SLEEC performance. Our modifications yield higher computation efficiency by shortening running time by $\frac{1}{3}$, but result in worse overall ranking accuracy. This result gives us an intuition that algorithm design is more of an elaborate art than science.

Others Traditional adapted multi-label classifiers like Multi-label Random Forest and Multi-label-KNN yield very low LRAP due to their incapability of handling sparse data in extreme multi-label setting.

5. Conclusions

In this paper, we have reviewed different classes of methods to solve extreme multi-label classification problems. We implemented the representatives of each algorithm groups and conducted experiments on EURLex-4K for comparison of performance. The results stand perfectly with our expectations from methodology analysis. We also proposed minor innovations for two embedding methods, PLST and SLEEC, and proved the improvement of performance. Finally, we concluded that the leading extreme classification model Parabel performs the best on this dataset, as it stands out from other models for both accuracy and efficiency.

Reproductivity

Our codes and implementation could be found at:
https://github.com/TRokieG/Extreme_Multilabel_Classification

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