EEMC: Embedding Enhanced Multi-tag Classification

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The recently occurred representation learning make an attractive performance in NLP and complex network, it is becoming a fundamental technology in machine learning and data mining. How to use representation learning to improve the performance of classifiers is a very significance research direction. We using representation learning technology to map raw data(node of graph) to a low-dimensional feature space. In this space, each raw data obtained a lower dimensional vector representation, we do some simple linear operations for those vectors to produce some virtual data, using those vectors and virtual data to training multitag classifier. After that we measured the performance of classifier by F1 score(Macro% F1 and Micro% F1). Our method make Macro F1 rise from 28 % - 450% and make avergae F1 score rise from 12 % - 224%. By contrast, we trained the classifier directly with the lower dimensional vector, and measured the performance of classifiers. We validate our algorithm on three public data sets, we found that the virtual data helped the classifier greatly improve the F1 score. Therefore, our algorithm is a effective way to improve the performance of classifiers. These result suggest that the virtual data generated by simple linear operation, in representation space, still retains the information of the raw data. It’s also have great significance to the learning of small sample data sets.

1 Introduction

Learning also called embedding. Such as "word embedding", "graph embedding". We can think of representation learning as a mapping technology. Many people using data, with the form of vector, to fit their model. Obviously vectors is the main "language" in the Machine Learning world. But real world’s data "language" are multitudinous. How to translate the real world's data to a vector is a primary task for representation learning. A good "translate" should be include the underlying structure information. RL is generated from the actual demand on one hand, almost whole online data is structured, it’s hard to learning knowledge economically and fit machine learning model conveniently. People need to find dense and low dimensional vectors to represents graph. On the other hand, the embeded graph have many useful properties: distance for embeded feature space own latent meaning. Researchers found the distance between "China" and "Beijing" equal to the distance between "Japan" and "Tokyo" [EEMC8]. Words with the same label, will occur at the same region in the embedded feature space.

In 2013, R. Al-Rfou [EEMC8] proposed word2vec model, that is a extended skipgram model which mapped words to some vectors. In the vector space, words have the same semantics have to located on same region. Even the distance between two different class word vectors has a specific meaning. All this shows a powerful potention for representation learning. In word2vec, the relationalship between words be considered as a conditional probability, the trainning objective of word2vec is to maximum this probability,

\[
\frac{1}{T} \sum_{t=1}^{T} \sum_{c<j} \log P(\omega_{t+j} | \omega_t)
\]

where \(c\) is the size of the training context. \(\omega_1, \omega_2, \omega_3, \ldots, \omega_T\) are a sequence of training words. \(\omega_t\) is called
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In another area of research, analysis graph data is an important work for big data application. Graph is structured data, usually using adjacent matrix to represent the relationship for nodes. With the continuous growth in graph size, using adjacent matrix to represent graph data becomes more unrealistic, since when \( n \) nodes are added, the size of adjacent matrix will increase \( n^2 \). DeepWalk [EEMC9] inspired by word2vec, this algorithm considers nodes as words, and takes a random walk on graph to sample a sequence of nodes, the sequence can be treated like a sentence. In this model, the optimization problem is similarity as formula 1, and training process is almost the same as word2vec.

\[
\min_{\Phi} -\log P(v_i - \omega, \ldots, v_i + \omega \mid v_i \mid \Phi(v_i)) \tag{2}
\]

where, \( \Phi(v_i) \) is the mapping of the node \( v_i \), that is an embedded node. \( v_i \) is like a center word in a training window. \( \omega \) is the width of training window. This discovery leads to the wider use of structured data in machine learning.

Multilabel classification methods are fundamental required in graph embedding experiment, it also have great uses in structured data classification, such as social network analysis, protein function classification, and intelligent recommendation and photo classification. Grigorios Tsoumakas et al. consider that multilabel classification methods can be divided into two main categories:

1) Problem transformation methods. Problem transformation methods transform the multilabel classification problem either into one or more single-label classification or regression problems. In this way, single-label classifiers are employed; and their single-label predictions are transformed into multi-label predictions. Problem transformation is attractive on account of both scalability and flexibility: any off-the-shelf single-label classifier can be used to suit requirements.

2) Algorithm adaptation methods. The algorithm adaptation methods, that extend specific learning algorithms in order to handle multi-label data directly [EEMC1]. Well-known approaches include AdaBoost, decision trees. Such methods are usually chosen to work specifically in certain domains.

Multi-tag classification tasks are commonly used methods for evaluating embedding quality. This method is usually trained in semi-supervised mode. Semi-supervised means that only part of the data is labeled. In actual data, part of the data is usually selected as labeled data, and the remaining data labels are predicted by the trained model. Actually, underfitting or non-working of a certain sub-classifier can easily occur, when the number of samples is not large.

This situation actually affects the evaluation of embedded quality. Even the best classifier, the output result in the absence of data is disastrous. The imbalance of the data set is the macro cause of this phenomenon. As show in figure 2, the number of samples belonging to one label in the data set is likely to be hundreds or even thousands of times that of another. A simple idea to deal with the problem is to copy the data directly, so that the label classes with a small sample will meet the training requirements. Actually the result were not ideal, this is because simply copying data does not increase the diversity of data in a label class. As we’ll see later in the experiment, the benefits of simply adding data are minimal.
2 Algorithm Framework

2.1 Embedding Node to Feature Space

General, the random walk category model reference the SkipGram of Word2vec which is the classic NLP algorithm. We take the node as a word, take the sampling node sequence as sentence. We formulate the model as a maximum likelihood optimization problem just like a langure model. Let \( G = (V, E) \) be a given network. Let \( f : V \rightarrow R^d \) be the mapping function from node to feature space. \( d \) is a parameter specifying the number of dimensions of the feature space. Actually, \( f \) is an \( |V| \times d \) matrix. Our goal is to learn a vectors to every node, we using an auto-encoder to learn the topological of the networks from the "sentence" of the nodes, then seek to optimize the following objective function:

\[
\max_f \sum_{v \in V} \log P(N_i(v)|f(v))
\]

Where \( N_i(v) \) is the neighbor nodes set of source node \( v \). We assume that the neighborhood of the source node are independence for each other. Then we can simplify the likelihood probability function:

\[
P(N_i(v)|f(v)) = \prod_{n_i \in N_i(v)} P(n_i|f(v))
\]

We using a sigmod function to map the dot product of the mapped vectors to a probability between 0 and 1:

\[
P(n_i|f(v)) = \frac{1}{1 + \exp(f(v) \cdot f(n_i))}
\]

The equation represents the similarities between source node and neighborhood node.

2.2 Autocoder Model

Generally, autocoders can be used for dimensionality reduction. It’s consists of encoder and decoder. The autocoder can be described as:

\[
g(f(\bar{x})) = \bar{x}
\]

The training process can be described as:

\[
\min_{\theta} L(\bar{x}, g(f(\bar{x}))
\]

\( L \) is a loss function, used to indicate the gap between \( \bar{x} \) and \( g(f(\bar{x})) \). The training process is minimizing \( L \) function.

2.3 Multitag Classification And Virtual Data

Multitag classification is the basic task for bigdata application. Node classification is a benchmark to evaluate the embedding quality in the field of complex network and network embedding. A large number of scholars only focus on the quality of embedding, but ignore the impact of the data itself on the performance of the classifier. In fact, it is difficult for classifiers to work properly when the data itself is seriously unbalanced. For example, the dataset only have one sample is labeled "A", at the same time, hundreds of samples are labeled as "B", so the classifier in charge of data labeled "A" will work badly, since we have no enough data to fit it. This phenomenon is very common in small and medium-sized networks.

Based on the observation of previous work, we notice that the embedded data has nice properties. For instance, the nodes have same label will embed more closer in feature space. Meanwhile, distance represents the degree of similarity between samples. In other words, the distance between two samples with same label far less than the sample with different label. The same labeled samples have almost same distance far from origin. Base on these phenomena, we make the following hypothesis:

- Same label samples will be embedded in a compacted space.

\[
D(x_L^0, y_L^0) \ll D(x_L^0, y_L^0')
\]

- Distance is the only measure of samples’ similarity.

\[
x \in L, \quad y \in L \iff D(x, 0) \approx D(y, 0)
\]

- The distance between different label samples much bigger than same labe samples.

\[
|D(x_L^0, 0) - D(y_L^0, 0)| \gg 0
\]

We know the embedding model only have one single hidden layer, this can be express as fellow:

\[
g(\bar{x}) = f(\omega * \bar{x} + b)
\]

\( g(\bar{x}) \) is a function in embedded space. \( f(\bar{x}) \) is sigmod function.

\[
g(\theta x_1' + (1 - \theta)x_2') = f(\omega(\theta x_1' + (1 - \theta)x_2') + b)
\]

\[
= f(\theta(\omega x_1 + b) + (1 - \theta)(\omega x_2 + b))
\]

Since \( f(\bar{x}) \) is convex, when \( \bar{x} < 0 \),

\[
f(\theta(\omega x_1 + b) + (1 - \theta)(\omega x_2 + b)) \leq \theta f(\omega x_1 + b) + (1 - \theta)f(\omega x_2 + b)
\]

\[
= \theta g(x_1) + (1 - \theta)g(x_2)
\]
3 Experiment

In this section we present an experimental analysis of our method. We test our algorithm in PPI, Wiki, and Blogcatalog graph to classify nodes. In this graph, every node get one or more labels from a label set $L$. We use semi-supervised method to training the classifier. All experiments started from the number of 400 nodes and gradually increased 200 nodes per step. We set the parameter: $size = 120$, $window = 5$, read sampled files, in this file store sampled sequence by random walk.

3.1 PPI Classification

Protein-Protein Interactions: PPI is a subgraph of Homo Sapiens. The subgraph corresponds to the graph induced by nodes for which we could obtain labels from the hallmark gene sets and represent biological states. The PPI graph has 3890 nodes and 76584 edges and 50 class labels. In our test, we trained data start from 400 nodes to 3800 nodes, every step increase 200 nodes. We set the parameter: $addcoeff = 1$ to add the virtual nodes and set $nodenum = 3890$. As show in figure 4, comparing with normal method (trained with no virtual nodes), our method make a significant improvement in F1 score, it achieve a gain of 43.9% in Macro_F1 score and 11.17% in Micro_F1 score over normal method.

3.2 WIKI Classification

WIKI is a cooccurrence network of words appearing in the first million bytes of the Wikipedia dump. The labels represent the Part-of-Speech (POS) tags inferred using the Stanford POS-Tagger. The graph has 4,777 nodes, 184,812 edges, and 40 different labels. We set the parameter: $addcoeff = 0.35$ to add the virtual nodes and set $nodenum = 4777$. As show in figure 5 comparing with normal method (trained with no virtual nodes), our algorithm achieve a tremendous gain of 452% in Macro_F1 score even with a slight reduction 3.16% in Micro_F1 score. To sum up, our method giving us 224% gain over normal method in average F1 score.

3.3 BLOG Classification

This is a graph of social relationships of the bloggers showed on the BlogCatalog website. The labels represent blogger interests inferred through the metadata provided by the bloggers. The network has 10,312 nodes, 333,983 edges, and 39 different labels. We set the parameter: $addcoeff = 0.15$ to add the virtual nodes and set $nodenum = 10312$. As show in figure 6 comparing with normal method (trained with no virtual nodes), our algorithm achieve a distinct gain of 28.7% in Macro_F1 score even with a slight reduction 3.56% in Micro_F1 score. To sum up, our method giving us 12.5% gain over normal method in average F1 score.
3.4 Experiment Analyzing

In our experiments, an obvious rule is, the small for data, the better for result. This situation is also understandable, a smaller dataset have a high probability of getting underfitting sub-classifiers. Conversely, a big dataset have low probability of getting underfitting sub-classifiers. Experiment result shows that, our method is effective in improving the accuracy of classifier. In our experiment, we set different value to addcoeff to achieve the best result. This parameter determines the size of virtual nodes need to be add in training dataset. A certain fact will be mentioned, this parameter is not proportional to F1 score. An reasonable value will got higher score.

3.5 Parameter Sensitivity

In order to evaluate the impact of parameters for classification performance of EEMC. We design experiments on three multi-label classification tasks. Actually the parameter addcoeff is a factor from 0 to 1. Since, only the addcoeff directly related to the fixed dataset, so we fixed the embeded parameter(window size and the walk length) and training number of nodes (train,um=1200). We then vary the size of factor addcoeff to observing it's impact on the classification performance. As show in Figure4. With the increase of virtual data, macro F1 and micro F1 scores are all increasing. In Figure5, the macro F1 score first soared sharply, then gradually decrease with the parameter addcoeff increases. The micro F1 score gradually decrease with the parameter addcoeff increases, this suggests that it is important to select an appropriate parameter on some dataset. In Figure6 the macro F1 score and micro F1 score are also change slow, macro F1 first rise and then leveled off, with the parameter addcoeff increases. micro F1 score make a slow decline then leveling off. Although the micro F1 in Figure5 and Figure6 are all slow decline, but the accuracy of the classification can still benefit from macro F1 and average F1. Such as in wiki expriment, when we set addcoeff = 0.35, the micro F1 score decline 3% but macro F1 score gain of 452%. This experiment also suggests that our approach works best for small and middle datasets with more class tags.

Refer to figure2 in PPI dataset, the label class with the most data has about 200 samples. In Wiki and Blog this number are about 2400 and 1600. In PPI we set addcoeff = 1 in WIKI addcoeff = 0.35, in Blog addcoeff = 0.15. Combined with experimental results, we can infer that the number of training samples less than 600 and more than 200 is appropriate for classifiers. More than this number will cause overfitting. In Blog dataset, most label class have enough samples to fit classifiers, so the benefits from our algorithm are minimal.

4 Conclusion

In this paper, we propose a general method to boost the performance for off-the-shelf classifier, our method try to generate some virtual data for those labels that include few sample. Use this data to training classifier, then we have proved the validity of our method through three expriments, experimental results show that our method is remarkably effective in improving the performance of classifier. We also test the sensitivity of the parameters, the experimental results shows that on partial dataset, bigger parameter is not always better, set an appropriate parameter is very import. Since the embedding process does not require a large sample, and after embedding, meaningful virtual data can be easily obtained. So our method also have great significance to the learning of small sample data sets. In conclusion, our method can significantly improve the performance of the classifier, meanwhile, our method explored another way of how improving the performance of classifier.

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Figure 4: PPI classify result1

Figure 5: Wikipedia classify result1

Figure 6: Blogcatalog classify result1

Figure 7: Impact of virtual data number in PPI
Figure 8: Impact of virtual data number in WIKI

Figure 9: Impact of virtual data number in BLOG

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