Using Neural Network Formalism to Solve Multiple-Instance Problems

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Abstract. Many objects in the real world are difficult to describe by means of a single numerical vector of a fixed length, whereas describing them by means of a set of vectors is more natural. Therefore, \textit{Multiple instance learning} (MIL) techniques have been constantly gaining in importance throughout the last years. MIL formalism assumes that each object (sample) is represented by a set (bag) of feature vectors (instances) of fixed length, where knowledge about objects (e.g., class label) is available on bag level but not necessarily on instance level. Many standard tools including supervised classifiers have been already adapted to MIL setting since the problem got formalized in the late nineties. In this work we propose a neural network (NN) based formalism that intuitively bridges the gap between MIL problem definition and the vast existing knowledge-base of standard models and classifiers. We show that the proposed NN formalism is effectively optimizable by a back-propagation algorithm and can reveal unknown patterns inside bags. Comparison to 14 types of classifiers from the prior art on a set of 20 publicly available benchmark datasets confirms the advantages and accuracy of the proposed solution.

1 Motivation

The constant growth of data sizes and data complexity in real world problems has increasingly put strain on traditional modeling and classification techniques. Many assumptions cease to hold; it can no longer be expected that a complete set of training data is available for training at once, models fail to reflect information in complex data unless a prohibitively high number of parameters is employed, availability of class labels for all samples can not be realistically expected, and particularly the common assumption about each sample to be represented by a fixed-size vector seems to no longer hold in many real world problems.

\textit{Multiple instance learning} (MIL) techniques address some of these concerns by allowing samples to be represented by an arbitrarily large set of fixed-sized vectors instead of a single fixed-size vector. Any explicit ground truth information (e.g., class label) is assumed to be available on the (higher) level of samples but not on the (lower) level of instances. The aim is to utilize unknown patterns on instance-level to enable sample-level modeling and decision making. Note that
MIL does not address the Representation Learning problem. Instead it aims at better utilization of information in cases when ground truth knowledge about a dataset may be granular and available on various levels of abstraction only.

From a practical point of view MIL promises to i) save ground truth acquisition cost – labels are needed on sample-level, i.e., on higher-level(s) of abstraction only, ii) reveal patterns on instance level based on the available sample-level ground truth information, and eventually iii) achieve high accuracy of models through better use of information present in data.

Despite significant progress in recent years, the current battery of MIL tools is still burdened with compromises. The existing models (see next Section for a brief discussion) clearly leave open space for more efficient utilization of information in samples and for a clearer formalism to provide easily interpretable models with higher accuracy. The goal of this paper is to provide a clean formalism bridging the gap between the MIL problem formulation and classification techniques of neural networks (NNs). This opens the door to applying latest results in NNs to MIL problems.

2 Prior art on multi-instance problem

The pioneering work [11] coined multiple-instance or multi-instance learning as a problem where each sample $b$ (called bag in the following) consists of a set of instances $x$, i.e., $b = \{x_i \in \mathcal{X} | i \in \{1, \ldots, |b|\}\}$, equivalently $b \in \mathcal{B} = \bigcup_{k>1} \{x_i \in \mathcal{X} | i \in \{1, \ldots, k\}\}$ and each instance $x$ can be attributed a label $y_x \in \{-1, +1\}$, but these instance-level labels are not known even in the training set. The sample $b$ is deemed positive if at least one of its instances had a positive label, i.e., label of a sample $b$ is $y = \max_{x \in b} y_x$. Most approaches solving this definition of MIL problem belong to instance-space paradigm, in which the classifier is trained on the level of individual instances $f : \mathcal{X} \mapsto \{-1, +1\}$ and the label of the bag $b$ is inferred as $\max_{x \in b} f(x)$. Examples of such methods include: Diverse-density [17], EM-DD [23], MILBoost [22], and MI-SVM [2].

Later works (see reviews [1,2]) have introduced different assumptions on relationships between labels on the instance level and labels of bags or even dropped the notion of instance-level labels and considered only labels on the level of bags, i.e., it is assumed that each bag $b$ has a corresponding label $y \in \mathcal{Y}$, which is for simplicity assumed to be binary, i.e., $\mathcal{Y} = \{-1, +1\}$ in the following. Most approaches solving this general definition of the problem follow either the bag-space paradigm and define a measure of distance (or kernel) between bags [4,6,13] or the embedded-space paradigm and define a transformation of the bag to a fixed-size vector [21,65].

Prior art on neural networks for MIL problems is scarce and aimed for instance-space paradigm. Ref. [19] proposes a smooth approximation of the maximum pooling in the last neuron as $\frac{1}{|b|} \ln \left( \sum_{x \in b} \exp(f(x)) \right)$, where $f(x) : \mathcal{X} \mapsto \mathbb{R}$ is the output of the network before the pooling. Ref. [24] drops the requirement on smooth pooling and uses the maximum pooling function in the last neuron. Both approaches optimize the $L_2$ error function.
Due to space limits, the above review of the prior art was brief. The interested reader is referred to [1,12,4] for a more thorough discussion of a problem and algorithms.

3 Neural network formalism

The proposed neural network formalism is intended for a general formulation of MIL problems introduced in [18]. It assumes a non-empty space $\mathcal{X}$ where instances live with a set of all probability distributions $\mathcal{P}^\mathcal{X}$ on $\mathcal{X}$. Each bag corresponds to some probability distribution $p_b \in \mathcal{P}^\mathcal{X}$ with its instances being realizations of a random variable with distribution $p_b$. Each bag $b$ is therefore assumed to be a realization of a random variable distributed according to $P(p_b, y)$, where $y \in \mathcal{Y}$ is the bag label. During the learning process each concrete bag $b$ is thus viewed as a realization of a random variable with probability distribution $p_b$ that can only be inferred from a set of instances $\{x \in b | x \sim p_b\}$ observed in data. The goal is to learn a discrimination function $f : B \mapsto \mathcal{Y}$, where $B$ is the set of all possible realizations of distributions $p \in \mathcal{P}^\mathcal{X}$, i.e., $B = \{x_i | p \in \mathcal{P}^\mathcal{X}, x_i \sim p, i \in \{1, \ldots, l\}, l \in \mathbb{N}\}$. This definition includes the original used in [11], but it also includes the general case where every instance can occur in positive and negative bags, but some instances are more frequent in one class.

The proposed formalism is based on the embedded-space paradigm representing bag $b$ in an $m$-dimensional Euclidean space $\mathbb{R}^m$ through a set of mappings

$$\left(\phi_1(b), \phi_2(b), \ldots, \phi_m(b)\right) \in \mathbb{R}^m \tag{1}$$

with $\phi : B \mapsto \mathbb{R}$. Many existing methods implement embedding function as

$$\phi_i = g\left(\{k(x, \theta_i)\}_{x \in b}\right), \tag{2}$$

where $k : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}^+_{0}$ is a suitably chosen distance function, $g : \bigcup_{k=1}^{\infty} \mathbb{R}^k \mapsto \mathbb{R}$ is the pooling function (e.g. minimum, mean or maximum), and finally $\Theta = \{\theta_i \in \mathcal{X} | i \in \{1, \ldots, m\}\}$ is the dictionary with instances as items. Prior art methods differ in the choice of aggregation function $g$, distance function $k$, and finally in the selection of dictionary items, $\Theta$. A generalization was recently proposed in [6] defining $\phi$ using a distance function (or kernel) over the bags $k : B \times B \mapsto \mathbb{R}$ and dictionary $\Theta$ containing bags rather instances. This generalization can be seen as a crude approximation of kernels over probability measures used in [18].

The computational model defined by (1) and (2) can be viewed as a neural network sketched in Figure 1. One (or more) lower layers implement a set of distance functions $\{k(x, \theta_i)\}_{i=1}^{m}$ (denoted in Fig. 1 in vector form as $k(x, \theta)$) projecting each instance $x_i$ from the bag $\{x_i\}_{i=1}^{m}$ from the input space $\mathbb{R}^d$ for $\mathbb{R}^m$. The pooling layer implementing the pooling function $g$ produces a single vector $\bar{x}$ of the same dimension $\mathbb{R}^m$. Finally subsequent layers denoted in the figure as $f(\bar{x})$ implement the classifier that already uses a representation of the bag as a feature vector of fixed length $m$. The biggest advantage of this
formalism is that with a right choice of pooling function $g(\cdot)$ (e.g. mean or maximum) all parameters of the embedding functions $k(x, \theta)$ can be optimized by the standard back-propagation algorithm. Therefore embedding at the instance-level (layers before pooling) is effectively optimized while requiring labels only on the bag-level. This mechanism identifies parts of the instance-space $\mathcal{X}$ with the largest differences between probability distributions generating instances in positive and negative bags with respect to the chosen pooling function. This is also the most differentiating feature of the proposed formalism to most prior art, which typically optimizes embedding parameters $\theta_i$ regardless of the labels.

The choice of a pooling function depends on the type of the MIL problem. If the bag’s label depends on a single instance, as it is the case for the instance-level paradigm, then the maximum pooling function is appropriate, since its output also depends on a single instance. On the other hand if a bag’s label depends on properties of all instances, then the mean pooling function is appropriate, since its output depends on all instances and therefore it characterizes the overall distribution.

Remark: the key difference of the above approach to the prior art [24] is in performing pooling inside the network as opposed to after the last neuron or layer as in the cited reference. This difference is key to the shift from instance-centric modeling in prior art to bag-centric advocated here. However the proposed formalism is general and includes [24] as a special case, where instances are projected into the space of dimension one ($m = 1$), pooling function $g$ is set to maximum, and layers after the pooling functions are not present ($f$ is equal to identity).

4 Experimental evaluation

The evaluation of the proposed formalism uses publicly available datasets from a recent study of properties of MIL problems [8], namely BrownCreeper, CorelAfrican, CorelBeach, Elephant, Fox, Musk1, Musk2, Mutagenesis1, Mutagenesis2.
Fig. 2. Critical difference diagram shows average rank of each method over 20 problems. The thick black line shows the confidence interval of corrected Bonferroni-Dunn test with significance 0.05 testing whether two classifiers have equal performance.

esis2, Newsgroups1, Newsgroups2, Newsgroups3, Protein, Tiger, UCSBBreast-Cancer, Web1, Web2, Web3, Web4, and WinterWren. The supplemental material [9] contains equal error rate (EER) of 28 MIL classifiers (and their variants) from prior art implemented in the MIL matlab toolbox [20] together with the exact experimental protocol and indexes of all splits in 5-times repeated 10-fold cross-validation. Therefore the experimental protocol has been exactly reproduced and results from [9] are used in the comparison to prior art.

The proposed formalism has been compared to those algorithms from prior art that has achieved the lowest error on at least one dataset. This selection yielded 14 classifiers for 20 test problems, which demonstrates diversity of MIL problems and difficulty to choose suitable method. Selected algorithms include representatives of instance-space paradigm: MIL Boost [22], SimpleMIL, MI-SVM [2] with Gaussian and polynomial kernel, and prior art in Neural Networks (denoted prior NN) [24]; bag-level paradigm: k-nearest neighbor with citation distance [21] using 5 nearest neighbors; and finally embedded-space paradigm: Miles [5] with Gaussian kernel, Bag dissimilarity [6] with minmin, meanmin, meanmean, Hausdorff, and Earth-moving distance (EMD), cov-coef [9] embedding bags by calculating covariances of all pairs of features over the bag, and finally extremes and mean embedding bags by using extreme and mean values of each feature over instances of the bag. All embedded space paradigm methods except Miles used logistic regression classifier.

The proposed MIL neural network consists of a single layer of rectified linear units (ReLU) [15] with transfer function $\max\{0, x\}$, followed by a mean-pooling layer and a single linear output unit. The training minimized a hinge loss function using the Adam [16] variant of stochastic gradient descend algorithm with mini-batch of size 100, maximum of 10,000 iterations, and default settings. L1 regularization on weights of the network was used to decrease overfitting. The topology had two parameters — the number of neurons in the first
Table 1. Average equal error rate of the proposed NN formalism on training and testing set and average equal error rate on the testing set of the best prior art for the given problem. Abbreviations of the prior art are as introduced in Section 4.

| Problem                  | Error of NN on training set | prior art error algorithm |
|--------------------------|----------------------------|--------------------------|
| BrownCreeper             | 0                          | 11.2 MILBoost            |
| CorelAfrican             | 2.6                        | 11.2 minmin              |
| CorelBeach               | 0.2                        | 17 extremes              |
| Elephant                 | 0                          | 16.2 minmin              |
| Fox                      | 0.4                        | 36.1 meanmin             |
| Musk1                    | 0                          | 12.8 Citation            |
| Musk2                    | 0                          | 11.8 Hausdorff           |
| Mutagenesis1             | 7.5                        | 16.9 cov-coef            |
| Mutagenesis2             | 14.9                       | 17.2 emd                 |
| Newsgroups1              | 0                          | 18.4 meanmean            |
| Newsgroups2              | 0                          | 27.5 prior NN            |
| Newsgroups3              | 0                          | 31.2 meanmean            |
| Protein                  | 2.5                        | 15.5 minmin              |
| Tiger                    | 0                          | 19 MILES                 |
| UCSBBreastCancer         | 0                          | 13.6 MI-SVM g            |
| Web1                     | 0                          | 20.9 MILES               |
| Web2                     | 0                          | 7.1 MI-SVM p             |
| Web3                     | 0                          | 13.6 MI-SVM g            |
| Web4                     | 0                          | 1.5 mean-inst            |
| WinterWren               | 0                          | 2.1 emd                  |

Exact values of EER of the best algorithm from the prior art and that of the proposed NN formalism is summarized in Table 1. From the results it is obvious that the proposed neural network formalism have scored poorly on problems.
with a large dimension and a small number of samples, namely Newsgroups and Web (see Table 1 of [7] for details on the data). The neural network formalism has easily overfit to the training data, which is supported by zero errors on the training sets.

5 Conclusion

This work has presented a generalization of neural networks to multi-instance problems. Unlike the prior art, the proposed formalism embeds samples consisting of multiple instances into vector space, enabling subsequent use with standard decision-making techniques. The key advantage of the proposed solution is that it simultaneously optimizes the classifier and the embedding. This advantage was illustrated on a set of real-world examples, comparing results to a large number of algorithms from the prior art. The proposed formalism seems to outperform the majority of standard MIL methods in terms of accuracy. It should be stressed though that results were compared to those published by authors of survey benchmarks; not all methods in referred tests may have been set in the best possible way. However, as many such cases would be very computationally expensive, the proposed formalism becomes competitive also due to its relatively modest computational complexity that does not exceed that of a standard 3-layer neural network. The proposed formalism opens up a variety of options for further development. A better and possibly more automated choice of pooling functions is one of the promising ways to improve performance on some types of data.

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