ABSTRACT

In this work, we consider the task of classifying the binary positive-unlabeled (PU) data. The existing discriminative learning based PU models attempt to seek an optimal re-weighting strategy for U data, so that a decent decision boundary can be found. In contrast, we provide a totally new paradigm to attack the binary PU task, from perspective of generative learning by leveraging the powerful generative adversarial networks (GANs). Our generative positive-unlabeled (GPU) learning model is devised to express P and N data distributions. It comprises of three discriminators and two generators with different roles, producing both positive and negative samples that resemble those come from the real training dataset. Even with rather limited labeled P data, our GPU framework is capable of capturing the underlying P and N data distribution with infinite realistic sample streams. In this way, an optimal classifier can be trained on those generated samples using a very deep neural networks (DNNs). Moreover, an useful variant of GPU is also introduced for semi-supervised classification.

1 INTRODUCTION

Positive-unlabeled (PU) classification (Denis, 1998; Denis et al., 2005; Ward et al., 2009) has gained great popularity in dealing with limited partially labeled data and achieved its success in a broad range of applications. For instance, PU classification can be used for the detection of outliers in an unlabeled dataset with knowledge only from a collection of inlier data (Hido et al., 2008; Smola et al., 2009). PU classification also finds its usefulness in ‘one-vs-rest’ classification task such as land-cover classification (urban vs non-urban) where non-urban data are too diverse to be labeled than urban data (Li et al., 2011). The automatic label identification is another important application of PU learning, such as automatically tagging photos by providing a collection of photos being of the same class.

The most commonly used PU models for binary classification can typically be categorized, in terms of the way of handling U data, into two types (Kiryo et al., 2017). One type of approaches such as (Liu et al., 2002; Li & Liu, 2003) attempt to recognize negative samples in U data and then feed them to classical PN models. However, these methods depend heavily on the heuristic strategies and often yield a poor solution. The other type of approaches, including (Liu et al., 2003; Lee & Liu, 2003), provide a better solution by treating U data to be N data with a decayed weight. Nevertheless, finding an optimal weight turns out to be computationally expensive. Additionally, the classifier trained based on all methods mentioned above suffer from a systematic estimation bias (Du Plessis et al., 2015; Kiryo et al., 2017).

To overcome the drawbacks of previous methods, the authors of (du Plessis et al., 2014) lately investigated the strategy of considering U data as a weighted combination of P data and N data (Elkan & Noto, 2008), and proposed an unbiased risk estimator by using a non-convex symmetric ramp loss.
Motivated by the weakness of non-convex training of unbiased risk estimator, the same authors studied a more generic class of convex formulation of loss functions (e.g., the convex composite loss derived from double hinge loss) (Du Plessis et al., 2015). They theoretically argued the proposed loss functions still yield unbiased estimation yet with more appealing learning properties than the non-convex counterpart.

More recently, Kiryo and his colleagues observed the fact that the risk of previous estimators can go negative without lower bound, which will lead to serious overfitting if the model becomes too flexible (Kiryo et al., 2017). They introduced a non-negative risk estimator to fix the problem and demonstrated their estimator can be adapted to very flexible model like deep neural networks (DNNs) and convolutional neural networks (CNNs).

All these recent approaches make their efforts to seek an optimal re-weighting strategy for U data, so that a decent decision boundary can be obtained. Despite their breakthrough on PU task, they are all based on the discriminative learning. However, discriminative based models concentrate on learning useful representations of the data, failing to capture the underlying data distributions. Given quite limited P data, the existing traditional discriminative PU learning models, including the state of the art non-negative risk estimator (Kiryo et al., 2017), could not be able to perform as reasonably well as they do when P samples are sufficiently large.

Generative models, on the other hand, have the advantage in expressing complex data distribution. Apart from distribution density estimation, generative models are often applied to learn a function that is able to create more samples from that distribution. Lately, a large body of successful deep generative models have emerged, especially generative adversarial networks (GANs) (Goodfellow et al., 2014; Denton et al., 2015; Reed et al., 2016; Salimans et al., 2016). GANs intend to solve the task of generative modeling by making two agents play a game against each other. One agent is called generator that tries to generate data from random noise; the other agent, named discriminator, examines both real and fake data and determines whether the data is real or fake. Both agents keep evolving over time and get better and better at their jobs. Eventually, the generator is forced to create synthetic data which is as realistic as possible to those that come from the training data distribution.

Inspired by the tremendous success and expressive power of GANs, we novelly attack the PU classification task by resorting to generative modeling. In this work, we propose a deep generative model, called generative positive-unlabeled learning (GPU), for the binary PU classification. Building upon the GANs framework, our GPU model consists of an array of generators and discriminators competing against among them. It is devised to simultaneously generate positive and negative samples that resemble those come from the true data distribution. Then, a standard PN classifier can be trained on the generated samples. Given a quite small portion of labeled P data as seeds, our GPU framework is capable of capturing the underlying P and N data distributions, with the capacity to produce infinite P and N samples streams. As long as GANs, which GPU relies on, are sophisticated to generate high-quality samples, the optimal accuracy could be achieved by training a very deep neural networks (DNNs). Moreover, our approach does not need to explicitly estimate the class prior, unlike the existing PU models assume class prior is available or need to estimate it from data.

Our main contribution, in contrast to the conventional discriminative PU learning, is that we innovate a totally new paradigm to effectively solve the PU task through deep generative models. Furthermore, we also introduce a closely related variant of GPU but for semi-supervised classification.

Overall, our novel work opens a door to possibly many new solutions other than the traditional discriminative learning based approaches for the weakly supervised learning problems.

2 Preliminaries and Problem Setting

In what follows, we start by formulating the task of PU classification. Then, we review the fundamental idea of the standard GANs. Finally, we introduce some notations and the problem setting for our proposed framework.
2.1 Positive-Unlabeled (PU) classification

Given as input \(d\)-dimensional random variable \(\mathbf{x} \in \mathbb{R}^d\) and scalar random variable \(y \in \{\pm 1\}\) as class label, and let \(\mathbb{P}(\mathbf{x}, y)\) be the joint density, the class-conditional densities are defined as

\[
\mathbb{P}_p(\mathbf{x}) = \mathbb{P}(\mathbf{x} | y = 1) \quad \mathbb{P}_n(\mathbf{x}) = \mathbb{P}(\mathbf{x} | y = -1),
\]

while \(\mathbb{P}(\mathbf{x})\) refers to as the unlabeled marginal density. The standard PU classification task (Ward et al., 2009) consists of a positive dataset \(\mathcal{X}_p\) and an unlabeled dataset \(\mathcal{X}_u\) with i.i.d samples drawn from \(\mathbb{P}_p(\mathbf{x})\) and \(\mathbb{P}(\mathbf{x})\) respectively:

\[
\mathcal{X}_p = \{\mathbf{x}_p^i \}_{i=1}^{n_p} \sim \mathbb{P}_p(\mathbf{x}) \quad \mathcal{X}_u = \{\mathbf{x}_u^i \}_{i=1}^{n_u} \sim \mathbb{P}(\mathbf{x}).
\]

Due to the fact that the unlabeled dataset is in fact a mixture of both positive and negative samples, the marginal density turns out to be

\[
\mathbb{P}(\mathbf{x}) = \pi \mathbb{P}(\mathbf{x} | y = 1) + (1 - \pi) \mathbb{P}(\mathbf{x} | y = -1),
\]

where \(\pi = p(y = 1)\) is denoted as class-prior probability, which is usually unknown in advance and can be estimated from the given data (Jain et al., 2016; Ramaswamy et al., 2016). The objective of PU task is to train a classifier on \(\mathcal{X}_p\) and \(\mathcal{X}_u\) so as to classify the new unseen pattern \(\mathbf{x}^{\text{new}}\).

In contrast to PU classification, positive-negative (PN) classification assumes all negative samples, \(\mathcal{X}_n = \{\mathbf{x}_n^i \}_{i=1}^{n_n} \sim \mathbb{P}_n(\mathbf{x}),\) are labeled beforehand, so that the classifier can be trained in an ordinary supervised learning fashion.

2.2 Generative Adversarial Networks (GANs)

GANs, originated in (Goodfellow et al., 2014), is one of the most recent successful generative models that is equipped with the power of producing distributional outputs. GANs obtains this capability through an adversarial competition between a generator \(G\) and a discriminator \(D\) that involves optimizing a min-max objective:

\[
\min_G \max_D V(D, G) = \min_G \mathbb{E}_{\mathbf{x} \sim \mathbb{P}_x(\mathbf{x})} \log(D(\mathbf{x})) + \mathbb{E}_{\mathbf{z} \sim \mathbb{P}_z(\mathbf{z})} \log(1 - D(G(\mathbf{z})))
\]

(1)

where \(\mathbb{P}_x(\mathbf{x})\) represents the true data distribution; \(\mathbb{P}_z(\mathbf{z})\) is typically a simple fixed distribution (e.g., \(\mathcal{N}(0, 1)\)) for latent code \(\mathbf{z}\), while distribution \(\mathbb{P}_g(\mathbf{x})\) associated with generator \(G\) is induced by the transformation \(G(\mathbf{z}) : \mathbf{z} \rightarrow \mathbf{x}\).

To find the optimal solution, (Goodfellow et al., 2014) resorted to simultaneous stochastic gradient descent (SGD) for alternately updating discriminator \(D\) and generator \(G\). The authors argued that the gradient descent on \(\mathbb{P}_g(\mathbf{x})\) minimizes the distribution distance between \(\mathbb{P}_x(\mathbf{x})\) and \(\mathbb{P}_g(\mathbf{x})\). When some equilibrium point is reached, GANs is able to perfectly recover the true data distribution \(\mathbb{P}_x(\mathbf{x}) = \mathbb{P}_g(\mathbf{x})\), provided the optimal discriminator \(D^* = \arg \max_D V(D, G)\) is obtained.

2.3 Problem Setting

Throughout the paper, \(\{\mathbb{P}_p(\mathbf{x}), \mathbb{P}_n(\mathbf{x}), \mathbb{P}(\mathbf{x})\}\) are denoted as real positive, real negative and real entire data distribution, respectively. We make an assumption that \(\mathbb{P}_p(\mathbf{x}) \cup \mathbb{P}_n(\mathbf{x}) = \mathbb{P}(\mathbf{x}),\) \(\mathcal{X}_p\) represents the positively labeled dataset, \(\mathcal{X}_n\) represents the negatively labeled dataset, while \(\mathcal{X}_u\) serves as unlabeled dataset. \(\{\mathbb{P}_{gp}(\mathbf{x}), \mathbb{P}_{gn}(\mathbf{x})\}\) describe the distributions formed by the fake examples from the generated set \(\mathcal{X}_{gp}\) and \(\mathcal{X}_{gn}\). \(\{G_p, G_n\}\) stand for the respective positive and negative generators, targeting to produce positive and negative examples. Correspondingly, \(\{D_p, D_n, D_u\}\) denote the positive, negative and unlabeled discriminators. Finally, \(D_{pn}\) is referred to as the PN classifier.

For this work, we focus on the two-sample problem setting of PU learning task in which only two classes are taken into account. In particular, we also assume each class mainly concentrates on one major mode.
In brief, our GPU framework comprises of two generators \( \{ G_p, G_n \} \) which are jointly trained against three discriminators \( \{ D_p, D_u, D_n \} \). Guided by the adversarial supervision of three discriminators, \( \{ G_p, G_n \} \) are tasked with generating positive and negative samples that are indistinguishable with corresponding positive and negative data drawn from \( \{ \mathbb{P}_p(x), \mathbb{P}_n(x) \} \).

As being their competitive opponents, three discriminators \( \{ D_p, D_u, D_n \} \) are developed to play distinct role in supervising \( \{ G_p, G_n \} \) when learning to discern the real data from fake data given by \( \{ G_p, G_n \} \). Among these discriminators, the discriminator \( D_p \) tries to differentiate the real positive sample from the synthetic sample of \( G_p \), whereas the business of discriminator \( D_u \) is aimed at separating the real unlabelled sample from both synthetic \( G_p \) sample and synthetic \( G_n \) sample at the same time. The discriminator \( D_n \), nevertheless, is conducted in a way that it can easily make a distinction between the real positive sample and the generated negative sample from \( G_n \).

More formally, the generators \( \{ G_p, G_n \} \) are trained against the discriminators \( \{ D_p, D_u, D_n \} \) with the objective decomposing as:

\[
\min_{G_p, G_n} \max_{D_p, D_u, D_n} V(D, G) = \min_{G_p} \max_{D_p, D_u} V_{G_p}(D, G) + \min_{G_n} \max_{D_n} V_{G_n}(D, G),
\]

(2)

where the first term in (2) corresponds to

\[
\min_{G_p} \max_{D_p, D_u} V_{G_p}(D, G) = \max_{G_p} \min_{D_p, D_u} V_{G_p}(D, G) + \max_{G_n} \min_{D_n} V_{G_n}(D, G).
\]

(3)

In particular,

\[
\min_{G_p} \max_{D_p, D_u} V_{G_p}(D, G) = \min_{G_p} \mathbb{E}_{x \sim \mathbb{P}_p(x)} \log(D_p(x)) + \mathbb{E}_{z \sim \mathbb{P}_z(z)} \log(1 - D_p(G_p(z))),
\]

(4)

\[
\min_{G_p} \max_{D_u, D_n} V_{G_n}(D, G) = \min_{G_p} \mathbb{E}_{x \sim \mathbb{P}_p(x)} \log(D_u(x)) + \mathbb{E}_{z \sim \mathbb{P}_z(z)} \log(1 - D_u(G_p(z))),
\]

(5)

which indicate the generator \( G_p \), co-supervised by both the discriminator \( D_p \) and the discriminator \( D_u \), tries to minimize the distance between \( \mathbb{P}_{gp}(x) \) and \( \mathbb{P}_p(x) \) while striving to stay around the true
data distribution $\mathbb{P}(x)$. Equations (4) and (5) imply that $G_p$ endeavours to fool both $D_p$ and $D_u$ by creating examples that resemble the positive ones in $\mathcal{X}_p$ and the positive ones in $\mathcal{X}_u$ at the same time. As a result, the loss incurred by $D_p$ for $G_p$ in (4) together with the loss incurred by $D_u$ for $G_p$ in (5) jointly guide $P_{gp}(x)$ gradually moves towards and finally converges to $P_{p}(x)$.

On the other hand, the second term in (2) refers to as

$$\min_{G_n} \max_{D_n,D_u} V_{G_n}(D,G) = \min_{G_n} \max_{D_n,D_u} V_{G_n,D_n}(D,G) + \min_{G_n} \max_{D_u} V_{G_n,D_u}(D,G)$$

(6)

in which the former part in (6) reads as

$$\max_{D_n} V_{G_n,D_n}(D,G) = \mathbb{E}_{x \sim P_p(x)} \log(D_n(x)) + \mathbb{E}_{z \sim P_z(z)} \log(1 - D_n(G_n(z)))$$

(7)

and

$$\min_{G_n} V_{G_n,D_n}(D,G) = \min_{G_n} \mathbb{E}_{z \sim P_z(z)} \log(D_n^*(G_n(z))),$$

(8)

where $D_n^*$ in (8) is the optimal discriminator obtained after we execute the ‘D step’ in (7). Notice that we use different losses for $D_n$ in (7) and for $G_n$ in (8), by contrast with ‘zero-sum’ loss applied elsewhere. The latter part in (6) is given by

$$\min_{G_n} \max_{D_n} V_{G_n,D_n}(D,G) = \min_{G_n} \mathbb{E}_{x \sim P_n(x)} \log(D_n(x)) + \mathbb{E}_{z \sim P_z(z)} \log(1 - D_n(G_n(z))).$$

(9)

Above formulations (6)-(8) suggest the generator $G_n$, when facing both the discriminator $D_n$ and the discriminator $D_u$, struggles to make $P_{gn}(x)$ stay away from the positive distribution $\mathbb{P}_{p}(x)$, and meanwhile makes its effort to settle $P_{gn}(x)$ within the data distribution $\mathbb{P}(x)$. This will eventually push $P_{gn}(x)$ towards $P_{n}(x)$.

To achieve that, the loss term $\log(D_n^*(G_n(z)))$ in (8) favors discriminator $G_n$ to produce negative examples. On the opposite side, the loss term $\log(D_n^*(x))$ plus $\log(1 - D_n(G_n(z)))$ in (7) helps $D_n$ to distinguish the real positive examples from the fake ones, especially fake negative examples. Consequently, discriminator $D_n$ will send uniformly negative feedback to the generator $G_n$. In this way, the gradient information derived from negative feedback drives down $P_{gn}(x)$ near the positive data region $\mathbb{P}_{p}(x)$. In the mean time, the gradient signals from $D_u$ increase $P_{gn}(x)$ outside the positive region yet within the true data distribution $\mathbb{P}(x)$.

3.2 Variant for Semi-Supervised Classification

The objective of semi-supervised classification is to learn a classifier from positive, negative and unlabeled data. In such setting, besides dataset $\mathcal{X}_p$ and $\mathcal{X}_u$, we assume a partially labeled negative dataset $\mathcal{X}_n$ is also available, with samples drawn from negative distribution $P_{n}(x)$.
In fact, the very same architecture of GPU can be applied to the semi-supervised classification task by just modifying the loss function for $G_n$. A closely related variant of GPU, called generative positive negative unlabeled (GPNU) learning framework, is depicted in Figure 2. In stead of using the loss in (8), we go back to the standard ‘zero-sum’ loss like

$$\min_{G_n} \max_{D_n} V_{G_n, D_n}(D, G) = \min_{G_n} \mathbb{E}_{x \sim \mathbb{P}_n(x)} \log(D_n(x)) + \mathbb{E}_{z \sim \mathbb{P}_i(z)} \log(1 - D_n(G_n(z))). \quad (10)$$

Under the loss formulation (10), the discriminator $D_n$ discerns the real negative examples from the synthetic negative examples given by $G_n$. Now the generator $G_n$ tries to fool $D_n$ and $D_u$ in the meantime by outputting realistic examples. Being attracted by both $\mathbb{P}(x)$ and $\mathbb{P}_n(x)$ , the generated distribution $\mathbb{P}_{gn}(x)$ will slightly approach to $\mathbb{P}_n(x)$ and finally recovers the true $\mathbb{P}_n(x)$.

Motivated by the argument given in (Goodfellow et al., 2014), it is not hard to show that the optimal $G_p$ and $G_n$, which minimize the composite loss incurred by $\{D_p, D_u\}$ and the composite loss incurred by $\{D_n, D_u\}$, can be achieved if and only if the three conditions

$$\mathbb{P}_p(x) = \mathbb{P}_{gp}(x)$$
$$\mathbb{P}_n(x) = \mathbb{P}_{gn}(x)$$
$$\mathbb{P}(x) = \mathbb{P}_{gp}(x) \cup \mathbb{P}_{gn}(x) \quad (11)$$

are simultaneously satisfied.

3.3 Related Work

A few existing work have explored several approaches that involves training ensembles of GANs. (Wang et al., 2016) introduced an heuristic strategy based on the cascade of GANs to mitigate the missing modes problem. For the purpose of stabilizing GANs training, (Neyshabur et al., 2017) proposed to train one generator against a set of discriminators, each of which pays attention to a different random projection of the data, trying to avoid perfectly identifying the generated samples from the real ones. By doing so, the issue of vanishing gradients for discriminator could be effectively alleviated since the low-dimensional projections of the true data distribution are less concentrated.

A similar $N$-discriminator extension to GANs framework is adopted in (Durugkar et al., 2016) with the objective to accelerate training of generator to a more stable state with higher quality output, by exploring different strategies of aggregating feedback from multiple discriminators.

By contrast, our framework fundamentally differs from theirs in terms of motivation, application and architecture. Our model is specified in PU classification (or semi-supervised classification) task, while theirs are focused on improving the training of GANs. In addition, our architecture contains two generators that are used for purpose of producing examples in different categories, in comparison to theirs with only one generator generating examples of all kinds. Nevertheless, we do share a point in common in a way that multiple discriminators are exploited, which is shown to be more stable and easier to train than the single case.

4 Discussion

One key factor to the success of GPU relies heavily on the capability of GANs in generating realistic samples with high quality standard. In this way, the expected performance could be achieved by a classifier trained on the generated P and N data. However, it is widely known that the training of the original GANs to produce high-dimensional data (e.g. high-quality large images) is extremely challenging. GANs suffers from issues of mode collapse and mode oscillation, especially when applied to large-size images whose distribution lies in a high-dimensional spaces with multiple output modes. For this reason, the similar issue of GANs might happen to our GPU as well.

To mitigate this problem and further stabilize the GPU training, we can try multiple negative discriminators $\{D^i_u\}_{i=1}^L$ to jointly guide the negative generator $G_n$ instead of single negative discriminator $D_n$ (also try to employ multiple positive discriminators $\{D^i_p\}_{i=1}^L$ to together supervise the positive generator $G_p$).
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