Discriminative adversarial networks for positive-unlabeled learning

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Abstract

As an important semi-supervised learning task, positive-unlabeled (PU) learning aims to learn a binary classifier only from positive and unlabeled data. In this article, we develop a novel PU learning framework, called discriminative adversarial networks, which contains two discriminative models represented by deep neural networks. One model $\Phi$ predicts the conditional probability of the positive label for a given sample, which defines a Bayes classifier after training, and the other model $D$ distinguishes labeled positive data from those identified by $\Phi$. The two models are simultaneously trained in an adversarial way like generative adversarial networks, and the equilibrium can be achieved when the output of $\Phi$ is close to the exact posterior probability of the positive class. In contrast with existing deep PU learning approaches, DAN does not require the class prior estimation, and its consistency can be proved under very general conditions. Numerical experiments demonstrate the effectiveness of the proposed framework.

1 Introduction

In many real-life applications, we are confronted with the task of building a binary classification model from a number of positive data and plenty of unlabeled data without extra information on the negative data. For example, it is common in disease gene identification \cite{1} that only known disease genes and unknown genes are available, because the reliable non-disease genes are difficult to obtain. Similar scenarios occur in deceptive review detection \cite{2}, web data mining \cite{3}, inlier-based outlier detection \cite{4}, etc. Such a task is certainly beyond the scope of the standard supervised machine learning, and where positive-unlabeled (PU) learning comes in handy.

A straightforward approach for PU learning is to employ a two-step strategy: First reliable negative data are identified from the unlabeled data by some

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heuristic techniques [5, 6, 7, 8], then the classifier can be trained by traditional supervised learning or expectation-maximization-like semi-supervised learning algorithms [9, 10]. Furthermore, the two steps can be iteratively executed so that more negative data can be accurately identified [11]. Most of the two-step strategy based methods assume that the positive and negative data distributions can be well separated with almost non-overlapping supports, which is difficult to satisfy in complex practical problems. Recently, applications of generative adversarial networks (GAN) in PU learning have received growing attention [12, 13], where the generative models learn to generate fake positive and negative samples (or only negative samples), and the classifier is trained by using the fake samples. Experiments show that GAN can improve the performance of PU learning when the size of positive labeled data is extremely small, but some strong assumptions of data distributions, including the data separability, are still required for the GAN based methods.

Another widely used approach is to train the classifier by minimizing a weighted loss function, where unlabeled data are interpreted as negative samples with noisy labels, and the weights can be constant hyperparameters [14, 15] or modeled as a continuous weight function according to the estimated mislabeling probabilities [16, 17]. In [18], a universal framework for classification with noisy labels are developed under the data separability assumption, and the PU learning can be efficiently performed by the presented rank pruning algorithm as a special case within this framework.

One solution to the PU learning problem with general data distributions is given by [19, 20], where an unbiased estimator for the misclassification risk of supervised learning is derived for PU data, and the classifier can be trained through minimizing the estimate. However, the direct minimization of the estimated risk easily leads to severe overfitting. In order to address this difficulty, a non-negative risk estimator is presented in [21], which is biased but more robust to statistical noise. The main limitation of this approach is that the class prior, i.e., the proportion of positive data (including labeled and unlabeled) to the whole data, is needed. In practical applications, the class prior can be estimated by some class prior estimation methods [22, 23, 24, 25], but the classification performance could be badly affected by an inaccurate estimate.

In this paper, we propose a novel PU learning framework called discriminative adversarial networks (DAN). The key idea of DAN is to approximate the ideal Bayes classifier via reducing the distribution distance between the labeled positive data and those identified by the classifier from the whole dataset. DAN measures and minimizes the distance through a minimax game between the classifier and another discriminative model by analogy to the well-known generative adversarial networks (GAN) [26], and provides a more efficient way to recover the positive and negative data distributions from unlabeled data than GAN based PU learning methods. Moreover, it can effectively avoid the phenomenon of mode collapse, from which GAN easily suffers. Both theoretical analysis and experimental results show that the proposed framework can achieve high classification accuracy in general cases without the class prior or the common assumption of data separability in PU learning. The paper is organized as fol-
lows. The next section is devoted to problem statement. Section 3 presents DAN and its detailed mathematical formulation. Section 4 compares our approach and some related works, and experiment results are provided in Section 5. Finally, further discussion and some future research directions of DAN are given in Section 6.

2 Problem statement

Let \( \mathcal{X} = \{x_1, \ldots, x_N\} \subset \mathbb{R}^d \) be \( N \) independent samples drawn from an underlying distribution density \( f(x) \) with labels \( y_1, \ldots, y_N \in \{ \pm 1 \} \), where only the first \( M \) samples \( \mathcal{P} = \{x_1, \ldots, x_M\} \) are labeled as positive, i.e., \( y_n = +1 \) for \( n \leq M \), and the labels of the other samples \( \mathcal{U} = \{x_{M+1}, \ldots, x_N\} \) are unavailable. We further assume that the empirical distribution of the positive data in \( \mathcal{P} \) is consistent with the ground truth \( f_P(x) = \mathbb{P}(x|y = +1) \). The goal of PU learning is to learn a binary classification model from the positive dataset \( \mathcal{P} \) and the unlabeled dataset \( \mathcal{U} \), which can predict the label \( y \) of a new instance \( x \sim f \).

It is well-known that the optimal classifier in the sense of minimum misclassification probability can be given by \( y = \text{sign}(\Phi^*(x) - 0.5) \) with \( \Phi^*(x) = \mathbb{P}(y = +1|x) \) being the conditional probability of the positive label. In the case of positive-negative (PN) learning, where all training samples are labeled, \( \Phi^* \) can be effectively approximated by minimizing some empirical misclassification risk (e.g., cross-entropy loss). But such an approximation is difficult for PU learning due to the absence of labeled negative training data.

Remark 1. We only consider here the single-training-set scenario of PU learning with \( \mathcal{X} \overset{iid}\sim f \). Another common scenario in the literature is called case-control \([27]\), where samples in \( \mathcal{P} \) and \( \mathcal{U} \) are drawn from \( f_P \) and \( f \) independently, and the method proposed in this paper can be naturally extended to this scenario (see Section C in Supplementary Information).

3 Discriminative adversarial networks

3.1 Motivation

Unlike some popular PU learning methods \([19, 21, 12]\), the class prior \( \pi_P = \mathbb{P}(y = +1) \) of the positive class is not assumed to be known in this paper, and only distributions of positive data and the whole dataset are available. According to the Bayes’ theorem, the two distributions are connected via \( \Phi^* \) as \( f_P = f_{\Phi^*} \), where

\[
f_{\Phi^*}(x) \triangleq \frac{f(x) \cdot \Phi(x)}{\int f(x) \cdot \Phi(x)dx}
\]  

represents the positive data distribution reconstructed by a function \( \Phi : \mathbb{R}^d \rightarrow [0,1] \). Furthermore, by replacing \( f(x) \) with the empirical distribution of \( \mathcal{X} \),
Eq. (1) can be rewritten as
\[ f_\Phi(x) = \frac{1}{N} \sum_{n=1}^{N} \bar{\Phi}^{-1} \Phi(x_n) \delta(x - x_n), \tag{2} \]
where \( \delta \) denotes the Dirac function and \( \bar{\Phi} \) is the mean value of \( \Phi(x) \) over \( X \). Hence, we can generate samples \( x \sim f_\Phi \) via resampling \( X \) with probability proportional to \( \Phi(x) \).

The above analysis suggests that a parametric model \( \hat{\Phi} \) of \( \Phi^* \) can be trained via minimizing the distance between \( f_\Phi \) and \( f_P = f_\Phi^* \). However, it is worth pointing out that \( f_\Phi = f_{c\Phi} \) for \( c > 0 \) according to (1). So, we can only get the value of \( \Phi^*(x) \) up to a proportional constant even if \( f_\Phi = f_P \) holds exactly. The scale invariance of \( f_\Phi \) has been thoroughly discussed in the research of mixture proportion estimation, and some theoretical conclusions can be seen in [28, 29]. Here, we make the following assumption so that \( \Phi^* \) is identifiable for given \( f \) and \( f_P \):
\[ \max_{x \in X} \Phi^*(x) = 1, \tag{3} \]
i.e., at least one sample can be predicted to be positive with probability one, which comprises many practical cases. Under this assumption, we can obtain
\[ \frac{\Phi(x)}{\max_{x' \in X} \Phi(x')} = \Phi^*(x) \tag{4} \]
if \( f_\Phi = f_P \).

### 3.2 Method

Inspired by the remarkable success of generative adversarial networks (GAN) [30], here we represent \( \Phi \) as a deep neural network, and define a second deep discriminative model \( D \), which maps a sample \( x \) to the probability that \( x \) came from \( f_P \) rather than \( f_\Phi \). Then the distance between \( f_P \) and \( f_\Phi \) can be measured and minimized through the following game between \( \Phi \) and \( D \):
\[ \min_{\Phi} \max_D J_{\text{dist}}(\Phi, D) = \mathbb{E}_{x \sim f_P} \left[ \log D(x) \right] + \mathbb{E}_{x \sim f_\Phi} \left[ \log (1 - D(x)) \right] \]
\[ = \frac{1}{M} \sum_{x \in P} \log D(x) + \frac{1}{N} \sum_{x \in X} \bar{\Phi}^{-1} \Phi(x) \log (1 - D(x)) \tag{5} \]
Intuitively, as illustrated in Fig. 1, \( D \) intends to separate the samples uniformly drawn from \( P \) and those obtained by resampling from \( X \) with weights given by \( \Phi \), whereas \( \Phi \) is trained to correctly identify positive samples in \( X \) so as to fool \( D \). Under some technical assumptions, it can be shown that for a fixed \( \Phi \),
\[ \max_D J_{\text{dist}}(\Phi, D) = 2\text{JSD}(f_P || f_\Phi) - \log 4 \tag{6} \]
at the limit of infinite data size (see Proposition 2 in Supplementary Information), where \( \text{JSD}(\cdot || \cdot) \) denotes the Jensen-Shannon divergence. Hence, in the
ideal situation, the training procedure converges to the equilibrium point where \( f_\Phi = f_P \) and \( D \) cannot distinguish the two distributions with \( D(x) \equiv 0.5 \), and \( \Phi^* = \Phi \) can be obtained after the normalization described in (4).

The adversarial training method described in above can provide satisfying performance when \( d \) is small. But for high-dimensional PU learning tasks, the training procedure defined by (5) also suffers from mode collapse like training of GAN, i.e., \( \Phi \) tends to predict \( \mathbb{P}(y = +1| x) \approx 0 \) for a part of positive samples especially when the positive data distribution has multiple modes. In order to address this problem, we introduce a penalty factor

\[
J_{\text{pen}}(\Phi) = \frac{1 - \log \Phi_P}{\max \{\log \Phi_P - \log \Phi, 0\} + \epsilon},
\]

and change the learning objective as

\[
\min_{\Phi} \max_{D} J(\Phi, D) = (J_{\text{dist}}(\Phi, D) + \log 4) \cdot J_{\text{pen}}(\Phi)
\]

so that JSD\((f_P || f_\Phi) = 0\) is still satisfied by the optimal solution, where \( \log \Phi_P \) is the average of \( \log \Phi(x) \) over \( \mathcal{P} \), and \( 0 < \epsilon \ll 1 \) is a small constant to avoid singularity. The numerator of \( J_{\text{pen}} \) penalizes small values of \( \Phi(x) \) for \( x \in \mathcal{P} \), and can effectively prevent the phenomenon of model collapse because \( J_{\text{pen}}(\Phi) \to \infty \) as \( \Phi(x) \to 0 \) for some \( x \in \mathcal{P} \). Furthermore, the normalization constraint (3) of model \( \Phi \) can be automatically satisfied by solving (6) since \( J_{\text{pen}}(c \cdot \Phi) < J_{\text{pen}}(\Phi) \) for \( c > 1 \). The denominator of \( J_{\text{pen}} \) is designed according to our experimental experience (see Section B in Supplementary Information for some other choices), which increases the gap between \( \log \Phi(x) \) for \( x \) in \( \mathcal{P} \) and \( \mathcal{X} \), and can improve the classification performance. More detailed analysis of \( J_{\text{pen}} \) and \( J \) is given in Section A of Supplementary Information.

The learning framework developed in this section is similar to GAN, and is based on a zero-sum game between two discriminators instead of a generator and a discriminator. Thus, we call this framework discriminative adversarial networks (DAN).
Algorithm 1 DAN learning

INPUT: Training data $X = \mathcal{P} \cup \mathcal{U}$, initial weights $W_D, W_\Phi$ of $D$ and $\Phi$, hyperparameter $\epsilon$.

OUTPUT: Classifier $y = \text{sign}(\Phi(x) - 0.5)$ defined by $\Phi$.

1: for $t = 1, \ldots, T$ do
2: Randomly sample mini-batches $B_X$ and $B_P$ from $X$ and $\mathcal{P}$ with batch size $B$.
3: Compute

$$J_{\text{dist}} = B^{-1} \sum_{x \in B_P} \log D(x) + \left( \sum_{x \in B_X} \Phi(x) \right)^{-1} \sum_{x \in B_X} \Phi(x) \log (1 - D(x)), $$

$$J_{\text{pen}} = \frac{1 - B^{-1} \sum_{x \in B_P} \log \Phi(x)}{\max \left\{ B^{-1} \sum_{x \in B_P} \log \Phi(x) - \log B^{-1} \sum_{x \in B_X} \Phi(x), 0 \right\} + \epsilon}. $$

4: Update weights $W_D$ and $W_\Phi$ with step-sizes $\eta_D$ and $\eta_\Phi$:

$$W_D \leftarrow W_D + \eta_D \frac{\partial J_{\text{dist}}}{\partial W_D}, \quad (9)$$

$$W_\Phi \leftarrow W_\Phi - \eta_\Phi \frac{\partial (|J_{\text{dist}} + \log 4| \cdot J_{\text{pen}})}{\partial W_\Phi}. \quad (10)$$

5: end for
6: Normalize $\Phi$ as

$$\Phi(x) \leftarrow \min \left\{ \frac{\Phi(x)}{\max_{x \in X} \Phi(x)}, 1 \right\}. \quad (11)$$

3.3 Implementation

The detailed DAN learning algorithm adopted in this paper is summarized by Algorithm 1 where $\Phi, D$ are both deep networks with weights denoted by $W_\Phi, W_D$, and the Sigmoid output neurons (or the other bounded output neurons) can be used so that $\Phi(x), D(x) \in [0, 1]$ for all $x$. For applications in big data scenarios, all mean values involved in the objective function are approximated by mini-batches in each iteration. Notice that $W_D$ is updated only by using the gradient of $J_{\text{dist}}$ in Step 9 because $J_{\text{pen}}$ is independent of $D$. For $W_\Phi$, the value of $(J_{\text{dist}}(D, \Phi) + \log 4)$ is usually positive under the condition that $D$ performs better than random guess, which is usually satisfied in training process. But when the model $D$ is badly initialized with $J_{\text{dist}}(D, \Phi) + \log 4 < 0$, updating $W_\Phi$ according to the gradient of $J$ may yield the divergence of the algorithm. So we implement the update of $W_\Phi$ as shown in (10) for numerical stability.
4 Related work

An important idea of DAN is to approximate $\Phi^*(x) = P(y = +1|x)$ by matching $f_\Phi$ and $f_{P^*}$, which has in fact been investigated in literature (see, e.g., [31,32,33,34,24]). However, the direct approximation based on (1) involves the probability density estimation and is difficult for high-dimensional applications. In [34,24], by modeling the ratio between $f_P$ and $f$ as a linear combination of basis functions, this problem is transformed into a quadratic programming problem. But the approximation results cannot meet the requirement for classification, and are only applicable to estimation of the class prior of $\pi_P = P(y = +1)$.

One main contribution of our approach compared to the previous works is that we find a general and effective way to optimize the model of $\Phi^*$ by adversarial training.

It is also interesting to compare DAN to GenPU, a GAN based PU learning method [12], since they share the similar adversarial training architecture. In DAN, the discriminative model $\Phi$ plays the role of the generative model in GAN by approximating positive data distribution in an implicit way, and can be efficiently trained together with $D$. In contrast, GenPU is much more time-consuming and easily suffers from mode collapse as stated in [12] due to that it contains three generators and two discriminators. (Notice that the penalty factor $J_{pen}$ cannot be applied to GenPU for the probability densities of samples given by generators are unknown.) Furthermore, the consistency of the GenPU needs the assumptions that class prior is given and there is no overlapping between positive and negative data distributions, which are not necessary for DAN.

5 Experiments

In this section, we conduct a series of PU learning experiments on both synthetic and real-world datasets to evaluate the performance of DAN. The detailed settings of datasets and algorithms are provided in Section D of Supplementary Information, and the software code for DAN is also available.

We first visualize the learning results of DAN on four two-dimensional toy examples in Fig. 2, from which we can observe that an accurate classification boundary can be deduced from the conditional class probability approximated by DAN even if the positive and negative data cannot be well separated.

Next, we conduct experiments on three benchmark datasets taken from the UCI Machine Learning Repository [35,36], and the performance of DAN is compared to that of some recently developed PU learning methods, including the unbiased risk estimator based uPU and nnPU [19,21], the generative model based GenPU [12], and the rank pruning (RP) proposed in [18].

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1. The software code will be publicly available after the blind review process.
2. The software codes are downloaded from https://github.com/kiryor/nnPUlearning, https://github.com/cgnorthcutt/rankpruning, and https://qibinzhao.github.io/index.html.
Figure 2: Results of DAN learning on four two-dimensional datasets. First line: Samples in training sets, where each set contains 5000 positive samples (in yellow) and 5000 negative samples (in green), and 1000 positive samples are labeled. Second line: The estimated $\Phi(x)$ given by DAN.

that uPU and nnPU require the class prior $\pi_P$, we implement uPU and nnPU under two different conditions: (a) The exact value of $\pi_P$ is known, and (b) $\pi_P$ is estimated by KM2 proposed in [20], which is one of the state-of-the-art class prior estimation algorithms. For GenPU, the hyperparameters of the algorithm are determined by greedy grid search (see Section D.5 in Supplementary Information). The classification results are summarized in Table 1. It can be seen that DAN outperforms the other methods with high accuracies and low variances on almost all the datasets. Only the nnPU obtains a higher accuracy on the dataset of Grid Stability with “unstable vs stable” when the exact value of $\pi_P$ is given, and its accuracy decreases significantly with estimated $\pi_P$. In addition, RP interprets unlabeled data as noisy negative data and can get an accurate classifier when the proportion of positive data is small in unlabeled data. But in the opposite case where the proportion is too large, RP performs even worse than random guess. ($\pi_P = 0.896$ and $0.635$ in Page Blocks with ‘2,3,4,5’ vs ‘1’ and Grid Stability with ‘unstable’ vs ‘stable’.)

Finally, all the methods are compared on two image datasets: FashionMNIST and CIFAR-10[3] and the classification results are collected in Table 2 where the superior performance of DAN is also evident. Here uPU performs much worse than nnPU due to the overfitting problem [21] (see Fig. 4 in Supplementary Information). Moreover, the performance of GenPU is also not satisfying because of the mode collapse of generators as shown in Fig. 3. In contrast, different modes of positive and negative data can be successfully sampled.

[3]Datasets are downloaded from https://github.com/zalandoresearch/fashion-mnist and https://www.cs.toronto.edu/~kriz/cifar.html
Table 1: Classification accuracies (%) of compared methods on UCI datasets. The accuracies are evaluated on test sets, and the mean and standard deviation values are computed from 10 independent runs. Definitions of labels ('Positive' vs 'Negative') are as follows: Page Blocks\(^1\): '1' vs '2,3,4,5'. Page Blocks\(^2\): '2,3,4,5' vs '1'. Grid Stability\(^1\): 'stable' vs 'unstable'. Grid Stability\(^2\): 'unstable' vs 'stable'. Avila\(^1\): 'A' vs the rest. Avila\(^2\): 'A, F' vs the rest. Labeled positive data are randomly selected from the training data with \(M = 100, 1000, 2000\) and \(N = 3284, 6000, 10430\).

| Dataset       | DAN      | mPU      | mPU(KM2) | uPU      | uPU(KM2) | GenPU    | RP       |
|---------------|----------|----------|----------|----------|----------|----------|----------|
| Page Blocks\(^1\) | 95.1 ± 0.1 | 92.3 ± 1.2 | 93.4 ± 1.1 | 93.0 ± 1.2 | 92.8 ± 1.3 | 93.2 ± 0.3 | 91.2 ± 1.4 |
| Page Blocks\(^2\) | 94.0 ± 0.1 | 91.7 ± 0.6 | 90.2 ± 2.6 | 90.0 ± 2.8 | 86.8 ± 4.7 | 90.2 ± 0.1 | 9.96 ± 0.7 |
| Grid Stability\(^1\) | 93.0 ± 0.2 | 91.5 ± 1.7 | 80.8 ± 2.5 | 92.2 ± 0.1 | 92.6 ± 0.7 | 69.3 ± 0.6 | 84.7 ± 1.3 |
| Grid Stability\(^2\) | 90.3 ± 0.6 | 90.5 ± 0.3 | 84.1 ± 1.8 | 87.9 ± 0.9 | 86.8 ± 0.5 | 75.6 ± 1.8 | 36.7 ± 0.6 |
| Avila\(^1\)     | 81.6 ± 0.2 | 75.9 ± 2.2 | 73.3 ± 2.0 | 76.5 ± 1.0 | 75.0 ± 0.4 | 63.4 ± 1.1 | 75.8 ± 0.4 |
| Avila\(^2\)     | 86.2 ± 0.6 | 84.8 ± 0.5 | 83.1 ± 2.1 | 84.0 ± 1.0 | 82.7 ± 1.7 | 67.1 ± 0.8 | 77.2 ± 0.2 |

6 Discussion

The framework of DAN can be viewed as a mixture of discriminative learning and generative learning: A discriminative model is trained by minimizing a loss function defined by the distribution distance as a generative model. Due to the existence of unlabeled data, it is very difficult, if not impossible, to perform the PU learning in a pure discriminative manner. Even uPU and nnPU, which are developed based on the estimator of the discriminative loss, still need to model positive and negative data distributions for the approximation of class prior. But DAN demonstrates that, in PU learning, the classifier can be trained directly without solving the problem of probability density estimation as an intermediate step. It is interesting to extend this idea to more general semi-supervised learning problems, such as PNU learning, where some data are labeled as positive or negative while most data are unlabeled, and DAN has the potential to address such classification challenges especially in application scenarios where labeled positive and negative data cannot cover all modes of datasets.

It is also worthy to note that DAN is a very flexible framework, and the performance can be expected to be further improved by utilizing many advanced GAN techniques developed in recent years. For example, by analogy to WGAN and MMD-GAN, we can simply establish DAN models based on the Wasserstein metric and maximum mean discrepancy between distributions. Another research direction in future is to investigate robust DAN for semi-supervised learning with noisy labels.
Table 2: Classification accuracies (%) of compared methods on FashionMNIST and CIFAR-10 datasets. The accuracies are evaluated on test sets. Definitions of labels ('Positive' vs 'Negative') are as follows: FashionMNIST\textsuperscript{1}: '1,4,7' vs '0,2,3,5,6,8,9'. FashionMNIST\textsuperscript{2}: '0,2,3,5,6,8,9' vs '1,4,7'. CIFAR-10\textsuperscript{1}: '0,1,8,9' vs '2,3,4,5,6,7'. CIFAR-10\textsuperscript{2}: '2,3,4,5,6,7' vs '0,1,8,9'. Labeled positive data are randomly selected from the training data with $M = 3000$.

| Dataset    | DAN  | nnPU | nnPU(KM2) | uPU  | nPU(KM2) | GenPU | RP  |
|------------|------|------|-----------|------|----------|-------|-----|
| FashionMNIST\textsuperscript{1} | 93.4 | 92.4 | 90.4      | 88.8 | 86.9     | 48.3  | 91.9|
| FashionMNIST\textsuperscript{2} | 91.9 | 90.6 | 90.1      | 66.2 | 78.5     | 78.5  | 73.6|
| CIFAR-10\textsuperscript{1}    | 89.7 | 89.2 | 87.8      | 64.2 | 63.7     | 67.9  | 85.7|
| CIFAR-10\textsuperscript{2}    | 89.1 | 88.2 | 87.2      | 43.8 | 43.7     | 71.7  | 83.7|

Figure 3: Samples generated by using $\Phi$ in DAN and generative models in GenPU. (a, b) Images resampled from training set with probability proportional to $\Phi(x)$ and $1 - \Phi(x)$. (c, d) Images generated by positive and negative generators in GenPU. True labels ('Positive' vs 'Negative') are given by '1,4,7' (Trouser, Coat, Sneaker) vs '0,2,3,5,6,8,9' (T-shirt/Top, Pullover, Dress, Sandal, Skirt, Bag, Ankle boot).
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Supplementary Information

A Theoretical analysis of DAN learning

In this section, we analyze the properties of (8) and its optimal solution under the following assumptions.

Assumption 1. $\Phi, D$ have enough capacity and both $N$ and $M$ tends to infinity with $h = N/M$ being fixed.

Assumption 2. The marginal distribution $f(x) > 0$ for all $x \in \mathbb{R}^d$.

Assumption 3. There exists a measurable set $\Omega \subset \mathbb{R}^d$ so that $\Phi^*(x) \equiv 1$ for all $x \in \Omega$.

Proposition 1. $J_{\text{pen}}$ defined by (7) satisfies: (i) $J_{\text{pen}}(c\Phi) < J_{\text{pen}}(\Phi)$ for $c > 1$. (ii) $J_{\text{pen}} \geq (\epsilon + \log h)^{-1}$. (iii) $J_{\text{pen}} \to \infty$ as $\Phi(x) \to 0$ for some $x \in P$.

Proof. The proof of (i) is trivial, and (ii) and (iii) are direct conclusions of the following inequality:

$$\log \Phi_P - \log \Phi \leq \log \Phi_P - \log \left( \frac{M}{N} \cdot \frac{1}{M} \sum_{x \in P} \Phi(x) \right)$$

$$= \log \Phi_P - \log \left( \frac{1}{M} \sum_{x \in P} \Phi(x) \right) + \log \frac{N}{M}$$

$$\leq \log h.$$  \hspace{1cm} (12)

Proposition 2. For a given $\Phi$,

$$\max_D J_{\text{dist}}(\Phi, D) = 2J_{\text{SD}}(f_P \| f_\Phi) - \log 4,$$  \hspace{1cm} (13)

and the maximum is achieved when

$$D(x) = \frac{f_P(x)}{f_P(x) + f_\Phi(x)}.$$  \hspace{1cm} (14)

Proof. According to the definition, $J_{\text{dist}}$ is maximized when

$$\frac{\partial (f_P(x) \log D(x) + f_\Phi(x) \log (1 - D(x)))}{\partial D(x)} = 0.$$  \hspace{1cm} (15)

Then, the optimal $D$ is given by (14) and the maximum is

$$J_{\text{dist}}(\Phi, D) = \int f_P(x) \cdot \log \frac{f_P(x)}{\frac{1}{2} (f_P(x) + f_\Phi(x))} \, dx + \log \frac{1}{2}$$

$$+ \int f_\Phi(x) \cdot \log \frac{f_\Phi(x)}{\frac{1}{2} (f_P(x) + f_\Phi(x))} \, dx + \log \frac{1}{2}$$

$$= 2J_{\text{SD}}(f_P \| f_\Phi) - \log 4.$$  \hspace{1cm} (16)
Proposition 3. If $\Phi^*(x) = 1$ for some area $\Omega \subset \mathbb{R}^d$ with $\int_\Omega f(x)dx > 0$, and $(\Phi, D)$ is an optimal solution to (8). Then

$$
\frac{\Phi(x)}{\max_{x \in \mathcal{X}} \Phi(x)} \to \Phi^*(x)
$$

in probability and $D(x) \equiv 0.5$.

Proof. It can be known from Propositions [1] and [2] that the optimal $(\Phi, D)$ satisfies $D(x) \equiv 0.5$ and $f_\Phi = f_{\Phi^*}$. Therefore

$$
\Phi(x) \propto \frac{f_\Phi(x)}{f(x)} = \frac{f_{\Phi^*}(x)}{f(x)} \propto \Phi^*(x).
$$

(18)

We can then obtain (17) according to Assumption 3.

Notice that Proposition 3 shows the consistency of DAN learning with normalization step (11).

B Penalty factors

Besides the penalty factor given in (7), we also considered the following factors:

$$
J^{(1)}_{\text{pen}} = 1 - \log \Phi^p,
$$

(19)

$$
J^{(2)}_{\text{pen}} = \frac{1 - \log \Phi^p}{\max \{ \log \Phi^p - \log \bar{\Phi}, 0 \}} + \epsilon,
$$

(20)

$$
J^{(3)}_{\text{pen}} = \frac{1 - \log \Phi^p}{\text{MI}(\Phi)},
$$

(21)

where

$$
\text{MI}(\Phi) = \text{KL}(P(x,y)||P(x)P(y))|_{P(y=+1|x)=\Phi(x),P(y=-1|x)=1-\Phi(x)}
$$

(22)

$$
= \Phi \log \Phi - \Phi \log \bar{\Phi} + (1-\Phi) \log (1-\Phi) - \bar{\Phi} \log (1-\bar{\Phi})
$$

(22)

denotes the mutual information between sample $x$ and its label $y$ defined by $\Phi$, and $\bar{g}$ denotes the average of $g(x)$ over $\mathcal{X}$ in (22). All the above choices of the penalty factor can lead to consistency of learning. We choose $J_{\text{pen}}$ defined by (7) because it achieves the best performance in our experiments.
Table 3: Parameters of toy examples.

| Dataset                  | parameters                      |
|--------------------------|---------------------------------|
| Concentric circles       | factor=0.5 noise=0.1            |
| Half moons               | noise=0.1                       |
| Blobs                    | cluster_std=1.0                 |
| Gaussian mixture model   | covariance matrix=0.16 ⋅ I      |

C Case-control scenario

Under the scenario of case-control, the empirical approximation \( f_Φ \) of \( f_Φ \) becomes

\[
f_Φ(x) = \frac{1}{N - M} \sum_{n=M+1}^{N} \bar{Φ}^{-1}Φ(x_n)δ(x - x_n),
\]

where \( \bar{Φ} \) is the mean value of \( Φ(x) \) over \( U \). Therefore, the method and theory presented in this paper can be extended to the case-control scenario by defining

\[
J_{dist}(Φ, D) = \mathbb{E}_{x \sim f_P} [\log D(x)] + \mathbb{E}_{x \sim f_Φ} [\log (1 - D(x))]
\]

\[
= \frac{1}{M} \sum_{x \in P} \log D(x) + \frac{1}{N - M} \sum_{x \in U} \bar{Φ}^{-1}Φ(x) \log (1 - D(x))
\]

D Experiment details

In FashionMNIST, CIFAR-10 and Avila, datasets have been separated into training and test sets. For the two UCI datasets, we adopt the train_test_split function in scikit-learn to get test sets.

D.1 Toy examples

The former three toy examples in our experiments are generated by functions of make_circles, make_moons, make_blobs in the package of scikit-learn, where the centers of blobs are \((1, 5), (5, 1), (0, 0), (6, 6)\). The dataset of the fourth example are given by a Gaussian mixture model with centers \((0, -\sqrt{2}), (-1, -1), (-\sqrt{2}, 0), (-1, 1), (0, \sqrt{2}), (1, 1), (\sqrt{2}, 0), (1, -1)\). The other details are shown in Table 3.

D.2 UCI datasets

We first clarify the UCI datasets used in our experiments in Table 4. Then, we give the detailed experimental settings of each experiment in Table 5.
Table 4: Description of UCI datasets used in experiments.

| Dataset          | $N$  | size of test set | $d$ |
|------------------|------|------------------|-----|
| Page Blocks      | 3284 | 2189             | 10  |
| Grid Stability   | 6000 | 4000             | 14  |
| Avila            | 10430| 10437            | 10  |

Table 5: Experimental settings for UCI datasets, where $N_P$ denotes the number of all labeled and unlabeled positive data in training sets.

| Experiment setting | Data amount | $\pi_P$ |
|--------------------|-------------|---------|
| Page Blocks$^1$ '2,3,4,5' vs '1' | $N_P=342$ $M=100$ | 0.104 |
| Page Blocks$^2$ '1' vs '2,3,4,5' | $N_P=2942$ $M=100$ | 0.896 |
| Grid Stability$^1$ 'stable' vs 'unstable' | $N_P=2187$ $M=1000$ | 0.365 |
| Grid Stability$^2$ 'unstable' vs 'stable' | $N_P=3813$ $M=1000$ | 0.635 |
| Avila$^1$ 'A' vs The rest | $N_P=4286$ $M=2000$ | 0.411 |
| Avila$^2$ 'A,F' vs The rest | $N_P=6247$ $M=2000$ | 0.599 |

D.3 FashionMNIST and CIFAR-10

The details of the experiments are shown in Table 6. Classification errors of nnPU, uPU and DAN on CIFAR-10 test data with different numbers of epochs are plotted in Fig. 4.

D.4 Other details

We choose Adam as the optimizer for DAN in our experiments, and the hyperparameters in Adam are $(\beta_1, \beta_2) = (0.5, 0.99)$. The architectures for models in DAN are shown in Table 7. The epoch number of DAN for image datasets is 60, and 100 for the other datasets. Moreover, the hyperparameter $\epsilon = 10^{-8}$.

D.5 Choice of hyperparameters of GenPU

GenPU contains four hyperparameters: $\pi_P \lambda_p$, $\pi_P \lambda_u$, $\pi_N \lambda_n$, $\pi_N \lambda_u$. Although the parameters are coupled for given $\pi_P$ in [12], our experience shows that the better performance can be achieved by selecting the four parameters independently. Table 8 shows the best hyperparameters which lead to the largest classification accuracies on test sets. They are selected in $\{0.01, 0.05, 0.1, 0.5, \ldots, 1000, 5000\}$ by greedy grid search.
Figure 4: Test errors of DAN, nnPU-KM2 and uPU-KM2 on CIFAR-10 with different numbers of epochs. The left one: Classes 2,3,4,5,6,7 are positive. The right one: Classes 0,1,8,9 are positive.

Table 6: Experimental settings for FashionMNIST and CIFAR-10, where $N_P$ denotes the number of all labeled and unlabeled positive data in training sets.

| Experiment   | Setting                  | Data amount   | $\pi_P$ | KM2 |
|--------------|--------------------------|---------------|--------|-----|
| FashionMNIST | '1,4,7' vs '0,2,3,5,6,8,9' | $N_P=18000$   | 0.300  | 0.267 |
|              | '0,2,3,5,6,8,9' vs '1,4,7' | $N_P=42000$   | 0.700  | 0.756 |
| CIFAR-10     | '0,1,8,9' vs '2,3,4,5,6,7' | $N_P=20000$   | 0.400  | 0.532 |
|              | '2,3,4,5,6,7' vs '0,1,8,9' | $N_P=30000$   | 0.600  | 0.690 |

Table 7: The architectures details for experiments.

| Dataset   | Network | Model               | Initial learning rate |
|-----------|---------|---------------------|-----------------------|
| Toy examples | D       | 5-layers MLP with ReLU | $10^{-3}$ |
|            | $\Phi$  | 5-layers MLP with ReLU | $10^{-3}$ |
| UCI datasets | D       | 8-layers MLP with ReLU | $10^{-4}$ |
|            | $\Phi$  | 8-layers MLP with ReLU | $10^{-4}$ |
| Fashion-MNIST | D       | 7-layers CNN with ReLU | $10^{-4}$ |
|            | $\Phi$  | 7-layers CNN with ReLU | $10^{-4}$ |
| CIFAR-10   | D       | 7-layers CNN with ReLU | $10^{-4}$ |
|            | $\Phi$  | 7-layers CNN with ReLU | $10^{-4}$ |
Table 8: Choice of hyperparameters for GenPU.

| Dataset | FashionMNIST | CIFAR-10 | Page Blocks | Grid Stability | Avila |
|---------|--------------|----------|-------------|----------------|-------|
| $\pi_P \lambda_p$ | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 |
| $\pi_P \lambda_u$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $\pi_N \lambda_n$ | 100 | 1000 | 100 | 1000 | 200 | 1000 | 1000 |
| $\pi_N \lambda_u$ | 1 | 50 | 1 | 1 | 1 | 500 | 500 |