Transductive Adversarial Networks (TAN)

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Abstract

TAN is a novel domain-adaptive semi-supervised machine learning framework that is designed for learning a conditional probability distribution on unlabelled data in a target domain, while only having access to: (1) easily obtained labelled data in a related, yet likely simpler, source domain and (2) a prior distribution on the labels for the target domain. TAN leverages a fully adversarial training procedure and a unique generator/encoder architecture which approximates the transductive combination of the source- and target-domain data. A benefit of TAN is that it allows the distance between the source- and target-domain label vector distributions to be greater than 0 whereas other domain-adaptive semi-supervised learning algorithms require this distance to equal 0. TAN can, however, still handle the latter case and is a more generalised approach to this case. Another benefit of TAN is that due to being a fully adversarial algorithm, it has the ability to accurately approximate highly complex distributions. Theoretical and experimental analyses demonstrate the viability of the TAN framework.

1. Introduction

The scenario of having access to a small amount of labeled data but a large amount of unlabelled data is a common one in practice. In an idealised learning situation, the joint probability distribution between the input vector and the label vector across the sets of labeled and unlabelled data are equal. However, typically this does not occur in practice. Instead, the small amount of labeled data that is accessible is usually either significantly simpler than the encountered unlabelled data, or comes from a different domain with a different joint probability distribution between its input vector and label vector. These two practical cases can be considered the same from a learning point-of-view as the latter practical case.

In the standard domain-adaptive semi-supervised learning scenario, it is expected that the labelled and unlabelled input vectors can be drawn from unique marginal probability distributions. However, it is required that the label-vector marginal probability distribution for the labelled and unlabelled sets of data are equal and match the available labelled set of data [CITE]. This is demonstrated in the following example involving the MNIST (hand-drawn digits) and SVHN (house numbers from Google StreetView images) datasets.
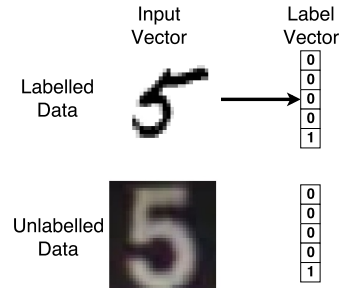

Figure 1. The standard domain-adaptive semi-supervised learning scenario where the label-vector marginal probability distributions across domains are expected to be equal. In this example learning scenario, the labelled data are pairs of both an image of a hand-drawn number from 1 through 5 and a 5-dimensional one-hot encoded vector that encodes the numerical representation of the input image. The unlabelled data are images of house numbers from 1 through 5. There are common features in the input vectors across domains that allow a domain-adaptive semi-supervised learning algorithm to assign labels to the unlabelled input vectors using the available labelled and unlabelled data.

Now consider a generalised domain-adaptive semi-supervised learning scenario where both the input-vector and the label-vector marginal probability distributions across domains are not expected to be equal. This generalised scenario motivates the design of TAN. The scenario is demonstrated in the following example involving the MNIST and SVHN datasets.

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Code and hyperparameters are available at:
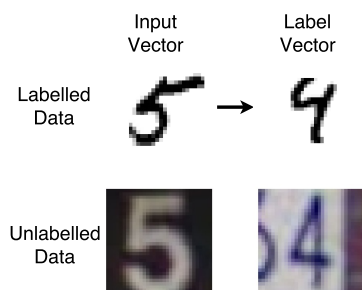https://github.com/sean-rowan/tan

Figure 2. A generalised domain-adaptive semi-supervised learning scenario where both the input-vector and the label-vector marginal probability distributions across domains are not expected to be equal. In this example learning scenario, the labelled data are pairs of a hand-drawn single-digit image of an odd number and a hand-drawn single-digit image of the previous even number. The unlabelled data pairs are the same except they are images of house numbers.

This generalised domain-adaptive semi-supervised learning scenario is distinct from the style-transfer learning problem. In style transfer, learning occurs only on a single marginalised input vector across domains, and does not involve a corresponding label vector, thus significantly simplifying the learning procedure [CITE].

We now further motivate the usefulness of an algorithm that can learn a conditional probability distribution within the generalised domain-adaptive semi-supervised learning scenario with a real-world application. Consider the problem of human drug discovery. In a human drug discovery scenario, there is no data available about how an experimental drug molecule might bind to known human protein structures due to the difficulty in testing new drugs on live human subjects. However, there is ample data available on how an experimental drug molecule can bind to known yeast cell protein structures due to the free ability to test new drugs on these cells. In this scenario, the yeast cell experiments represent the source domain and the human experiments represent the target domain. The yeast cell protein structure is the input vector of the source domain and the experimental drug for yeast cells is the label vector of the source domain. Likewise, the human protein structure is the input vector of the target domain and the experimental drug for humans is the unknown label vector of the target domain. The learning goal is to generate a shortlist of potential candidate drugs for further human testing. Such an algorithm would be highly valuable in discovering new drugs for humans with fewer drug trials.

2. Related Work

- GAN overview and impact

- ALI details

- Limitations of GAN and ALI; reason for TAN

- Similar work to TAN, same limitations

3. TAN Algorithm

3.1. TAN Model

3.2. TAN Training Procedure

4. Experiments

5. Conclusions