Theoretical Perspective of Deep Domain Adaptation

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Abstract
Deep domain adaptation has recently undergone a big success. Compared with shallow domain adaptation, deep domain adaptation has showed higher predictive performance and stronger capacity to tackle structural data (e.g., image and sequential data). The underlying idea of deep domain adaptation is to bridge the gap between source and target domains in a joint feature space so that a supervised classifier trained on labelled source data can be nicely transferred to the target domain. This idea is certainly appealing and motivating, but under the theoretical perspective none of theory has been developed to support this. In this paper, we have developed a rigorous theory to explain why we can bridge the relevant gap in an intermediate joint space. Under the light of our proposed theory, it turns out that there is a strong connection between deep domain adaptation and Wasserstein (WS) distance. More specifically, our theory revolves the following points: i) first, we propose a context wherein we can perfectly perform a transfer learning and ii) second, we further prove that by means of bridging the relevant gap and minimizing some reconstruction errors we are minimizing a WS distance between the pushforward source distribution and the target distribution via a transport that maps from the source to target domains.

1. Introduction
Learning a discriminative classifier or other predictor in the presence of a shift between source (training) and target (testing) distributions is known as domain adaptation (DA). Domain adaptation, also known as the covariate shift problem or a special case of transfer learning, aims to devise automatic methods that make it possible to perform transfer learning from the source domain with labels to the target domains without labels. Studies in domain adaptation can be broadly categorized into two themes: shallow and deep domain adaptations. A number of approaches to domain adaptation have been suggested in the context of shallow learning when data representations/features are given and fixed, notably via reweighing or selecting samples from the source domain (Borgwardt et al., 2006; Huang et al., 2007; Gong et al., 2013) or seeking an explicit feature space transformation that would map source distribution into the target ones (Pan et al., 2009; Gopalan et al., 2011; Baktashmotlagh et al., 2013).

To further advance shallow domain adaptation, deep domain adaptation has recently been proposed to encourage the learning of new representations for both source and target data in order to minimize the divergence between them (Ganin & Lempitsky, 2015; Tzeng et al., 2015; Long et al., 2015; Shu et al., 2018; French et al., 2018). Source and target data are mapped to a joint feature space via a generator and the gap between source and target distributions is bridged in this joint space by minimizing the divergence between the forwarded distributions. For instance, the works of (Ganin & Lempitsky, 2015; Tzeng et al., 2015; Long et al., 2015; Shu et al., 2018; French et al., 2018) minimize the Jensen-Shannon divergence between the two relevant distributions relying on the GAN principle (Goodfellow et al., 2014), while the work of (Long et al., 2015) minimizes the maximum mean discrepancy (MMD) (Gretton et al., 2007) and the work of (Courty et al., 2017) minimizes the Wasserstein distance between them. The idea of bridging the gap of the source and target domains in a joint feature space is intuitive, motivating and appealing. However, there has been none of theoretical work proposed to further mathematically explain and support this idea.

In this paper, we develop a rigorous theory to explain why we can bridge the gap between the source and target domains in the joint feature space for deep domain adaptation. The theory indicates a strong connection between deep domain adaptation and WS distance. More specifically, our theory first answers the question under which circumstance we can ideally perform deep domain adaptation to transfer learning from the source to target domains. Under the light of this theory, it turns out that we need to learn a bijection map that pushforwards the source to target distributions which can be further obtained by minimizing a WS distance...
between them. Inspecting this minimization further leads us to a theory which specifies that we need to bridge the gap between the source and target distributions in a joint space in conjunction with minimizing some reconstruction errors. This theory certainly sheds light on why we can bridge the gap in the joint feature space. Furthermore, this theory also introduces some new principled terms: i) we should use different generator network for source and target domains and ii) in addition to minimizing the divergence between the source and target distributions in the joint space, we need to minimize some reconstruction errors. We conduct the corresponding experiments to investigate the behavior and influence of additional components when plugging into the model for deep domain adaptation.

2. Related Background

In this section, we present the related background for our paper. We depart with the introduction of pushforward measure followed by the definition of optimal transport and the introduction of a standard machine learning setting.

2.1. Pushforward Measure

Given two probability spaces \((\mathcal{X}, \mathcal{F}, \mu)\) and \((\mathcal{Y}, \mathcal{G})\) where \(\mathcal{X}, \mathcal{Y}\) are two sample spaces, \(\mathcal{F}, \mathcal{G}\) are two \(\sigma\)-algebras over \(\mathcal{X}, \mathcal{Y}\) respectively, and \(\mu\) is a probability measure, a map \(T: \mathcal{X} \to \mathcal{Y}\) is said to be \((\mathcal{Y}, \mathcal{G})\)-or \((\mathcal{X}, \mathcal{F})\)-measurable if for every \(A \in \mathcal{G}\), the inverse \(T^{-1}(A) \in \mathcal{F}\). The \((\mathcal{Y}, \mathcal{G})\)-or \((\mathcal{X}, \mathcal{F})\) measurable map \(T\) when applied to \((\mathcal{X}, \mathcal{F}, \mu)\) induces a distribution \(\nu\) over \((\mathcal{Y}, \mathcal{G})\) which is defined as:

\[
\nu(A) = \mu(T^{-1}(A)), \quad \forall A \in \mathcal{G}
\]

We also say that the map \(T\) transport the probability measure \(\mu\) to \(\nu\) and denote as \(\nu = T#\mu\). Furthermore, if \(\mu\) and \(\nu\) are two given atomless probability measures over \((\mathcal{X}, \mathcal{F})\) and \((\mathcal{Y}, \mathcal{G})\), there exists a bijection \(T: \mathcal{X} \to \mathcal{Y}\) that transports \(\mu\) to \(\nu\). This is formally stated in the following theorem.

**Theorem 1.** Given two probability spaces \((\mathcal{X}, \mathcal{F}, \mu)\) and \((\mathcal{Y}, \mathcal{G}, \nu)\) with two atomless probability \(\mu, \nu\) over two Polish spaces \(\mathcal{X}, \mathcal{Y}\) (i.e., separably complete metric spaces), there exist a bijection \(T: \mathcal{X} \to \mathcal{Y}\) that transports \(\mu\) to \(\nu\), i.e., \(T#\mu = \nu\).

2.2. Optimal Transport

Given two probability measures \((\mathcal{X}, \mu)\) and \((\mathcal{Y}, \nu)\) and a cost function \(c(x, x')\), the Earth Mover (EM) distance between these two distributions is defined as:

\[
\text{EM}_c(\mu, \nu) = \inf_{T#\mu = \nu} \mathbb{E}_{x \sim \mu}[c(x, T(x))]
\]

Although in the theoretical analysis we only use the above definition originated from Gaspard Monge, there is another equivalent definition of EM distance originated from Kantorovich:

\[
\text{EM}_c(\mu, \nu) = \inf_{\pi \in \Gamma(\mu, \nu)} \mathbb{E}_{(x, x') \sim \pi}[c(x, x')]
\]

where \(\Gamma(\mu, \nu)\) specifies the set of joint distributions over \(\mathcal{X} \times \mathcal{Y}\) which admits \(\mu\) and \(\nu\) as marginals.

The WS distance is an extension of the EM distance and defined as follows:

\[
\text{WS}_c(\mu, \nu) = \inf_{T#\mu = \nu} \mathbb{E}_{x \sim \mu}[c(x, T(x))^p]^{1/p}
\]

\[
\text{WS}_c(\mu, \nu) = \inf_{\pi \in \Gamma(\mu, \nu)} \mathbb{E}_{(x, x') \sim \pi}[c(x, x')^p]^{1/p}
\]

where \(p > 0\).

2.3. Machine Learning Setting and General Loss

According to (Vapnik, 1999), a standard machine learning system consists of three components: the generator, the supervisor, and the function class.

**Generator** The generator is the mechanism to generate data examples \(x \in \mathbb{R}^d\) and is mathematically formulated by an existed but unknown distribution \(p(x)\).

**Supervisor** The supervisor is the mechanism to assign labels \(y\) (e.g., \(y \in \{1, 2, \ldots, M\}\)) for the classification problem and \(y \in \mathbb{R}\) for the regression problem) to a data example \(x\) and is mathematically formulated as a conditional distribution \(p(y | x)\).

**Family class** This specifies the family class \(\{f_\theta : \theta \in \Theta\}\) parameterized by \(\theta\) which is used to predict label for the data examples \(x\).

Given a loss function \(l(x, y; \theta) = \ell(y, f_\theta(x))\) where \(\ell: \mathbb{R}^2 \to \mathbb{R}\) and \(\ell(y, y')\) specifies the loss suffered if predicting the data example \(x\) with the label \(y'\) while its true label is \(y\), the general loss of the decision function \(f_\theta\) is defined as the expected loss caused by \(f_\theta\):

\[
R(\theta) = \mathbb{E}_{p(x, y)}[l(x, y; \theta)] = \int l(x, y; \theta) p(x, y) \, dx \, dy
\]

The optimal parameter \(\theta^* \in \Theta\) is sought by minimizing the general loss as:

\[
\theta^* = \arg\min_{\theta \in \Theta} R(\theta)
\]

3. Theoretical Results

We first introduce the ideal circumstance wherein we can perfectly learn and later develop further theory
Theorem 2. Let $T$ be a bijective transformation that transports $P_s$ to $P_t$ (i.e., $T \# P_s = P_t$). Assume that source and target supervisors are harmonic in the sense that $p_t(y \mid T(x)) = p_s(y \mid x)$, or in the other words the target supervisor assigns labels to $T(x)$ in the same way as the source supervisor does for $x$. Then, we can perfectly do transfer learning.

Proof. Let us consider using any discriminative function $f_\theta$ in the function class with $\Theta$. Assume that we are using a marginal loss function where $l(x, y; \theta) = \ell(y, f_\theta(x))$. For any $x^t \sim P_t$, we employ $g_\theta = T^{-1} \circ f_\theta$ to predict it, i.e., $g_\theta(x^t) = f_\theta(T^{-1}(x^t))$. We now inspect the general error of $g_\theta$ incurred on the target distribution.

\[
R^t(\theta) = \int \ell(y, g_\theta(x^t)) p^t(x^t, y) \, dx^t \, dy = \int \ell(y, g_\theta(x^t)) p_t(y \mid x^t) \, dy p_t(x^t) \, dx^t = \int \ell(y, g_\theta(x^t)) p_t(y \mid x^t) \, dy \, dP_t(x^t) = \int \ell(y, g_\theta(T(x^t))) p_t(y \mid T(x^t)) \, dy dP_t(x^t)
\]

Recall that $g_\theta(T(x^t)) = f_\theta(T^{-1}(T(x^t))) = f_\theta(x^t)$ and $p_t(y \mid T(x^t)) = p_s(y \mid x^t)$, we can further derive:

\[
R^t(\theta) = \int \ell(y, f_\theta(x^t)) p_s(y \mid x^t) \, dy dP_s(x^t) = \int \ell(y, f_\theta(x^t)) p_s(y \mid x^t) \, dy dP_s(x^t) = \int \ell(y, f_\theta(x^t)) p_s(y \mid x^t) \, dy dP_s(x^t) = \int \ell(y, f_\theta(x^t)) p_s(x^t, y) \, dy dx^t = R^s(\theta)
\]

This suggests to learn a bijective transformation $T$ that transports $P_s$ to $P_t$. To this end, we cast the relevant problem as minimizing a WS distance w.r.t a cost function $c$ from $T \# P_s$ to $P_t$:

\[
\min_T WS_c(T \# P_s, P_t)
\]

Assume that we are using a deep NN class with the same architecture to formulate $T$. Let us consider an intermediate layer and decompose $T$ to $T(x) = g(G(x))$ where $G : \mathbb{R}^d \rightarrow \mathbb{Z}$ maps from the input to an intermediate layer or a joint space $\mathcal{Z}$. We now cast the problem of learning $T$ to:

\[
\min_G \min_g WS_c((G \circ g) \# P_s, P_t)
\]

In the following theorem, we indicate that the above min-min problem can be equivalently transformed to another form involving the joint space (See Figure 1 for details).

Theorem 3. Consider the following optimization problem:

\[
\min_G \min_g WS_c((G \circ g) \# P_s, P_t)
\]

This optimization problem is equivalent to the following optimization problem:

\[
\min_{G,g} H:G \# P_s = H \# P_t \quad \min_{L:L \# P_t = T \# P_s} \quad \min_{E:E \sim \mathbb{P}_t} c(x, g(H(x)))^{1/p}
\]

Proof. We start with

\[
WS_c((G \circ g) \# P_s, P_t) = \min_{L:L \# P_t = T \# P_s} \min_{E:E \sim \mathbb{P}_t} c(x, L(x))^{1/p}
\]

We thus obtain the following equality:

\[
\min_G \min_{g} WS_c((G \circ g) \# P_s, P_t)
\]

Given $G,g$, for any $H$ satisfying $H \# P_t = G \# P_s$, let $H' = H \circ g$, then $H' \# P_t = T \# P_s$; therefore, we arrive:

\[
E_{x \sim \mathbb{P}_s} c(x, g(H(x)))^{1/p} = E_{x \sim \mathbb{P}_t} c(x, H'(x))^{1/p} \geq \min_{L:L \# P_t = T \# P_s} \min_{E:E \sim \mathbb{P}_t} c(x, L(x))^{1/p}
\]

\[
E_{x \sim \mathbb{P}_s} c(x, g(H(x)))^{1/p} \geq \min_{H:G \# \mathbb{P}_s = H \# \mathbb{P}_t} \min_{E:E \sim \mathbb{P}_t} c(x, g(H(x)))^{1/p}
\]

\[
\min_{G,g} H:G \# P_s = H \# P_t \quad \min_{L:L \# P_t = T \# P_s} \quad \min_{E:E \sim \mathbb{P}_t} c(x, g(H(x)))^{1/p}
\]

\[
\min_{G,g} H:G \# P_s = H \# P_t \quad \min_{L:L \# P_t = T \# P_s} \quad \min_{E:E \sim \mathbb{P}_t} c(x, L(x))^{1/p}
\]
Finally, we reach the conclusion as:

\[
\frac{L}{\text{E} \mathbb{P}_{x} \sim \left[ c \left( x, L \left( x \right) \right) \right]^{1/p}} = \frac{E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, g' \left( h' \left( x \right) \right) \right) \right]^{1/p}}{\min_{g} \min_{H : G \mathbb{P}_{x} = T \mathbb{P}_{x}} \frac{E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, g \left( H \left( x \right) \right) \right) \right]^{1/p}}{}}
\]

We then have:

\[
\begin{align*}
\frac{E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, L \left( x \right) \right) \right]^{1/p}}{\text{min}_{g} \min_{H : G \mathbb{P}_{x} = T \mathbb{P}_{x}} \frac{E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, g \left( H \left( x \right) \right) \right) \right]^{1/p}}{}} & \geq \frac{E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, g \left( H \left( x \right) \right) \right) \right]^{1/p}}{\min_{g} \min_{H : G \mathbb{P}_{x} = T \mathbb{P}_{x}} \frac{E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, g \left( H \left( x \right) \right) \right) \right]^{1/p}}{}} \\
& \geq \min_{g} \min_{H : G \mathbb{P}_{x} = T \mathbb{P}_{x}} \frac{E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, g \left( H \left( x \right) \right) \right) \right]^{1/p}}{}}
\end{align*}
\]

where \( \lambda > 0 \) is a non-negative parameter and \( D \) could be any divergence between two distributions. In addition, since we minimize the reconstruction error:

\[
E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, g \left( H \left( x \right) \right) \right) \right]^{1/p} = \min_{g} \min_{H : G \mathbb{P}_{x} = T \mathbb{P}_{x}} \frac{E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, g \left( H \left( x \right) \right) \right) \right]^{1/p}}{}
\]

Finally, we reach the conclusion as:

\[
\begin{align*}
\frac{E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, g \left( H \left( x \right) \right) \right) \right]^{1/p}}{\text{min}_{G, g} \text{WS}_{c} \left( \left( G \circ g \right) \mathbb{P}_{x}, \mathbb{P}_{t} \right)} & \geq \frac{E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, g \left( H \left( x \right) \right) \right) \right]^{1/p}}{}}
\end{align*}
\]

In the term

\[
\begin{align*}
\frac{L}{\text{E} \mathbb{P}_{x} \sim \left[ c \left( x, g \left( L \left( x \right) \right) \right) \right]^{1/p}} = \frac{E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, g \left( H \left( x \right) \right) \right) \right]^{1/p}}{\min_{g} \min_{H : G \mathbb{P}_{x} = T \mathbb{P}_{x}} \frac{E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, g \left( H \left( x \right) \right) \right) \right]^{1/p}}{}}
\end{align*}
\]

, we can think \( G \) and \( H \) as two different generators that map \( \mathbb{P}_{s} \) and \( \mathbb{P}_{t} \) to a joint space wherein \( G \mathbb{P}_{s} = H \mathbb{P}_{t} \). Besides, the map \( g \) is trained to minimize the reconstruction error:

\[
E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, g \left( H \left( x \right) \right) \right) \right]^{1/p}
\]

We now do relaxation this term and come with the following optimization problem

\[
\begin{align*}
\min_{G, g, H} E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, g \left( H \left( x \right) \right) \right) \right]^{1/p} + \lambda D \left( G \mathbb{P}_{s}, H \mathbb{P}_{t} \right)
\end{align*}
\]

To enable the transfer learning, we can train a supervised classifier \( C \) on either \( D_{s} = \{ (x_{1}, y_{1}), \ldots, (x_{N}, y_{N}) \} \) or \( G \left( D_{s} \right) = \{ (G(x_{1}), y_{1}), \ldots, (G(x_{N}), y_{N}) \} \). The final optimization problem is hence as follows:

\[
\begin{align*}
\min_{C, G, g, H} \min_{L} E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, g \left( H \left( x \right) \right) \right) \right]^{1/p} + \lambda D \left( G \mathbb{P}_{s}, H \mathbb{P}_{t} \right) + E_{x \sim \mathcal{P}_{x}} \left[ c \left( x, k \left( G \left( x \right) \right) \right) \right]^{1/p} + E_{(x, y) \sim D_{s}} \left[ \ell \left( yC \left( A \left( x \right) \right) \right) \right]
\end{align*}
\]

where \( A \) is either the identity map or \( G \).

4. Experiment

5. Conclusion

Deep domain adaptation aims to address the problem of scarcity of qualified labelled data for supervised learning. To enable transferring the learning across the source and target domains, deep domain adaptation tries to bridge the gap between the source and target distributions in a joint feature space. Although this idea is appealing and motivating, none of theory has been proposed to mathematically explain its rational. In this paper, we have developed a rigorous theory to establish a firm theoretical foundation for deep...
domain adaptation. This turns out that bridging the gap of two relevant distributions or minimizing their divergence is only a brick in a building. This theory indicates other bricks for obtaining an ideal deep domain adaptation model. We conduct the corresponding experiments to investigate the behavior and influence of additional components when plugging into the model for deep domain adaptation.

References

Baktashmotlagh, M., Harandi, M. T., Lovell, B. C., and Salzmann, M. Unsupervised domain adaptation by domain invariant projection. In 2013 IEEE International Conference on Computer Vision, pp. 769–776, Dec 2013.

Borgwardt, Karsten M., Gretton, Arthur, Rasch, Malte J., Kriegel, Hans-Peter, Schölkopf, Bernhard, and Smola, Alex J. Integrating structured biological data by kernel maximum mean discrepancy. Bioinformatics, 22(14): e49–e57, July 2006. ISSN 1367-4803.

Courty, N., Flamary, R., Tuia, D., and Rakotomamonjy, A. Optimal transport for domain adaptation. IEEE transactions on pattern analysis and machine intelligence, 39(9): 1853–1865, 2017.

French, G., Mackiewicz, M., and Fisher, M. Self-ensembling for visual domain adaptation. In International Conference on Learning Representations, 2018.

Ganin, Y. and Lempitsky, V. Unsupervised domain adaptation by backpropagation. In Proceedings of the 32nd International Conference on International Conference on Machine Learning - Volume 37, ICML’15, pp. 1180–1189, 2015.

Gong, Boqing, Grauman, Kristen, and Sha, Fei. Connecting the dots with landmarks: Discriminatively learning domain-invariant features for unsupervised domain adaptation. In Dasgupta, Sanjoy and McAllester, David (eds.), Proceedings of the 30th International Conference on Machine Learning, volume 28 of Proceedings of Machine Learning Research, pp. 222–230, Atlanta, Georgia, USA, 17–19 Jun 2013.

Goodfellow, Ian, Pouget-Abadie, Jean, Mirza, Mehdi, Xu, Bing, Warde-Farley, David, Ozair, Sherjil, Courville, Aaron, and Bengio, Yoshua. Generative adversarial nets. In Advances in neural information processing systems, pp. 2672–2680, 2014.

Gopalan, Raghuaraman, Li, Ruonan, and Chellappa, Rama. Domain adaptation for object recognition: An unsupervised approach. In Proceedings of the 2011 International Conference on Computer Vision, ICCV ’11, pp. 999–1006, Washington, DC, USA, 2011. IEEE Computer Society. ISBN 978-1-4577-1101-5.

Gretton, A., Borgwardt, K. M., Rasch, M., Schölkopf, B., and Smola, A. J. A kernel method for the two-sample-problem. In Advances in neural information processing systems, pp. 513–520, 2007.

Huang, Jiayuan, Gretton, Arthur, Borgwardt, Karsten M., Schölkopf, Bernhard, and Smola, Alex J. Correcting sample selection bias by unlabeled data. In Schölkopf, B., Platt, J. C., and Hoffman, T. (eds.), Advances in Neural Information Processing Systems 19, pp. 601–608. MIT Press, 2007.

Long, M., Cao, Y., Wang, J., and Jordan, M. Learning transferable features with deep adaptation networks. In Bach, F. and Blei, D. (eds.), Proceedings of the 32nd International Conference on Machine Learning, volume 37 of Proceedings of Machine Learning Research, pp. 97–105, Lille, France, 2015.

Pan, Sinno Jialin, Tsang, Ivor W., Kwok, James T., and Yang, Qiang. Domain adaptation via transfer component analysis. In Proceedings of the 21st International Joint Conference on Artificial Intelligence, IJCAI’09, pp. 1187–1192, San Francisco, CA, USA, 2009. Morgan Kaufmann Publishers Inc.

Shu, R., Bui, H., Narui, H., and Ermon, S. A DIRT-t approach to unsupervised domain adaptation. In International Conference on Learning Representations, 2018.

Tzeng, E., Hoffman, J., Darrell, T., and Saenko, K. Simultaneous deep transfer across domains and tasks. CoRR, 2015.

Vapnik, Vladimir N. The Nature of Statistical Learning Theory. Springer, second edition, November 1999. ISBN 0387987800.