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Maximizing Conditional Independence for Unsupervised Domain Adaptation

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Appendix A Main Proofs

Appendix A.1 Class-conditional Distribution Alignment

Theorem 1. Assume that the product $k_{\ddot{\mathcal{X}}}k_{\mathcal{Z}}$ is a characteristic kernel on $\mathcal{X}\times\mathcal{Y}\times\mathcal{Z}$, and $\mathcal{F}_{\mathcal{Y}}+\mathbb{R}$ is dense in $L^2(P_{\mathcal{Y}})$. For any conditional distributions $P^S_{X|Y}$, $P^T_{X|Y}\in \Pr^S(\mathcal{X}|\mathcal{Y})$, we have

$$V_{\ddot{Z}\ddot{X}|Y}=0\Longrightarrow P^S_{X|Y}=P^T_{X|Y}.$$

Proof. Based on Lemma 1, we have

$$V_{\ddot{Z}\ddot{X}|Y}=0\Longrightarrow X\perp\!\!\!\perp Z\mid Y.$$

With the property of conditional independence, we have

$$P(X\mid Z,Y)=P(X\mid Y).$$

Thus,

$$P^S_{X|Y}=P^T_{X|Y}.$$

Appendix A.2 Empirical Estimation

The empirical estimation of the dependence can be expressed as

$$\hat{I}_n^{NOCCO}(X,Z)=\mathrm{Tr}(\mathbf{R_Z}\mathbf{I}_n\mathbf{R_X}\mathbf{I}_n).$$

Proof. Provided that V_{YX} is Hilbert-Schmidt, the dependence of X and Z is measured by

$$I^{NOCCO}(X,Z)=\|V_{ZX}\|^2_{HS}. \tag{A1}$$

Denote $\mathbf{X}\in\mathbb{R}^{d_1\times n}$ and $\mathbf{Z}\in\mathbb{R}^{d_2\times n}$ as the observations of random variables X and Z, respectively. The kernel feature maps $\phi(\cdot)$ and $\lambda(\cdot)$ are used to map $\mathbf{X}$ and $\mathbf{Z}$ into the Reproducing Kernel Hilbert Space (RKHS). Then, we obtain kernel matrices

$$\mathbf{K_X}=\mathbf{\Phi}^T\mathbf{\Phi},\quad \mathbf{K_Z}=\mathbf{\Lambda}^T\mathbf{\Lambda},$$

where $\mathbf{K_X}$, $\mathbf{K_Z}\in\mathbb{R}^{n\times n}$, and

$$\mathbf{\Phi}=[\phi(\mathbf{x}_1),\phi(\mathbf{x}_2),\cdots,\phi(\mathbf{x}_n)],$$
$$\mathbf{\Lambda}=[\lambda(\mathbf{z}_1),\lambda(\mathbf{z}_2),\cdots,\lambda(\mathbf{z}_n)].$$

Thus, the empirical estimation of the cross-covariance operator Σ_{ZX} is written as

$$\widehat{\Sigma}^{(n)}_{ZX}=\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Phi}^T}{n},$$

where $\mathbf{H}_n=\mathbf{I}_n-\frac{\mathbf{1}\mathbf{1}^T}{n}$ is the centering matrix and $\mathbf{1}\in\mathbb{R}^n$ is the all-ones vector. Similarly, the estimations of covariance operators $\widehat{\Sigma}^{(n)}_{XX}$ and $\widehat{\Sigma}^{(n)}_{ZZ}$ can be written as

$$\widehat{\Sigma}^{(n)}_{XX}=\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Phi}^T}{n},\qquad \widehat{\Sigma}^{(n)}_{ZZ}=\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Lambda}^T}{n}.$$

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Thus, by regularizing the singular covariance operators with ε_n [51], the normalized cross-covariance operator (NOCCO) V_{ZX} can be estimated by

$$\widehat{V}_{ZX}^{(n)} = \left(\Sigma_{ZZ}^{(n)} + \varepsilon_n I\right)^{-1/2} \widehat{\Sigma}_{ZX}^{(n)} \left(\widehat{\Sigma}_{XX}^{(n)} + \varepsilon_n I\right)^{-1/2} \tag{A2}$$

$$= \mathrm{Tr}\left(\left(\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Lambda}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1/2} \frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Phi}^T}{n} \left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Phi}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1/2}\right). \tag{A3}$$

Based on (A3), we can provide an empirical estimation of (A1) as

$$\begin{aligned}
\hat{I}_n^{NOCCO} =& \|\widehat{V}_{ZX}^{(n)}\|_{HS}^2 \\
=& \mathrm{Tr}\left(\widehat{V}_{ZX}^{(n)*}\widehat{V}_{ZX}^{(n)}\right) \\
=& \mathrm{Tr}\left(\left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Phi}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1/2} \frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Lambda}^T}{n} \left(\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Lambda}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1/2} \left(\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Lambda}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1/2} \frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Phi}^T}{n} \left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Phi}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1/2}\right) \\
=& \mathrm{Tr}\left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Lambda}^T}{n} \left(\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Lambda}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1} \frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Phi}^T}{n} \left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Phi}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1}\right).
\end{aligned} \tag{A4}$$

Here we have

$$\left(\frac{\mathbf{\Phi}\mathbf{\Phi}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1} = \frac{1}{\varepsilon_n}\left(\mathbf{I} - \mathbf{\Phi}\left(\varepsilon_n n\mathbf{I}_n + \mathbf{K}_X\right)^{-1}\mathbf{\Phi}^T\right),$$

where $\mathbf{K}_X = \mathbf{\Phi}^T\mathbf{\Phi}$. $\mathbf{I}$ and $\mathbf{I}_n$ are different in this equation, the former can be regarded as an operator and the latter is the identity matrix with dimension n. $\mathbf{H}_n$ is a symmetric idempotent matrix, which satisfies $\mathbf{H}_n\mathbf{H}_n = \mathbf{H}_n$. Denote $\mathbf{G}_X = \mathbf{H}_n\mathbf{K}_X\mathbf{H}_n$. Therefore,

$$\begin{aligned}
\left(\widehat{\Sigma}_{XX}^{(n)} + \varepsilon_n\mathbf{I}\right)^{-1} &= \left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Phi}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1} \\
&= \left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{H}_n^T\mathbf{\Phi}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1} \\
&= \frac{1}{\varepsilon_n}\left(\mathbf{I} - \mathbf{\Phi}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{H}_n^T\mathbf{\Phi}^T\mathbf{\Phi}\mathbf{H}_n\right)^{-1}\mathbf{H}_n^T\mathbf{\Phi}^T\right) \\
&= \frac{1}{\varepsilon_n}\left(\mathbf{I} - \mathbf{\Phi}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{H}_n^T\mathbf{K}_X\mathbf{H}_n\right)^{-1}\mathbf{H}_n^T\mathbf{\Phi}^T\right) \\
&= \frac{1}{\varepsilon_n}\left(\mathbf{I} - \mathbf{\Phi}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_X\right)^{-1}\mathbf{H}_n^T\mathbf{\Phi}^T\right).
\end{aligned} \tag{A5}$$

Thus, we can employ (A5) to calculate (A4) as

$$\begin{aligned}
\hat{I}_n^{NOCCO} =& \|\widehat{V}_{ZX}^{(n)}\|_{HS}^2 \\
=& \mathrm{Tr}\left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Lambda}^T}{n}\frac{1}{\varepsilon_n}[\mathbf{I} - \mathbf{\Lambda}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_Z\right)^{-1}\mathbf{H}_n^T\mathbf{\Lambda}^T]\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Phi}^T}{n}\frac{1}{\varepsilon_n}[\mathbf{I} - \mathbf{\Phi}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_X\right)^{-1}\mathbf{H}_n^T\mathbf{\Phi}^T]\right) \\
=& \mathrm{Tr}\left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{H}_n\mathbf{\Lambda}^T}{n}\frac{1}{\varepsilon_n}[\mathbf{I} - \mathbf{\Lambda}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_Z\right)^{-1}\mathbf{H}_n^T\mathbf{\Lambda}^T]\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{H}_n\mathbf{\Phi}^T}{n}\frac{1}{\varepsilon_n}[\mathbf{I} - \mathbf{\Phi}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_X\right)^{-1}\mathbf{H}_n^T\mathbf{\Phi}^T]\right) \\
=& \mathrm{Tr}\left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{H}_n\mathbf{\Lambda}^T}{n}\frac{1}{\varepsilon_n}[\mathbf{I} - \mathbf{\Lambda}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_Z\right)^{-1}\mathbf{H}_n^T\mathbf{\Lambda}^T]\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{H}_n\mathbf{\Phi}^T}{n}\frac{1}{\varepsilon_n}[\mathbf{I} - \mathbf{\Phi}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_X\right)^{-1}\mathbf{H}_n^T\mathbf{\Phi}^T]\right) \\
=& \mathrm{Tr}\left(\mathbf{H}_n\mathbf{\Lambda}^T[\mathbf{I} - \mathbf{\Lambda}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_Z\right)^{-1}\mathbf{H}_n^T\mathbf{\Lambda}^T]\frac{\mathbf{\Lambda}\mathbf{H}_n}{n\varepsilon_n}\mathbf{H}_n\mathbf{\Phi}^T[\mathbf{I} - \mathbf{\Phi}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_X\right)^{-1}\mathbf{H}_n^T\mathbf{\Phi}^T]\frac{\mathbf{\Phi}\mathbf{H}_n}{n\varepsilon_n}\right) \\
=& \mathrm{Tr}\left(\frac{\mathbf{G}_Z - \mathbf{G}_Z\left(\mathbf{G}_Z + \varepsilon_n n\mathbf{I}_n\right)^{-1}\mathbf{G}_Z}{n\varepsilon_n}\frac{\mathbf{G}_X - \mathbf{G}_X\left(\mathbf{G}_X + \varepsilon_n n\mathbf{I}_n\right)^{-1}\mathbf{G}_X}{n\varepsilon_n}\right) \\
=& \mathrm{Tr}\left(\mathbf{G}_Z\left(\mathbf{G}_Z + \varepsilon_n n\mathbf{I}_n\right)^{-1}\mathbf{G}_X\left(\mathbf{G}_X + \varepsilon_n n\mathbf{I}_n\right)^{-1}\right) \\
=& \mathrm{Tr}\left(\mathbf{R}_Z\mathbf{R}_X\right) \\
=& \mathrm{Tr}(\mathbf{R}_\mathbf{Z}\mathbf{I}_n\mathbf{R}_\mathbf{X}\mathbf{I}_n).
\end{aligned}$$

Note: $\mathbf{I}_n - \left(\mathbf{G} + n\varepsilon_n\mathbf{I}_n\right)^{-1}\mathbf{G} = \varepsilon_n n\left(\mathbf{G} + \varepsilon_n n\mathbf{I}_n\right)^{-1}$.

Theorem 2. Denote $\mathbf{S} = \mathbf{I}_n - \mathbf{R}_\mathbf{Y}$. The empirical estimation of the conditional dependence is

$$\hat{I}_n^{COND}(X, Z|Y) = \mathrm{Tr}(\mathbf{R}_{\ddot{\mathbf{Z}}}\mathbf{S}\mathbf{R}_{\ddot{\mathbf{X}}}\mathbf{S}). \tag{A6}$$

Proof. Denote $\ddot{X} = (X, Y)$, $\ddot{Z} = (Z, Y)$ with the kernel product $k_{\ddot{\mathcal{X}}} = k_\mathcal{X}k_\mathcal{Y}$ and $k_{\ddot{\mathcal{Z}}} = k_\mathcal{Z}k_\mathcal{Y}$. Lemma 1 implies that $X \perp\!\!\!\perp Z \mid Y$ if and only if $V_{\ddot{Z}\ddot{X}|Y} = 0$. Provided that $V_{\ddot{Z}\ddot{X}|Y}$ is Hilbert-Schmidt, the conditional dependence of X and Z given Y is measured by

$$I^{COND}(X, Z \mid Y) = \|V_{\ddot{Z}\ddot{X}|Y}\|_{HS}^2. \tag{A7}$$

Denote $\mathbf{X} \in \mathbb{R}^{d_1 \times n}$, $\mathbf{Y} \in \mathbb{R}^{K \times n}$, and $\mathbf{Z} \in \mathbb{R}^{d_2 \times n}$ as the observations of random variables X, Y and Z, respectively. The kernel feature maps $\phi(\cdot)$, $\lambda(\cdot)$ and $\psi(\cdot)$ are used to map $\ddot{\mathbf{X}}$, $\ddot{\mathbf{Z}}$ and $\mathbf{Y}$ into RKHSs, where $\ddot{\mathbf{X}} = (\mathbf{X}_{re}; \mathbf{Y}) \in \mathbb{R}^{(d'+K)\times n}$, $\ddot{\mathbf{Z}} = (\mathbf{Z}; \mathbf{Y}) \in \mathbb{R}^{(d_2+K)\times n}$. Then, we obtain kernel matrices

$$\mathbf{K}_{\ddot{\mathbf{X}}} = \mathbf{\Phi}^T\mathbf{\Phi}, \quad \mathbf{K}_{\ddot{\mathbf{Z}}} = \mathbf{\Lambda}^T\mathbf{\Lambda}, \quad \mathbf{K}_{\mathbf{Y}} = \mathbf{\Psi}^T\mathbf{\Psi},$$

where $\mathbf{K}_{\ddot{\mathbf{X}}}$, $\mathbf{K}_{\ddot{\mathbf{Z}}}$, $\mathbf{K}_{\mathbf{Y}} \in \mathbb{R}^{n\times n}$, and

$$\begin{aligned}
\mathbf{\Phi} &= [\phi(\ddot{\mathbf{x}}_1), \phi(\ddot{\mathbf{x}}_2), \cdots, \phi(\ddot{\mathbf{x}}_n)],\\
\mathbf{\Lambda} &= [\lambda(\ddot{\mathbf{z}}_1), \lambda(\ddot{\mathbf{z}}_2), \cdots, \lambda(\ddot{\mathbf{z}}_n)],\\
\mathbf{\Psi} &= [\psi(\mathbf{y}_1), \psi(\mathbf{y}_2), \cdots, \psi(\mathbf{y}_n)].
\end{aligned}$$

Similarly with the estimation of the NOCCO, we have

$$\begin{aligned}
\widehat{V}^{(n)}_{\ddot{Z}\ddot{X}} &= \left(\widehat{\Sigma}^{(n)}_{\ddot{Z}\ddot{Z}} + \varepsilon_n I\right)^{-1/2} \widehat{\Sigma}^{(n)}_{\ddot{Z}\ddot{X}} \left(\widehat{\Sigma}^{(n)}_{\ddot{X}\ddot{X}} + \varepsilon_n I\right)^{-1/2}\\
&= \left(\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Lambda}^T}{n} + \varepsilon_n I\right)^{-1/2} \frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Phi}^T}{n} \left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Phi}^T}{n} + \varepsilon_n I\right)^{-1/2},
\end{aligned}$$

$$\begin{aligned}
\widehat{V}^{(n)}_{\ddot{Z}Y} &= \left(\widehat{\Sigma}^{(n)}_{\ddot{Z}\ddot{Z}} + \varepsilon_n I\right)^{-1/2} \widehat{\Sigma}^{(n)}_{\ddot{Z}Y} \left(\widehat{\Sigma}^{(n)}_{YY} + \varepsilon_n I\right)^{-1/2}\\
&= \left(\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Lambda}^T}{n} + \varepsilon_n I\right)^{-1/2} \frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Psi}^T}{n} \left(\frac{\mathbf{\Psi}\mathbf{H}_n\mathbf{\Psi}^T}{n} + \varepsilon_n I\right)^{-1/2},
\end{aligned}$$

$$\begin{aligned}
\widehat{V}^{(n)}_{Y\ddot{X}} &= \left(\widehat{\Sigma}^{(n)}_{YY} + \varepsilon_n I\right)^{-1/2} \widehat{\Sigma}^{(n)}_{Y\ddot{X}} \left(\widehat{\Sigma}^{(n)}_{\ddot{X}\ddot{X}} + \varepsilon_n I\right)^{-1/2}\\
&= \left(\frac{\mathbf{\Psi}\mathbf{H}_n\mathbf{\Psi}^T}{n} + \varepsilon_n I\right)^{-1/2} \frac{\mathbf{\Psi}\mathbf{H}_n\mathbf{\Phi}^T}{n} \left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Phi}^T}{n} + \varepsilon_n I\right)^{-1/2}.
\end{aligned}$$

Based on the estimation of the cross-covariance operators $\widehat{V}^{(n)}_{\ddot{Z}\ddot{X}}$, $\widehat{V}^{(n)}_{\ddot{Z}Y}$, and $\widehat{V}^{(n)}_{Y\ddot{X}}$, the estimation of $V_{\ddot{Z}\ddot{X}|Y}$ is written as

$$\widehat{V}^{(n)}_{\ddot{Z}\ddot{X}|Y} = \widehat{V}^{(n)}_{\ddot{Z}\ddot{X}} - \widehat{V}^{(n)}_{\ddot{Z}Y}\widehat{V}^{(n)}_{Y\ddot{X}}.$$

Therefore, the empirical estimation of (A7) is

$$\begin{aligned}
\hat{I}^{COND}_n &\equiv \| \widehat{V}^{(n)}_{\ddot{Z}\ddot{X}|Y} \|^2_{HS}\\
&= \mathrm{Tr}\left(\widehat{V}^{(n)^*}_{\ddot{Z}\ddot{X}|Y} \widehat{V}^{(n)}_{\ddot{Z}\ddot{X}|Y}\right)\\
&= \mathrm{Tr}\left(\left(\widehat{V}^{(n)^*}_{\ddot{Z}\ddot{X}} - \widehat{V}^{(n)^*}_{Y\ddot{X}}\widehat{V}^{(n)^*}_{\ddot{Z}Y}\right)\left(\widehat{V}^{(n)}_{\ddot{Z}\ddot{X}} - \widehat{V}^{(n)}_{\ddot{Z}Y}\widehat{V}^{(n)}_{Y\ddot{X}}\right)\right)\\
&= \mathrm{Tr}\left(\widehat{V}^{(n)^*}_{\ddot{Z}\ddot{X}}\widehat{V}^{(n)}_{\ddot{Z}\ddot{X}} - \widehat{V}^{(n)^*}_{Y\ddot{X}}\widehat{V}^{(n)^*}_{\ddot{Z}Y}\widehat{V}^{(n)}_{\ddot{Z}\ddot{X}} - \widehat{V}^{(n)^*}_{\ddot{Z}\ddot{X}}\widehat{V}^{(n)}_{\ddot{Z}Y}\widehat{V}^{(n)}_{Y\ddot{X}} + \widehat{V}^{(n)^*}_{Y\ddot{X}}\widehat{V}^{(n)^*}_{\ddot{Z}Y}\widehat{V}^{(n)}_{\ddot{Z}Y}\widehat{V}^{(n)}_{Y\ddot{X}}\right),
\end{aligned} \tag{A8}$$

where

$$\begin{aligned}
&\mathrm{Tr}\left(\widehat{V}^{(n)^*}_{\ddot{Z}\ddot{X}}\widehat{V}^{(n)}_{\ddot{Z}\ddot{X}}\right)\\
=&\mathrm{Tr}\left(\left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Lambda}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1/2} \frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Lambda}^T}{n} \left(\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Lambda}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1/2} \left(\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Lambda}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1/2} \frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Phi}^T}{n} \left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Phi}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1/2}\right)\\
=&\mathrm{Tr}\left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Lambda}^T}{n}\left(\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Lambda}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1} \frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Phi}^T}{n} \left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Phi}^T}{n} + \varepsilon_n\mathbf{I}\right)^{-1}\right)\\
=&\mathrm{Tr}\left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{\Lambda}^T}{n}\frac{1}{\varepsilon_n}\left(\mathbf{I} - \mathbf{\Lambda}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_{\ddot{Z}}\right)^{-1}\mathbf{H}_n^T\mathbf{\Lambda}^T\right)\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{\Phi}^T}{n}\frac{1}{\varepsilon_n}\left(\mathbf{I} - \mathbf{\Phi}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_{\ddot{X}}\right)^{-1}\mathbf{H}_n^T\mathbf{\Phi}^T\right)\right)\\
=&\mathrm{Tr}\left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{H}_n\mathbf{\Lambda}^T}{n}\frac{1}{\varepsilon_n}\left(\mathbf{I} - \mathbf{\Lambda}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_{\ddot{Z}}\right)^{-1}\mathbf{H}_n^T\mathbf{\Lambda}^T\right)\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{H}_n\mathbf{\Phi}^T}{n}\frac{1}{\varepsilon_n}\left(\mathbf{I} - \mathbf{\Phi}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_{\ddot{X}}\right)^{-1}\mathbf{H}_n^T\mathbf{\Phi}^T\right)\right)\\
=&\mathrm{Tr}\left(\frac{\mathbf{\Phi}\mathbf{H}_n\mathbf{H}_n\mathbf{\Lambda}^T}{n}\frac{1}{\varepsilon_n}\left(\mathbf{I} - \lambda\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_{\ddot{Z}}\right)^{-1}\mathbf{H}_n^T\mathbf{\Lambda}^T\right)\frac{\mathbf{\Lambda}\mathbf{H}_n\mathbf{H}_n\mathbf{\Phi}^T}{n}\frac{1}{\varepsilon_n}\left(\mathbf{I} - \mathbf{\Phi}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_X\right)^{-1}\mathbf{H}_n^T\mathbf{\Phi}^T\right)\right)\\
=&\mathrm{Tr}\left(\mathbf{H}_n\mathbf{\Lambda}^T\left(\mathbf{I} - \mathbf{\Lambda}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_{\ddot{Z}}\right)^{-1}\mathbf{H}_n^T\mathbf{\Lambda}^T\right)\frac{\mathbf{\Lambda}\mathbf{H}_n}{n\varepsilon_n}\mathbf{H}_n\mathbf{\Phi}^T\left(\mathbf{I} - \mathbf{\Phi}\mathbf{H}_n\left(\varepsilon_n n\mathbf{I}_n + \mathbf{G}_{\ddot{X}}\right)^{-1}\mathbf{H}_n^T\mathbf{\Phi}^T\right)\frac{\mathbf{\Phi}\mathbf{H}_n}{n\varepsilon_n}\right)\\
=&\mathrm{Tr}\left(\frac{\mathbf{G}_{\ddot{Z}} - \mathbf{G}_{\ddot{Z}}\left(\mathbf{G}_{\ddot{Z}} + \varepsilon_n n\mathbf{I}_n\right)^{-1}\mathbf{G}_{\ddot{Z}}}{n\varepsilon_n}\frac{\mathbf{G}_{\ddot{X}} - \mathbf{G}_{\ddot{X}}\left(\mathbf{G}_{\ddot{X}} + \varepsilon_n n\mathbf{I}_n\right)^{-1}\mathbf{G}_{\ddot{X}}}{n\varepsilon_n}\right)\\
=&\mathrm{Tr}\left(\mathbf{G}_{\ddot{Z}}\left(\mathbf{G}_{\ddot{Z}} + \varepsilon_n n\mathbf{I}_n\right)^{-1}\mathbf{G}_{\ddot{X}}\left(\mathbf{G}_{\ddot{X}} + \varepsilon_n n\mathbf{I}_n\right)^{-1}\right)\\
=&\mathrm{Tr}\left(\mathbf{R}_{\ddot{Z}}\mathbf{R}_{\ddot{X}}\right),
\end{aligned}$$

$$
\begin{aligned}
&\operatorname{Tr}\left(\widehat{V}_{Y\ddot{X}}^{(n)*}\widehat{V}_{\ddot{Z}Y}^{(n)*}\widehat{V}_{\ddot{Z}\ddot{X}}^{(n)}\right)\\
&=\operatorname{Tr}\left(\left(\frac{\mathbf{\Phi H}_n\mathbf{\Phi}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1/2}\frac{\mathbf{\Phi H}_n\mathbf{\Psi}^T}{n}\left(\frac{\mathbf{\Psi H}_n\mathbf{\Psi}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1}\frac{\mathbf{\Psi H}_n\mathbf{\Lambda}^T}{n}\left(\frac{\mathbf{\Lambda H}_n\mathbf{\Lambda}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1}\frac{\mathbf{\Lambda H}_n\mathbf{\Phi}^T}{n}\left(\frac{\mathbf{\Phi H}_n\mathbf{\Phi}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1/2}\right)\\
&=\operatorname{Tr}\left(\frac{\mathbf{\Phi H}_n\mathbf{\Psi}^T}{n}\left(\frac{\mathbf{\Psi H}_n\mathbf{\Psi}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1}\frac{\mathbf{\Psi H}_n\mathbf{\Lambda}^T}{n}\left(\frac{\mathbf{\Lambda H}_n\mathbf{\Lambda}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1}\frac{\mathbf{\Lambda H}_n\mathbf{\Phi}^T}{n}\left(\frac{\mathbf{\Phi H}_n\mathbf{\Phi}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1}\right)\\
&=\operatorname{Tr}\left(\left(\frac{\mathbf{G}_Y-\mathbf{G}_Y\left(\varepsilon_n n\mathbf{I}_n+\mathbf{G}_Y\right)^{-1}\mathbf{G}_Y}{\varepsilon_n n}\right)\left(\frac{\mathbf{G}_{\ddot{Z}}-\mathbf{G}_{\ddot{Z}}\left(\varepsilon_n n\mathbf{I}_n+\mathbf{G}_{\ddot{Z}}\right)^{-1}\mathbf{G}_{\ddot{Z}}}{\varepsilon_n n}\right)\left(\frac{\mathbf{G}_{\ddot{X}}-\mathbf{G}_{\ddot{X}}\left(\varepsilon_n n\mathbf{I}_n+\mathbf{G}_{\ddot{X}}\right)^{-1}\mathbf{G}_{\ddot{X}}}{\varepsilon_n n}\right)\right)\\
&=\operatorname{Tr}\left(\left(\mathbf{G}_Y\left(\varepsilon_n n\mathbf{I}_n+\mathbf{G}_Y\right)^{-1}\right)\left(\mathbf{G}_{\ddot{Z}}\left(\varepsilon_n n\mathbf{I}_n+\mathbf{G}_{\ddot{Z}}\right)^{-1}\right)\left(\mathbf{G}_{\ddot{X}}\left(\varepsilon_n n\mathbf{I}_n+\mathbf{G}_{\ddot{X}}\right)^{-1}\right)\right)\\
&=\operatorname{Tr}\left(\mathbf{R}_Y\mathbf{R}_{\ddot{Z}}\mathbf{R}_{\ddot{X}}\right),
\end{aligned}
$$

$$
\begin{aligned}
&\operatorname{Tr}\left(\widehat{V}_{\ddot{Z}\ddot{X}}^{(n)*}\widehat{V}_{\ddot{Z}Y}^{(n)}\widehat{V}_{Y\ddot{X}}^{(n)}\right)\\
&=\operatorname{Tr}\left(\left(\frac{\mathbf{\Phi H}_n\mathbf{\Phi}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1/2}\frac{\mathbf{\Phi H}_n\mathbf{\Lambda}^T}{n}\left(\frac{\mathbf{\Lambda H}_n\mathbf{\Lambda}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1}\frac{\mathbf{\Lambda H}_n\mathbf{\Psi}^T}{n}\left(\frac{\mathbf{\Psi H}_n\mathbf{\Psi}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1}\frac{\mathbf{\Psi H}_n\mathbf{\Phi}^T}{n}\left(\frac{\mathbf{\Phi H}_n\mathbf{\Phi}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1/2}\right)\\
&=\operatorname{Tr}\left(\frac{\mathbf{\Phi H}_n\mathbf{\Lambda}^T}{n}\left(\frac{\mathbf{\Lambda H}_n\mathbf{\Lambda}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1}\frac{\mathbf{\Lambda H}_n\mathbf{\Psi}^T}{n}\left(\frac{\mathbf{\Psi H}_n\mathbf{\Psi}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1}\frac{\mathbf{\Psi H}_n\mathbf{\Phi}^T}{n}\left(\frac{\mathbf{\Phi H}_n\mathbf{\Phi}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1}\right)\\
&=\operatorname{Tr}\left(\left(\frac{\mathbf{G}_{\ddot{Z}}-\mathbf{G}_{\ddot{Z}}\left(\varepsilon_n n\mathbf{I}_n+\mathbf{G}_{\ddot{Z}}\right)^{-1}\mathbf{G}_{\ddot{Z}}}{\varepsilon_n n}\right)\left(\frac{\mathbf{G}_Y-\mathbf{G}_Y\left(\varepsilon_n n\mathbf{I}_n+\mathbf{G}_Y\right)^{-1}\mathbf{G}_Y}{\varepsilon_n n}\right)\left(\frac{\mathbf{G}_{\ddot{X}}-\mathbf{G}_{\ddot{X}}\left(\varepsilon_n n\mathbf{I}_n+\mathbf{G}_{\ddot{X}}\right)^{-1}\mathbf{G}_{\ddot{X}}}{\varepsilon_n n}\right)\right)\\
&=\operatorname{Tr}\left(\left(\mathbf{G}_{\ddot{Z}}\left(\varepsilon_n n\mathbf{I}_n+\mathbf{G}_{\ddot{Z}}\right)^{-1}\right)\left(\mathbf{G}_Y\left(\varepsilon_n n\mathbf{I}_n+\mathbf{G}_Y\right)^{-1}\right)\left(\mathbf{G}_{\ddot{X}}\left(\varepsilon_n n\mathbf{I}_n+\mathbf{G}_{\ddot{X}}\right)^{-1}\right)\right)\\
&=\operatorname{Tr}\left(\mathbf{R}_{\ddot{Z}}\mathbf{R}_Y\mathbf{R}_{\ddot{X}}\right),
\end{aligned}
$$

$$
\begin{aligned}
&\operatorname{Tr}\left(\widehat{V}_{Y\ddot{X}}^{(n)*}\widehat{V}_{\ddot{Z}Y}^{(n)*}\widehat{V}_{\ddot{Z}Y}^{(n)}\widehat{V}_{Y\ddot{X}}^{(n)}\right)\\
&=\operatorname{Tr}\left(\frac{\mathbf{\Psi H}_n\mathbf{\Psi}^T}{n}\left(\frac{\mathbf{\Psi H}_n\mathbf{\Psi}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1}\frac{\mathbf{\Psi H}_n\mathbf{\Lambda}^T}{n}\left(\frac{\mathbf{\Lambda H}_n\mathbf{\Lambda}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1}\frac{\mathbf{\Lambda H}_n\mathbf{\Psi}^T}{n}\left(\frac{\mathbf{\Psi H}_n\mathbf{\Psi}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1}\frac{\mathbf{\Psi H}_n\mathbf{\Phi}^T}{n}\left(\frac{\mathbf{\Phi H}_n\mathbf{\Phi}^T}{n}+\varepsilon_n\mathbf{I}\right)^{-1}\right)\\
&=\operatorname{Tr}\left(\mathbf{R}_Y\mathbf{R}_{\ddot{Z}}\mathbf{R}_Y\mathbf{R}_{\ddot{X}}\right).
\end{aligned}
$$

Note: $\mathbf{I}_n-\left(\mathbf{G}+n\varepsilon_n\mathbf{I}_n\right)^{-1}\mathbf{G}=\varepsilon_n n\left(\mathbf{G}+\varepsilon_n n\mathbf{I}_n\right)^{-1}$.

Thus, we can calculate (A8) as

$$
\begin{aligned}
\hat{I}_n^{COND}&=\operatorname{Tr}\left(\widehat{V}_{\ddot{Z}\ddot{X}}^{(n)*}\widehat{V}_{\ddot{Z}\ddot{X}}^{(n)}-\widehat{V}_{Y\ddot{X}}^{(n)*}\widehat{V}_{\ddot{Z}Y}^{(n)*}\widehat{V}_{\ddot{Z}\ddot{X}}^{(n)}-\widehat{V}_{\ddot{Z}\ddot{X}}^{(n)*}\widehat{V}_{\ddot{Z}Y}^{(n)}\widehat{V}_{Y\ddot{X}}^{(n)}+\widehat{V}_{Y\ddot{X}}^{(n)*}\widehat{V}_{\ddot{Z}Y}^{(n)*}\widehat{V}_{\ddot{Z}Y}^{(n)}\widehat{V}_{Y\ddot{X}}^{(n)}\right)\\
&=\operatorname{Tr}\left(\mathbf{R}_{\ddot{Z}}\mathbf{R}_{\ddot{X}}-\mathbf{R}_Y\mathbf{R}_{\ddot{Z}}\mathbf{R}_{\ddot{X}}-\mathbf{R}_{\ddot{Z}}\mathbf{R}_Y\mathbf{R}_{\ddot{X}}+\mathbf{R}_Y\mathbf{R}_{\ddot{Z}}\mathbf{R}_Y\mathbf{R}_{\ddot{X}}\right)\\
&=\operatorname{Tr}\left(\mathbf{R}_{\ddot{Z}}\mathbf{R}_{\ddot{X}}-\mathbf{R}_{\ddot{Z}}\mathbf{R}_{\ddot{X}}\mathbf{R}_Y-\mathbf{R}_{\ddot{Z}}\mathbf{R}_Y\mathbf{R}_{\ddot{X}}+\mathbf{R}_{\ddot{Z}}\mathbf{R}_Y\mathbf{R}_{\ddot{X}}\mathbf{R}_Y\right)\\
&=\operatorname{Tr}\left(\left(\mathbf{R}_{\ddot{Z}}-\mathbf{R}_{\ddot{Z}}\mathbf{R}_Y\right)\left(\mathbf{R}_{\ddot{X}}-\mathbf{R}_{\ddot{X}}\mathbf{R}_Y\right)\right)\\
&=\operatorname{Tr}\left(\mathbf{R}_{\ddot{Z}}\mathbf{S}\mathbf{R}_{\ddot{X}}\mathbf{S}\right)
\end{aligned}
$$

where $\mathbf{S}=\mathbf{I}_n-\mathbf{R}_Y$.

Proposition 1. Assuming that $k_{\ddot{\mathcal{X}}}$ and $k_{\ddot{\mathcal{Z}}}$ are radial kernels. If Y is a constant random variable, then the empirical estimations of the conditional dependence and dependence are equal. Then,

$$\hat{I}_n^{NOCCO}(X,Z)=\hat{I}_n^{COND}(X,Z|Y),$$

where the radial kernel is $k(x,y)=k(\|x-y\|)$.

Proof. Recall that

$$
\begin{aligned}
\hat{I}_n^{NOCCO}(X,Z)&=\operatorname{Tr}\left(\mathbf{R}_Z\mathbf{I}_n\mathbf{R}_X\mathbf{I}_n\right),\\
\hat{I}_n^{COND}(X,Z|Y)&=\operatorname{Tr}\left(\mathbf{R}_{\ddot{Z}}\mathbf{S}\mathbf{R}_{\ddot{X}}\mathbf{S}\right).
\end{aligned}
$$

The main differences are the weighting matrix $\mathbf{S}$ and the kernel-based matrix $\mathbf{R}_{\ddot{X}}$ with extended-variable Y. Note that Y takes a constant value, regardless of any event that occurs. Since radial kernel $k(\mathbf{x}_1,\mathbf{x}_2)=k(\|\mathbf{x}_1-\mathbf{x}_2\|)$ is employed, then we have

$$
\mathbf{K_Y}=\begin{bmatrix}k(0)&k(0)&\cdots&k(0)\\k(0)&k(0)&\cdots&k(0)\\\vdots&\vdots&\ddots&\vdots\\k(0)&k(0)&\cdots&k(0)\end{bmatrix}_{n\times n}
$$

and the centered Gram matrices $\mathbf{G_Y}=\mathbf{0}$. Thus, we obtain the first identity $\mathbf{S}=\mathbf{I}_n-\mathbf{R}_Y=\mathbf{I}_n-\mathbf{G}_Y\left(\varepsilon_n n\mathbf{I}_n+\mathbf{G}_Y\right)^{-1}=\mathbf{I}_n$. For the extended variable $\ddot{X}$, its kernel follows that

$$
\|\ddot{\mathbf{x}}_i-\ddot{\mathbf{x}}_j\|=\left\|\begin{bmatrix}\mathbf{x}_i-\mathbf{x}_j\\\mathbf{y}-\mathbf{y}\end{bmatrix}\right\|=\left\|\begin{bmatrix}\mathbf{x}_i-\mathbf{x}_j\\\mathbf{0}\end{bmatrix}\right\|=\|\mathbf{x}_i-\mathbf{x}_j\|,
$$

Thus, we obtain the second identity $\mathbf{K}_{\ddot{\mathbf{X}}} = \mathbf{K}_{\mathbf{X}}$ and $\mathbf{R}_{\ddot{X}} = \mathbf{R}_X$, where $\mathbf{R}_{\ddot{Z}} = \mathbf{R}_Z$ is similar. By combining these two identities, we have

$$\hat{I}_n^{COND}(X, Z|Y) \;=\; \mathrm{Tr}\left(\mathbf{R}_{\ddot{Z}}\mathbf{S}\mathbf{R}_{\ddot{X}}\mathbf{S}\right) \;=\; \mathrm{Tr}\left(\mathbf{R}_Z\mathbf{I}_n\mathbf{R}_X\mathbf{I}_n\right) \;=\; \hat{I}_n^{NOCCO}(X, Z).$$

Convergency. In the following, the convergency proof of COND $\widehat{V}_{XZ|Y}^{(n)}$ [38] is presented. Assume that V_{ZX}, V_{ZY}, and V_{YX} are Hilbert-Schmidt, and that the regularization constant ε_n satisfies $\varepsilon_n \to 0$ and $\varepsilon_n^3 n \to \infty$, then we have

$$\|\widehat{V}_{XZ|Y}^{(n)} - V_{XZ|Y}\|_{HS} \to 0 \quad (n \to \infty) \tag{A9}$$

in probability with rate $\varepsilon_n^{-\frac{3}{2}} n^{-\frac{1}{2}}$.

Proof. From the expressions in (A2) and (2), it is easy to obtain

$$\begin{aligned}
&\|\widehat{V}_{ZX|Y}^{(n)} - V_{ZX|Y}\|_{HS} \\
=&\|\widehat{V}_{ZX}^{(n)} - \widehat{V}_{ZY}^{(n)}\widehat{V}_{YX}^{(n)} - V_{ZX} + V_{ZY}V_{YX}\|_{HS} \\
=&\|\widehat{V}_{ZX}^{(n)} - V_{ZX} + V_{ZY}V_{YX} - V_{ZY}\widehat{V}_{YX}^{(n)} + V_{ZY}\widehat{V}_{YX}^{(n)} - \widehat{V}_{ZY}^{(n)}\widehat{V}_{YX}^{(n)}\|_{HS} \\
\leqslant&\|\widehat{V}_{ZX}^{(n)} - V_{ZX}\|_{HS} + \|V_{ZY}\|_{HS}\|V_{YX} - \widehat{V}_{YX}^{(n)}\|_{HS} + \|V_{ZY} - \widehat{V}_{ZY}^{(n)}\|_{HS}\|\widehat{V}_{YX}^{(n)}\|_{HS}
\end{aligned}$$

From the proof of Theorem 5 in [38], we have

$$\|\widehat{V}_{YX}^{(n)} - V_{YX}\|_{HS} = O_p(\varepsilon_n^{-3/2}n^{-1/2}) \quad \text{as} \quad n \to \infty.$$

Similarly, we have $\|\widehat{V}_{ZX}^{(n)} - V_{ZX}\|_{HS} = O_p(\varepsilon_n^{-3/2}n^{-1/2})$, $\|\widehat{V}_{ZY}^{(n)} - V_{ZY}\|_{HS} = O_p(\varepsilon_n^{-3/2}n^{-1/2})$ as $n \to \infty$. Since $\|V_{ZY}\|_{HS} \leqslant 1$ and $\|\widehat{V}_{YX}^{(n)}\|_{HS} \leqslant 1$, we have

$$\|\widehat{V}_{ZX|Y}^{(n)} - V_{ZX|Y}\|_{HS} = O_p(\varepsilon_n^{-3/2}n^{-1/2}).$$

Appendix A.3 Upper Bounds on the Target Error

Lemma A.1. For any hypothesis h, $h' \in \mathcal{H}$,

$$|\epsilon_S(h, h') - \epsilon_T(h, h')| \leqslant \frac{1}{2}\mathbb{E}_Y[d_{\mathcal{H}\Delta\mathcal{H}}(P_{X|Y}^S, P_{X|Y}^T)] + \|P_Y^S - P_Y^T\|_1.$$

Proof.

$$\begin{aligned}
|\epsilon_S(h, h') - \epsilon_T(h, h')| &\leqslant \sup_{h,h'\in\mathcal{H}} |\epsilon_S(h, h') - \epsilon_T(h, h')| \\
&= \sup_{h,h'\in\mathcal{H}} |\int_{\mathcal{Y}}\int_{\mathcal{X}} \mathbf{1}_{h(x)\neq h'(x)} p_{X|Y}^S p_Y^S dxdy - \int_{\mathcal{Y}}\int_{\mathcal{X}} \mathbf{1}_{h(x)\neq h'(x)} p_{X|Y}^T p_Y^T dxdy| \\
&= \sup_{h,h'\in\mathcal{H}} \int_{\mathcal{Y}}\int_{\mathcal{X}} \mathbf{1}_{h(x)\neq h'(x)} |p_{X|Y}^S p_Y^S - p_{X|Y}^T p_Y^S + p_{X|Y}^T p_Y^S - p_{X|Y}^T p_Y^T| dxdy \\
&= \sup_{h,h'\in\mathcal{H}} \int_{\mathcal{Y}}\int_{\mathcal{X}} \mathbf{1}_{h(x)\neq h'(x)} |(p_{X|Y}^S - p_{X|Y}^T)p_Y^S + p_{X|Y}^T(p_Y^S - p_Y^T)| dxdy \\
&\leqslant \int_{\mathcal{Y}} \sup_{h,h'\in\mathcal{H}} \int_{\mathcal{X}} \mathbf{1}_{h(x)\neq h'(x)} |p_{X|Y}^S - p_{X|Y}^T| p_Y^S dxdy + \int_{\mathcal{Y}}\int_{\mathcal{X}} p_{X|Y}^T |p_Y^S - p_Y^T| dxdy \\
&\leqslant \int_{\mathcal{Y}} \sup_{h,h'\in\mathcal{H}} \int_{\mathcal{X}} \mathbf{1}_{h(x)\neq h'(x)} |p_{X|Y}^S - p_{X|Y}^T| p_Y^S dxdy + \int_{\mathcal{Y}} |p_Y^S - p_Y^T| dxdy \\
&= \frac{1}{2}\mathbb{E}_Y[d_{\mathcal{H}\Delta\mathcal{H}}(P_{X|Y}^S, P_{X|Y}^T)] + \|P_Y^S - P_Y^T\|_1
\end{aligned}$$

Lemma A.2 (Lemma 6, [2])**.** For the domain $\mathcal{D}$, let S be a labeled sample set of size m drawn from $\mathcal{D}$ and labeling them according to the gourndtruth labeling function f. Let $\hat{\epsilon}(h)$ be the empirical error of some fixed hypothesis h on this sample set, and let $\epsilon(h)$ be the true error, then

$$P[|\hat{\epsilon}(h) - \epsilon(h)| \geqslant \varepsilon_n] \leqslant 2\exp(-2m{\varepsilon_n}^2)$$

Theorem 3. Let $\mathcal{H}$ be a hypothesis space of VC dimension d, m be the sample size of source domain and f_s be the ground truth labeling function for the source domain. If $\hat{h} \in \mathcal{H}$ is the empirical minimizer of $\hat{\epsilon}_S(h)$ and $h_T^* = \operatorname*{argmin}_{h\in\mathcal{H}} \epsilon_T(h)$ is the target error minimizer, then for any $\delta \in (0, 1)$, with probability at least $1 - \delta$,

$$\epsilon_T(\hat{h}) \leqslant \epsilon_T(h^*) + 2(\lambda + \frac{1}{2}\mathbb{E}_Y[d_{\mathcal{H}\Delta\mathcal{H}}(P_{X|Y}^S, P_{X|Y}^T)] + \|P_Y^S - P_Y^T\|_1) + 2\eta_{d,m,\delta}, \tag{A10}$$

where $\eta_{d,m,\delta} = \sqrt{\frac{1}{2m}(\log\frac{d}{\delta})}$, $\lambda = \min_{h\in\mathcal{H}}\{\epsilon_S(h) + \epsilon_T(h)\}$.

Proof. Let $h^* = \operatorname{argmin}_{h\in\mathcal{H}} \epsilon_T(h) + \epsilon_S(h)$. Then,

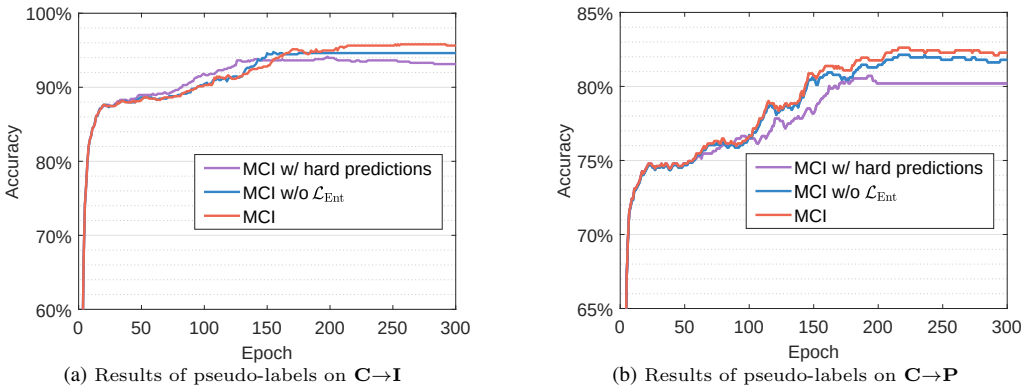
$$\begin{aligned}
|\epsilon_S(h) - \epsilon_T(h)| &= |\epsilon_S(h, f_s) - \epsilon_T(h, f_t)| \\
&= |\epsilon_S(h, f_s) - \epsilon_S(h, h^*) + \epsilon_S(h, h^*) - \epsilon_T(h, h^*) + \epsilon_T(h, h^*) - \epsilon_T(h, f_t)| \\
&\leqslant |\epsilon_S(h, f_s) - \epsilon_S(h, h^*)| + |\epsilon_S(h, h^*) - \epsilon_T(h, h^*)| + |\epsilon_T(h, h^*) - \epsilon_T(h, f_t)| \\
&\leqslant \epsilon_S(h^*) + \epsilon_T(h^*) + |\epsilon_S(h, h^*) - \epsilon_T(h, h^*)| \\
&\leqslant \lambda + \frac{1}{2}\mathbb{E}_Y[d_{\mathcal{H}\Delta\mathcal{H}}(P^S_{X|Y}, P^T_{X|Y})] + \|P^S_Y - P^T_Y\|_1. \qquad \text{(A11)}
\end{aligned}$$

The second inequality follows from the triangle inequality [40]. The last inequality follows from the definition of λ and Lemma A.1. Now applying Lemma A.2 on (A11), we have for any $\delta \in (0, 1)$, with probability $1 - \delta$,

$$\begin{aligned}
\epsilon_T(\hat{h}) &\leqslant \epsilon_S(\hat{h}) + \lambda + \frac{1}{2}\mathbb{E}_Y[d_{\mathcal{H}\Delta\mathcal{H}}(P^S_{X|Y}, P^T_{X|Y})] + \|P^S_Y - P^T_Y\|_1 \\
&\leqslant \hat{\epsilon}_S(\hat{h}) + \eta(d, m, \delta) + \lambda + \frac{1}{2}\mathbb{E}_Y[d_{\mathcal{H}\Delta\mathcal{H}}(P^S_{X|Y}, P^T_{X|Y})] + \|P^S_Y - P^T_Y\|_1 \\
&\leqslant \hat{\epsilon}_S(h^*_T) + \eta(d, m, \delta) + \lambda + \frac{1}{2}\mathbb{E}_Y[d_{\mathcal{H}\Delta\mathcal{H}}(P^S_{X|Y}, P^T_{X|Y})] + \|P^S_Y - P^T_Y\|_1 \\
&\leqslant \epsilon_S(h^*_T) + 2\eta(d, m, \delta) + \lambda + \frac{1}{2}\mathbb{E}_Y[d_{\mathcal{H}\Delta\mathcal{H}}(P^S_{X|Y}, P^T_{X|Y})] + \|P^S_Y - P^T_Y\|_1 \\
&\leqslant \epsilon_T(h^*) + 2\eta(d, m, \delta) + 2(\lambda + \frac{1}{2}\mathbb{E}_Y[d_{\mathcal{H}\Delta\mathcal{H}}(P^S_{X|Y}, P^T_{X|Y})] + \|P^S_Y - P^T_Y\|_1).
\end{aligned}$$

The first and the last inequalities follows from (A11). The second and the fourth inequalities follows from Lemma A.2. The third inequality follows the definition of $\hat{h}$.

Appendix B Experimental Results



(a) Results of pseudo-labels on **C→I** (b) Results of pseudo-labels on **C→P**

Figure B1 (Color online) The accuracy of pseudo-labels in the training process.

Table B1 Accuracies (%) on Office-31. CDTrans* and SHOT* uses DeiT-Base backbone. TVT° uses ViT-Base backbone. "-B" indicates ViT-Base backbone.

Backbone	Methods	A→W	D→W	W→D	A→D	D→A	W→A	Mean
AlexNet	Source-Only [48]	61.6	95.4	99.0	63.8	51.1	49.8	70.1
	DAN [4]	68.5	96.0	99.0	67.0	54.0	53.1	72.9
	DANN [7]	73.0	96.4	99.2	72.3	53.4	51.2	74.3
	CDAN+E [9]	78.3	97.2	**100.0**	76.3	57.3	57.3	77.7
	ATM [14]	**80.2**	97.9	**100.0**	**77.5**	62.1	61.3	**79.6**
	MCI	78.5	**98.6**	99.6	75.9	**62.5**	**62.2**	**79.6**
ViT	ViT-B [46]	91.2	99.2	**100.0**	90.4	81.1	80.6	90.4
	CDTrans* [26]	96.7	99.0	**100.0**	97.0	81.1	81.9	92.6
	SHOT* [24]	94.3	99.0	**100.0**	95.3	79.4	80.2	91.4
	TVT° [27]	96.4	**99.4**	**100.0**	96.4	84.9	**86.1**	93.8
	SSRT-B [18]	**97.7**	99.2	**100.0**	**98.6**	83.5	82.2	93.5
	MCI	94.7	**99.4**	**100.0**	97.9	**86.5**	85.6	**94.0**

Table B2 Accuracies (%) on Office-Home (ResNet-50).

Office-Home	Ar→Cl	Ar→Pr	Ar→Rw	Cl→Ar	Cl→Pr	Cl→Rw	Pr→Ar	Pr→Cl	Pr→Rw	Rw→Ar	Rw→Cl	Rw→Pr	Mean
Source-Only [47]	34.9	50.0	58.0	37.4	41.9	46.2	38.5	31.2	60.4	53.9	41.2	59.9	46.1
DAN [4]	43.6	5.0	67.9	45.8	56.5	60.4	44.0	43.6	67.7	63.1	51.5	74.3	56.3
DANN [7]	45.6	59.3	70.1	47.0	58.5	60.9	46.1	43.7	68.5	63.2	51.8	76.8	57.6
KGOT [29]	36.2	59.4	65.0	48.6	56.5	60.2	52.1	37.8	67.1	59.0	41.9	72.0	54.7
ETIC [31]	49.3	71.3	76.3	58.6	70.5	71.0	59.7	47.4	77.3	66.0	50.4	79.6	64.8
CDAN+E [9]	50.7	70.6	76.0	57.6	70.0	70.0	57.4	50.9	77.3	70.9	56.7	81.6	65.8
DSAN [13]	54.4	70.8	75.4	60.4	67.8	68.0	62.6	55.9	78.5	73.8	60.6	83.1	67.6
DMP [34]	52.3	73.0	77.3	64.3	72.0	71.8	63.6	52.7	78.5	72.0	57.7	81.6	68.1
ATM [14]	52.4	72.6	80.2	61.1	72.0	72.6	59.5	52.0	79.1	73.3	58.9	83.4	67.9
BuresNet [35]	54.7	74.4	77.1	63.7	72.2	71.8	64.1	51.7	78.4	73.1	58.0	82.4	68.5
WCEL [36]	56.3	75.1	77.6	60.5	68.6	70.2	61.2	49.6	76.6	68.7	59.8	83.6	67.3
SymmNets-V2 [22]	48.1	74.3	78.7	64.6	71.8	74.1	64.4	50.0	80.2	74.3	53.1	83.2	68.1
SHOT [24]	57.1	**78.1**	81.5	68.0	**78.2**	78.1	67.4	54.9	82.2	73.3	58.8	84.3	71.8
DCAN+SCDA [17]	**60.7**	76.4	**82.8**	**69.8**	77.5	**78.4**	**68.9**	**59.0**	**82.7**	**74.9**	**61.8**	**84.5**	**73.1**
MCI	51.7	76.3	80.1	60.6	75.2	76.3	64.8	51.4	81.7	69.3	54.8	83.3	68.8

Table B3 Accuracies (%) on Office-Home (ViT). CDTrans* and SHOT* uses DeiT-Base backbone. TVT° uses ViT-Base backbone. "-B" indicates ViT-Base backbone.

Office-Home	Ar→Cl	Ar→Pr	Ar→Rw	Cl→Ar	Cl→Pr	Cl→Rw	Pr→Ar	Pr→Cl	Pr→Rw	Rw→Ar	Rw→Cl	Rw→Pr	Mean
ViT-B [46]	54.7	83.0	87.2	77.3	83.4	85.5	74.4	50.9	87.2	79.6	53.8	88.8	75.5
CDtrans* [26]	68.8	85.0	86.9	81.5	87.1	87.3	79.6	63.3	88.2	82.0	66.0	90.6	80.5
TVT° [27]	74.89	86.82	89.47	82.78	87.95	88.27	79.81	71.94	90.13	85.46	74.62	90.56	83.56
SSRT-B [18]	**75.2**	89.0	**91.1**	**85.1**	88.3	**90.0**	**85.0**	**74.2**	**91.3**	**85.7**	**78.6**	**91.8**	**85.4**
SHOT* [24]	67.1	83.5	85.5	76.6	83.4	83.7	76.3	65.3	85.3	80.4	66.7	83.4	78.1
MCI	71.2	**89.8**	89.5	82.4	**89.4**	89.2	81.0	68.0	90.3	83.2	75.6	90.9	83.4

Table B4 Accuracies (%) on VisDA-2017 (ResNet-101).

VisDA-2017	plane	bcycl	bus	car	horse	knife	mcycl	person	plant	sktbrd	train	truck	Mean
Source-Only [47]	72.3	6.1	63.4	**91.7**	52.7	7.9	80.1	5.6	90.1	18.5	78.1	25.9	49.4
DAN [4]	68.1	15.4	76.5	87.0	71.1	48.9	82.3	51.5	88.7	33.2	88.9	42.2	62.8
DANN [7]	81.9	77.7	82.8	44.3	81.2	29.5	65.1	28.6	51.9	54.6	82.8	7.8	57.4
ETIC [31]	49.3	71.3	76.3	58.6	70.5	71.0	59.7	47.4	77.3	66.0	50.4	79.6	64.8
CDAN [9]	85.2	66.9	83.0	50.8	84.2	74.9	88.1	74.5	83.4	76.0	81.9	38.0	73.9
DSAN [13]	90.9	66.9	75.7	62.4	88.9	77.0	**93.7**	75.1	92.8	67.6	89.1	39.4	75.1
CTSN [21]	92.3	65.1	84.2	68.4	90.4	61.2	92.3	74.1	88.7	66.9	82.3	19.4	75.4
DMP [34]	92.1	75.0	78.9	75.5	91.2	81.9	89.0	77.2	93.3	77.4	84.8	35.1	79.3
ATM [14]	93.9	65.1	83.7	72.1	92.2	**92.5**	92.4	79.7	86.1	47.8	86.1	22.0	76.1
WCEL [36]	**95.2**	**82.5**	81.2	73.5	93.4	82.6	89.8	80.2	86.3	76.4	85.4	45.6	78.2
SUDA [19]	88.3	79.3	66.2	64.7	87.4	80.1	85.9	78.3	86.3	87.5	78.8	74.5	79.8
SymmNets-V2 [22]	87.3	62.2	79.1	66.7	80.3	79.7	87.8	75.6	88.9	31.4	**90.7**	25.8	71.3
SHOT [24]	94.3	88.5	80.1	57.3	93.1	94.9	80.7	80.3	91.5	89.1	86.3	**58.2**	**82.9**
MCI	94.1	66.4	**85.7**	69.2	93.2	**91.8**	93.6	78.9	90.1	**85.4**	87.7	26.8	80.3

Table B5 Accuracies (%) on DomainNet (ResNet-101). In each sub-table, the column-wise means source domain and the row-wise means target domain.

Source-Only [47]	clp	inf	pnt	qdr	rel	skt	Avg.
clp	-	19.3	37.5	11.1	52.2	41.0	32.2
inf	30.2	-	31.2	3.6	44.0	27.9	27.4
pnt	39.6	18.7	-	4.9	54.5	36.3	30.8
qdr	7.0	0.9	1.4	-	4.1	8.3	4.3
rel	48.4	22.2	49.4	6.4	-	38.8	33.0
skt	46.9	15.4	37.0	10.9	47.0	-	31.4
Avg.	34.4	15.3	31.3	7.4	40.4	30.5	26.6

DANN [7]	clp	inf	pnt	qdr	rel	skt	Avg.
clp	-	15.5	34.8	9.5	50.8	41.4	30.4
inf	31.8	-	30.2	3.8	44.8	25.7	27.3
pnt	39.6	15.1	-	5.5	54.6	35.1	30.0
qdr	11.8	2.0	4.4	-	9.8	8.4	7.3
rel	47.5	17.9	47.0	6.3	-	37.3	31.2
skt	47.9	13.9	34.5	10.4	46.8	-	30.7
Avg.	35.7	12.9	30.2	7.1	41.4	29.6	26.1

CDAN [9]	clp	inf	pnt	qdr	rel	skt	Avg.
clp	-	20.4	36.6	9.0	50.7	42.3	31.8
inf	27.5	-	25.7	1.8	34.7	20.1	22.0
pnt	42.6	20.0	-	2.5	55.6	38.5	31.8
qdr	21.0	4.5	8.1	-	14.3	15.7	12.7
rel	51.9	23.3	50.4	5.4	-	41.4	34.5
skt	50.8	20.3	43.0	2.9	50.8	-	33.6
Avg.	38.8	17.7	32.8	4.3	41.2	31.6	27.7

DCAN [25]	clp	inf	pnt	qdr	rel	skt	Avg.
clp	-	18.5	43.6	17.1	60.3	45.8	37.1
inf	39.7	-	38.4	5.9	54.6	28.5	33.4
pnt	48.6	19.7	-	9.9	61.7	41.2	36.2
qdr	33.2	5.6	16.1	-	18.4	16.2	17.9
rel	53.7	18.5	50.5	4.0	-	33.4	32.0
skt	57.6	17.3	47.3	10.1	55.3	-	37.5
Avg.	46.6	15.9	39.2	9.4	50.1	33.0	32.4

MDD+SCDA [17]	clp	inf	pnt	qdr	rel	skt	Avg.
clp	-	20.4	43.3	15.2	59.3	46.5	36.9
inf	32.7	-	34.5	6.3	47.6	29.2	30.1
pnt	46.4	19.9	-	8.1	58.8	42.9	35.2
qdr	31.1	6.6	18.0	-	28.8	22.0	21.3
rel	55.5	23.7	52.9	9.5	-	45.2	37.4
skt	55.8	20.1	46.5	15.0	56.7	-	38.8
Avg.	44.3	18.1	39.0	10.8	50.2	37.2	33.3

MCI	clp	inf	pnt	qdr	rel	skt	Avg.
clp	-	19.2	43.9	18.9	63.9	47.2	38.6
inf	56.4	-	43.0	10.7	62.3	41.8	42.8
pnt	50.9	24.3	-	14.4	65.1	47.4	40.4
qdr	27.6	2.5	7.9	-	15.2	18.7	14.4
rel	57.5	26.4	55.8	22.2	-	47.8	41.9
skt	59.3	22.1	51.8	27.4	56.7	-	43.4
Avg.	50.3	18.9	40.5	18.7	52.7	40.6	**36.9**

Table B6 Computational time (s) and accuracy (%) of HSIC, ETIC, and MCI.

Method	Image-CELF task **C→I**			Office-31 task **W→A**		
	HSIC	ETIC	MCI	HSIC	ETIC	MCI
Time	0.0333	0.0027	0.0556	0.3333	0.0157	0.7000
Accuracy (%)	95.1	90.9	95.5	72.7	69.0	83.4

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