Invariance Learning based on Label Hierarchy

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case

Deep Neural Networks inherit spurious correlations embedded in training data and hence may fail to predict desired labels on unseen domains (or environments), which have different distributions from the domain used in training. Invariance Learning (IL) has been developed recently to overcome this shortcoming; using training data in many domains, IL estimates such a predictor that is invariant to a change of domain. However, the requirement of training data in multiple domains is a strong restriction of IL, since it often needs high annotation cost. We propose a novel IL framework to overcome this problem. Assuming the availability of data from multiple domains for a higher level of classification task, for which the labeling cost is low, we estimate an invariant predictor for the target classification task with training data in a single domain. Additionally, we propose two cross-validation methods for selecting hyperparameters of invariance regularization to solve the issue of hyperparameter selection, which has not been handled properly in existing IL methods. The effectiveness of the proposed framework, including the cross-validation, is demonstrated empirically, and the correctness of the hyperparameter selection is proved under some conditions.

1 Introduction

Training data used in machine learning unintentionally contain unrelated factors to the objective of the task, which are called spurious correlations. Deep Neural Networks (DNNs) often inherit the spurious correlations embedded in the data in training domains and hence may fail to predict desired labels in domains which have different distributions from the training domains, namely unseen domains. For example, in a problem of classifying images of cows, DNNs tend to misclassify cows in sandy beaches; most training pictures are taken in green pastures and DNNs inherit context information in training [3, 9]. Systems trained with medical data collected in one hospital do not generalize well to other health centers; DNNs unintentionally extract environmental factors specific to a particular hospital in training [16, 17, 18].

Invariance Learning (IL) is an approach developed rapidly to overcome the issue of spurious correlation or short-cut learning [10, 14, 13, 12, 11, 15, 21, 33, 34, 35, 36]. Let $e \in \mathcal{E}$ be a domain (or environment) index, and $X^e \in \mathcal{X}$ and $Y^e \in \mathcal{Y}$ be an input object and its label in domain $e \in \mathcal{E}$, respectively. Using training data in multiple training domains $\mathcal{E}_{tr} \subset \mathcal{E}$, IL estimates a predictor $f : \mathcal{X} \to \mathcal{Y}$ that performs as...
well in unseen domains $e \in \mathcal{E} - \mathcal{E}_t$, as in the training domain, that is, a predictor \textit{invariant} to change of domains. In IL, the training data must be annotated with labels of $\mathcal{Y}$ completely.

While the IL approach has attracted much attention as a solution to the spurious correlation, requiring training data with exact labeling from multiple domains may hinder wide applications in practice; preparing training data in many domains are often expensive with data annotation. Even when we can draw data from multiple domains, they are often only available in an incompletely labeled form, which are called \textit{pseudo label data} \cite{12, 13, 14, 15}, \textit{partial label data} \cite{10, 18, 17} and \textit{complementary label data} \cite{51, 50, 49}.

We propose a novel IL framework to reduce the need of training data with exact labels from multiple domains. We estimate the invariance by the coarser labeled data, which need lower annotation cost. Specifically, in addition to the target task of classification, we consider another classification task of a higher level in the label hierarchy, that is, we suppose that the additional task has a coarser label set than the target task. We consider the situation where the training data of the target task is given in only one domain, while the task of higher label hierarchy has data from multiple domains. This significantly reduces the annotation cost since the data with coarser labels are much easier to obtain. More formally, assuming the availability of additional data $(X^e, Z^e)$ from multiple domains $e \in \mathcal{E}_{ad} \subset \mathcal{E}$ for the higher level of classification task, we estimate an invariant predictor for the target task with training data of a single domain $\{e^*\}$. Here, the higher level of classification task means that its label is given by $Z^e = g(Y^e)$ with some surjective function $g: \mathcal{Y} \to Z$ to define the label hierarchy. For example, consider the case where $\mathcal{Y} := \{\text{bird}_1, \ldots, \text{bird}_{10000}, \text{no birds}\}$, labels with 10,000 kinds of birds and no birds, and $\mathcal{Z} := \{\text{there are birds}, \text{no birds}\}$, $g(y) = \text{no birds}$ if $y = \text{no birds}$ and $g(y) = \text{there are birds}$ otherwise. Then, the binary labels $\mathcal{Z}$ are much more easily annotated than the original 10001 class labels $\mathcal{Y}$. This may be done by humans with crowd-sourcing or a binary classifier of high accuracy.

Another important issue in IL is hyperparameter selection. Most IL methods involve some hyperparameters to balance the classification accuracy and the degree of invariance. As \cite{21} and \cite{19} point out, in the literature of IL, the best performances of invariance have often been achieved by selecting the hyperparameters using test data from unseen domains. Moreover, \cite{19} numerically demonstrated that, without using test data, simple methods of hyperparameter selection fail to find a preferable hyperparameter. This illustrates a strong need for establishing an appropriate method of hyperparameter selection for IL.

We propose two methods of cross-validation (CV) for hyperparameter selection in our new IL framework. Since we assume training data of a single domain for the target task, it is impossible to estimate the deviation of the risks over the domains. We make use of the additional data from multiple domains in the higher level and provide methods of CV, which is applicable in the current setting. Theoretical analysis reveals that our methods select hyperparameter correctly with some condition.

The main contributions of this paper are as follows:

- We establish a novel framework of invariant learning, which estimates an invariant predictor from a single domain data, assuming additional data from multiple domains for a higher level of classification task.

- We propose two methods of cross-validation under the framework for selecting hyperparameters without accessing any samples from unseen target domains.
Experimental studies verify that the proposed framework extracts an invariant predictor more effectively than other existing methods.

We mathematically prove that the proposed CV methods select the correct hyperparameter under some settings.

2  Invariance Learning based on Label Hierarchy

Notations
Throughout this paper, the space of input features and finite class labels are denoted by $\mathcal{X}$ and $\mathcal{Y}$, respectively. For given predictor $f : \mathcal{X} \to \mathcal{Y}$ and random variable $(X,Y)$ on $\mathcal{X} \times \mathcal{Y}$ with its probability $P_{X,Y}$, $R^{(X,Y)}(f)$ denotes the risk of $f$ on $(X,Y)$; i.e., $R^{(X,Y)}(f) := \int l(f(x), y) dP_{X,Y}$, where $l : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ is a loss function. For $m \in \mathbb{N}_{>0}$, $[m]$ denotes the set $\{1, \ldots, m\}$. For a finite set $A$, $|A| \in \mathbb{N}$ denotes the number of elements in $A$.

2.1 Review of Invariance Learning

Following [10], to formulate the out-of-distribution (o.o.d.) generalization, we assume that the joint distribution of data $(X^e, Y^e)$ depends on the domain (or environment) $e \in \mathcal{E}$, and consider the dependence of a predictor $f$ on the domain variable $e$. Suppose we are given training data sets $D^e := \{(x^e_i, y^e_i)\}_{i=1}^n \sim P_{X^e, Y^e}$ i.i.d. from multiple domains $e \in \mathcal{E}_{tr}$. The final goal of the o.o.d. problem is to predict a desired label $Y^e \in \mathcal{Y}$ from $X^e \in \mathcal{X}$ for larger target domains $\mathcal{E} \supset \mathcal{E}_{tr}$. To discuss the o.o.d. performance, [10] introduced the o.o.d. risk

\[ R^{\text{o.o.d.}}(f) := \max_{e \in \mathcal{E}} R^e(f), \quad (1) \]

where $R^e(f) := R^{(X^e, Y^e)}(f)$. This is the worst case risk over the domains $\mathcal{E}$, including unseen domains $\mathcal{E} - \mathcal{E}_{tr}$.

To solve (1), [10] estimates such a predictor $w \circ \Phi$ that is invariant to change of domains, where the invariance $\Phi : \mathcal{X} \to \mathcal{H}$ and the predictor $w : \mathcal{H} \to \mathcal{Y}$ function as eliciting the invariant representation from $X^e \in \mathcal{X}$, and estimating a label of the invariant representation $\Phi(X^e)$ respectively. The estimation are implemented by solving the following optimization problem:

\[
\min_{\Phi \in \mathcal{I}_{tr}, w : \mathcal{H} \to \mathcal{Y}} \sum_{e \in \mathcal{E}_{tr}} R^e(w \circ \Phi),
\]

where $\mathcal{I}_{tr}$ is the set of invariances captured by $\bigcup_{e \in \mathcal{E}_{tr}} D^e$. All of IL, including [10], estimate the invariance using the difference among $\mathcal{E}_{tr}$, assuming the availability of multiple training domains in common.

While how to capture the invariance varies slightly among IL, we adopt the method based on conditional independence as done by [40], [11] and [15]:

\[ \mathcal{I}_{tr} := \{ \Phi : \mathcal{X} \to \mathcal{H} \mid P(Y^e|\Phi(X^e)) \text{ does not depend on } e \in \mathcal{E}_{tr} \}. \]
2.2 Invariance estimation by higher label data

Our goal is to make an invariant predictor from a single training domain $E_{tr} = \{e^*\}$. In this case, (2) is reduced to the empirical risk minimization $\min_{f} \mathcal{R}^{e^*}(f)$ on $e^*$, and therefore the standard IL is not able to extract invariance.

In this paper, we introduce an assumption that additional data $D^e_{ad}$ from $(X^e, Z^e)$ with coarser label $Z^e \in \mathcal{Z}$ is available for multiple domains $E_{ad} \subset E$. This means that we have data for another task in a higher label hierarchy than the target task. More formally, the label $Z^e$ is assumed to follow $Z^e = g(Y^e)$ with surjective label mapping $g: \mathcal{Y} \rightarrow \mathcal{Z}$ from the lower to the higher level in the hierarchy. For example, in the problem of animal recognition from images, $\mathcal{Y}$ is $\{\text{cow}, \text{horse}, \text{dog}, \ldots, \text{no animal}\}$ and $\mathcal{Z}$ may be $\{\text{animal, no animal}\}$. The domain $e$ specifies the background of the image: pasture, sand, room, and so on.

By making use of the data $\bigcup_{e \in E_{ad}} D^e_{ad}$ in the higher level, our objective for the invariant prediction of $Y^e$ is given by

$$\min_{\Phi \in \mathcal{I}_{ad}, w: \mathcal{H} \rightarrow \mathcal{Y}} \mathcal{R}^{e^*}(w \circ \Phi),$$

where $\mathcal{I}_{ad}$ is the set of invariances:

$$\mathcal{I}_{ad} := \{\Phi: \mathcal{X} \rightarrow \mathcal{H} | P(g(Y^e)|\Phi(X^e)) \text{ does not depend on } e \in E_{ad}\}.$$

The condition of $\mathcal{I}_{ad}$ is necessary to the invariance condition of the target task $(X^e, Y^e)$, that is,

"$P(Y^e|\Phi(X^e))$ does not depend on $e \in E$" $\Rightarrow$

"$P(g(Y^e)|\Phi(X^e))$ does not depend on $e \in E_{ad}$"

holds.

2.3 Construction of objective function

While there are many possible variations in the design of losses and models, we focus a probabilistic output case and evaluate its error by the cross entropy loss; that is, we model $w$ by maps to $p^\theta: \mathcal{H} \rightarrow \mathcal{P}_Y$, where $\mathcal{P}_Y$ denotes the set of probabilities on $\mathcal{Y}$. The risk is then written by

$$\mathcal{R}^e(p^\theta \circ \Phi) = \int -\log p^\theta(Y^e|\Phi(X^e))dP_{X^e, Y^e}.$$

We aim to solve (3) by minimizing the following objective function:

$$Objective(\theta, \Phi) := \hat{\mathcal{R}}^{e^*}(p^\theta \circ \Phi) + \lambda \cdot (\text{Dependence measure of } P(Z^e|\Phi(X^e))) \text{ on } e \in E_{ad}).$$

Here, $\hat{\mathcal{R}}^{e^*}(p^\theta \circ \Phi)$ denotes the empirical risk of $p^\theta \circ \Phi$ evaluated by $D^{e^*}$:

$$\hat{\mathcal{R}}^{e^*}(p^\theta \circ \Phi) := -\frac{1}{|D^{e^*}|} \sum_{(x^{e^*}, y^{e^*}) \in D^{e^*}} \log p^\theta(y^{e^*}|\Phi(x^{e^*}))$$
The above equivalence follows immediately.

Invariance coincide, and therefore we may use \( \sum \) where \( \hat{\theta} \).

**Proof.**

where \( \parallel \nabla \parallel_{\text{argmin}} \Theta \cdot X \) \( (ii) \) \argmin \( \hat{\lambda} \) \( \left\{ \sum_{(x,y) \in D_{x,y}^{[k]}} \log p_{p_{[k]}}(y|x, s) \right\} \) \( \text{for } Z \). Set the hyperparameter candidates \( \Lambda \).

**Algorithm 1** Two Cross Validation Methods.

\textbf{Require: :} Split \( D_{x,y}^{[k]} \) into \( K \) parts. Set the hyperparameter candidates \( \Lambda \).

\textbf{Require: :} \( \hat{P}(Z^e = z) \leftarrow \frac{\left| \hat{D} \right|}{|D_{x,y}^{[k]}|} \) where \( |D_{x,y}^{[k]}| \) \( \forall e \in \mathcal{E}_{x,y} \)  in \( Z \).

\begin{enumerate}
    \item for \( \lambda \in \Lambda \)
    \item for \( k \) from 1 to \( K \) do
    \item Learn \( \theta_{[k]}^{\lambda} \).
    \item \( \hat{R}^{[k]}(p_{\theta_{[k]}^{\lambda}} \circ \Phi_{[k]}^{\lambda}) \leftarrow \frac{1}{|D_{x,y}^{[k]}|} \sum_{(x,y) \in D_{x,y}^{[k]}} \log p_{p_{[k]}}(y|x, s) \) \( \text{for } Z \).
    \item \( \hat{R}^{[k]}(p_{\theta_{[k]}^{\lambda}} \circ \Phi_{[k]}^{\lambda}) \leftarrow \hat{R}^{[k]}(p_{\theta_{[k]}^{\lambda}} \circ \Phi_{[k]}^{\lambda}) + \sum_{(x,y) \in D_{x,y}^{[k]}} \log p_{p_{[k]}}(y|x, s) \) \( \text{for } Z \).
    \item end for
    \item if CORRECTION = True
    \item \( \hat{R}^{[k]}(p_{\theta_{[k]}^{\lambda}} \circ \Phi_{[k]}^{\lambda}) \leftarrow \frac{1}{|D_{x,y}^{[k]}|} \sum_{(x,y) \in D_{x,y}^{[k]}} \log p_{p_{[k]}}(y|x, s) \) \( \text{for } Z \).
    \item end if
    \item end for
    \item (I) \( \hat{R}^{[k]}(p_{\theta_{[k]}^{\lambda}} \circ \Phi_{[k]}^{\lambda}) \leftarrow \frac{1}{K} \sum_{k=1}^{K} \hat{R}^{[k]}(p_{\theta_{[k]}^{\lambda}} \circ \Phi_{[k]}^{\lambda}) \).
    \item (I) \( \hat{R}^{[k]}(p_{\theta_{[k]}^{\lambda}} \circ \Phi_{[k]}^{\lambda}) \leftarrow \frac{1}{K} \sum_{k=1}^{K} \hat{R}^{[k]}(p_{\theta_{[k]}^{\lambda}} \circ \Phi_{[k]}^{\lambda}) \).
    \item Select \( \lambda^* := \argmin \lambda \hat{R}^{[k]}(p_{\theta_{[k]}^{\lambda}} \circ \Phi_{[k]}^{\lambda}) \).
\end{enumerate}

For the regularization term, among others, we adopt the one introduced in [10], noting that their definition of invariance agrees with ours in our setting, as we see below. [10] call \( \Phi \) invariant when \( \argmin \text{in } \mathbb{E} \text{ runs over all probability densities.} \) The following lemma ensures that our and their definition of the invariance coincide, and therefore we may use \( \sum_{e \in \mathcal{E}_{x,y}} \| \nabla \|_{\text{argmin}} \Theta \cdot X \) \( \text{for } Z \).

**Lemma 2.1.** When modeling \( w \) by conditional probabilities, the following statements are equivalent:

\begin{enumerate}
    \item \( P(Z^e|\Phi(X^e)) \) does not depend on \( e \in \mathcal{E} \).
    \item \( \argmin \mathcal{R}(X^e, Z^e)(p_{\theta_{[k]}^{\lambda}} \circ \Phi_{[k]}^{\lambda}) \) does not depend on \( e \in \mathcal{E} \), \( p_{\theta_{[k]}^{\lambda}}^{Z^e|H} \rightarrow p_{\hat{X}}^{Z^e|H} \) \( \text{for } Z \).
\end{enumerate}

where \( p_{\theta_{[k]}^{\lambda}}^{Z^e|H} \) in (ii) runs over all probability densities.

**Proof.** Noting that \( \argmin \mathcal{R}(X^e, Z^e)(p_{\theta_{[k]}^{\lambda}} \circ \Phi_{[k]}^{\lambda}) \) coincides with the probability density function of \( P(Z^e|\Phi(X^e)) \), the above equivalence follows immediately.

In summary, we construct an objective function by

\[ \text{Objective}(\theta, \theta_{[k]}^{\lambda}) := \mathcal{R}^{[k]}(p_{\theta_{[k]}^{\lambda}} \circ \Phi_{[k]}^{\lambda}) + \lambda \cdot \sum_{e \in \mathcal{E}_{x,y}} \| \nabla \|_{\text{argmin}} \Theta \cdot X \mathcal{R}^{[k]}(p_{\theta_{[k]}^{\lambda}} \circ \Phi_{[k]}^{\lambda}) \|^2, \quad (4) \]
where \( p^Z[H] : H \rightarrow \mathcal{P}_Z \) is the logistic regression model, same as [10], and \( \hat{R}(X^e,Z^e)(p^Z[H] \circ \Phi) := -\frac{1}{|D_{ad}|} \sum_{(x^e,z^e) \in D_{ad}} \log p^Z[H] (z^e|\Phi(x^e)) \).

### 3 Hyperparameter selection method

#### 3.1 Hyperparameter Selection in Invariance Learning

Most IL methods involve hyperparameters to control the trade-off between the classification accuracy and invariance. Thus, hyperparameter selection is essential in IL methods.

The hyperparameter selection in IL has special difficulty. Since the o.o.d. problem needs to predict \( Y^e \) on unseen domains, the hyperparameter must be chosen without accessing any data in the unseen domains. It was reported [19] that the success of IL methods depends strongly on the careful choice of hyperparameters; some of the results used data from unseen domains in the choice. [19] reported also experimental results of various IL methods with two CV methods, training-domain validation (Tr-CV) and leave-one-domain-out validation (LOD-CV), and showed that the CV methods failed to select preferable hyperparameters. In Colored MNIST experiment, for example, the accuracy of Invariant Risk Minimization [10] is 52.0% at best, which is about the random guess level.

The failure of the CV methods are caused by the improper design of the objective function for CV; they do not simulate the o.o.d. risk, which is the maximum risk over the domains. Tr-CV splits data in each training domain into training and validation subsets, and takes the sum of the validated risks over the training domains. Obviously, this is not an estimate of the o.o.d. risk. LOD-CV holds out one domain among the training domains in turn and validates models with the average of the validated risks over the held-out domains. Again, this average does not correspond to the o.o.d. risk. In summary, the problem we need to solve is: How can we construct an evaluation function of the o.o.d. risk from validation data? In the sequel, we will propose two methods of CV, which are summarized in Algorithm [1].

#### 3.2 Method I: using data of higher level task

We divide each of \( D_{ad}^c, D_{ad}[k], \ldots, D_{ad}[k] \) into \( K \) parts, and use the \( k \)-th sample \( \{D_{ad}[k], D_{ad}[k], \ldots, D_{ad}[k]\} \) and the rest \( \{D_{ad}[k], D_{ad}[k], \ldots, D_{ad}[k]\} \) for validation and training, respectively. To approximate the o.o.d. risk of the predictor \( p_{\theta_{[-k],k}}(p_{\Phi^\lambda_{[-k],k}} \circ \Phi^\lambda_{[k]}) \) for \( e \in E_{ad} \cup \{e^*\} \). For \( e^* \), we use the standard empirical estimate \( \hat{R}^c(p_{\theta_{[-k],k}} \circ \Phi^\lambda_{[-k],k}) := \frac{1}{|D_{ad}|} \sum_{(x^e,z^e) \in D_{ad}} \log p_{\theta_{[-k],k}} (y^e|\Phi^\lambda_{[-k]}(x^e)) \). For \( e \in E_{ad} \), we substitute unavailable \( Y^e \) with \( Z^e \) and use \( \hat{R}^c(X^e,Z^e)(p_{\theta_{[-k],k}} \circ \Phi^\lambda_{[-k],k}) := \frac{1}{|D_{ad}|} \sum_{(x^e,z^e) \in D_{ad}} \log p_{\theta_{[-k],k}} (z^e|\Phi^\lambda_{[-k]}(x^e)) \).

#### 3.3 Method II: using correction term

Method I can be improved by considering the difference \( \hat{R}^c(p_{\theta_{[-k],k}} \circ \Phi^\lambda_{[-k],k}) - \hat{R}^c(X^e,Z^e)(p_{\theta_{[-k],k}} \circ \Phi^\lambda_{[-k],k}) \), for which we deduce the following theorem. The proof is given in Appendix [A].
Theorem 3.1. Let $Z^c := \{ z \in Z \mid \| g^{-1}(z) \| > 1 \}$. For any map $\Phi : X \rightarrow H$, $p_\theta : H \rightarrow \mathcal{P}_Y$, and random variable $(X, Y)$ on $\mathcal{X} \times \mathcal{Y}$, the following equality holds:

$$
R^{(X,Y)}(p_\theta \circ \Phi) - R^{(X,g(Y))}(p_\theta \circ \Phi) = \sum_{z^c' \in Z^c} \left\{ P(g(Y) = z^c') \times \int -\log p_\theta(Y|\Phi(X), Y \in g^{-1}(z^c')) dP_{X,Y|Y \in g^{-1}(z^c')} \right\},
$$

(5)

Here, $P_{X,Y|Y \in g^{-1}(z^c)}$ denotes the conditional distribution of $(X, Y)$ given the event $Y \in g^{-1}(z^c)$, and $p_\theta(y|\Phi(x), Y \in g^{-1}(z^c)) := \frac{p_\theta(y|\Phi(x))}{\sum_{y \in g^{-1}(z^c)} p_\theta(y|\Phi(x))}$.

The theorem shows that, to estimate $R^e(p_{\theta,p_{\lambda}} \circ \Phi_{[\lambda],[k]}^\lambda) - R^{(X^e,Z^e)}(p_{\theta,p_{\lambda}} \circ \Phi_{[\lambda],[k]}^\lambda)$, we need to estimate the following two values:

(i) $P(g(Y^c) = z^c) = P(Z^c = z^c)$ for every $z^c \in Z^c$,

(ii) $\int -\log p_{\theta,p_{\lambda}}(Y^c|\Phi_{[\lambda],[k]}^\lambda(X^c), g^{-1}(z^c)) dP_{X^c,Y^c|Y^c \in g^{-1}(z^c)}$ for every $z^c \in Z^c$.

(i) is naturally estimated by $D_{ad}^e \hat{P}(Z^c = z) := \frac{|D_{ad,z^c}^e|}{|D_{ad}^e|}$, where $D_{ad,z^c}^e := \{(x, z) \in D_{ad}^e \mid z = z^c\}$. (ii) is not directly estimable, as $Y^c$ is not observed. For an approximation of (ii), we substitute $Y^c$ with $Y^c^*$ and use

$$
\frac{1}{|D_{[k],z^c}^e|} \sum_{(x,y) \in D_{[k],z^c}^e} -\log p_{\theta,p_{\lambda}}(y|\Phi_{[\lambda],[k]}^\lambda(x), g^{-1}(z^c)),
$$

where

$$
D_{[k],z^c}^* := \{(x,y) \in D_{[k]}^e \mid g(y) = z^c\} \subset D_{[k]}^e.
$$

3.4 Theoretical analysis of our cross validation methods

In Sections 3.2 and 3.3, we approximate $R^{(X^e,Y^c)}$ using $Z^c$. While the approximation is not exact, we will prove that the proposed CV methods still select a correct hyperparameter under some conditions. We will also elucidate the difference of the two CV methods theoretically. In this paper, to avoid discussing non-trivial effects of nonlinear $\Phi$, we focus the case of variable selection, which appears in the invariance problem of causal inference [11, 12] and regression [40].

Let $\mathcal{X} := \mathcal{X}_1 \times \mathcal{X}_2$ where $\mathcal{X}_1 := \mathbb{R}^{n_1}$ and $\mathcal{X}_2 := \mathbb{R}^{n_2}$ with $n_1, n_2 \in N$, and assume that the projection $\Phi_{\mathcal{X}_1}$ from $\mathcal{X}$ onto $\mathcal{X}_1$ yields the invariance to $\{(X^e, Y^e)\}_{e \in \mathcal{E}}$, that is, $P(Y^c|\Phi_{\mathcal{X}_1}(X^e))$ are the same over $\forall(X^e, Y^e) \in \{(X^e, Y^e)\}_{e \in \mathcal{E}}$. Suppose that we have a model $\{\Phi\}$ for the feature map, where $\Phi$ is a projection of $\mathcal{X}$ onto some subset of $n_1$ + $n_2$ variables of $\mathcal{X}$. Minimizing (4) with its hyperparameter $\lambda$ over the model yields the feature map as a projection $\Phi_{\lambda} : \mathcal{X} \rightarrow \mathbb{R}^{n_{\lambda}}$ $(n_{\lambda} \leq n_1 + n_2)$. Let $\Phi_2^\lambda$ denote the $\mathcal{X}_2$-component of $\Phi_{\lambda}$ and, if $\Phi_{\lambda}$ does not have any $\mathcal{X}_2$-component, we write $\text{Im}\Phi_2^\lambda = \emptyset$. For simplicity of theoretical analysis, we assume that minimization with its hyperparameter $\lambda$ learns perfectly $p_\lambda^e(y|\Phi_{\lambda}(x))$, the conditional probability density function of $P_{Y^c\mid\Phi_{\lambda}(X^e)}$. Then, neglecting the estimations, the approximated o.o.d. risk of $p_\lambda^e \circ \Phi_{\lambda}$ used by Methods I and II are represented by the following $R^I(\lambda)$ and $R^{II}(\lambda)$, respectively:
\[ R^I(\lambda) := \max \left\{ \max_{e \in E_{ad}} R^{(X^*,g(Y^*)})(p^{e,\lambda} \circ \Phi^\lambda), R^{(X^*,Y^*)}(p^{e,\lambda} \circ \Phi^\lambda) \right\}, \]

\[ R^{II}(\lambda) := \max_{e \in E_{ad}, \lambda} \left\{ R^{(X^*,g(Y^*))}(p^{e,\lambda} \circ \Phi^\lambda) + \sum_{z^* \in \mathcal{Z}} \left\{ P(g(Y^*) = z^*) \times \int -\log p^{e,\lambda}(Y^*|\Phi^\lambda(X^*), Y^* \in g^{-1}(z^*)) \right\} \right\}. \]

We have the following theoretical justification of our CV methods: the chosen \( \lambda \) gives a minimizer of the correct CV criterion. For the proofs, see Appendices \[B\] and \[C\].

**Theorem 3.2** (Effectiveness of Method I). Assume that the following four conditions of \( \mathcal{E}, \mathcal{E}_{ad} \) and \( \Lambda \) hold:

(a) \( P_{\Phi,X_1(X^*)} \) does not depend on \( e \in \mathcal{E} \).

(b) For any random variable \((X,Y)\) with \( P_{\Phi,X_1(X),Y} = P_{\Phi,X_1(X^*),Y^*} \), there exists \( e \in \mathcal{E} \) such that \((X,Y) = (X^*,Y^*)\).

(c) \( \exists \lambda^j \in \Lambda \) s.t. \( \Phi^{\lambda^j} = \Phi^{\lambda_1} \).

(d) \( \forall \lambda \) with \( \text{Im} \Phi^\lambda \neq \emptyset \), \( \exists e_\lambda \in \mathcal{E}_{ad} \) such that \( P\left(g(Y^*)|\Phi^\lambda(X^*)\right) \leq e^{-\beta} - \varepsilon, P_{X^*,Y^*,-a.e} \). i.e., \( P_{X^*,Y^*}(B) = 1 \), where

\[ B := \left\{ (x,y) \in \mathcal{X} \times \mathcal{Y} \mid P\left(g(Y^*) = g(y)|\Phi^\lambda(X^*) = \Phi^\lambda(x)\right) \leq e^{-\beta} - \varepsilon \right\}. \]

Here \( \beta := H(Y^*|\Phi^{\lambda_1}(X^*)) \) is the conditional entropy of \((\Phi^{\lambda_1}(X^*), Y^*)\).

Then, we have

\[ \arg\min_{\lambda \in \Lambda} R^I(\lambda) \subset \arg\min_{\lambda \in \Lambda} R^{a.a.d.}(p^{e,\lambda} \circ \Phi^\lambda). \]

**Theorem 3.3** (Effectiveness of Method II). Assume that (a), (b), (c) and the following condition (d)' hold:

(d)' \( \forall \lambda \) with \( \text{Im} \Phi^\lambda \neq \emptyset \), \( \exists e_\lambda \in \mathcal{E}_{ad} \) such that \( P\left(g(Y^*)|\Phi^\lambda(X^*)\right) \leq e^{-\beta_\lambda} - \varepsilon, P_{X^*,Y^*,-a.e}. \)

\[ \beta_\lambda := H(Y^*|\Phi^{\lambda_1}(X^*)) - \sum_{z^* \in \mathcal{Z}} \left\{ P(g(Y^*) = z^*) \times \int -\log p^{e,\lambda}(Y^*|\Phi^\lambda(X^*), g^{-1}(z^*)) dP_{X^*,Y^*}(Y^*) \right\}. \]

Then, we have

\[ \arg\min_{\lambda \in \Lambda} R^{II}(\lambda) \subset \arg\min_{\lambda \in \Lambda} R^{a.a.d.}(p^{e,\lambda} \circ \Phi^\lambda). \]

The assumptions (d) and (d)' mean that labeling rules on \( \mathcal{E}_{ad} \) and \( e^* \) are different due to a domain-specific factor (i.e., an \( X_2 \)-component). (d) and (d)' mean that, if \( \lambda \) fails to remove environment factors
(i.e., \( \text{Im } \Phi_2^\lambda \neq \emptyset \)), for some \( \epsilon_\lambda \in \mathcal{E}_{\text{ad}} \), either of the following two inequalities

\[
P(g(Y^e\lambda) = g(y)|\Phi^\lambda(X^e\lambda) = \Phi^\lambda(x)) \leq e^{-\beta} - \varepsilon
\]

\[
P(g(Y^e^\ast) = g(y)|\Phi^\lambda(X^e^\ast) = \Phi^\lambda(x)) \leq e^{-\beta_\lambda} - \varepsilon
\]

hold on a set of \((x, y)\) with probability 1 w.r.t. \(P(\Phi^\lambda(X^e\lambda), Y^e\lambda)\). Noting that \((\Phi^\lambda(X^e\lambda), Y^e\lambda)\) attaches a label \(z\) to \(\Phi^\lambda(x)\) such that \(P(g(Y^e\lambda) = z|\Phi^\lambda(X^e\lambda) = \Phi^\lambda(x))\) is large, the inequalities in (d) and (d)' mean that \(Y^e\lambda\) and \(Y^e^\ast\) attach different labels to the same \(x \in \mathcal{X}\) with high probability due to its \(X_2\)-component.

The theoretical analysis shows, while Method I is simpler than Method II, Method II is more applicable than Method I; that is because Method II eases the sufficient condition (d) for Method I to succeed. Noting that \(\beta \geq \beta_\lambda\) and hence, \(e^{-\beta} - \varepsilon \leq e^{-\beta_\lambda} - \varepsilon\), the condition (d)' is milder than (d). The fact implies that we can apply Method II even when labeling rules on \(\mathcal{E}_{\text{ad}}\) and \(e^*\) due to domain-specific factors are too similar to apply Method I.

We also show one of the sufficient conditions of \(e^*\) for there to exist \((X^e\lambda, Y^e\lambda)\) which satisfies the inequalities in (d) or (d)' for \(\forall \lambda\) with \(\text{Im } \Phi_2^\lambda \neq \emptyset\) in Appendix D.

4 Related work

Fine-tuning The proposed framework uses additional data from multiple domains as well as the training data for the target task so that it may be relevant to Transfer learning (TL) [22, 23, 24] and meta-learning [30, 41], which realize fast and accurate learning for a new target task based on a model pretrained with additional data sets or tasks. For example, after initial learning with a large data set, fine-tune [22, 23] re-trains the model with the target task, while frozen feature [24] fixes the pre-trained model and tunes a head network. Although they show advantages in many learning problems, they may not work effectively in the current setting; in the fine-tuning with the target task \((X^e^\ast, Y^e^\ast)\), the model tends to learn spurious correlation in the data set and does not generalize to o.o.d. domains. Some fine-tuning methods will be compared with the proposed approach experimentally in Section 5.

Domain adaptation by deep feature learning Domain adaptation strategies by deep feature learning [25, 26, 27, 31, 32] assume that we can access input data on a test domain in advance, and try to obtain data representation \(\Phi(X^e)\) that follows the same distribution for the training and test domains. While the strategies lead to high predictive performance on a test domain similar to a training domain, such \(\Phi\) does not function by discarding environmental factors from \(X^e \in \mathcal{X}\) as noted in [10]. Experimental comparisons will be shown in Section 5.

5 Experiments

We study the effectiveness of the proposed framework and CV methods through experiments, comparing them with several conventional methods: empirical risk minimization (ERM), fine-tuning methods, and
Table 1: Average Test Accuracies and SEs of Synthesized Data on $e = -e^*$ (5 runs): Oracle shows the results of the experiments with the first component. The best scores are **bolded**.

| Method          | $e = 1$ | $e = 3$ | $e = 10$ | $e = 15$ | $e = 20$ | $e = 30$ | $e = 40$ | $e = 45$ | $e = 50$ |
|-----------------|---------|---------|----------|----------|----------|----------|----------|----------|----------|
| Oracle          | 0.482 (0.113) | 0.789 (0.218) | 0.899 (0.000) | 0.906 (0.007) | 0.905 (0.004) | 0.904 (0.003) | 0.905 (0.002) | 0.905 (0.001) | 0.906 (0.001) |

Table 2: Comparison of Two CV methods. Average Test Accuracies and SEs of the estimates (10 runs). Best scores are **bolded**.

| Method      | $\lambda_{a(t)}$ = 10 | $\lambda_{a(t)}$ = 20 | $\lambda_{a(t)}$ = 30 | $\lambda_{a(t)}$ = 40 | $\lambda_{a(t)}$ = 50 |
|-------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|
| Oracle      | 0.529 (1.489)           | 0.556 (1.441)           | 0.568 (1.480)           | 0.581 (1.418)           | 0.560 (1.395)           |
| CV I        | 0.527 (1.522)           | 0.574 (0.889)           | 0.565 (0.889)           | 0.574 (0.792)           | 0.522 (1.103)           | 0.523 (1.102) | 0.482 (1.113) | 0.506 (1.155) | 0.430 (1.148) | 0.437 (1.157) | 0.502 (1.149) |
| CV II       | 0.527 (1.522)           | 0.574 (0.889)           | 0.565 (0.889)           | 0.574 (0.792)           | 0.522 (1.103)           | 0.523 (1.102) | 0.482 (1.113) | 0.506 (1.155) | 0.430 (1.148) | 0.437 (1.157) | 0.502 (1.149) |

Deep domain adaptation strategies. As fine-tuning methods, we employ two typical types of transfer learning: fine tune (FT) and frozen feature (FF) [22, 23, 24]. As a deep domain adaptation technique, we adopt the state-of-the-art method DSAN [31]. We also compare our two CV methods (CVI and CVII) with conventional CV methods: training-domain validation (Tr-CV) and leave-one-domain-out cross-validation (LOD-CV) [19]. We have two hyperparameters to be selected by CV. In the training with [4], we set $\lambda = 1$ when the training epoch is less than a certain threshold $t$, and $\lambda = \lambda_{a(t)}$ if the epoch is larger than $t$. From a set of candidates, each of the CV methods selects a pair $(t, \lambda_{a(t)})$. To know the best possible performance among the candidates, we also apply the test-domain validation (TDV) [19], which selects the hyperparameters with the unseen test domain. Note that TDV is not applicable in practical situations. The details on the experiments can be found in Appendix E.

**Synthesized Data 1** We compared the proposed method with the other approaches using synthesized data with $X = \mathbb{R}^2$, $Y = [3]$ and $Z = [2]$. We used distributions $N_0 := \mathcal{N}(0, 10^2) \times \mathcal{N}(e, 10^2)$, $N_1 := \mathcal{N}(30, 10^2) \times \mathcal{N}(-4e, 10^2)$ and $N_2 := \mathcal{N}(-30, 10^2) \times \mathcal{N}(-e, 10^2)$, where $\mathcal{N}(a,b)$ denotes a normal distribution with its (mean, variance) = $(a,b)$. Given $x \sim N_i$, the task is to predict $N_i$ among $i = 0, 1, 2$. The aim of IL is to ignore the second component of $x$, as it works as an environmental factor. Given $e^* \in \mathbb{N}_{\geq 0}$ ranging from 0 to 50, each experiment draws $D^e \sim P_{X^*, Y^*, Z^*}$ with its sample size $n^e = 2000$, and then predicts $Y^* - e^*$ from $X^* - e^*$. Setting $g$ by $g(0) = 0$ and $g(1) = g(2) = 1$, we draw $D^e_{ad} \sim P_{X^*, Z^*}$ from $\mathcal{E}_{ad} = \{ -100, -50, 0, 50, 100 \}$ with its sample size $n^e = 1000 \ (\forall e \in \mathcal{E}_{ad})$. We model $\Phi$ by a 3-layer neural net. Setting the maximum epoch 500, we select $(t, \lambda_{a(t)})$ from $3 \times 5$ candidates with $t \in \{0, 100, 200\}$ and $\lambda_{a(t)} \in \{10^0, 10^1, ..., 10^4\}$ by each of the CV methods. Table 1 shows the test accuracy of the estimates for $e = -e^*$ over 2000 random samples $(x, y) \sim P_{X^*, Y^*, Z^*}$. When $e^* = 0$ and 5, the environmental bias of training ($e^*$) are similar to the one of test ($-e^*$), and hence, the fine-tuning methods yield high performances, which may use spurious correlation. As $e^*$ increases, the difference between the training ($e^*$) and test ($-e^*$) distributions becomes larger, and the previous methods fail to achieve high accuracy. The proposed methods (Ours) keep higher performance than the others even for large $e^*$. Among the CV methods, our two methods (CVI, CVII) significantly outperform the others for larger $e^*$. For this data set, CVI and CVII show almost the same performance.
Table 3: Average Test Accuracies and SEs of Hierarchical Colored MNIST (5runs). TDV selects $\lambda$ which yields the highest performance on $e = 0.9$. Best scores are **bolded**.

|                  | $e = 0.1$       | $e = 0.9$       |
|------------------|----------------|----------------|
| **Best possible**| .800           | ...            |
| Oracle (grayscale)| .780 (.002)   |                |
| ERM              | .796 (.000)    | .177 (.006)    |
| FT               | **.800 (.001)**| .201 (.004)    |
| FE               | .796 (.001)    | .200 (.007)    |
| DSAN             | .789 (.004)    | .091 (.005)    |
| Ours +Our CV I   | .773 (.003)    | .644 (.011)    |
| Ours +Our CV II  | .745 (.008)    | **.707 (.012)**|
| Ours +Tr-CV      | .794 (.004)    | .541 (.007)    |
| Ours +LOD CV     | .338 (.048)    | .334 (.029)    |
| Ours +TDV        | .738 (.018)    | .732 (.008)    |

Table 4: Means and SEs of $\{\text{(Accuracy of TDV on } e = 0.9) - \text{(Accuracy of Each CV on } e = 0.9)\}$ (5runs). Lowest errors are **bolded**.

| CVI | CVII | Tr-CV | LOD-CV |
|-----|------|-------|--------|
| .088 (.004) | **.025 (.006)** | .191 (.019) | -.398 (.025) |

**Synthesized Data 2** To highlight the difference of the proposed CVI and CVII, we compare them regarding the difference between domains $E_{\text{ad}}$ and $e^*$. We used synthesized data with $X = \mathbb{R}^2$, $Y = [10]$ and $Z := [2]$, preparing ten distributions $\{N_i\}_{i=1}^{10}$ on $\mathbb{R}^2$, which include an environmental bias in the second component depending $e \in Z$ (see Appendix E.1 for explicit representations of $\{N_i\}_{i=1}^{10}$). The task is to predict $N_i$ ($i = 1, \ldots, 10$) for $x \sim N_i$. Setting $e^* := 20$ with $n^* = 60000$, the test task is to predict the label for domain $e = -20$. Regarding the task with label of higher level, we use $g(y) = 0$ if $y$ is odd and $g(y) = 0$ if $y$ is even. We draw $D_{e^*} \sim P_{X^*,Z^*} (n^* = 20000)$ from $E_{\text{ad}} = \{e_{\text{ad}}, 40\}$, where $e_{\text{ad}}$ ranges from $-9$ to $1$. As $e_{\text{ad}}$ increases, the domains $E_{\text{ad}}$ approach to $e^*$, and thus the labeling rule on $E_{\text{ad}}$ becomes similar to one of $e^*$. The model $\Phi$ is a 3-layer neural net. We set the maximum epoch 500, and select the hyperparameter $(t, \lambda_{\text{after}})$ from 4 candidates with $t \in \{0\}$ and $\lambda_{\text{after}} \in \{0, 0.001, 0.01, 100\}$ by each CV method. Table 2 shows the test accuracy of the estimates for $e = -e^*$ over 2000 random samples $(x, y) \sim P_{X^{e^*}, Y^{e^*}}$. The results show that, while CVI fails to select optimal hyperparameters as $e$ increases, CVII keeps higher performance, which accords with the theoretical implication in Section 3.4.

**Hierarchical Colored MNIST** We apply our framework to *Hierarchical Colored MNIST*, which is an extended version of Colored MNIST [10] with $Y = [3]$ and $Z := [2]$. We aim to predict $Y^e$ from digit image data $X^e$, which is in the three categories $0 - 2$ ($y = 0$), $3$ or $4$ ($y = 1$) and $5 - 9$ ($y = 2$). The label is changed randomly to one of the rest with a probability of $20\%$, which is denoted by $\hat{y}$. The environment $e$ controls the color of the digit; for $\hat{y} = 0, 1$, the digit is colored in red with probability $e$ and for $\hat{y} = 2$ colored in green with probability $1 - e$. In the experiment, $D^{e^*} \sim P_{X^{e^*}, Y^{e^*}}$ is drawn with sample size
Fig 1: Visualization of Bird recognition problem

Table 5: Average Test Accuracies and SEs of Bird recognition problem (5 runs). Oracle shows a result of ERM with samples from both $e_1$ and $e_2$ given. TDV selects $\lambda$ which yields the highest performance on $e_2$. Best scores are bolded.

|                      | Test Acc. on $e_1$ | Test Acc. on $e_2$ |
|----------------------|--------------------|--------------------|
| Oracle               | .875 (.018)        |                    |
| ERM                  | .902 (.008)        | .317 (.044)        |
| FT                   | .909 (.012)        | .364 (.028)        |
| FE                   | .767 (.024)        | .052 (.013)        |
| Ours +Our CV I       | .897 (.020)        | .727 (.062)        |
| Ours +Our CV II      | .897 (.020)        | .727 (.062)        |
| Ours +Tri-CV         | .919 (.006)        | .651 (.031)        |
| Ours +LOD CV         | .338 (.048)        | .334 (.029)        |
| Ours +TDV            | .886 (.035)        | .782 (.020)        |

$n^e = 5000$, and $Y^e$ is predicted based on $X^e$ for $e = 0.1$ and 0.9. Regarding $Z^e$, we consider the task where we predict $z = 0$ for $X^e$ in 0–2 and $z = 1$ for 3–9 (that is, $g(0) = 0$ and $g(1) = g(2) = 1$). We obtain the final label $\hat{z}$ by flipping $z$ with 20%. As the environment factor, we color the digit red for $\hat{z} = 0$ with probability $e$ and green for $\hat{z} = 1$ with probability $1 - e$. We set $E_{ad} = \{0.1, 0.3, 0.5, 0.7, 0.9\}$ with $n^e = 5000$ for $\forall e \in E_{ad}$. We model $\Phi$ by a 3-layer neural net. With the maximum epoch 500, we select $(t, \lambda_{after})$ from $3 \times 10$ candidates with $t \in \{0, 100, 200\}, \lambda_{after} \in \{10^0, 10^1, ..., 10^9\}$ by each CV method. Table 3 shows test accuracies for 2000 random samples in the environment $e = 0.1$ and $e = 0.9$. The results, together with Appendix E.3, demonstrate that the proposed methods significantly outperform the others for $e = 0.9$. Among the two proposed methods, CV II yields the higher test accuracy. Table 4 shows the difference between accuracies by TDV and each CV for the same data set with $e = 0.9$. The results, together with Appendix E.3, verify that CVII selects preferable hyperparameters with smaller errors.
Bird recognition  

Our method is applied to the Bird recognition problem \cite{28}, which aims to predict three labels $Y^e$ of images $X^e$: waterbird ($Y^e = 0$), landbird ($Y^e = 1$) and no bird ($Y^e = 2$). The dataset is made by combining background images from the Places dataset \cite{39} and bird images from the CUB dataset \cite{38} in two different ways $E := \{e_1, e_2\}$. In domain $e_1$, we prepare three types of image: landbird image with land background, waterbird image with water background, and no bird with land background (Figure 1 left). In domain $e_2$, we have landbird images with water background, waterbird images with land background, and no bird with water background (Figure 1 right). For the sample of the target task, we used the domain $e^* = e_1$ and generated $n^* = 8649$ data $D^{e^*} \sim P_{X^e, Y^e}$. The sample in the higher level $D^{e}_ad$ of $(X^e, Z^e)$, whose label is landbird ($Z^e = 0$) and no landbird ($Z^e = 1$) (i.e., $g(1) = 0$ and $g(0) = g(2) = 1$), is drawn from both $e_1$ and $e_2$ with $n^{e_1} = n^{e_2} = 8649$. Here, we use $D^{e^*}$ as $D^{e}_ad$ with labels of $D^{e^*}$ re-annotated by $g$. We made a predictor of $Y^e$ based on $X^e$, and evaluated the test accuracy in the two domains $e = e_1, e_2$. We model $\Phi$ by ResNet50 \cite{29}. Setting the maximum epoch 5, we select $(t, \lambda_{after})$ from $5 \times 5$ candidates with $t \in [5], \lambda_{after} \in \{10^0, 10^1, ..., 10^4\}$ by each CV method. Table 1 shows test accuracies with 2162 random samples for $e_1$ and $e_2$. We can see that the proposed framework together with CV methods succeeded in capturing the predictor invariant to the change of background, while the other methods failed. ERM and FT show much higher accuracy for $e_1$ than Oracle and worst results for $e_2$, which implies that these methods learn spurious correlation in $D^{e^*}$.

6 Conclusion

We have proposed a new framework of invariance learning – assuming the availability of datasets for another task in higher label hierarchy, we obtain an invariant predictor for the target classification task using training data in a single domain with the help of the multiple data sets for the higher task. This framework mitigates the difficulty of annotating many labels for the target task. Additionally, we have proposed two CV methods for hyperparameter selection, which has been an outstanding problem of previous methods for invariant learning. Theoretical analysis has revealed that our methods select hyperparameter correctly under some settings. The experimental results on synthesized and object recognition tasks have demonstrated the effectiveness of the proposed framework and CV methods.

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A Proof of Theorem 3.1

\[ R^{(X,Y)}(p_\theta \circ \Phi) - R^{(X,g(Y))}(p_\theta \circ \Phi) = \int - \log p_\theta(Y|\Phi(X)) dP_{Y,\Phi(X)} + \int \log p_\theta(g(Y)|\Phi(X)) dP_{g(Y),\Phi(X)} \]

\[ = - \int \log \frac{p_\theta(Y|\Phi(X))}{p_\theta(g(Y)|\Phi(X))} dP_{Y,\Phi(X)} \]

\[ = - \int dP_{g(Y)} \int \log \frac{p_\theta(Y|\Phi(X))}{p_\theta(g(Y)|\Phi(X))} dP_{Y,\Phi(X)|g(Y)} \quad (6) \]

By the definition of \( p_\theta(y|\Phi(x), Y \in g^{-1}(z)) \) in Theorem 3.1, \( \frac{p_\theta(y|\Phi(x))}{p_\theta(g(y)|\Phi(x))} = p_\theta(y|\Phi(x), Y \in g^{-1}(z)) \) holds, where \( z = g(y) \). Therefore, we obtain

\[ [6] = - \int dP_{g(Y)} \int \log \frac{p_\theta(Y|\Phi(X))}{p_\theta(g(Y)|\Phi(X))} dP_{Y,\Phi(X)|g(Y)} \]

\[ = - \int dP_{g(Y)} \int \log p_\theta(Y|\Phi(X), Y = g(Y)) dP_{Y,\Phi(X)|g(Y)} \]

\[ = - \sum_{z \in Z} P(g(Y) = z) \int \log p_\theta(Y|\Phi(X), Y \in g^{-1}(z)) dP_{Y,\Phi(X)|g(Y) = z} \]

\[ = - \sum_{z \in Z^\Phi} P(g(Y) = z) \int \log p_\theta(Y|\Phi(X), Y \in g^{-1}(z)) dP_{Y,\Phi(X)|g(Y) = z} \quad (7) \]

Noting that, for all \( z^- \notin Z^\Phi \) and \( y := g^{-1}(z^-) \), \( p_\theta(y|\Phi(x), Y \in g^{-1}(z^-)) = 1 \) holds, we can see that \( \log p_\theta(y, |\Phi(x), Y = g^{-1}(z^-)) = 0 \). It leads us to the equality \( \sum_{z^- \notin Z^\Phi} P(g(Y) = z^-) \int \log p_\theta(Y|\Phi(X), Y \in g(z^-)) dP_{Y,\Phi(X)|g(Y) = z^-} = 0 \), which concludes the proof. \( \square \)

B Proof of Theorem 3.2

We restate Theorem 3.2 with some notation arrangements.

**Theorem B.1.** Let \( X := X_1 \times X_2 \) where \( X_1 := \mathbb{R}^{n_1} \) and \( X_2 := \mathbb{R}^{n_2} \) with \( n_1, n_2 \in \mathbb{N} \). For any random variable \( X \) on \( \mathcal{X} \), \( X_1 \) and \( X_2 \) denote its \( X_1 \)- and \( X_2 \)-component of \( X \), respectively. Assume that, for \( \lambda \in \Lambda \), there corresponds a projection \( \Phi^\lambda : \mathcal{X} \to \mathbb{R}^{n_\lambda} \) \((n_\lambda \leq n_1 + n_2)\). \( \Phi_1^\lambda \) and \( \Phi_2^\lambda \) denote the \( X_1 \) and \( X_2 \)-components of \( \Phi^\lambda \). For \( i = 1, 2 \), if \( \Phi^\lambda \) does not have an \( X_i \)-component, we denote \( \text{Im} \Phi_i^\lambda = \emptyset \). \( \Phi(X), \Phi(X)_1, \Phi(X)_2 \) are abbreviated by \( X^\lambda, X^\lambda_1, X^\lambda_2 \), respectively. Fixing a random variable \( (X^\lambda_1, Y^I) \)

\(^1\)\( z^- \notin Z^\Phi \) implies that \(|g^{-1}(z^-)| = 1 \) and therefore, \( g^{-1}(z^-) \) is determined uniquely. Note that there is no chance that \(|g^{-1}(z^-)| = 0 \) by the surjectivity of \( g \).
on $X_1 \times Y$, set

$$T_{all} := \left\{ (X,Y) : \text{random variable on } X \times Y \bigg| P_{Y|X_1} = P_{Y'|X_1} \right\}.$$ 

Fix $(X^*, Y^*) \in T_{all}$ and $T_{ad} \subset T_{all}$. For $\lambda \in \Lambda$, $p^{*\lambda} : \mathbb{R}^{n_x} \to \mathcal{P}_Y$ denotes the conditional probability density function of $P(Y^*|\Phi^{\lambda}(X^*)) = P(Y^*|X^*\lambda)$. For $\lambda \in \Lambda$, define $R^{o.o.d.}(\lambda)$ and $R^I(\lambda)$ by

$$R^{\text{o.o.d.}}(\lambda) := \max_{(X,Y) \in T_{all}} R^{(X,Y)}(p^{*\lambda} \circ \Phi^{\lambda}),$$

$$R^I(\lambda) := \max \left\{ \max_{(X,Y) \in T_{ad}} R^{(X,Y)}(p^{*\lambda} \circ \Phi^{\lambda}), R^{(X^*,Y^*)}(p^{*\lambda} \circ \Phi^{\lambda}) \right\}$$

respectively. Assume that the following two conditions hold:

(I) $\exists \lambda^I \in \Lambda$ s.t. $\Phi^{\lambda^I} = \Phi^{X_1}$.

(II) For sufficiently small $\varepsilon \ll 1$, the following statement holds:

$$\forall \lambda \text{ with } \text{Im}\Phi^{\lambda} \neq \emptyset, \text{ there exists } (X^{e_1}, Y^{e_2}) \text{ such that } P(g(Y^*)|X^{e_1}) \leq e^{-\beta} - \varepsilon \text{ holds } P_{X^{e_1}, Y^{e_2}} - \text{almost everywhere.}$$

Then, $\text{argmin}_{\lambda \in \Lambda} R^I(\lambda) \subset \text{argmin}_{\lambda \in \Lambda} R^{\text{o.o.d.}}(\lambda)$ holds.

$T_{all}$, $T_{ad}$ and $(X^*, Y^*)$ correspond to $\{(X^e, Y^e)\}_{e \in E}, \{(X^e, Y^e)\}_{e \in E_{ad}}$ and $(X^e, Y^e)$ in Theorem 3.2 respectively. (a) and (b) in Theorem 3.2 are represented by the construction of $T_{all}$. (c) and (d) in Theorem 3.2 are represented by (I) and (II) respectively.

To prove Theorem B.1, we prepare three lemmas. In the lemmas, notations are same as in Theorem B.1 and conditions (I) and (II) in Theorem B.1 are also imposed on.

**Lemma B.2.** $\lambda^I \in \text{argmin}_{\lambda \in \Lambda} R^{\text{o.o.d.}}(\lambda)$.

**Lemma B.3.** Assume that $\hat{\lambda} \in \text{argmin}_{\lambda \in \Lambda} R^I(\lambda)$. Then $\text{Im}\Phi^\lambda_2 = \emptyset$.

**Lemma B.4.** If $\hat{\lambda} \in \Lambda$ satisfies $\text{Im}\Phi^\lambda_2 = \emptyset$, $R^I(\hat{\lambda}) = R^{\text{o.o.d.}}(\hat{\lambda})$.

Before proving the above lemmas, we prove Theorem B.1 suppose that they hold.

**proof of Theorem B.1**

Take $\hat{\lambda} \in \text{argmin}_{\lambda \in \Lambda} R^I(\lambda)$. Then, $\text{Im}\Phi^\lambda_2 = \emptyset$ holds by Lemma B.3 and therefore, $R^I(\hat{\lambda}) = R^{\text{o.o.d.}}(\hat{\lambda})$ holds by Lemma B.4. Moreover, $R^{\text{o.o.d.}}(\hat{\lambda}) \geq R^{\text{o.o.d.}}(\lambda^I)$ holds by Lemma B.2 and $R^{\text{o.o.d.}}(\lambda^I) = R^I(\lambda^I)$ holds by B.4. By the assumption $\hat{\lambda} \in \text{argmin}_{\lambda \in \Lambda} R^I(\lambda^I)$, $R^I(\lambda^I) \geq R^I(\hat{\lambda})$ holds. Arranging these inequalities, we obtain

$$R^I(\hat{\lambda}) = R^{\text{o.o.d.}}(\hat{\lambda}) \geq R^{\text{o.o.d.}}(\lambda^I) = R^I(\lambda^I) \geq R^I(\hat{\lambda}).$$  \hspace{1cm} (9)

Since the left and right ends of (9) are connected by the same value $R^I(\hat{\lambda})$, the inequalities in (9) must be equalities. Hence, we obtain the equality $R^{\text{o.o.d.}}(\hat{\lambda}) = R^{\text{o.o.d.}}(\lambda^I)$. By the minimality of $\lambda^I$ (Lemma

\footnote{Note that, since $\Phi^{\lambda^I}$ is the projection onto $X_1$, $\text{Im}\Phi^{\lambda^I}_2 = \emptyset$.}
Let us prove the contraposition of Lemma B.3. Take \( \hat{\lambda} \in \arg\min \mathcal{R}^{\lambda} \) and \( (\tilde{X},\tilde{Y}) \in T_{all} \) such that \( \int -\log p_{\hat{\lambda}}(\tilde{Y} | \Phi(\tilde{X})) dP_{\tilde{X},\tilde{Y}} \geq \int -\log p_{\hat{\lambda}}(Y | \Phi(\hat{\lambda} \hat{X})) dP_{\hat{X},\hat{Y}} \). Take \( (\hat{X},\hat{Y}) \in T_{all} \) such that its distribution is \( P_{X_1',Y_1'} \times P_{X_2} \). Here, \( P_{X_2} \) denotes a marginal distribution of \( (\hat{X},\hat{Y}) \in T_{all} \) on \( X_2 \) and \( P_{X_1',Y_1'} \times P_{X_2} \) denotes the product of \( P_{X_1',Y_1'} \) and \( P_{X_2} \).

\[
\int -\log p_{\hat{\lambda}}(\tilde{Y} | \Phi(\tilde{X})) dP_{\tilde{X},\tilde{Y}} = \int -\log p_{\hat{\lambda}}(Y | \Phi(\hat{\lambda} \hat{X})) dP_{\hat{X},\hat{Y}} = \int dP_{X_2} \int -\log p_{\hat{\lambda}}(Y | \Phi(\hat{\lambda} \hat{X})) dP_{\hat{X},\hat{Y}} \tag{10}
\]

Note that, for \( \forall x \in \text{Im} \Phi(\hat{\lambda}) \), \( \int -\log p_{\hat{\lambda}}(Y | X_1',X_2') = x_2' \) holds since a minimum of the cross entropy loss is attained if and only if \( p_\theta \) corresponds to the conditional distribution function \( p_{\hat{\lambda}}(Y|X_1') \) of \( P_{Y'|X_1'} \). Therefore, we can see that

\[
\int -\log p_{\hat{\lambda}}(Y | \Phi(\hat{\lambda} \hat{X})) dP_{\hat{X},\hat{Y}} \geq \int dP_{X_2} \int -\log p_{\hat{\lambda}}(Y | X_1') dP_{X_1',Y_1'} \tag{10}
\]

and therefore, it concludes the proof. Here, the first equality holds because \( -\log p_{\hat{\lambda}}(Y | X_1') \) is not affected by \( X_2 \).

Let us prove the contraposition of Lemma B.3. Take \( \hat{\lambda} \in \Lambda \) with \( \text{Im} \Phi(\hat{\lambda}) \neq \emptyset \). To prove that \( \hat{\lambda} \notin \arg\min \mathcal{R} \), we may prove that \( \mathcal{R} (\hat{\lambda}) > \mathcal{R} (\lambda') \) since \( \lambda' \in \Lambda \) (Assumption (I) in the statement). To show this, it suffices to prove the following statement:

\[
\exists (\hat{X},\hat{Y}) \in T_{ad} \ s.t. \ \int -\log p_{\hat{\lambda}}(g(\hat{Y}) | \hat{X}) dP_{\hat{X},g(\hat{Y})} > \mathcal{R} (\lambda'). \tag{11}
\]

From Condition (II), we can take \((X_2',Y_2') \in T_{ad} \) such that the following statement holds:

\[
\exists (\hat{X},\hat{Y}) \in T_{ad} \ s.t. \ \int -\log p_{\hat{\lambda}}(g(\hat{Y}) | \hat{X}) dP_{\hat{X},g(\hat{Y})} > \mathcal{R} (\lambda'). \tag{11}
\]
\[ P(g(Y^*)|X^{*,\hat{\lambda}}) \leq e^{-\beta} - \varepsilon \text{ holds } P_{X^{*,\delta},Y^{*,\lambda}} - \text{almost everywhere.} \]

Before proving (11), we prepare one supplementary inequality:

**Supplementary Inequality**

\[ \int -\log p^{*,\hat{\lambda}}(g(Y^{e_{\hat{\lambda}}})|X^{e_{\hat{\lambda}},\hat{\lambda}})dP_{X^{*,\delta},g(Y^{*,\lambda})} \geq -\log \{e^{-\beta} - \varepsilon\}. \]

To prove the inequality, note that \( P_{X^{*,\delta},g(Y^{*,\lambda})}(A) = 0 \), where

\[ A := \{(x, y) \in X \times Y \mid P(g(Y^*) = g(y)|X^{*,\hat{\lambda}} = \Phi_{\lambda}^\lambda(x)) > e^{-\beta} - \varepsilon\} \]

since \( P(g(Y^*)|X^{*,\hat{\lambda}}) \leq e^{-\beta} - \varepsilon \) holds \( P_{X^{*,\delta},Y^{*,\lambda}} - \text{almost everywhere} \) holds.

Therefore, we can see that

\[ \int -\log p^{*,\hat{\lambda}}(g(Y^{e_{\hat{\lambda}}})|X^{e_{\hat{\lambda}},\hat{\lambda}})dP_{X^{*,\delta},g(Y^{*,\lambda})} = \int_{X\times Y-A} -\log p^{*,\hat{\lambda}}(g(Y^{e_{\hat{\lambda}}})|X^{e_{\hat{\lambda}},\hat{\lambda}})dP_{X^{*,\delta},g(Y^{*,\lambda})} \]

. Note that for any \((x, y) \in X \times Y - A\), \( -\log p^{*,\hat{\lambda}}(g(y)|x^{\hat{\lambda}}) \geq e^{-\beta} - \varepsilon\); indeed, since

\[ X \times Y - A = \{(x, y) \in X \times Y \mid P(g(Y^*) = g(y)|X^{*,\hat{\lambda}} = \Phi_{\lambda}^\lambda(x)) \leq e^{-\beta} - \varepsilon\} \],

for any \((x, y) \in X \times Y - A\),

\[ -\log p^{*,\hat{\lambda}}(g(y)|x^{\hat{\lambda}}) = -\log P(g(Y^*) = g(y)|X^{*,\hat{\lambda}} = \Phi_{\lambda}^\lambda(x)) \geq -\log \{e^{-\beta} - \varepsilon\}. \]

Then, we obtain

\[ \int -\log p^{*,\hat{\lambda}}(g(Y^{e_{\hat{\lambda}}})|X^{e_{\hat{\lambda}},\hat{\lambda}})dP_{X^{*,\delta},g(Y^{*,\lambda})} = \int_{X\times Y-A} -\log p^{*,\hat{\lambda}}(g(Y^{e_{\hat{\lambda}}})|X^{e_{\hat{\lambda}},\hat{\lambda}})dP_{X^{*,\delta},g(Y^{*,\lambda})} \]

\[ \geq -\log \{e^{-\beta} - \varepsilon\}. \]

**Proof of Inequality (11).**

\[ \int -\log p^{*,\hat{\lambda}}(g(Y^{e_{\hat{\lambda}}})|X^{e_{\hat{\lambda}},\hat{\lambda}})dP_{X^{*,\delta},g(Y^{*,\lambda})} \geq -\log \{e^{-\beta} - \varepsilon\} > -\log \{e^{-\beta}\} = \beta = H(Y^*|X^*_1) \] (12)

Note that \( H(Y^*|X^*_1) = \mathcal{R}^{o.o.d.}(\lambda^f) \); indeed,

\[ \mathcal{R}^{o.o.d.}(\lambda^f) = \max_{(X,Y) \in \mathcal{T}_{od}} \mathcal{R}^{(X,Y)}(p^{*,\lambda^f} \circ \Phi^\lambda) = \max_{(X,Y) \in \mathcal{T}_{od}} \int -\log p^{*,\lambda^f}(Y|\Phi^\lambda(X))dP_{X,Y} \]

\[ = \max_{(X,Y) \in \mathcal{T}_{od}} \int -\log p^{*,\lambda^f}(Y|\Phi^\lambda(X))dP_{\Phi^\lambda(X),Y} \]

\[ = \max_{(X,Y) \in \mathcal{T}_{od}} \int -\log p^{*,\lambda^f}(Y|X_1)dP_{X_1,Y}. \] (13)
Noting that \( P_{X_1,Y} = P_{X_1^*,Y^*} = P_{X_1,Y^*} \) for any \((X,Y) \in T_{all}\) and \(p^{*,\lambda'}\) coincides with the conditional probability density function of \( P_{Y^*|X_1^*}\), we can see that

\[
\mathbb{I}_3 = \int -\log p^{*,\lambda'}(Y^*|X_1^*)dP_{X_1^*,Y^*} = H(Y^*|X_1^*).
\]

Hence, we can derive \( \int -\log p^{*,\lambda}(g(Y^*)|X_1^*,\lambda)dP_{X_1^*,Y^*,\lambda} > H(Y^*|X_1^*) = \mathcal{R}^{o.o.d.}(\lambda') \), which concludes the proof. □

**proof of Lemma B.4**

Take \( \lambda \in \Lambda \) that satisfies \( \text{Im}\Phi_2 = \emptyset \). Then, \( P_{\phi(X,Y)} = P_{\phi(X,Y),Y^*} \) holds for \( \forall (X,Y) \in T_{all} \) because of \( P_{X_1,Y} = P_{X_1^*,Y^*} \), and therefore, \( \mathcal{R}^{(X,g(Y))}(p^{*,\lambda} \circ \Phi) = \mathcal{R}^{(X,g(Y))}(p^{*,\lambda} \circ \Phi'_{\Lambda}) \) and \( \mathcal{R}^{(X,Y^*)}(p^{*,\lambda} \circ \Phi) = \mathcal{R}^{(X,Y^*)}(p^{*,\lambda} \circ \Phi'_{\Lambda}) \) hold. These two equalities lead the following equality:

\[
\mathcal{R}^{(X,I)}(p^{*,\lambda} \circ \Phi) = \max \left\{ \max_{(X,Y) \in T_{all}} \mathcal{R}^{(X,g(Y))}(p^{*,\lambda} \circ \Phi), \mathcal{R}^{(X,Y^*)}(p^{*,\lambda} \circ \Phi) \right\}
\]

By Theorem 3.1

\[
\mathcal{R}^{(X,I)}(p^{*,\lambda} \circ \Phi) = \mathcal{R}^{(X,g(Y))}(p^{*,\lambda} \circ \Phi) + \sum_{z^* \in \mathbb{Z}^d} P(Y^* = g^{-1}(z^*)) \int -\log p^{*,\lambda}(Y^*|\Phi(X),Y^* \in g^{-1}(z^*)) dP_{X,Y^*}
\]

\[
\geq \mathcal{R}^{(X,g(Y))}(p^{*,\lambda} \circ \Phi')
\]

holds and therefore, \( \mathbb{I}_4 = \mathcal{R}^{(X,I)}(p^{*,\lambda} \circ \Phi) \). Since \( P_{\phi(X),Y} \) are the same for \( T_{all} \),

\[
\mathcal{R}^{(X,I)}(p^{*,\lambda} \circ \Phi) = \max_{(X,Y) \in T_{all}} \mathcal{R}^{(X,Y)}(p^{*,\lambda} \circ \Phi) = \mathcal{R}^{o.o.d.}(p^{*,\lambda} \circ \Phi)
\]

which concludes the proof.

**C Proof of Theorem 3.3**

**Theorem C.1.** Notations are same as in the statement of Theorem B.4 Define \( \mathcal{R}_{II}(\lambda) \) by

\[
\mathcal{R}_{II}(\lambda) := \max_{(X,Y) \in T_{all} \setminus \{(X^*,Y^*)\}} \left\{ \mathcal{R}^{(X,g(Y))}(p^{*,\lambda} \circ \Phi_{\lambda}) + \sum_{z^* \in \mathbb{Z}^d} \left\{ P(g(Y) = z^*) \right\} \int -\log p^{*,\lambda}(Y^*|X^*\lambda, Y^* \in g^{-1}(z^*)) dP_{X^*,Y^*}|Y^* \in g^{-1}(z^*) \right\}
\]

In addition to the condition (I), the following condition (II) hold:
(II) For a sufficiently small $\varepsilon \ll 1$, the following statement holds:

\[\forall \lambda \in \Lambda \text{ with } \text{Im}\Phi^\lambda_2 \neq \emptyset, \text{ there exists } (X^{\varepsilon_\lambda}, Y^{\varepsilon_\lambda}) \text{ such that } P(g(Y^*)|X^{*,\lambda}) \leq e^{-\beta_\lambda} - \varepsilon \text{ holds } P_{X^{\varepsilon_\lambda}, Y^{\varepsilon_\lambda}}\text{-almost everywhere.} \]

Here,

\[\beta_\lambda := H(Y^*|X_1^*) - \sum_{z^{*\varepsilon} \in \mathcal{Z}} \left\{ P(g(Y^*) = z^{*\varepsilon}) \cdot \int -\log p^{*,\lambda}(Y^*|X^{*,\lambda}, Y^* \in g^{-1}(z^{*\varepsilon}))dP_{X^*, Y^*}|Y^* \in g^{-1}(z^{*\varepsilon}) \right\}. \]

Then, \(\arg\min_{\lambda \in \Lambda_{\varepsilon}} R^{II}(\lambda) \subset \arg\min_{\lambda \in \Lambda_{\varepsilon}} R^{o.o.d.}(\lambda)\).

**Lemma C.2.** Assume that \(\hat{\lambda} \in \arg\min_{\lambda \in \Lambda_{\varepsilon}} R^{II}(\lambda)\). Then \(\text{Im}\Phi^\lambda_2 = \emptyset\).

**Lemma C.3.** If \(\hat{\lambda} \in \Lambda\) satisfies \(\text{Im}\Phi^\lambda_2 = \emptyset\), \(R^{II}(\hat{\lambda}) = R^{o.o.d.}(\hat{\lambda})\).

**proof of Theorem C.1**

Combining the above two lemmas and Lemma B.2, we can show the desired statement essentially the same as the one in the proof of Theorem C.1.

**proof of Lemma C.2**

Let us prove the contraposition of Lemma B.3. Take \(\hat{\lambda} \in \Lambda\) with \(\text{Im}\Phi^\lambda_2 \neq \emptyset\). To prove that \(\hat{\lambda} \notin \arg\min_{\lambda} R^{II}(\lambda)\), we may prove that \(R^{II}(\hat{\lambda}) > R^{II}(\lambda')\) since \(\lambda' \in \Lambda\) (Assumption (I) in the statement).

To show this, it suffices to prove the following statement:

\[
\exists (\hat{X}, \hat{Y}) \in T_{ad} \text{ s.t. } \\
\int -\log p^{*,\hat{\lambda}}(g(\hat{Y})|\hat{X}^{\hat{\lambda}})dP_{X^*g(\hat{Y})} + \sum_{z^{*\varepsilon} \in \mathcal{Z}} P(g(\hat{Y}) = z^{*\varepsilon}) \cdot \int -\log p^{*,\hat{\lambda}}(Y^*|X^{*,\lambda}, Y^* \in g^{-1}(z^{*\varepsilon}))dP_{X^*, Y^*}|Y^* \in g^{-1}(z^{*\varepsilon}) \\
> R^{II}(\lambda'). \quad (15)
\]

Take \((X^{\varepsilon_\lambda}, Y^{\varepsilon_\lambda}) \in T_{ad}\) such that the following statement holds:

\[P(g(Y^*)|X^{*,\hat{\lambda}}) \leq e^{-\beta_\hat{\lambda}} - \varepsilon \text{ holds } P_{X^{\varepsilon_\lambda}, Y^{\varepsilon_\lambda}}\text{-almost everywhere.}\]

Before proving (15), we prepare one supplementary inequality:

**Supplementary Inequality**

\[
\int -\log p^{*,\hat{\lambda}}(g(Y^{\varepsilon_\lambda})|X^{\varepsilon_\lambda}, Y^{\varepsilon_\lambda})dP_{X^{\varepsilon_\lambda}, g(Y^{\varepsilon_\lambda})} \geq -\log \left\{ e^{-\beta_\hat{\lambda}} - \varepsilon \right\}.
\]

We can prove the inequality same as in the proof of Lemma B.3 and therefore, omit the proof.

**Proof of Inequality (15).**

\[
\int -\log p^{*,\hat{\lambda}}(g(Y^{\varepsilon_\lambda})|X^{\varepsilon_\lambda}, Y^{\varepsilon_\lambda})dP_{X^{\varepsilon_\lambda}, g(Y^{\varepsilon_\lambda})} + \sum_{z^{*\varepsilon} \in \mathcal{Z}} P(g(Y^{\varepsilon_\lambda}) = z^{*\varepsilon}) \cdot \int -\log p^{*,\hat{\lambda}}(Y^*|X^{*,\lambda}, Y^* \in g^{-1}(z^{*\varepsilon}))dP_{X^*, Y^*}|Y^* \in g^{-1}(z^{*\varepsilon}) \\
\geq -\log \left\{ e^{-\beta_\hat{\lambda}} - \varepsilon \right\} + \sum_{z^{*\varepsilon} \in \mathcal{Z}} P(g(Y^{\varepsilon_\lambda}) = z^{*\varepsilon}) \cdot \int -\log p^{*,\hat{\lambda}}(Y^*|X^{*,\hat{\lambda}}, Y^* \in g^{-1}(z^{*\varepsilon}))dP_{X^*, Y^*}|Y^* \in g^{-1}(z^{*\varepsilon})
\]

22
\[
> - \log \{e^{-\beta\Lambda}\} + \sum_{\hat{z}^* \in \mathcal{Z}} P(g(\hat{z}^*) = \hat{z}^*) \cdot \int \log p_{\hat{z}^*}(Y|X^*,\hat{z}^*,Y^* \in g^{-1}(\hat{z}^*))dP(X^*,Y^*)|Y^* \in g^{-1}(\hat{z}^*)
\]
\[
= \beta\Lambda + \sum_{\hat{z}^* \in \mathcal{Z}} P(g(\hat{z}^*) = \hat{z}^*) \cdot \int \log p_{\hat{z}^*}(Y|X^*,\hat{z}^*,Y^* \in g^{-1}(\hat{z}^*))dP(X^*,Y^*)|Y^* \in g^{-1}(\hat{z}^*)
\]
\[
= H(Y^*|X^*_1) - \sum_{\hat{z}^* \in \mathcal{Z}} \left\{ P(g(\hat{z}^*) = \hat{z}^*) \cdot \int \log p_{\hat{z}^*}(Y|X^*,\hat{z}^*,Y^* \in g^{-1}(\hat{z}^*))dP(X^*,Y^*)|Y^* \in g^{-1}(\hat{z}^*) \right\}
\]
\[
+ \sum_{\hat{z}^* \in \mathcal{Z}} P(g(\hat{z}^*) = \hat{z}^*) \cdot \int \log p_{\hat{z}^*}(Y|X^*,\hat{z}^*,Y^* \in g^{-1}(\hat{z}^*))dP(X^*,Y^*)|Y^* \in g^{-1}(\hat{z}^*)
\]\[
(16)
\]
Since \(P_{X^*_1,g(Y^*)} = P_{X^*_1,g(Y^*)} = P_{X^*_1,g(Y^*)}\) holds by the construction of \(T_{all}\), we can see that \(P(g(\hat{z}^*) = \hat{z}^*) = P(g(\hat{z}^*) = \hat{z}^*)\) for any \(\hat{z}^* \in \mathcal{Z}\). Therefore, we obtain
\[
- \sum_{\hat{z}^* \in \mathcal{Z}} \left\{ P(g(\hat{z}^*) = \hat{z}^*) \cdot \int \log p_{\hat{z}^*}(Y|X^*,\hat{z}^*,Y^* \in g^{-1}(\hat{z}^*))dP(X^*,Y^*)|Y^* \in g^{-1}(\hat{z}^*) \right\}
\]
\[
+ \sum_{\hat{z}^* \in \mathcal{Z}} P(g(\hat{z}^*) = \hat{z}^*) \cdot \int - \log p_{\hat{z}^*}(Y|X^*,\hat{z}^*,Y^* \in g^{-1}(\hat{z}^*))dP(X^*,Y^*)|Y^* \in g^{-1}(\hat{z}^*) = 0.
\]
Hence, we can conclude \((16) = H(Y^*|X^*_1)\). Moreover, \(H(Y^*|X^*_1) = R^{o.o.d.}(\lambda^f)\); indeed,
\[
R^{o.o.d.}(\lambda_f) = \max_{(X,Y) \in T_{all}} R^{(X,Y)}(p_{\lambda^f} \circ \Phi^X) = \max_{(X,Y) \in T_{all}} \int - \log p_{\lambda^f}(Y|\Phi^X(X))dP_{X,Y}
\]
\[
= \max_{(X,Y) \in T_{all}} \int - \log p_{\lambda^f}(Y|\Phi^X(X))dP_{\Phi^X(X),Y}
\]
\[
= \max_{(X,Y) \in T_{all}} \int - \log p_{\lambda^f}(Y|X_1)dP_{X_1,Y}
\]\[
(17)
\]
Noting that \(P_{X_1,Y} = P_{X_1,Y^*} = P_{X_1,Y^*}\) for any \((X,Y) \in T_{all}\) and \(p_{\lambda^f}\) coincides with the conditional probability density function of \(P_{Y^*|X^*_1}\), we can see that
\[
(17) = \int - \log p_{\lambda^f}(Y^*|X^*_1)dP_{X_1,Y} = H(Y^*|X^*_1).
\]
Hence, we can derive \((16) = H(Y^*|X^*_1) = R^{o.o.d.}(\lambda^f)\), which concludes the proof. \(\square\)

**proof of Lemma C.3**

Take \(\hat{\lambda} \in \Lambda\) which satisfies \(\text{Im}\hat{\Phi}_2 = 0\). Since \(\text{Im}\hat{\Phi}_2 = 0\), \(P_{\Phi(X^*_1),Y} = P_{\Phi(X^*_1),Y^*}\) holds for \(\forall (X,Y) \in T_{all}\) because of the construction of \(T_{all}\). Therefore,
\[
R^{o.o.d.}(\hat{\lambda}) := \max_{(X,Y) \in T_{all}} R^{(X,Y)}(p_{\hat{\lambda}^\prime} \circ \Phi^X) = \max_{(X,Y) \in T_{all}} R^{(X,Y)}(p_{\hat{\lambda}^\prime} \circ \Phi^X)
\]
23
\[ \max_{(X,Y) \in T_{\text{all}} \cup \{(X^*,Y^*)\}} \left\{ R^{(X,g(Y))}(p^{*\lambda} \circ \Phi^{\lambda}) + \sum_{z^* \in \mathcal{Z}} \left( P(g(Y) = z^*) \int - \log p^{*\lambda}(Y|X^{*\lambda}, Y \in g^{-1}(z^*)) dP_{(X,Y)|Y \in g^{-1}(z^*)} \right) \right\} = \max_{(X,Y) \in T_{\text{all}} \cup \{(X^*,Y^*)\}} \left\{ R^{(X,g(Y))}(p^{*\lambda} \circ \Phi^{\lambda}) + \sum_{z^* \in \mathcal{Z}} \left( P(g(Y) = z^*) \int - \log p^{*\lambda}(Y|X^{*\lambda}, Y \in g^{-1}(z^*)) dP_{(X,Y)|Y \in g^{-1}(z^*)} \right) \right\} = R^{(X^*,Y^*)} \]

and therefore, it concludes the proof. Here, the third equality holds by Theorem 3.1; the first and forth equalities hold because of the fact that \( P_{\Phi(X^{*\lambda}),Y} = P_{\Phi(X^{*\lambda}),Y^*} \) holds for \( \forall (X,Y) \in T_{\text{all}}. \)

\section{Sufficient Conditions of \( e^* \) for there to exist \( (X^{e\lambda},Y^{e\lambda}) \) which satisfies (d) and (d)'}

\textbf{Theorem D.1.} Notations are same as in Theorem 3.1 and 4.1, \((X^*,Y^*)\) satisfies the following condition:

\begin{enumerate}[(A)]
    \item For a sufficiently small \( \varepsilon \ll 1 \), the following statement holds:
        \[ \forall \lambda \text{ with } \text{Im} \Phi_2^{\lambda} \neq \emptyset, \forall \alpha \in \text{Im} \Phi_1^{\lambda}, \forall b \in \mathcal{Y}, \exists c(\lambda,a,b) \text{ s.t. } P(Y^* = b|X_1^{*\lambda} = a, X_2^{*\lambda} = c) \geq (1 - e^{-\beta}) + \varepsilon. \]
\end{enumerate}

Then, \( \forall \lambda \text{ with } \text{Im} \Phi_2^{\lambda} \neq \emptyset, \) there exists \((X^{e\lambda},Y^{e\lambda})\) in \( T_{\text{all}} \) such that the inequality in (d) holds.

\textbf{Remark.} The condition (A) means that, in the environment \( e = e^* \), the affection of environmental factors (i.e., \( X_2 \)) to the response variable \( Y^{e^*} \) is large; indeed, the inequality in (A) means that, if \( \lambda \) fails to remove environment factors (i.e., \( \text{Im} \Phi_2^{\lambda} \neq \emptyset \)), we can control the probability of \( Y^{e^*} = b \) by the selection \( c \) for any \( b \in \mathcal{Y} \).

\textbf{Proof.} Fix \( \forall \lambda \text{ with } \text{Im} \Phi_2^{\lambda} \neq \emptyset. \) Take \((\tilde{X},\tilde{Y}) \in T_{\text{all}} \) such that its probability measure corresponds to \( \tilde{P}_{X_2|Y,X_1} \times P_{Y^*,X_1}, \) where \( \tilde{P}_{X_2|Y,X_1} \) is defined by, setting \( \hat{c}(\lambda,a,b) \) by

\[ \hat{c}(\lambda,a,b) \in \arg \min_{c \in \mathcal{X}_2} P(g(Y^*) = g(b)|X_1^{*\lambda} = \Phi_1^{\lambda}(a), X_2^{*\lambda} = \Phi_2^{\lambda}(c)), \]

\[ \tilde{P}_{X_2|Y=b,X_1=a} := \delta_{X_2=\hat{c}(\lambda,a,b)}. \] Here, for \( c \in \mathcal{X}_2, \) the probability measure \( \delta_{X_2=c} \) on \( \mathcal{X}_2 \) denotes a Dirac measure at \( c \in \mathcal{X}_2. \)

Before proving Theorem D.1, we prepare the following inequalities:

\textbf{Supplementary Inequality 1.}

\[ \forall a \in \mathcal{X}_1, \forall b \in \mathcal{Y}, P\left( g(Y^*) = g(b) \left| X_1^{*\lambda} = \Phi_1^{\lambda}(a), X_2^{*\lambda} = \Phi_2^{\lambda}(\hat{c}(\lambda,a,b)) \right. \right) \leq e^{-\beta} - \varepsilon. \]

\( ^4 \)c(\lambda,a,b) means \( c \in \mathcal{X}_2 \) is determined by given \( \lambda \in \Lambda, a \in \mathcal{X}_1, b \in \mathcal{Y}. \)
To see the fact, take $b^* \in \mathcal{Y}$ such that $g(b^*) \neq g(b)$\footnote{Such $b^*$ always exists by the following reason. Since $|\mathcal{Z}| \geq 2$ (which is imposed on in Chapter 2.1), we can take $\mathcal{Z} \ni z^* \neq g(b)$. By the surjectivity of $g$, $g^{-1}(z^*) \neq \emptyset$. Taking $b^* \in g^{-1}(z^*)$, $g(b^*) = z^* \neq g(b)$.}. Then, by the condition (ii) of Theorem 3.3 and $\text{Im} \Phi^\lambda_2 \neq \emptyset$, there exists $(\lambda, a, b) \in \mathcal{X}_2$ such that
\[
\left. P \left( Y^* = b^* \bigg| X_1^*, \hat{\lambda} = \Phi^\lambda_1(a), X_2^*, \hat{\lambda} = \Phi^\lambda_2(c(\lambda, a, b)) \right) \right\} \geq 1 - e^{-\beta} + \epsilon.
\]
Therefore,
\[
P \left( g(Y^*) = g(b) \bigg| X_1^*, \hat{\lambda} = \Phi^\lambda_1(a), X_2^*, \hat{\lambda} = \Phi^\lambda_2(c(\lambda, a, b)) \right)
\]
\[
= \min_{c \in \mathcal{X}_2} P \left( g(Y^*) = g(b) \bigg| X_1^*, \hat{\lambda} = \Phi^\lambda_1(a), X_2^*, \hat{\lambda} = \Phi^\lambda_2(c) \right)
\]
\[
\leq P \left( g(Y^*) = g(b) \bigg| X_1^*, \hat{\lambda} = \Phi^\lambda_1(a), X_2^*, \hat{\lambda} = \Phi^\lambda_2(c(\lambda, a, b)) \right)
\]
\[
\leq 1 - \sum_{\hat{\lambda} \neq g(b)} P \left( g(Y^*) = \hat{\lambda} \bigg| X_1^*, \hat{\lambda} = \Phi^\lambda_1(a), X_2^*, \hat{\lambda} = \Phi^\lambda_2(c(\lambda, a, b)) \right)
\]
\[
\leq 1 - \left( 1 - e^{-\beta} + \epsilon \right)
\]
\[
\leq e^{-\beta} - \epsilon.
\]

**Proof of Theorem D.1**
We may prove that $P_{X,Y}(A) = 1$ where
\[
\left\{ (x, y) \in \mathcal{X} \times \mathcal{Y} \bigg| P \left( g(Y^*) = g(b) \bigg| X_1^*, \hat{\lambda} = \Phi^\lambda(x) \right) \leq e^{-\beta} - \epsilon \right\}.
\]

Then,
\[
P_{X,Y}(A) = \int 1_A dP_{X,Y} = \int 1_A d(\tilde{P}_{X_2|Y,X_1} \times P_{Y^t,X_1})
\]
\[
= \int dP_{Y^t,X_1} \int 1_A d\tilde{P}_{X_2|Y,X_1} = \int dP_{Y^t,X_1}(x_1, y) \delta_{X_2 = \hat{c}(\lambda,x_1,y)}(A(x_1,y))
\]
holds where $A_{(x_1,y)} := \{ x_2 \in \mathcal{X}_2 | (x_1, x_2, y) \in \mathcal{X} \times \mathcal{Y} \}$. By the Supplementary Inequality 1, $\hat{c}(\lambda, x_1, y) \in A_{(x_1, y)}$ holds and therefore, $\delta_{X_2 = \hat{c}(\lambda,x_1,y)}(A(x_1,y)) = 1$, which leads us to the equation
\[
\int dP_{Y^t,X_1}(x_1, y) \delta_{X_2 = \hat{c}(\lambda,x_1,y)}(A(x_1,y)) = 1
\]
\[
\square
\]
Theorem D.2. Notations are same as in Theorem B.1 and C.1, 

\[(X^*, Y^*)\] satisfies the following condition:

\[(A)' \text{ For a sufficiently small } \epsilon \ll 1, \text{ the following statement holds:} \]
\[\forall \lambda \text{ with } \text{Im}\Phi_2^\lambda \neq \emptyset, \forall \alpha \in \text{Im}\Phi_1^\lambda, \forall b \in Y, \exists c(\lambda, a, b) \text{ s.t. } P(Y^* = b|X_1^{*\lambda} = a, X_2^{*\lambda} = c) \geq (1 - e^{-\beta_\lambda}) + \epsilon.\]

Then, \(\forall \lambda \text{ with } \text{Im}\Phi_2^\lambda \neq \emptyset, \text{ there exists } (X^{c_\lambda}, Y^{c_\lambda}) \in T_{\text{all}} \text{ such that the inequality in (d)' holds.}\)

The proof of Theorem D.2 is essentially same as the one of Theorem D.1 and therefore, we omit.
E Additional Experiment explanations

E.1 Visualizations of Experiment Results

Synthesized data of first experiment is visualized as in Figure 2. Synthesized data of second experiment is visualized as in Figure 3.

E.2 Explicit representation of Second Synthetic data

\[ N_1 = \mathcal{N}(-180, 20^2) \times \mathcal{N}(-5e, 30^2), \]
\[ N_2 = \mathcal{N}(-100, 20^2) \times \mathcal{N}(-3e, 30^2), \]
\[ N_3 = \mathcal{N}(-20, 20^2) \times \mathcal{N}(-1e, 30^2), \]
\[ N_4 = \mathcal{N}(60, 20^2) \times \mathcal{N}(-2e, 30^2), \]
\[ N_5 = \mathcal{N}(140, 20^2) \times \mathcal{N}(-4e, 30^2), \]
\[ N_6 = \mathcal{N}(-140, 20^2) \times \mathcal{N}(4e, 30^2), \]
\[ N_7 = \mathcal{N}(-60, 20^2) \times \mathcal{N}(2e, 30^2), \]
\[ N_8 = \mathcal{N}(20, 20^2) \times \mathcal{N}(1e, 30^2), \]
\[ N_9 = \mathcal{N}(100, 20^2) \times \mathcal{N}(3e, 30^2), \]
\[ N_{10} = \mathcal{N}(180, 20^2) \times \mathcal{N}(5e, 30^2). \]

E.3 Additional Experiment of Hierarchical Colored MNIST

Although Hierarchical Colored MNIST in Chapter 6 fix its flip rate 20%, we additionally demonstrate by changing its flip rate among \{0.1, 0.15, 0.2, 0.25\}. Table 6 shows that our methods outperform other
Fig 3: Visualization of Synthesized Data 2. Left figure illustrates the training and test data of second
eperiment. Right figure illustrates $D_{ad}^{40}$ and $D_{ad}^{e_{ad}}$ with $e_{ad} = -9$.

methods. Table 6 and 7 show that, among several CV methods, our method II outperform other methods.
Table 8 the difference between accuracies by TDV and each CV for the same data set with $e = 0.9$. The
result verify that CVII selects preferable hyperparameters with smaller errors.

E.4 Experiment Details

Through the experiment in the present paper, all models of competitors are composed of neural networks
where its loss function, activation function, and optimizer are cross entropy, ReLU Networks and Adam [53]. In the following explanation, NN with its model architecture $a \rightarrow h_1 \rightarrow \cdots \rightarrow h_k \rightarrow h_n \rightarrow P(m)$ means
that its input and hidden dimensions are $a$ and $(h_1, \ldots, h_n)$ respectively, and its output is probability
density functions on $[m]$. NN with its model architecture $a \rightarrow h_1 \rightarrow \cdots \rightarrow h_k \rightarrow b$ means that its
input, hidden and output dimensions are $a$, $(h_1, \ldots, h_n)$ and $b$ respectively. All the experiment, we add
$L^2$-regularized term to our objective function.

We add explanations of previous CV methods. Tr-CV implements cross-validation with using only $D^*$. In LOD-CV, a model is learnt with excluding one of the $D^e \in D^{ad}$ from $D^{ad}$, and evaluate its
performance by $D^e$. Changing the role of $e \in E^{ad}$, and taking their mean, we evaluate final CV-value.
Table 7: Baselines of CV methods

|       | Tr-CV       | LOD-CV      |
|-------|-------------|-------------|
| 0.25  | .759 (.008) | .362 (.008) |
|       | .459 (.012) | .372 (.012) |
| 0.20  | .794 (.004) | .338 (.004) |
|       | .541 (.007) | .334 (.007) |
| 0.15  | .834 (.002) | .348 (.002) |
|       | .634 (.008) | .358 (.008) |
| 0.10  | .876 (.003) | .502 (.196) |
|       | .708 (.006) | .497 (.194) |

Table 8: Means and SEs of \{\text{(Accuracy of TDV on } e = 0.9) - \text{(Accuracy of Each CV on } e = 0.9) \} (5runs).

|       | CV I         | CV II        | Tr-CV       | LOD-CV      |
|-------|--------------|--------------|-------------|-------------|
| 0.25  | .068 (.007)  | .046 (.023)  | .231 (.013) | .319 (.033) |
| 0.20  | .088 (.004)  | .025 (.006)  | .191 (.014) | .398 (.025) |
| 0.15  | .059 (.012)  | .039 (.022)  | .148 (.019) | .430 (.028) |
| 0.10  | .037 (.010)  | .037 (.010)  | .121 (.008) | .332 (.196) |

E.4.1 Synthesized Data I

We set model architecture of \( \Phi \) used in our method \( 2 \to 20 \to 20 \to 1 \). We set model architecture of CB-ERM and ERM \( 2 \to 20 \to 20 \to \mathcal{P}_3 \). When we use FT and FE, its model architecture on pre-train phase and retraining phase are \( 2 \to 20 \to 20 \to \mathcal{P}_2 \) and \( 2 \to 20 \to 20 \to \mathcal{P}_3 \) respectively. We set running rate and hyperparameters of \( L^2 \)-regularized term 0.0115 and 0.01 respectively. When we use DSAN [31], we inherit learning condition in the Amazon Review dataset experiment. When training, we use batch learning. We set \( K = 10 \) of each CV method.

E.4.2 Synthesized Data II

We set model architecture of \( \Phi \) used in our method \( 2 \to 8 \to 8 \to 1 \). We set running rate and hyperparameters of \( L^2 \)-regularized term 0.05 and 0.001 respectively. When training, we use minibatch learning with dividing \( \mathcal{D}^*, \mathcal{D}^{adv} \) and \( \mathcal{D}^{40} \) into 50 equal parts respectively. We set \( K = 10 \) of each CV method.

E.4.3 Hierarchical Colored MNIST

We set model architecture of \( \Phi \) used in our method \( 2 \to 440 \to 440 \to 440 \). We set model architecture of CB-ERM and ERM \( 2 \to 440 \to 440 \to \mathcal{P}_3 \). When we use FT and FE, its model architecture on pre-train phase and retraining phase are \( 2 \to 440 \to 440 \to \mathcal{P}_2 \) and \( 2 \to 440 \to 440 \to \mathcal{P}_3 \) respectively. We set running rate and hyperparameter of \( L^2 \)-regularized term 0.0004 and 0.002 respectively. When we use DSAN, we inherit learning condition in the Amazon Review dataset experiment. When training, we use batch learning. We set \( K = 10 \) of our CV method.
E.4.4 Birds recognition

We set model architecture of $\Phi$ used in our method ResNet50 [29] with changing its output dimension 256. We set model architecture of CB-ERM and ERM ResNet50 [29] with changing its output $P_3$. When we use FT and FE, its model architecture on pre-train phase and retraining phase are ResNet50 [29] with changing its output dimension 2 and 3 respectively. We set running rate and hyperparameter of $L^2$-regularized term 0.00004 and 0.001 respectively. When training, we use minibatch learning with its minibatch size 56. We set $K = 5$ of each CV method.