ZIN: When and How to Learn Invariance by Environment Inference?

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Abstract

It is commonplace to encounter heterogeneous data, of which some aspects of the data distribution may vary but the underlying causal mechanisms remain constant. When data are divided into distinct environments according to the heterogeneity, recent invariant learning methods have proposed to learn robust and invariant models based on this environment partition. It is hence tempting to utilize the inherent heterogeneity even when environment partition is not provided. Unfortunately, in this work, we show that learning invariant features under this circumstance is fundamentally impossible without further inductive biases or additional information. Then, we propose a framework to jointly learn environment partition and invariant representation, assisted by additional auxiliary information. We derive sufficient and necessary conditions for our framework to provably identify invariant features under a fairly general setting. Experimental results on both synthetic and real world datasets validate our analysis and demonstrate an improved performance of the proposed framework over existing methods. Finally, our results also raise the need of making the role of inductive biases more explicit in future works, when considering learning invariant models without environment partition.

1 Introduction

Machine learning algorithms with empirical risk minimization (ERM) generally assume independent and identically distributed (i.i.d.) data in training and testing set. Due to changing circumstances, selection bias, or time shifts, data distributions are often heterogeneous across different environments in practical applications. When the distributions of training and testing data are indeed different, model performance can severely degrade \cite{Szegedy et al. 2014, Hendrycks and Dietterich 2019, Recht et al. 2019}, as ERM based algorithms may exploit the spurious correlations that are particularly useful to ERM in the training data but do not exist in the test data.

To tackle the distribution-shift or out-of-distribution generalization problem, a recent line of methods propose to utilize the causally invariant mechanisms (rather than the spurious correlations in the training data) that are supposed to be stable across different environments. For example, \cite{Peters et al. 2016} propose to exploit the invariance principle to learn a linear model that merely relies on the direct causes of the target. Such a model is shown to be robust to potential interventions on any variable except the target itself. \cite{Arjovsky et al. 2019} propose invariant risk minimization (IRM) to capture invariant correlations by learning representations

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that elicit an optimal invariant predictor across multiple training environments. Ahuja et al. [2020], Jin et al. [2020], Krueger et al. [2021], Xie et al. [2020] further develop several variants of IRM by introducing game theory, regret minimization, variance penalization, etc., and Xu and Jaakkola [2021], Chang et al. [2020], Lin et al. [2021] try to learn invariant features by coupled adversarial neural networks.

Noticeably, the aforementioned invariant learning methods require datasets to be partitioned into distinct environments and their effectiveness relies heavily on the quality of environment assignment—the environments should implicitly define variations of the spurious correlations. However, environment labels may be unavailable due to privacy issues or because they are difficult to obtain, e.g., some commonly used benchmark datasets are assembled by merging data from multiple sources without explicit source labels. It is hence tempting to utilize the inherent heterogeneity in this circumstance. Indeed, several works have proposed to directly learn invariant models. For instance, Creager et al. [2021] propose environmental inference for invariant learning (EIIL), a two-stage method by firstly inferring the environments with an ERM based trained biased model and then performing invariant learning on inferred environments. Liu et al. [2021b] devise an interactive mechanism, called heterogeneous risk minimization (HRM), with environment inference and invariant learning on raw feature level, and Liu et al. [2021c] extend it to representation level with kernelized trick.

However, as we will show in this work, learning causally invariant features under this circumstance can be risky, both empirically and theoretically. For example, EIIL relies on the assumption that the model trained by ERM purely relies on spurious features, which however is not guaranteed. As our first contribution, in Section 4, we show that learning invariant features from heterogeneous data without environment labels is in theory impossible without further inductive biases or additional information. This impossibility result, which is perhaps not very surprising to readers who are familiar with the identifiability issue in causal discovery [Spirtes et al., 2000, Peters et al., 2017], independent component analysis (ICA) [Hyvarinen et al., 2019], and unsupervised learning of disentangled representations [Locatello et al., 2019], motivates us to consider when and how we can indeed learn causally invariant features.

In Section 5, we proceed to propose a framework to jointly learn environment partition and invariant representation, based on additionally observed variables like time index or other concurrent observations. This is in contrast with inductive biases that may depend on particular tasks and may not be easy to characterize explicitly. Under a fairly general setting, we derive both sufficient and necessary conditions for our framework to identify invariant features.

Finally, Section 6 presents experimental analysis on both synthetic and real world datasets to validate our theoretic results. Our proposed framework achieves an improved performance over existing methods like EIIL and HRM, and has a comparable performance to IRM with ground-truth environment partition.

## 2 Other Related Work

Invariant learning methods can be interpreted as robust to certain interventions or heterogeneity from a causal perspective. On the other hand, heterogeneous data have also placed challenges and potential benefits in causal inference tasks. For example, Huang et al. [2020b] consider heterogeneous datasets to identify variables with changing local mechanism and further the causal directions. Here confounders are assumed as functions of the domain index or time. Tillman and Spirtes [2011], Danks et al. [2009], Huang et al. [2020a] study the multiple dataset setting with non-identical sets of variables for causal discovery, where the datasets may have different exogenous noise distributions and only part of the variables is present in each dataset.

Besides the invariant learning methods described in Section 1, another large class of methods for generalizing beyond training data is distributionally robust optimization (DRO) [Ben-Tal et al., 2013, Shapiro, 2017, Lee...
DRO methods propose to optimize the worst-case risk over a set of distributions close to the training distribution, or the so-called uncertainty set, defined by some probabilistic distances like Wasserstein distance or $f$-divergence. Picking a suitable probability distance and range of uncertainty set is usually difficult in practice [Duchi and Namkoong, 2021], and may result in the over-pessimism issue of DRO methods. A notable instance of DRO methods is group DRO, which optimizes the worst-case loss over groups or environments in the training data [Sagawa et al., 2020]. As with most invariant learning methods, group DRO generally requires a partition of groups obtained according to group annotation and label of each data sample.

However, obtaining group annotations can be costly or even impossible in practice. For example, we may not know a priori the inherent spurious features associated with data. Thus, a number of works have proposed to infer group partition or identify the minority group by looking at features produced by biased models, e.g., Sohoni et al. [2020], Ahmed et al. [2021], Creager et al. [2021], Liu et al. [2021a]. Notice that sometimes a small number of labelled annotations are still needed to find a proper trained model, which is different from the setting considered in this work. For instance, Liu et al. [2021a] upweights samples with high losses from the initial ERM model and relies on a small validation set of annotated data to tune parameters. Alternatively, Nam et al. [2020], Sanh et al. [2021] try to obtain a more robust model by boosting from the wrongly specified samples, based on the observation that models with limited capacity tend to learn spurious correlations or shortcuts. Unfortunately, as we will show in Section 4, it is in theory impossible to distinguish spurious or invariant features from only the observed data consisting of input-label pairs.

3 Preliminaries

Throughout this paper, upper-cased letters such as $X \in \mathbb{R}^d$ and $Y \in \mathbb{R}$ denote random variables. Lower-cased letters such as $x$ and $y$ denote deterministic instances. We consider there exist invariant features $X_v \in \mathbb{R}^{d_v}$ and spurious (non-invariant) features $X_s \in \mathbb{R}^{d_s}$, and we have a scrambled observation $X = q(X_v, X_s) \in \mathbb{R}^d$ with $q$ being an injective function. Consider the dataset $D := \{(x_i, y_i)\}_{i=1}^n$ where data may be collected from multiple environments $e \in E_{supp}$. We use superscript $e$ to indicate the environment index with a variable, e.g., $X^e$ and $Y^e$, when it is useful to make the index explicit. Notice that the true environment index $e$ is not provided in training, unless otherwise stated.

We consider the model as the composition of a feature extractor $\Phi$ and a classifier (or predictor) $f_\omega$ that is parameterized by $\omega$. To seek for out-of-distribution generalization ability, we hope that $\Phi$ merely encodes the information of invariant features. Let $\ell(\cdot, \cdot)$ denote a loss function such as cross entropy loss or squared error. Our goal is to learn a robust and invariant model that minimizes the following objective over all possible environments $e \in E_{supp}$:

$$\sup_{e \in E_{supp}} \mathbb{E}_{X^e, Y^e} [\ell (f_w(\Phi(X^e)), Y^e)].$$

While there is no single, common definition of invariant feature in the literature, in this work we consider an underlying structural causal model [Spirtes et al., 2000, Peters et al., 2017] governing the data generation process and treat the direct causal parents of $Y$ as invariant features, as in Peters et al. [2016], Arjovsky et al. [2019]. This is because the conditional probability of the outcome $Y$ given its parental variables or direct causes remains unchanged with any intervention (not on $Y$). In contrast, if a non-parental variable is included in the conditioned variables, then the conditional probability could change after some intervention.
As an example, we present the following data generation process:

\[
\begin{align*}
Y^e &= g_e(X_v^e, \epsilon_v), & X_v^e \perp \epsilon_v, \\
X_s^e &= g^e(Y^e, \epsilon_s^e), & Y^e \perp \epsilon_s^e, \\
X^e &= q(X_v^e, X_s^e),
\end{align*}
\]

(1)

where \( g_e, g^e \) denote some non-degenerate deterministic functions and \( \epsilon_v, \epsilon_s^e \) are independent noise variables. This data generation process is also considered in [Arjovsky et al., 2019, Aluja et al., 2021]. We observe data \( \{X^e, Y^e\}_{e=1}^E \) from multiple environments, each with probability \( P(X^e, Y^e) \). Then the marginal distribution of the mixed data can be represented as \( P(X, Y) = \sum_{e=1}^E \alpha_e P(X^e, Y^e) \) for some \( \alpha_e > 0 \) and \( \sum_{e=1}^E \alpha_e = 1 \).

4 Impossibility Result

The first question we ask is whether it is possible to learn invariant models from the heterogeneous data of multiple environments with unknown environmental indexes. The following toy example immediately gives a negative answer.

**Example 1.** Suppose that there are two environments \( e \in \{1, 2\} \) with \( \alpha_1 = \alpha_2 = 0.5 \), and we observe binary-valued features \( X_1, X_2 \) and label \( Y \). Consider the following data generation processes:

- \( X_1 \) is the invariant feature while \( X_2 \) is spurious:
  \[
  X_1 \sim \text{Bernoulli}(0.5), \quad Y = \begin{cases} 
  X_1, & \text{w.p. 0.8,} \\
  1 - X_1, & \text{w.p. 0.2,}
  \end{cases} \quad X_2^e = \begin{cases} 
  Y, & \text{w.p. } p_s^e, \\
  1 - Y, & \text{w.p. } 1 - p_s^e,
  \end{cases}
  \]

  where \( p_s^{e=1} = 0.7 \) and \( p_s^{e=2} = 0.9 \).

- \( X_2 \) is the invariant feature while \( X_1 \) is spurious:
  \[
  X_2 \sim \text{Bernoulli}(0.5), \quad Y = \begin{cases} 
  X_2, & \text{w.p. 0.8,} \\
  1 - X_2, & \text{w.p. 0.2,}
  \end{cases} \quad X_1^e = \begin{cases} 
  Y, & \text{w.p. } p_s^e, \\
  1 - Y, & \text{w.p. } 1 - p_s^e,
  \end{cases}
  \]

  with \( p_s^{e=1} = 0.7 \) and \( p_s^{e=2} = 0.9 \).

It can be shown that the joint distribution of mixed environments for each case is

\[
Y = \begin{cases} 
  1, & \text{w.p. 0.5,} \\
  0, & \text{w.p. 0.5,}
  \end{cases} \quad \begin{cases} 
  X_2 = X_1 = Y, & \text{w.p. 0.64,} \\
  X_2 \neq X_1 = Y, & \text{w.p. 0.16,} \\
  X_1 \neq X_2 = Y, & \text{w.p. 0.16,} \\
  X_2 = X_1 \neq Y, & \text{w.p. 0.04.}
  \end{cases}
\]

Thus, from the joint distribution over \( (X_1, X_2, Y) \), we cannot distinguish the two cases. Either case can be the underlying truth and the true invariant features cannot be identified.

Moreover and unfortunately, such an example is not rare. Indeed, for any data distribution \( P(X, Y) \) that can be generated by some data generation process like (1), we can find a different data generation process that induces the same distribution yet has different invariant/spurious features. Similarly, it is impossible to find the minority group that is determined by spurious features, based on only the data \( P(X, Y) \). This result is formally summarized in Theorem 1. A proof is provided in Appendix A.1.

**Theorem 1.** Let \( X_v \) and \( X_s \) be respectively invariant and spurious features, with label \( Y \). For the joint distribution \( P(X, Y) \) consisting of data from multiple environments with \( P(X_s, Y) \neq 0 \), we can find \( X'_v \) and \( X'_s \) as invariant and spurious features so that
\( X'_v \neq X_v \) and \( X'_v \cap X_s \neq \emptyset \).

\((X'_v, X'_s)\) together with some independent noise variables can generate the same distribution \( P(X, Y) \).

The above theorem may not be surprising to readers who are familiar with the identifiability issue in causal discovery and ICA literature. Also similar to causal discovery or ICA, in order to identify the invariant features we have to introduce additional assumptions/conditions or certain “inductive bias”. The latter may come implicitly from the proposed algorithm, model, and/or the data [Creager et al., 2021; Liu et al., 2021b,c]. We believe that this is the reason that makes the existing methods achieve improved empirical performance in their considered scenarios. For example, in HRM [Liu et al., 2021b,c], the discrepancy of spurious features among clusters should be larger than that of causal features, and in EIIIL [Creager et al., 2021], LFT [Nam et al., 2020; Sanh et al., 2021] and JTT [Liu et al., 2021a], the ERM model of the first stage should heavily or fully rely on the spurious feature; however, these inductive biases may not be always guaranteed. Thus, as suggested by Theorem 2, the role of inductive biases shall be discussed more explicitly when considering learning invariant models from heterogeneous data without environment labels.

Alternatively, in this work, we consider that there exist additionally observed variable \( Z \) with the data, which has been often considered in causal discovery and ICA literature [Huang et al., 2020b; Hyvarinen et al., 2019; Khemakhem et al., 2020]. The variable \( Z \) could be, for example, the time index in a time series, some kind of class labels, concurrently observed variables, or human annotations on potential unmeasured variable [Srivastava et al., 2020]. In the next section, we show how to utilize \( Z \) to learn invariant models from the mixed dataset.

5 ZIN: Learning Invariance with Additional Auxiliary Information

In this section, we first propose our framework to learn invariant models and then derive conditions for invariance identification. We show that these conditions are both sufficient and necessary under a fairly general setting. Extension to other cases is also discussed.

5.1 Method

We consider that there exists additional auxiliary information \( Z \in \mathbb{R}^{d_z} \) in company with the data \((X, Y)\). In the following, we propose ZIN, auxiliary information \( Z \) for environmental INference, for invariant learning from the mixture dataset \( D \) without environment labels:

\[
\min_{\omega, \Phi} \max_{\rho, \omega_1, \ldots, \omega_K} \mathcal{R}(\omega, \Phi) + \lambda \sum_{k=1}^{K} \left[ \mathcal{R}_{\rho(k)}(\omega, \Phi) - \mathcal{R}_{\rho(k)}(\omega_k, \Phi) \right] \\
=: \mathcal{L}(\Phi, \omega, \omega_1, \ldots, \omega_K, \rho),
\]

where \( K \in \mathbb{Z} \) is a pre-specified hyper-parameter, \( \rho(\cdot) : \mathbb{R}^{d_z} \to \mathbb{R}^K \) with \( \rho(k) \) denoting its \( k \)-th entry,

\[
\mathcal{R}(\omega, \Phi) = \frac{1}{n} \sum_{i=1}^{n} \ell(f_w(\Phi(x_i)), y_i), \\
\mathcal{R}_{\rho(k)}(\omega, \Phi) = \frac{1}{n} \sum_{i=1}^{n} \rho(k)(z_i)\ell(f_w(\Phi(x_i)), y_i),
\]

\[n\]
and $\mathcal{R}_{\rho(k)}(\omega, \Phi)$ is similarly defined by replacing $\omega$ with $\omega_k$ in $\mathcal{R}_{\rho(k)}(\omega, \Phi)$. Function $\rho(Z) \in [0, 1]^K$ with $\sum_k \rho(k)(Z) = 1$ is used to softly partition the training data into $K$ environments; the choice of $K$ will be empirically investigated in Section 5.1. Given a partition $\rho(Z)$, we can then measure how the model violates the invariance constraint due to the use of spurious information. In particular, we train $K$ independent classifiers $\{f_{\omega_k}\}_k$ and compare them with the classifier trained on the whole dataset (cf. the second term in Equation (2)). If $\Phi$ extracts spurious features that are unstable in the inferred environments, $\mathcal{R}_{\rho(k)}(\omega, \Phi)$ will be larger than $\mathcal{R}_{\rho(k)}(\omega, \Phi)$ and induce a non-zero penalty.

The idea of our method can be summarized as first inferring an environment partition and then learning invariant models based on the inferred environments. Creager et al. [2021] has used a similar intuition and adopted a pre-trained biased model to estimate the environments. However, their two-stage method cannot be jointly optimized, and the environment partition relies on the given model and lacks a theoretic guarantee. In contrast, we will first present sufficient conditions on $Z$ so that the proposed framework can provably identify the invariant features. We further show that these conditions are also necessary, and that violation of these conditions will lead to failure of invariance identification. Assigning independent weights to each data sample, which is the strategy adopted in Creager et al. [2021], is unfortunately an instance of such violations and may fail to identify invariant features.

5.2 Sufficient Conditions for Identifiability

We theoretically analyze our proposed method ZIN, to understand when it learns the invariant features. We temporarily consider a simple yet general setting: $X = [X_v; X_s]$ (i.e., no scramble on the observation) and $\Phi \in \{0, 1\}^d$ is an element-wise feature selection mask on $X$. Notice that $f_w$ can still be general non-linear functions. In this subsection, we also focus on classification tasks with $\ell(\cdot, \cdot)$ being the cross-entropy loss, as there is an interesting connection to (conditional) Shannon entropy. Extension to more general cases will be discussed in Section 5.4.

In this setting, our goal is equivalent to learning the optimal feature mask that merely selects invariant features, i.e., $\Phi_v = [1_d; 0^d]$. For a given feature mask $\Phi$, the objective function is equal to the following

$$\hat{L}(\Phi) = \min_{\omega, \rho, \{\omega_k\}_{k=1}^K} \max_{(\omega_1, \cdots, \omega_k)} \mathcal{L}(\Phi, \omega_1, \cdots, \omega_k, \rho).$$

Then ZIN can correctly identify the invariant features, or solution to Equation (2) is equivalent to $\Phi_v$, if and only if

$$\hat{L}(\Phi_v) < \hat{L}(\Phi), \quad \forall \Phi \neq \Phi_v. \tag{3}$$

Equation (3) will be used to establish our main theoretic result. With a little abuse of notation, we use $H(Y|X')$ to denote expected loss of an optimal classifier over some $X'$ and $Y$, and similarly $H(Y|\rho(Z), X')$ to denote the minimum risk of $\sum_{k=1}^K \mathcal{R}_{\rho(k)}(\omega_k, \Phi)$ for a given $\rho(Z)$. Notice that with cross-entropy loss and when $\rho(z_i)$ gives exactly one environment, i.e., $\rho(Z)$ is one-hot, it can be verified that the optimal loss $H(\cdot|\cdot)$ coincides with conditional entropy.

In the following we first state the assumptions for our identifiability result.

Assumption 1. The function space $\mathcal{F}$ is rich enough so that there is a model that can achieve the optimal expected risk to any precision. That is, for any feature mask $\Phi$ and any constant $\epsilon > 0$, there exists $f \in \mathcal{F}$ such that

$$\mathbb{E}[\ell(f(\Phi(X)), Y)] \leq H(Y|\Phi(X)) + \epsilon.$$
Assumption 2. If two features are invariant w.r.t. an environment partition, then the concatenated features are also invariant. This implies that for $X_1, X_2 \subset X$ and function $\rho(\cdot)$, if $H(Y|X_1) - H(Y|\rho(Z), X_1) = 0$ and $H(Y|X_2) - H(Y|\rho(Z), X_2) = 0$, we have

$$H(Y|X_1, X_2) - H(Y|\rho(Z), X_1, X_2) = 0.$$ 

Assumption 3. If a feature representation violates the invariance constraint, adding another feature into the representation would not make the penalty diminish. This implies that there exists a constant $\delta > 0$ so that for any $X_1, X_2 \subset X$,

$$H(Y|X_1, X_2) - H(Y|\rho(Z), X_1, X_2) \geq \delta (H(Y|X_1) - H(Y|\rho(Z), X_1)).$$

Assumption 4. There exists a constant $\gamma > 0$ so that

$$H(Y|X_1, X_2) \leq H(Y|X_1) - \gamma.$$ 

for any distant features $X_1$ and $X_2$.

Assumption 4 indicates that any feature contains some useful information w.r.t. $Y$, which cannot be explained by other features. If this is not true, we can simply remove such a feature from $X$ (e.g., by using preliminary variable selection methods [Vergara and Estevez 2014]), as it does not affect the classification performance.

With the above assumptions, we present our sufficient conditions for ZIN to identify invariant features. As we will show in Section 5.3, these conditions turn out to be necessary, too.

Condition 1 (Invariance Preserving Condition). For any feature $X^i_s \in X_s$ and any function $\rho(\cdot)$, it holds that

$$H(Y|X^i_s, \rho(Z)) = H(Y|X^i_s).$$

Condition 2 (Non-invariance Distinguishing Condition). For any feature $X^k_s \in X_s$, there exists a function $\rho(\cdot)$ and a constant $C > 0$ such that

$$H(Y|X^k_s) - H(Y|X^k_s, \rho(Z)) \geq C. \tag{4}$$

Condition 1 requires that invariant features should remain invariant based on any environment partition induced by $\rho(Z)$. Otherwise, if there exists an environment partition where an invariant feature becomes non-invariant, then this feature would induce a positive penalty. Condition 2 implies that for each spurious feature, there exists at least one partition so that this feature is non-invariant in the split environments. If a spurious feature does not incur any invariance penalty in all possible environment partitions, then we can never distinguish it from the true invariant features. Consequently, the additionally observed information $Z$ should capture the heterogeneity in the data, and $Z$ should be diverse enough so that every spurious feature can be identified.

Our main result on the identifiability is stated as follows.

Theorem 2 (Identifiability of Invariant Features). With Assumptions 2, 3, and Conditions 1, 2, if $\epsilon < \frac{C_\gamma \delta}{4\gamma + 2\gamma H(Y)}$ and $\lambda \in \left[ \frac{H(Y) + 1}{\delta C - 1} \lambda - \frac{1}{2}, \frac{\gamma}{4\epsilon} - \frac{1}{2} \right]$, then we have

$$\hat{\mathcal{L}}(\Phi_e) < \hat{\mathcal{L}}(\Phi), \quad \forall \Phi \neq \Phi_e,$$

where $H(Y)$ denotes the entropy of $Y$. That is, the solution to Problem 3 identifies the invariant features.
Proof (Sketch). Our proof consists of two steps. In the first step, we show that the invariance penalty of $\Phi_v$ will be upper bounded by $\epsilon$ according to Assumption 1 and that a feature mask selecting any spurious feature would induce another non-zero penalty depending on the constant $C$ in Condition 2. With a sufficiently large penalty weight $\lambda$, this feature mask will induce a larger loss $\hat{L}(\Phi)$ than $\hat{L}(\Phi_v)$ according to Assumption 4. Due to space limit, please see Appendix A.2 for a complete version.

5.3 Necessary Conditions for Identifiability

Conditions 1 and 2 may appear rather strong at first glance. In this section, we prove that they are also necessary conditions for ZIN to identify invariant features. Specifically, Proposition 1 shows that if Condition 1 is violated, then some invariant features will be excluded in the solution of Problem 2; and in Proposition 2, violation of Condition 2 results in some spurious features included in the solution.

Proposition 1. If Condition 1 is violated, i.e., there exists $X^i_v \in X_v$ and a function $\rho(\cdot)$ so that

$$H(y|X^i_v) - H(y|X^i_v, \rho(Z)) \geq C' > 0,$$

(5)

then there exists a feature mask $\Phi' \neq \Phi_v$ with

$$\hat{L}(\Phi_v) > \hat{L}(\Phi').$$

A proof is provided in Appendix A.3, which is similar to the first step of the proof of Theorem 2. A question is how Condition 1 could be violated when learning invariant models. On the other hand, while we introduce $Z$ as additional variables, it is also interesting to know whether we can obtain a valid partition based on only the data $(X,Y)$. Below we provide two examples regarding these questions.

Corollary 1. Condition 1 is violated for the following cases: if there is a function $\rho$ and an injective function $h$ so that

(a) $\rho(Z) = h(Y),$ 

(b) $\rho(Z) = h(X,Y),$ 

(c) $\rho(Z) = h(\text{Index}(X,Y)).$

Below we illustrate why this is case:

(a) Since $h$ is injective, then for any $X^i_v$

$$H(Y|X^i_v, h(Y)) = H(Y|X^i_v, Y) = 0.$$  

According to Assumption 4, we would have $H(Y|X^i_v) \geq H(Y|X) + \gamma \geq \gamma$. Then Proposition 1 indicates that we cannot identify all the invariant features. This example includes the case where $Z$ contains the information of $X$ and $Y$.

(b) The proof proceeds the same as above by noting $H(Y|X^i_v, h(X,Y)) = 0.$

(c) This case can be shown similarly to (a), because $H(Y|X^i_v, h(\text{Index}(X,Y))) = H(Y|X^i_v, X, Y) = 0.$ Since $h(\text{Index}(X,Y))$ can be interpreted as learning independent weights for each sample based on the dataset $\{(x_i, y_i)\}_i$, this case includes the strategy of Creager et al. [2021] as an instance.

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Proposition 2. If Condition 2 is violated, i.e., there exists a feature \( X^k_s \in X_s \) such that for any function \( \rho(\cdot) \),

\[
H(Y|X^k_s) - H(Y|X^k_s, \rho(Z)) = 0,
\]

then there exists a feature mask \( \Phi' \neq \Phi_v \) with

\[
\hat{L}(\Phi_v) > \hat{L}(\Phi').
\]

Since there exists a spurious feature \( X^k_s \) that is “invariant” in all possible environment partition, adding this feature to \( \Phi_v \) does not induce any penalty but increases the prediction power. Thus, such a feature mask can achieve smaller loss than \( \hat{L}(\Phi_v) \). For completeness, we provide a proof in Appendix A.4. Proposition 2 again indicates in theory that \( Z \) should be sufficiently diverse and informative so that each spurious feature can be recognized.

5.4 Discussions

Extension to Other Loss Functions. Sections 5.2 and 5.3 focus on classification task with cross-entropy loss, to establish sufficient and necessary conditions for invariance identification. Similar results can be shown for other loss functions or tasks in a straightforward manner. To see this, notice that \( H(\cdot|\cdot) \) in Assumptions 1-4 and Conditions 1-2 is used to represent the optimal expected risk, which coincides with the conditional entropy with cross-entropy loss and when \( \rho(z_i) \) gives exactly one environment. For other loss functions \( l(\cdot, \cdot) \) like squared error, we can use \( L(\cdot|\cdot) \) to represent the optimal expected risks, and \( L(\cdot) \) denotes the optimal expected risk with no predictor variables, e.g., variance for the squared error loss. Replacing \( H(\cdot|\cdot) \) with \( L(\cdot|\cdot) \), we can follow the same proof procedure to obtain similar sufficient and necessary conditions. This is summarized in Theorem 3 in Appendix B for completeness.

Beyond Feature Selection. Our theoretic analysis is mainly based on that, either adding a spurious feature or lacking an invariant feature would induce a larger loss than \( \hat{L}(\Phi_v) \). When extending this idea to cases with more general functions as feature extractor \( \Phi \), the difficulty lies in how to characterize the effect of an invariant/spurious feature in a quantitative way, which is required in our assumptions and conditions. A possible way is through the derivative of \( \Phi \) w.r.t. \( X \), and we leave further investigation as a future work. Nevertheless, the empirical result in Section 6 shows that ZIN can perform well on image classification tasks where \( \Phi \) adopts a ResNet-18 architecture [He et al., 2016].

Auxiliary Information for Related Methods. The proposed framework ZIN relies on additional auxiliary variables. It is interesting to ask whether this type of information is also useful to related methods such as EIIL and HRM. In many scenarios, the additional variable \( Z \) may have no or little information about the target, e.g., 1) in time series tasks, the time index is rarely used to predict the label; 2) in the CelebA classification task in Section 6.3 features like \( \text{Young} \) and \( \text{Eyeglasses} \) are likely to provide little information about predicting \( \text{Smiling} \). Then \( Z \) may not be useful to ERM and EIIL. In Section 6.3 we also provide \( Z \) to EIIL and HRM, and the experimental result shows that it does not help or even harms the test performance. How to find useful additional auxiliary information for other invariant learning methods like EIIL or HRM is an interesting direction, but is beyond the scope of the present work.

6 Experiments

In this section, we empirically verify our theoretic analysis and the effectiveness of ZIN on both synthetic and real world datasets.
6.1 Baselines

We compare ZIN with several existing methods:

- **Empirical risk minimization (ERM)**: ERM seeks to minimize the empirical loss over the training data.

- **Invariant risk minimization (IRM)** [Arjovsky et al., 2019]: its performance with ground-truth environment partition serves as an upper bound.

- **Environment inference for invariant learning (EIIL)** [Creager et al., 2021]: a two-stage algorithm where a trained biased model based on \((X, Y)\) is used for splitting environments, followed by applying IRM to the inferred environment partition.

- **Heterogeneous risk minimization (HRM)** [Liu et al., 2021b]: HRM iterates between environment inferring by clustering and invariance learning.

**Implementations.** We implement \(\rho(\cdot)\) in ZIN as a two-layer MLP with 32 hidden units. The number of inferred environments \(K\) is set to be 2 as default. For the task on synthetic datasets in Section 6.2 and the house price prediction task in Section 6.3, we also adopt a two-layer MLP with 32 hidden units for function \(f\). For the CelebA task in Section 6.3, feature extractor \(\phi\) uses ResNet-18 architecture [He et al., 2016]. We use Adam [Kingma and Ba, 2014] with learning rate 0.001 as our optimizer. More details can be found in Appendix C.

6.2 Synthetic Dataset

**Temporal Heterogeneity.** We first consider temporal heterogeneity where distributional shift occurs over time. Let \(t \in [0, 1]\) denote the time index and \(X_v(t) \in \mathbb{R}\) be the invariant feature at time \(t\). The data generation process is

\[
X_v(t) \sim \begin{cases} 
\mathcal{N}(1, \sigma^2), & \text{w.p. } 0.5, \\
\mathcal{N}(-1, \sigma^2), & \text{w.p. } 0.5,
\end{cases}
\]

\[
Y(t) = \begin{cases} 
\text{sign}(X_v(t)), & \text{w.p. } p_v, \\
-\text{sign}(X_v(t)), & \text{w.p. } 1 - p_v,
\end{cases}
\]

where probability \(p_v\) is a constant w.r.t. \(t\), indicating a stable correlation between \(Y(t)\) and \(X_v(t)\). The spurious feature \(X_s(t)\) is generated from \(Y(t)\) as follows:

\[
X_s(t) \sim \begin{cases} 
\mathcal{N}(Y(t), \sigma^2), & \text{w.p. } p_s(t), \\
\mathcal{N}(-Y(t), \sigma^2), & \text{w.p. } 1 - p_s(t),
\end{cases}
\]

Notice here probability \(p_s(t)\) varies with time index. Our goal is to learn a model that purely relies on the feature \(X_v\).

**Spatial Heterogeneity.** We next consider spatial heterogeneity that is also commonly encountered in practice, e.g., environments may be divided according to locations of latitude and longitude. We simulate spatial heterogeneity in the same way as Equations (6)-(8) but use a two-dimensional spatial variable \(r = [r_1, r_2] \in [0, 1]^2\).

**Experiment Setting.** For temporal heterogeneity, we simulate two heterogeneous environments along time, namely, \([0, 0.5], [0.5, 1]\), and \(p_v(t)\) will be set differently. We use tuple of \(p_s(t)\) in the two environments to denote a simulated case. For example, \((0.999, 0.7)\) stands for \(p_s(t) = 0.999, t \in [0, 0.5)\) and \(p_s(t) = 0.7, t \in [0.5, 1]\). As to spatial heterogeneity, we simulate four environments for training by equally splitting the space into four blocks, i.e., \([0, 0.5) \times [0, 0.5)\), \([0.5, 1] \times [0, 0.5)\), \([0.5, 1) \times [0.5, 1)\), \([0.5, 1] \times [0.5, 1)\). Similarly, we
denote a simulated case by tuple of $p_s(r)$ in the four elements. For both temporal and spatial heterogeneity, we evaluate the performance on four distinct test environments with $p_s \in \{0.999, 0.8, 0.2, 0.1\}$ and $p_v$ being constant. More details regarding the implementations are given in Appendix [C].

**Results.** Table 1 reports the test accuracy regarding temporal heterogeneity. In all simulated settings, the worst accuracy of ERM is much lower than the mean accuracy, indicating that ERM tends to rely on spurious feature $X_s$. EIIL can improve the worst accuracy in some cases, e.g., when $p_s(t) = (0.999, 0.8)$ and $p_s(t) = (0.999, 0.9)$. However, its performance is even worse than ERM for some other settings. This may be attributed to the first stage of EIIL, where the trained biased model is not guaranteed and may learn both spurious and invariant features, as also discussed by Creager et al. [2021]. The proposed method ZIN improves the worst test accuracy significantly. For instance, when $p_s(t) = (0.999, 0.7)$ and $p_v = 0.9$, ZIN achieves 85.36% worst accuracy, outperforming ERM and EIIL by over 28% and 65%, respectively. Moreover, ZIN is very close to IRM that knows the ground-truth environment partition, showing that ZIN can infer the environments effectively (see left panel of Figure 1 for an example). Finally, it seems that HRM does not learn a useful model here.

The experimental results of spatial heterogeneity in Table 2 show similar performances to those of temporal heterogeneity. An interesting observation is that ZIN outperforms IRM with ground-truth environments in this simulation, especially when “duplicated” environments exist, e.g., when $p_s(r) = (0.999, 0.999, 0.7, 0.7)$. We conjecture that in this case the “ground-truth” partition may not be the most effective for invariant learning due to the heavily overlapped environments. As shown in the right panel of Figure 1, ZIN automatically merges duplicated environments.

**Ablation Study on Z and K.** We now verify the theoretical results in Section 5 by choosing different inputs as $Z$. We adopt a setting of spatial heterogeneity with $p_s(r) = (0.999, 0.999, 0.8, 0.8)$ and $p_v = 0.8$. Note that the heterogeneity in this setting is only along the second dimension $r_2$. The results are shown in Table 3. One can verify that Conditions 1 and 2 are satisfied when $r$ or $r_2$ is chosen as $Z$. The mean and worst test accuracy implies that ZIN based on $r$ or $r_2$ can effectively remove the spurious feature. Since $p_s(r)$ does not change along $r_1$, choosing $r_1$ to infer environment partition violates Condition 2, which is reflected
by the poor performance of ZIN with $r_1$. Using $[X, Y]$ as input to $\rho(\cdot)$ is also a violation by Corollary 1 and the corresponding results in Table 3 confirm our analysis. Lastly, notice that $X \in X$ contains some information of $Y$ and there may exist a function $\rho(\cdot)$ so that $H(Y|X_v) > H(Y|X_v, \rho(X))$. This violates Condition 2 and leads to poor results when choosing $X$ as input to $\rho(\cdot)$.

We also empirically verify the choice of hyper-parameter $K$ using the same simulated setting. Figure 2 shows that $K$ has a relatively small impact, especially when $K \geq 4$.

### 6.3 Real World Datasets

**House Price Prediction.** This experiment considers a real world regression dataset of house sales prices from Kaggle (https://www.kaggle.com/c/house-prices-advanced-regression-techniques). The target variable is house price and each sample contains 17 predictive variables such as the built year of the house, number of bedrooms, etc. The dataset is split according to the built year, with training dataset in period [1900, 1950] and test dataset in period (1950, 2000]. We choose the built year as the auxiliary information for ZIN. As there is no well-defined ground-truth environment partition for IRM, we manually split the training dataset equally into 5 segments with 10-year range in each segment. Table 4 reports the mean squared error (MSE) and ZIN again outperforms other methods on test dataset.

Following the discussion in Section 5.4, we empirically investigate whether this type of additional information $Z$, together with $X$, helps EiIL and HRM. The corresponding results are marked with (+Z) in Table 4. We observe that the results of EiIL and HRM with additional information $Z$ are worse than those without using $Z$. This implies that such information may not be directly utilized by or even can harm the two methods.

**CelebA.** This task is to predict *Smiling* based on the image from CelebA [Liu et al., 2015], and by construction the target is spuriously correlated with *Gender*. We have access to the meta annotations of CelebA images and they serve as $Z$ in our framework. In particular, we pick the following seven features as potential auxiliary variables: \{Young, Blond Hair, Eyeglasses, High Cheekbones, Big Nose, Bags Under Eyes, Chubby\}. Notice
that the annotation of Gender is not provided to ZIN, EIIL, HRM and ERM, but is made available to IRM to create an oracle environment partition.

Empirical results are given in Table 5 where ZIN(#) represents ZIN using # of the seven features as $Z$. ERM achieves the highest training accuracy on average, while only has 47.58% worst test accuracy. EIIL has the worst performance on both training and test data, showing that it may not learn the causal features. Finally, we observe that ZIN performs better when more auxiliary information is provided: specifically, ZIN(7) achieves the best test performance based on the mixed dataset without environment labels.

7 Concluding Remarks

In this work, we investigate when and how to learn invariant models from heterogeneous data without explicit environment labels. We first show that learning invariant models in this case is impossible, without further inductive bias or additional information. Then, we propose ZIN to jointly learn environment partition and invariant representation based on some additional auxiliary variables. Under a fairly general setting, we

Table 5: Accuracy (%) on CelebA task.

| Method | Train | Test Mean | Test Worst |
|--------|-------|-----------|------------|
| ERM    | 90.97±0.66 | 70.76±0.26 | 47.58±0.46 |
| EIIL   | 44.78±5.85  | 55.26±1.17  | 43.12±8.98  |
| ZIN(1) | 90.62±0.78  | 70.79±0.61  | 47.62±0.98  |
| ZIN(4) | 83.57±1.40  | 75.20±0.71  | 63.47±1.41  |
| ZIN(7) | 83.06±1.28  | 76.29±0.60  | 67.27±1.15  |
| IRM    | 81.30±1.53  | 78.44±0.48  | 75.03±1.29  |
derive sufficient and necessary conditions for ZIN to provably identify invariant features. Experimental results verify our analysis and demonstrate an improved performance of ZIN over existing methods. A future work is to extend the theoretic results to more general feature extractor functions, as discussed in Section 5.4.

As in unsupervised learning of disentangled representations [Locatello et al., 2019], our results also raise the need of future works to make the role of inductive biases more explicit, when studying the task of learning invariance from heterogeneous data without environment labels. Alternatively, one may also take into account weak forms of supervision or additional structure information on the considered scenario.

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A Proofs

A.1 Proof of Theorem 1

Proof. First, we assume $Y$ and $X_v$ are univariate variables, i.e., $Y, X_v \in \mathbb{R}$. Let $\eta_1 \sim \text{Uniform}(0, 1)$ independent of $X_s$ and $Y$, and set $X'_v = X_s$. Define the conditional cumulative distribution function and its inverse as:

$$F_{Y|X_s=x_s}(y) = P(Y \leq y \mid X_s = x_s),$$
$$Y' = f'_1(X'_v, \eta_1) = F_{Y|X_s}^{-1}(\eta_1) = \inf\{y \in \mathbb{R} : F_{Y|X_s}(y) \geq \eta_1\} \text{ with } X_s = X'_v.$$

By definition, we would have

$$P(Y' \leq y \mid X'_v) = P(f'_1(X'_v, \eta_1) \leq y) = P(F_{Y|X_s}^{-1}(\eta_1) \leq y) = P(F_{Y|X_s} \circ F_{Y|X_s}^{-1}(\eta_1) \leq F_{Y|X_s}(y)) = P(\eta_1 \leq F_{Y|X_s}(y)) = P(Y \leq y \mid X_s).$$

Similarly, we can construct $X'_s = f'_2(X'_v, Y', \eta_2) = F_{X_s|X_s}^{-1}(\eta_2)$ so that $\Pr(X'_s|Y', X'_v) = \Pr(X_s|Y, X_s)$ with $\eta_2 \sim \text{Uniform}(0, 1)$. Thus, we have

$$\Pr(X'_v, X'_s, Y) = \Pr(X'_s|Y', X'_v)\Pr(Y'|X'_v)\Pr(X'_v) = \Pr(X_v|Y, X_s)\Pr(Y|X_s)\Pr(X_s) = \Pr(X_v, X_s, Y).$$

Next, we can easily find a function $q'()$ so that $X' = q'(X'_v, X'_s) = q(X_v, X_s)$, where we have chosen $X'_v = X_s$ and $X'_s = X_v$. Together with Equation (10), we conclude that $P(X', Y') = P(X, Y)$.

Second, we consider that $X_v$ has a multi-dimension. We may leave $Y$ to be a univariate variable as the label in many ML problems is scalar-valued. For this case, we can pick an entry of $X_v$, say, $X_v^{(j)}$ for some $j$. Then we set $X'_v = (X_v^{(-j)}, X_s)$ where $X_v^{(-j)}$ denotes the rest entries of $X_v$ except the $j$-th. Then we can similarly use the inverse conditional cumulative distribution function and an independent uniformly distributed noise variable $\eta_1$ to construct $Y' = f'(X'_v, \eta_1)$ so that $P(Y' \leq y \mid X'_v) = P(Y \leq y \mid X_v^{(-j)}, X_s)$. Similarly, we set $X'_s = X_v^{(j)}$ and we can construct $X'_s = f'_2(X'_v, Y', \eta_2)$ so that $P(X'_s|Y', X'_v) = P(X_v^{(j)} \mid Y, X_s)$. We can then get the same conclusion following the previous proof.

A.2 Proof of Theorem 2

Proof. Our proof proceeds by two steps. First, we show that any feature mask that selects at least one spurious feature would induce a penalty. With sufficiently large $\lambda$, the penalty will dominate the expected risk and then exceed $\hat{L}(\Phi_v)$. Second, we show that any proper subset of the invariant features induces a loss larger than $\hat{L}(\Phi_v)$.

Step 1 Suppose that the feature mask contains at least one spurious features. Denote the selected features as $X_{+s}$ and the corresponding feature mask as $\Phi_{+s}$. We aim to show that

$$\hat{L}(\Phi_{+s}) > \hat{L}(\Phi_v).$$
By Assumption 1 with a given $\epsilon > 0$, we have
\[
\hat{L}(\Phi_v) \leq (1 + 2\lambda)\epsilon + H(Y|X_v) + \lambda (H(Y|X_v) - H(Y|X_v, \rho(Z))) \\
= (1 + 2\lambda)\epsilon + H(Y|X_v) \\
\leq (1 + 2\lambda)\epsilon + H(Y). \quad \quad (11)
\]

One the other hand, we have
\[
L(\Phi_v + s) \geq -(1 + 2\lambda)\epsilon + H(Y|X_v + s) + \lambda (H(Y|X_v + s) - H(Y|X_v + s, \rho(Z))) \\
\geq -(1 + 2\lambda)\epsilon + \lambda (H(Y|X_v + s) - H(Y|X_v + s, \rho(Z))) \\
\geq -(1 + 2\lambda)\epsilon + \lambda \delta C, \quad \quad (12)
\]
where the last inequality is due to Assumption 3 and Condition 2. Thus, if we choose $\epsilon < \delta C/4$ and $\lambda > \frac{H(Y)+2\epsilon}{\delta C - 4\epsilon}$, we can get
\[
\hat{L}(\Phi_v) < \hat{L}(\phi) < \hat{L}(\Phi_v).
\]

**Step 2** Denote a proper subset of invariant features as $X_{-v} \subseteq X_v$, and similarly the feature mask as $\Phi_{-v}$.

In Step 1, we have shown that
\[
\hat{L}(\Phi_v) \leq (1 + 2\lambda)\epsilon + H(Y|X_v).
\]

Similar to Equation (12), we have
\[
\hat{L}(\Phi_{-v}) \geq -(1 + 2\lambda)\epsilon + H(Y|X_{-v}).
\]

Then according to Assumption 4 we have
\[
\hat{L}(\Phi_{-v}) - \hat{L}(\Phi_v) \geq -2(1 + 2\lambda)\epsilon + H(y|X_{-v}) - H(y|X_v) \\
\geq -2(1 + 2\lambda)\epsilon + \gamma.
\]

Thus, if $\epsilon < \gamma/(2(1 + 2\lambda))$, we have
\[
\hat{L}(\Phi_{-v}) > \hat{L}(\Phi_v).
\]

In conclusion, with $\lambda \in \left[\frac{H(Y)+1/2\delta C}{\delta C - 4\epsilon} - \frac{1}{2}, \frac{\gamma}{4\epsilon} - \frac{1}{2}\right]$, we can get
\[
\hat{L}(\Phi_v) < \hat{L}(\Phi_v), \quad \forall \Phi \neq \Phi_v.
\]

Notably, there exists a feasible $\lambda$ if $\epsilon < \frac{\gamma\lambda}{1 + 2\lambda + 2\delta C H(Y)}$. The proof is complete by noticing that $\epsilon$ can be chosen arbitrarily according to Assumption 1.

**A.3 Proof of Proposition 1**

**Proof.** Consider the following feature set
\[
X_v := \{X^j : H(Y|X^j, \rho(Z)) = H(Y|X^j) \quad \forall \rho(\cdot)\},
\]
and the corresponding feature mask is denoted as $\Phi_v$.\]
Note that feature \( \mathbf{X}_i \) in Proposition 1 is not in \( \mathbf{X}_v \), so \( \Phi_{\overline{v}} \neq \Phi_v \). By Assumption 1 with a given \( \epsilon \), we can have
\[
\hat{L}(\Phi_{\overline{v}}) \leq (1 + 2\lambda)\epsilon + H(Y|\mathbf{X}_{\overline{v}}) + \lambda(H(Y|\mathbf{X}_v) - H(Y|\mathbf{X}_v, \rho(Z)) = (1 + 2\lambda)\epsilon + H(Y|\mathbf{X}_v)
\]
\[
\leq (1 + 2\lambda)\epsilon + H(Y).
\]
One the other hand, we have
\[
L(\Phi_v) \geq -(1 + 2\lambda)\epsilon + H(Y|\mathbf{X}_v) + \lambda(H(Y|\mathbf{X}_v) - H(Y|\mathbf{X}_v, \rho(Z)))
\]
\[
\geq -(1 + 2\lambda)\epsilon + \lambda\delta(H(Y|\mathbf{X}^i_v) - H(Y|\mathbf{X}^i_v, \rho(Z)))
\]
\[
\geq -(1 + 2\lambda)\epsilon + \lambda\delta C',
\]
which can be shown similarly to Equation (12). Thus, if we choose \( \epsilon < \frac{\delta C'}{4} \) and \( \lambda > \frac{H(Y) + 2\epsilon}{\delta C' - 4\epsilon} \), we would get
\[
\hat{L}(\Phi_{\overline{v}}) < \hat{L}(\Phi_v).
\]

A.4 Proof of Proposition 2

Proof. Denote a feature set \( \mathbf{X}_{v(+)k} \), which contains the invariant feature set \( \mathbf{X}_v \) as well a spurious feature \( \mathbf{X}_{s} X_s \) in Proposition 2.

Similar to Equation (11), we can show that
\[
\hat{L}(\Phi_{v(+)k}) \leq (1 + 2\lambda)\epsilon + H(Y|\mathbf{X}_{v(+)k}).
\]
And similar to Equation (12), we also have
\[
\hat{L}(\Phi_v) \geq -(1 + 2\lambda)\epsilon + H(Y|\mathbf{X}_v).
\]
Then it follows that
\[
\hat{L}(\Phi_v) - \hat{L}(\Phi_{v(+)k}) \geq -2(1 + 2\lambda)\epsilon + H(Y|\mathbf{X}_v) - H(y|\mathbf{X}_{v(+)k})
\]
\[
\geq -2(1 + 2\lambda)\epsilon + \gamma.
\]
If \( \epsilon < \frac{\gamma}{2(1 + 2\lambda)} \), we have
\[
\hat{L}(\Phi_v) > \hat{L}(\Phi_{v(+)k}).
\]
Thus, we cannot identify all the invariant features from Problem 2.

B Additional Theoretical Results

Theorem 3. Consider Assumptions 1-4 and Conditions 1-2 where \( H(\cdot|\cdot) \) is replaced with \( L(\cdot|\cdot) \) accordingly. If \( \epsilon < \frac{C_{\gamma}^3}{4\gamma + 2C_{\delta}L(Y)} \) and \( \lambda \in \left[ \frac{L(Y) + 1/2\gamma}{\delta C' - 4\epsilon} - \frac{1}{2}, \frac{2\epsilon}{\gamma} - \frac{1}{2} \right] \), we have
\[
\hat{L}(\Phi_v) < \hat{L}(\Phi), \quad \forall \Phi \neq \Phi_v,
\]
where we assume \( L(Y) < \infty \). If Condition 1 or Condition 2 is violated, then there exists a feature mask \( \Phi' \neq \Phi_v \) so that
\[
\hat{L}(\Phi_v) > \hat{L}(\Phi').
\]
C More Experimental Details

For the synthetic datasets and the house price prediction dataset, we use the full batch gradient in optimizing. The ERM method is trained for 4000 epochs. The IRM/ZIN method is also trained for 4000 epochs, with annealing in the first 2000 epochs. We train EIIL for 4000 epochs which is divided equally, i.e., 2000 epochs, in the two stages. For the CelebA classification task, we use mini-batch training with batch size of 128. All the methods are trained for 50 epochs, with annealing strategy in the first 25 epochs.