Improving Group Robustness on Spurious Correlation Requires Preciser Group Inference

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Abstract

Standard empirical risk minimization (ERM) models may prioritize learning spurious correlations between spurious features and true labels, leading to poor accuracy on groups where these correlations do not hold. Mitigating this issue often requires expensive spurious attribute (group) labels or relies on trained ERM models to infer group labels when group information is unavailable. However, the significant performance gap in worst-group accuracy between using pseudo group labels and using oracle group labels inspires us to consider further improving group robustness through preciser group inference. Therefore, we propose GIC, a novel method that accurately infers group labels, resulting in improved worst-group performance. GIC trains a spurious attribute classifier based on two key properties of spurious correlations: (1) high correlation between spurious attributes and true labels, and (2) variability in this correlation between datasets with different group distributions. Empirical studies on multiple datasets demonstrate the effectiveness of GIC in inferring group labels, and combining GIC with various downstream invariant learning methods improves worst-group accuracy, showcasing its powerful flexibility. Additionally, through analyzing the misclassifications in GIC, we identify an interesting phenomenon called semantic consistency, which may contribute to better decoupling the association between spurious attributes and labels, thereby mitigating spurious correlation. The code for GIC is available at https://github.com/yujinhanml/GIC.

1. Introduction

The presence of spurious correlation causes machine learning models to fail on certain groups of samples, even when achieving high accuracy on average group (Ribeiro et al., 2016; Beery et al., 2018; Hashimoto et al., 2018; Duchi et al., 2019). Deep networks trained via standard empirical risk minimization (ERM) may be biased by the spurious attributes/features such as the image backgrounds (Beery et al., 2018; Geirhos et al., 2020), which admit different correlations with the true labels for the different groups of data. As a result, the model typically performs well on the majority group of data that aligns with the spurious attributes but performs poorly on certain groups of data that have no or even opposite correlations with spurious attributes. This critical issue is widespread in many fields, such as medical AI, facial recognition and sentiment analysis (Blodgett et al., 2016; Tatman, 2017; Gururangan et al., 2018; Badgeley et al., 2019; Sagawa et al., 2019).

There have emerged a series of previous works that aim to develop more robust training methods to improve the worstgroup performance when group information is available. For instance, one can focus on particularly training over the worst-group risk (Sagawa et al., 2019) via group distributional robust optimization (GroupDRO). Additionally, the spurious correlation can also be eliminated by balancing the risk in different groups, which can be achieved via feature reweighting (Kirichenko et al., 2022) or selective Mixup (Yao et al., 2022). These methods have been demonstrated to be effective to mitigate the spurious correlations, leading to substantial improvements over ERM.

However, group labeling is expensive, labor-intensive, and human-biased. It is more important and practical to develop robust algorithms for improving worst-group accuracy when the group information is unavailable (Liu et al., 2021; Zhang et al., 2022). In such a scenario, a line of recent works (Sohoni et al., 2020; Nam et al., 2020; Ahmed et al., 2020; Liu et al., 2021; Zhang et al., 2022; Chen et al., 2023) propose to first infer the data groups, and then seek to train a robust model according to the estimated group information. For instance, JTT (Liu et al., 2021) identifies the data being misclassified by the ERM as the minority group, and trains a more robust model via upweighting the examples in mi-

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nority groups; CnC (Zhang et al., 2022) infers pseudo group labels via ERM and develops a contrastive learning method across groups to train the final model.

The primary focus of the aforementioned research is on invariant learning, i.e., leveraging the group information obtained from ERM to learn the invariant attributes. However, the accuracy of group label inference has been overlooked, making the existing group inference-based methods perform significantly worse than those using oracle group labels. Very recently, some group inference methods have been developed as alternatives to ERM, such as EIIL (Creager et al., 2021), SSA (Nam et al., 2022), ZIN (Lin et al., 2022) and DISC (Wu et al., 2023). However, they may either struggle with complex spurious correlations (e.g., EIIL) (Lin et al., 2022), or require additional information (e.g., human inspection, few spurious annotations, etc) that is related to the group labels (e.g., SSA, ZIN, and DISC). Therefore, noticing the performance shortcomings and applicability limitations in existing group inference methods, we raise an important yet challenging question:

Can we develop a more accurate group inference method to mitigate spurious correlations without relying on any additional information?

In this work, we propose GIC (Group Inference via data Comparison), a novel, practical and accurate method to infer group labels, which can be then seamlessly incorporated into a variety of oracle group label-based robust learning methods to improve the worst-group performance. In particular, GIC adopts a (unlabeled) comparison dataset, which has (slightly) different group distribution compared to the training dataset, and infers the group information in a contrastive manner. More specifically, GIC trains an alternative classifier to assign spurious attribute labels to data points solely on their spurious attributes, where the training objective is designed to encourage discovering the distribution discrepancy between the comparison and training dataset while maintaining the high correlation between the spurious attribute label and true label in the training dataset. Notably, unlike previous methods that may rely on (partial) group labels or human inspections, obtaining the comparison data does not necessitate any assumptions. It does not need to be labeled and can be obtained from various sources, such as a validation set with true validation labels, a completely unlabeled subset sampled from the test data, or even directly resampled from the training dataset in a non-uniform manner. We highlight the main contributions as follows:

 We propose GIC, a principled method for more accurate group inference. It encourages the high correlation between predicted spurious attribute labels and true labels on the training set, while emphasizing the differences in this correlation between training and comparison data. Compared with existing group inference methods, GIC consistently achieves higher recall and precision in predicting groups for various datasets (see Section 4.4).

- 2. We show that the proposed GIC can seamlessly integrate with multiple invariant learning algorithms to improve the worst-group accuracy. In Section 4.3 and 4.4, GIC is successfully combined with Mixup (Yao et al., 2022), GroupDRO (Creager et al., 2021), Upsample (Liu et al., 2021), and Subsample (Kirichenko et al., 2022). It can be seen that GIC consistently outperform baselines in terms of the worst-group accuracy, for all candidate invariant learning algorithms. More importantly, when integrated with Mixup, our model improves over the state-of-the-art for nearly all tasks when the group label is unavailable. Additionally, the average and worst-group accuracy of our model can almost match that of using oracle group labels directly. This further justifies the effectiveness of our group inference method.
- 3. We illustrate that GIC can infer reasonable groups that differ from human decisions in Section 4.5. Analysis of misclassified examples reveals GIC's semantic consistency, where similar semantic instances are assigned to the same group, although they are not categorized into the same group by human decisions. This semantic consistency benefits methods like Mixup, which rely on distorting semantics for invariant learning, leading to improved worst-group accuracy compared to using oracle group labels. It highlights the potential effectiveness and improvements of integrating GIC with human decisions when group information defined by humans is accessible.

2. Related Work

Recent research shows that the traditional ERM can learn both spurious and invariant features (Kirichenko et al., 2022; Izmailov et al., 2022; Rosenfeld et al., 2022; Chen et al., 2023). However, with strong spurious correlations, ERM tends to prioritize learning the spurious features (Chen et al., 2023), which hinders its ability to generalize on data where these spurious correlations are absent. To tackle this issue, invariant feature learning, referred to as invariant learning for simplicity, has been introduced to learn invariant representations. A notable approach to invariant learning is the use of group robustness methods.

When group labels are available, some classical group robustness methods, such as GroupDRO (Sagawa et al., 2019), attempt to minimize the worst-group loss instead of the average loss using oracle group labels. Other methods aim to achieve invariant learning by balancing the majority and minority groups, such as reweighting (Sagawa et al., 2020), regularization (Cao et al., 2019), and downsampling (Kirichenko et al., 2022). Additionally, approaches like semi-supervised learning (Nam et al., 2022; Sohoni et al., 2021) or Mixup (Yao et al., 2022), which selectively combine samples with matching labels but differing spurious attributes or matching spurious attributes but differing labels, are also be considered to improve the the worst-group accuracy. Some methods attempt to infer group labels by training a simple ERM (Blodgett et al., 2016; Tatman, 2017; Gururangan et al., 2018; Badgeley et al., 2019; Sagawa et al., 2019), maximizing the GroupDRO loss (Creager et al., 2021), or even introducing human knowledge (Lin et al., 2022; Wu et al., 2023) when group information is unknown. However, these group inferred methods have performance gaps compared to group annotation utilized methods and may not be applicable when prior information is unavailable. In this work, we focus on group robustness without relying on any group labels or human-provided information.

We point out that, although we aims to learn invariant features to train more robust and generalizable models, similar to classical domain adaptation (Blanchard et al., 2011; Muandet et al., 2013) methods, such as UDA (Ganin & Lempitsky, 2015) and DANN (Ganin et al., 2016), our setting differs from them which divide the training data into source and target domains and use the source and target features, along with the source labels, to transfer knowledge to the specific target domain (Zhang et al., 2022). In contrast, we do not have a natural source and target domains and strive to enhance the accuracy of specific groups affected by spurious correlations, without prior knowledge of training sample domains or spurious attributes.

3. Method

3.1. Problem Setup

Consider the training dataset \mathcal{D} , which comprises n data point-label pairs, where each data point-label pair belongs to some group $g \in \mathcal{G}$, denoted as $\mathcal{D} = \{(\mathbf{x}_i, y_i, g_i)\}_{i=1}^n$. Following previous work (Liu et al., 2021; Zhang et al., 2022; Yao et al., 2022; Yang et al., 2023), we consider each group q = (y, a) to be jointly defined by the label $y \in \mathcal{Y}$ and unobserved spurious attributes $a \in \mathcal{A}$ (i.e., $\mathcal{G} = \mathcal{Y} \times \mathcal{A}$), where the spurious attribute a is spuriously correlated with the label y (e.g., the image background and the image label). We denote y_s as the spurious attribute label of a (e.g., the label of the image background, which can be "land" versus "water" or "red" versus "green"). The groups q in dataset \mathcal{D} often encounter the imbalance issue, where ERM training tends to mostly depend on majority groups, thus may memorize the spurious correlation contributed by these groups. However, such spurious correlations are often absent or even oppositely appearing in minority groups. Therefore, our ultimate objective is to train a robust model $f_{\rm robust}(\theta)$, parameterized by $\theta \in \Theta$, capable of classifying an input \mathbf{x}_i to a label y_i regardless of whether it belongs to the majority or minority group. This is referred to as the

worst-group accuracy defined as follows:

$$\max_{q \in \mathcal{G}} \mathbb{E}[\mathbb{1}[f_{\theta}(\mathbf{x}) \neq y]|g], \tag{1}$$

where \mathcal{G} denotes the set of groups. In this paper, we consider the setting in that the group information is unavailable, one can only train the robust classifier f_{robust} using the ungrouped data. Moreover, instead of using raw data point x, we can also make use of its feature representation, which is obtained by training a model from scratch via ERM or directly using a pretrained model. We define the feature representation of x as follows:

$$\mathbf{z} = \Phi(\mathbf{x}),\tag{2}$$

where $\Phi(\cdot)$ is a feature extractor.

3.2. GIC: Group Inference via data Comparison

We now introduce GIC (Groups Inference via data Comparison), a principled and novel method that infers spurious attribute (group) labels and contributes to mitigating spurious correlations. The *goal of GIC* is to train a spurious attribute classifier to predict the spurious attribute label y_s , i.e.,

$$\hat{y}_{s,\mathbf{w}} = f_{\text{GIC}}(\mathbf{z}; \mathbf{w}), \tag{3}$$

where **w** is weights of GIC model f_{GIC} . Then using the predicted $\hat{y}_{s,\mathbf{w}}$, GIC partitions the data into different groups, i.e., $\hat{g} = (y, \hat{y}_{s,\mathbf{w}})$. The inferred group \hat{g} can be integrated into downstream invariant learning methods, aiding in training the robust model f_{robust} .

Comparison data. Before formally introducing details of GIC, we first introduce the concept of comparison data. We assume access to a dataset C, where its group distribution (slightly) differs from the training data D, e.g., the group distribution of D is $(g_1, g_2) = (0.1, 0.9)$, while the group distribution of C is $(g_1, g_2) = (0.2, 0.8)$. We refer to C as *comparison data*, which can have true labels or be unlabeled. We remark that the comparison data is easy to obtain, which will be thoroughly discussed in Section 3.4.

Based on the definition of spurious attribute labels y_s , an ideal spurious attribute prediction $\hat{y}_{s,w}$ should exhibit the following two properties: (1) It should be highly correlated with the true label y. It is this high correlation between the spurious attribute label and the true label that biases the ERM-based model training. (2) The correlation between $\hat{y}_{s,w}$ and y varies across different datasets. Unlike the invariant attribute label, which is always equivalent to the true label, the correlation between the spurious attribute label is spurious, changing with the spurious attribute distribution across different datasets. Consider an extreme case, the spurious background attribute for both waterbirds and landbirds in the comparison data accounts for 50%, while in the training set, the spurious attribute label

is completely equivalent to the true label (e.g., $y_s = y$). The equivalence correlation that exists in the training data does not hold in the comparison data.

Based on the mentioned two properties, we design the optimization objective of GIC, which consists of two terms: (1) **Correlation Term**, used to describe the high correlation between $\hat{y}_{s,w}$ and y in the training data; (2) **Spurious Term**, used to describe the discrepancy in the correlation between the training and comparison data, aiming to emphasize the correlation is spurious rather than invariant. By jointly optimizing the above objectives, GIC is encouraged to train a spurious attribute classifier that yields the spurious attribute prediction $\hat{y}_{s,w}$, as shown in Equation (3).

Correlation Term. To encourage the high correlation between y and $\hat{y}_{s,\mathbf{w}}$ in the training set, we consider the following optimization objective:

$$\max_{\mathbf{w}} I(y^{tr}; \hat{y}^{tr}_{s, \mathbf{w}}), \tag{4}$$

where $\hat{y}_{s,\mathbf{w}}^{tr} = f_{\text{GIC}}(\mathbf{z}^{tr}; \mathbf{w})$ is the predicted spurious attribute label on training data. Here, mutual information is considered due to its widespread usage to measure the correlation or dependency between random variables (Li & Jurafsky, 2016; Kong et al., 2019; Pan et al., 2020; Su et al., 2023). We aim to maximize the mutual information between y_s and y, encouraging the predicted spurious attribute label y_s from GIC to be highly correlated with the true label y.

Solely satisfying Equation (4) is not enough as invariant attribute information contained in feature representations (Kirichenko et al., 2022; Chen et al., 2023) can also exhibit high correlation with true labels. To aid GIC in learning spurious attributes instead of invariant ones, we introduce an additional spurious term.

Spurious Term. We use conditional probability to describe the correlation between $\hat{y}_{s,\mathbf{w}}$ and y, i.e., $\mathbb{P}(y|\hat{y}_{s,\mathbf{w}})$. Then let $\mathbb{P}(y^{tr}|\hat{y}_s^{tr})$ and $\mathbb{P}(y^c|\hat{y}_s^c)$ be the conditional distributions in the training and comparison dataset respectively, we will characterize their discrepancy. Since we are comparing distributions with the same support, we opt for the simplest and widely used choice (Ahmed et al., 2020; Lee et al., 2022), the KL-divergence. Then, we maximize the following objective to encourage GIC to learn spurious attributes:

$$\max_{\mathbf{w}} \mathrm{KL}(\mathbb{P}(y^{tr}|\hat{y}_{s,\mathbf{w}}^{tr})||\mathbb{P}(y^{c}|\hat{y}_{s,\mathbf{w}}^{c})), \tag{5}$$

where $\hat{y}_{s,\mathbf{w}}^c = f_{\text{GIC}}(\mathbf{z}^c; \mathbf{w})$ is the estimated spurious attribute labels on the comparison data.

Note that a more formal expression for Equation (5) should use different distribution notations and the same variable names, i.e.,

$$\max_{\mathbf{w}} \operatorname{KL}(\mathbb{P}_{\operatorname{tr}}(y|\hat{y}_{s,\mathbf{w}})||\mathbb{P}_{\operatorname{c}}(y|\hat{y}_{s,\mathbf{w}}))$$
(6)

where $\mathbb{P}_{tr}(y|\hat{y}_{s,\mathbf{w}}) := \mathbb{P}(y^{tr}|\hat{y}_{s,\mathbf{w}}^{tr})$ and $\mathbb{P}_{c}(y|\hat{y}_{s,\mathbf{w}}) := \mathbb{P}(y^{c}|\hat{y}_{s,\mathbf{w}}^{c})$. Here, distinct variable names, such as $\hat{y}_{s,\mathbf{w}}^{tr}$ and $\hat{y}_{s,\mathbf{w}}^{c}$, are utilized to indicate their origins from different (training or comparison) datasets, thereby emphasizing GIC can achieve improved group inference via data comparison.

The essence of maximizing Equation (5) is to encourage GIC to learn spurious attributes by violating the invariant learning principle (Creager et al., 2021). If $\hat{y}_{s,\mathbf{w}}$ is inferred based on invariant attributes rather than spurious ones, then $\mathbb{P}(y^{tr}|\hat{y}_{s,\mathbf{w}}^{tr})$ and $\mathbb{P}(y^c|\hat{y}_{s,\mathbf{w}}^c)$ will be identical and then

$$\mathrm{KL}(\mathbb{P}(y^{tr}|\hat{y}_{s,\mathbf{w}}^{tr})||\mathbb{P}(y^c|\hat{y}_{s,\mathbf{w}}^c)) = 0.$$
(7)

Conversely, if $\hat{y}_{s,\mathbf{w}}$ is based on spurious attributes rather than invariant attributes, the inequality

$$\operatorname{KL}(\mathbb{P}(y^{tr}|\hat{y}_{s,\mathbf{w}}^{tr})||\mathbb{P}(y^{c}|\hat{y}_{s,\mathbf{w}}^{c})) \ge 0$$
(8)

holds, where the equality holds only when the training and comparison data share the same group distribution. Therefore, maximizing Equation (5) entails encouraging GIC to prioritize learning spurious attributes over invariant ones.

Algorithm 1 GIC

Input: Training data \mathcal{D} ; comparison data \mathcal{C} ; feature extractor $\Phi(\cdot)$; weighting parameters γ ; training epochs K of GIC **Stage 1: Extracting feature representations** Obtain $\mathbf{z}^{tr} = \Phi(\mathbf{x}^{tr}), \mathbf{z}^{c} = \Phi(\mathbf{x}^{c})$ where $\mathbf{x}^{tr} \in \mathcal{D}, \mathbf{x}^{c} \in \mathcal{D}$ С. Stage 2: Inferring group labels Initialize the parameters w for spurious attribute classifier f_{GIC}. for epoch 1 to K do if the true label of C is available then Optimizing Equation (11) to update w. else Optimizing Equation (12) to update w. end if end for Infer spurious attribute labels $\hat{y}_{s,\mathbf{w}}^{tr} = f_{\text{GIC}}(\mathbf{z}^{tr}; \mathbf{w}).$ **Return:** Pseudo group labels $\hat{g} = (y^{tr}, \hat{y}^{tr}_{s, \mathbf{w}})$.

Overall Objective. By combining Equation (4) and (5), we derive the overall objective of GIC as follows:

$$\max_{\mathbf{w}} I(y^{tr}; \hat{y}_{s,\mathbf{w}}^{tr}) + \gamma \mathrm{KL}(\mathbb{P}(y^{tr}|\hat{y}_{s,\mathbf{w}}^{tr}) || \mathbb{P}(y^c|\hat{y}_{s,\mathbf{w}}^c)), \quad (9)$$

where $\gamma \ge 0$ is a weighting parameter used to balance Correlation Term and Spurious Term.

However, the overall objective of GIC faces certain practical issues. Firstly, the mutual information term is difficult to accurately estimate (Paninski, 2003; Belghazi et al., 2018).



Figure 1. Decision boundary visualization. f_{ERM} underperforms f_{GIC} in recognizing spurious attributes and f_{robust} in identifying invariant attributes. Classes 0 and 1 are represented by colors (red and blue), respectively, with shapes marking spurious attributes.

Secondly, Equation (9) cannot handle the situation where the comparison data is unlabeled, which limits the applicability of GIC in various scenarios.

We first replace the mutual information $I(y^{tr}; \hat{y}_{s,\mathbf{w}}^{tr})$ with the cross-entropy $H(y^{tr}, \hat{y}_{s,\mathbf{w}}^{tr})$ to achieve accurate estimation. A detailed proof in Appendix A.1 demonstrates that $-H(y^{tr}, \hat{y}_{s,\mathbf{w}}^{tr})$ is, in fact, a lower bound of $I(y^{tr}; \hat{y}_{s,\mathbf{w}}^{tr})$. Therefore, maximizing $I(y^{tr}; \hat{y}_{s,\mathbf{w}}^{tr})$ can be achieved by minimizing $H(y^{tr}, \hat{y}_{s,\mathbf{w}}^{tr})$. This replacement aligns with intuition because maximizing mutual information between y^{tr} and $\hat{y}_{s,\mathbf{w}}^{tr}$ essentially encourages a closer alignment of their distributions, which is consistent with the objective of minimizing cross-entropy $H(y^{tr}, \hat{y}_{s,\mathbf{w}}^{tr})$.

We then extend GIC to the case where the true label y^c of the comparison data are not available. We substitute the true labels y^c with the comparison data's feature representation \mathbf{z}^c , which strongly associates with y^c and is always accessible. We present the following theorem:

Theorem 3.1. [Lower Bound of Spurious Term without y^c] Given representations \mathbf{z}^{tr} and \mathbf{z}^c , the spurious term is lower bounded by the following expression as:

$$\operatorname{KL}(\mathbb{P}(y^{tr}|\hat{y}_{s,\mathbf{w}}^{tr})||\mathbb{P}(y^{c}|\hat{y}_{s,\mathbf{w}}^{c}) \geq \operatorname{KL}(\mathbb{P}(\mathbf{z}^{tr}|\hat{y}_{s,\mathbf{w}}^{tr})||\mathbb{P}(\mathbf{z}^{c}|\hat{y}_{s,\mathbf{w}}^{c}))$$
(10)

In Theorem 3.1, when y^c is missing, we resort to maximizing the lower bound $\operatorname{KL}(\mathbb{P}(\mathbf{z}^{tr}|\hat{y}_{s,\mathbf{w}}^{tr})||\mathbb{P}(\mathbf{z}^c|\hat{y}_{s,\mathbf{w}}^c))$ as an alternative. We point out that maximizing a lower bound is meaningful as it provides the worst-case guarantee over the original objective. The detailed proof of Theorem 3.1 is provided in Appendix A.1.

Therefore, based on whether y^c is accessible, we propose the following two optimization objectives:

With y^c . The overall objective of GIC can be defined as:

$$\min_{\mathbf{w}} H(y^{tr}, \hat{y}_{s,\mathbf{w}}^{tr}) - \gamma \mathrm{KL}(\mathbb{P}(\mathbf{y}^{tr} | \hat{y}_{s,\mathbf{w}}^{tr}) || \mathbb{P}(\mathbf{y}^{c} | \hat{y}_{s,\mathbf{w}}^{c})).$$
(11)

Without y^c . The overall objective of GIC can be redefined



Figure 2. Evaluation of group label inference. Compared to baseline methods such as ERM and EIIL, GIC significantly improves the recall for minority group label inference while maintaining a relatively high precision.

as:

$$\min_{\mathbf{w}} H(y^{tr}, \hat{y}_{s,\mathbf{w}}^{tr}) - \gamma \mathrm{KL}(\mathbb{P}(\mathbf{z}^{tr} | \hat{y}_{s,\mathbf{w}}^{tr}) || \mathbb{P}(\mathbf{z}^{c} | \hat{y}_{s,\mathbf{w}}^{c})).$$
(12)

When implementing the objective (11) and (12), we further adopt a more computationally tractable form involving the difference between joint and marginal distributions to replace conditional probability distributions. Taking the case with the label y^c as an example, we consider

$$\begin{aligned} \operatorname{KL}(\mathbb{P}(y^{tr}|\hat{y}_{s,\mathbf{w}}^{tr})||\mathbb{P}(y^{c}|\hat{y}_{s,\mathbf{w}}^{c})) \\ &= \operatorname{KL}(\mathbb{P}(y^{tr},\hat{y}_{s,\mathbf{w}}^{tr})||\mathbb{P}(y^{c},\hat{y}_{s,\mathbf{w}}^{c})) - \operatorname{KL}(\mathbb{P}(\hat{y}_{s,\mathbf{w}}^{tr}))||\mathbb{P}(\hat{y}_{s,\mathbf{w}}^{c})) \end{aligned}$$
(13)

and then the MINE algorithm (Belghazi et al., 2018) is employed to estimate these $KL(\cdot||\cdot)$ terms. The pseudocode, outlined in Algorithm 1, presents a comprehensive procedure for utilizing GIC to infer group labels.

3.3. Learning Robust Classifier with GIC

After obtaining the spurious attribute label $\hat{y}_{s,\mathbf{w}}$, we then infer the group label as $\hat{g} = (y, \hat{y}_{s,\mathbf{w}})$. The inferred groups \hat{g} can be used with downstream invariant learning methods to learn invariant attributes and train a robust model f_{robust} . For example, we can use Subsample technique to construct a balanced dataset by retaining all data from the smallest group and subsampling the data from the other inferred groups to match the same size for training f_{robust} .

In Section 4, we experiment with various downstream learning algorithms, demonstrating that the inferred groups from GIC can be flexibly utilized by diverse invariant learning algorithms to learn invariant features. This facilitates the training of robust models, denoted by $f_{\rm robust}$, which effectively mitigate spurious correlations.

3.4. How to Obtain the Comparison Data

Comparison data C with different group distributions from the training data is crucial in implementing GIC. The



Figure 3. Visualization of evaluated datasets with minority groups marked by red boxes. The spurious attribute and targets exhibit strong spurious correlations, while these correlations typically does not hold for minority groups.

sources for comparison data are diverse, such as using a (labeled) validation data, or sampling from the unlabeled test data. In previous works, the validation set is often required to serve as a crucial basis for parameter selection (Liu et al., 2021; Zhang et al., 2022; Creager et al., 2021), and even directly participate in model training, aiding in group inference (Nam et al., 2022).

In challenging scenarios where both the validation set and the test set are inaccessible, we can manually create comparison data from the training set. This can be accomplished by resampling the training dataset in a non-uniform manner, such as adjusting the sampling weight based on the trained ERM's prediction, as shown in JTT (Liu et al., 2021). Specifically, the error set (missclassification set) of a trained ERM often represents minority groups where the spurious correlation no longer exists. By sampling from the error set and non-error set, we can artificially construct comparison data with different group distributions.

Although non-uniform sampling from the training set can ensure the availability of labeled comparison data, we still emphasize the reason we consider the unlabeled comparison data, such as sampling from the test set, is that in the real world, unlabeled data is often cheaper, abundant and easier to obtain (Shejwalkar et al., 2023; Göpfert et al., 2019). And subsequent analysis in Appendix C.4 supports that abundant comparison data is beneficial for the performance of GIC. By incorporating unlabeled comparison data, the applicability of GIC is enhanced.

3.5. The Relationship between GIC and ERM

In this section, we highlight the relationship between GIC and ERM. When there is no difference in group distribution between training and comparison data, or the weighting parameter $\gamma = 0$, GIC degenerates to ERM in terms of group label inference. the KL loss in (11) and (12) is minimal,

indicating a reduced impact of the spurious term. Consequently, the CE loss becomes predominant, causing GIC to effectively become an ERM-based group inference method.

Although ERM can still be used for inferring group labels, it lacks the crucial spurious term necessary to violate the principle of invariant learning and to effectively identify spurious features. Thus, ERM-based inference should serve as the performance baseline for GIC's group label performance which is validated by subsequent experiments. Moreover, GIC can also be viewed as a special ERM-based group inference method where the spurious term functions as a regularization term. By incorporating insights from the comparison data, the spurious term encourages the trained neural network to differentiate between spurious and invariant features, thus enhancing group label inference.

4. Experiments

Through our experimental evaluation, the primary goal is to address the following questions: (1) The effectiveness of GIC in mitigating spurious correlations: Can GIC successfully enhance worst-group accuracy and mitigate spurious correlation issues? (2) The accuracy of GIC in inferring group labels: Can GIC reliably predict group labels? (3) Analysis of misclassified cases: What factors contribute to misclassifications by GIC for certain instances?

Our experimental results will be presented in the order of the three questions mentioned above. In experiments, we use $\text{GIC}_{\mathcal{C}_y}$ to denote the scenario where the comparison data has true labels, and $\text{GIC}_{\mathcal{C}}$ to denote the scenario where the comparison data is unlabeled.

4.1. Experiments on Synthetic 2D Data

We start with a synthetic 2D dataset to demonstrate how GIC helps train a more robust model by learning spurious

<i>Table 1.</i> Average and worst-group accuracy comparison (%). Baselines are divided into two types based on whether group labels are
required, and we highlight the <u>1st</u> worst-group and the <u>2nd</u> worst-group results for the non-group label class. \checkmark denotes the use of
training/validation group labels for training. GIC demonstrates strong advantages in baselines without group labels, even competing with
methods with group labels on certain datasets.

Method	Group Labels	CMI	VIST	Wate	rbirds	Cel	ebA	CivilCor	nments
Method	Train / Val	Avg.	Worst	Avg.	Worst	Avg.	Worst	Avg.	Worst
			Oracle (Group labels	are require	d			
GroupDRO	√/×	74.4 ± 0.5	$69.8{\scriptstyle\pm2.6}$	$92.0\pm$ 0.6	89.9 ± 0.6	91.2 ± 0.4	87.2 ± 1.6	89.9±0.5	70.0 ± 2.0
LISA	$\sqrt{/\times}$	74.0 ± 0.1	$73.3{\scriptstyle \pm 0.2}$	91.8 ± 0.3	$89.2{\pm}0.6$	92.4 ± 0.4	$89.3{\scriptstyle\pm1.1}$	89.2±0.9	72.6 ± 0.1
DFR	\times/\checkmark	72.2 ± 1.1	70.6 ± 1.1	$94.2{\pm}_{0.4}$	$92.9{\scriptstyle \pm 0.2}$	91.3 ± 0.3	$88.3{\pm}_{1.1}$	87.2 ± 0.3	70.1 ± 0.8
SSA	×/√	$75.0{\scriptstyle \pm 0.3}$	$71.1{\pm}_{0.4}$	$92.2{\scriptstyle\pm0.9}$	$89.0{\pm}_{0.6}$	92.8 ± 0.1	$89.8{\scriptstyle\pm1.3}$	88.2 ± 2.0	$69.9{\scriptstyle\pm2.0}$
			Oracle Gr	oup labels a	re not requi	red			
ERM	\times / \times	12.9 ± 0.8	$3.4{\pm}0.9$	97.3 ± 1.0	62.6±0.3	94.9±0.3	$47.7{\scriptstyle\pm2.1}$	92.1±0.4	58.6±1.7
JTT	\times / \times	$76.4{\scriptstyle\pm3.3}$	$67.3{\pm}_{5.1}$	89.3 ± 0.7	$83.8{\pm}_{1.2}$	88.1 ± 0.3	$81.5{\scriptstyle \pm 1.7}$	91.1	69.3
EIIL	\times / \times	$74.1{\scriptstyle \pm 0.2}$	$65.5{\scriptstyle\pm5.1}$	96.5 ± 0.2	77.2 ± 1.0	85.7 ± 0.1	$81.7{\pm}0.8$	90.5 ± 0.2	$67.0{\scriptstyle \pm 2.4}$
CnC	\times / \times	-	-	$90.9{\scriptstyle \pm 0.1}$	<u>88.5</u> ±0.3	89.9 ± 0.5	$88.8{\pm}_{0.9}$	81.7 ± 0.5	$68.9{\pm}_{2.1}$
$\operatorname{GIC}_{\mathcal{C}_y}$ -M	\times/\times	$73.2{\pm}_{0.2}$	<u>72.2</u> ±0.5	89.6±1.3	<u>86.3</u> ±0.1	91.9±0.1	$\underline{89.4} \pm 0.2$	90.0±0.2	<u>72.5</u> ±0.3
$\operatorname{GIC}_{\mathcal{C}}$ -M	\times / \times	$73.1{\pm}_{0.5}$	$\underline{71.7}\pm0.3$	89.3 ± 0.8	85.4 ± 0.1	92.1 ± 0.1	<u>89.5</u> ±0.0	89.7±0.0	$\underline{72.3}\pm0.2$

attributes. The synthetic dataset consists of training (\mathcal{D}^{tr}) , validation $(\mathcal{D}^{val}$ which is the labeled comparison data \mathcal{D}^c), and test (\mathcal{D}^{ts}) sets. There is a spurious correlation in \mathcal{D}^{tr} , where true labels are highly correlated with the spurious attribute \mathbf{x}_1 , while \mathcal{D}^c and \mathcal{D}^{ts} have correlations with the invariant feature \mathbf{x}_2 . More details about the synthetic data can be found in Appendix B.1. Figure 1 shows the decision boundaries of the traditional ERM model f_{ERM} , the spurious attribute classifier f_{GIC} , and the retrained robust model f_{robust} using inferred group labels from f_{GIC} and the Subsample strategy. We also train ERM models exclusively on the invariant feature (denoted as $f_{\text{invariant}}$) and the spurious feature (denoted as f_{spurious}).

We observe that the spurious attribute has a significant negative impact on $f_{\rm ERM}$, resulting in its decision boundary that is far from $f_{\rm invariant}$. In contrast, the decision boundary of $f_{\rm robust}$ is much closer to $f_{\rm invariant}$, indicating its robustness achieved by leveraging the more balanced training data constructed by GIC. Furthermore, $f_{\rm GIC}$ has a decision boundary that is much closer to $f_{\rm spurious}$ compared to $f_{\rm ERM}$, indicating that GIC is better at capturing spurious attributes than ERM-based group inference methods.

4.2. Experiments on Real-World Data

Real-World Datasets. We explore datasets in image and text classification that exhibit spurious correlations. For instance, CMNIST (Arjovsky et al., 2019) involves digit recognition with spurious features where digit colors (red or green) are linked to digit values. Waterbirds (Sagawa et al.,

2019) associates bird types with a spurious background attribute (water or land). CelebA (Liu et al., 2015) focuses on hair color recognition influenced by spurious gender-related features. CivilComments-WILDS (Borkan et al., 2019; Koh et al., 2021) aims to distinguish toxic from non-toxic online comments, with labels spuriously correlated with mentions of demographic identities. Figure 3 represents the spurious attributes and training targets of these datasets. Appendix B.2.1 provides a detailed group distribution description of these datasets. In the main text, we primarily use labeled and unlabeled validation sets as comparison data to demonstrate the effectiveness of GIC when comparison data is directly available. The experimental evidence in Appendix C.4 further illustrates the effectiveness of constructing comparison data through non-uniform sampling from the training set.

Baselines. For methods that address spurious correlation while requiring group labels, we consider GroupDRO (Sagawa et al., 2019), DFR (Kirichenko et al., 2022), LISA (Yao et al., 2022), and SSA (Nam et al., 2022). We also compare against methods that tackle spurious correlation without requiring group labels, namely, ERM, JTT (Liu et al., 2021), CnC (Zhang et al., 2022), and EIIL (Creager et al., 2021). ERM serves as a lower bound baseline, representing a basic training method without specific techniques to improve the accuracy of the worst-group. Additionally, we evaluate the accuracy of GIC in inferring group labels by comparing it to ERM and EI (the inferring group method of EIIL) and assess the GIC's performance when using Mixup, Subsample, Upsample, and GrouDRO as downstream invariant learning methods. Detailed information on these methods can be found in Appendix B.2.2.

Model Training. Following stages outlined in Algorithm 1, we provide a details of models and parameters used, particularly the selection of crucial hyperparameters training epoch K and weight parameter γ in Appendix B.2.3.

Evaluation. In order to assess how well GIC tackles spurious correlations, we report the average and worst-group accuracy for all baselines. Furthermore, to evaluate the accuracy of GIC in inferring group labels, we report the precision (proportion of correctly inferred examples belonging to the true minority group) and recall (proportion of examples from the true minority group correctly inferred) of minority groups. We focus on minority groups because their small sample size presents challenges for accurate group inference and successfully identifying these minority groups is crucial as spurious correlations often do not hold for them.

4.3. The Effectiveness of GIC in Mitigating Spurious Correlations

Table 1 showcases the average and worst-group accuracies for all methods. We specifically highlight GIC's performance when combined with Mixup (denoted as GIC_{C_u} -M and $\operatorname{GIC}_{\mathcal{C}}$ -M). In comparison to methods that train without leveraging group information, GIC_{C_u} -M and GIC_{C} -M consistently achieve higher worst-group accuracy across all datasets. Notably, even when compared to methods that incorporate group information during training, GIC_{C_u} -M and $\operatorname{GIC}_{\mathcal{C}}\text{-}M$ deliver impressive results, particularly on CelebA and CivilComments datasets, where GIC_{C_u} -M almost matches the performance of baselines that utilize group labels. Furthermore, we observe that methods without group labels demonstrate weaker performance on worst-group accuracy compared to oracle group label-based methods. This discrepancy is especially pronounced when employing the same invariant learning algorithm (e.g., GroupDRO and EIIL, GIC_{C_{y}}-M and LISA). It underscores the necessity of further enhancing the accuracy of inferred group labels to boost the worst-group accuracy. The baselines, including JTT, CNC, EIIL, and SSA, tune hyperparameters and employ early stopping based on the highest worst-group accuracy observed on the validation set. Similarly, we also consider using the highest worst-group accuracy of the validation set with group labels as a criterion to ascertain the optimal number of training epochs. The ablation studies detailed in Appendix C.2 highlight the importance of early stopping as a strategy in the GIC framework.

4.4. The Accuracy of GIC in Inferring Group Labels

We then delve deeper into comparing the performance of GIC, ERM, and EI in inferring group labels of minority groups. In Figure 2, we find that GIC exhibits higher precision compared to the baselines on almost all datasets. This



Figure 4. Misclassified samples on CelebA. The semantic consistency in GIC leads to the misclassification of women with short hair (a typical characteristic of males) as males (91.7%), and men with long hair (a typical characteristic of females) as females (8.3%).

higher precision suggests that the minority groups estimated by GIC have low redundancy, thereby increasing the possibility of utilizing true minority group examples to assist in training robust models for downstream tasks. Furthermore, GIC's primary advantage lies in its high recall, consistently maintained at over 60% and even surpassing 80% in CM-NIST, CelebA, and CivilComments. The high recall rate indicates the estimated minority groups by GIC contain more diverse samples from true minority groups which can provide more discriminative information for downstream invariant learning tasks (Gong et al., 2019).

In Table 3, we present our findings on combining GIC, ERM, and EI with various invariant learning algorithms, including GroupDRO (Duchi et al., 2019), Subsample (Kirichenko et al., 2022), and Upsample (Liu et al., 2021). Our worstgroup results show that GIC consistently outperforms the baselines across different downstream algorithms, further emphasizing its superiority in group inference and worstgroup performance improvement. The ablation results concerning the use of the early stopping strategy when training robust models are also shown in the Appendix C.2.

4.5. Error Case Analysis

In this section, we then focus on the underlying factors contributing to these errors via visualizing the misclassified samples. Figure 4 shows examples from the CelebA dataset, where the spurious attribute is gender (woman and man), and the association between hair color and gender is considered spurious, such as blonde hair is correlated with women. We note an interesting phenomenon known as semantic consistency in GIC. For instance, GIC misclassifies women with short hair as men, who bear a strong semantic resemblance to correctly classified male samples with short

Method	+Group	DRO	+Subsc	ımple	+Upsa	mple	+Mix	кир
Method	Waterbirds	CelebA	Waterbirds	CelebA	Waterbirds	CelebA	Waterbirds	CelebA
ERM	$75.6 {\pm} 0.4$	77.2 ± 0.1	79.4 ± 0.3	78.5 ± 0.1	83.8 ± 1.2	81.5 ± 1.7	82.1±0.8	80.6 ± 1.7
EI	77.2 ± 1.0	81.7 ± 0.8	81.9 ± 1.4	$82.8{\pm}_{0.5}$	$81.3 {\pm} 0.7$	$84.8{\pm}_{0.2}$	85.7 ± 0.4	84.9 ± 3.7
$\operatorname{GIC}_{\mathcal{C}_y}$	80.2 ± 0.1	82.1 ± 0.3	83.5±0.8	86.1±2.2	84.1 ±0.0	87.2 ± 0.0	86.3 ±0.1	89.4 ± 0.2
$\operatorname{GIC}_{\mathcal{C}}$	79.2 ± 0.4	$79.7{\scriptstyle \pm 0.6}$	82.1 ± 1.1	$83.1{\pm}0.3$	82.1 ± 0.7	87.8±1.1	85.4 ± 0.1	89.5±0.0

Table 2. Worst-group accuracy comparison (%). We highlight the **1st** worst-group accuracy, mainly derived from GIC. The complete results including average-group accuracy are presented in Appendix C.1.



Figure 5. GIC generates better mixed images. By leveraging the high semantic consistency in image recognition, spurious attributes and true labels are decoupled in mixed images generated by GIC. Various mixing techniques are employed to handle different datasets, as detailed in Appendix B.2.2.

hair. This phenomenon is also evident in the waterbirds dataset, as detailed in Appendix 4.5, where GIC tends to classify water backgrounds with prominent land elements (such as trees) as land backgrounds. This semantic consistency significantly contributes to prediction errors in GIC and has a negative effect on downstream algorithms that rely on sampling. It can lead to an overrepresentation of majority group samples ([blond, women]) within the estimated minority group ([blond, men]), exacerbating group imbalances during resampling.

However, for invariant methods like Mixup (Yao et al., 2022) that aim to disrupt spurious correlations between spurious attributes and true labels for invariant learning, high semantic consistency is beneficial. We then show how GIC's semantic consistency leads to better mixed images compared to using oracle group labels. In Figure 5, Mixup disrupts the spurious correlation between blonde hair and women by mixing samples from the same class (blond) but with different spurious attributes (man). When sampling from the oracle blond man group, long-haired men may be selected, resulting in mixed images that still retain the typical woman attribute (long hair). However, by using the blond man sample inferred by GIC, such as the short-haired woman in Figure 5, the generated mixed samples is more closely

resemble blonde men compared to using oracle group labels. Similarly, advantages can also occur in the waterbirds dataset as shown in Figure 5. These findings may explain the better performance of GIC_{C_y} -M than LISA (which uses oracle group labels with Mixup) in Table 1, even though GIC's precision and recall are not at 100%.

5. Discussion

In this work, we introduce GIC, a novel method for better inferring group labels and mitigating spurious correlations without any additional information requirement. Experiments on synthetic and real data reveal the enhancement of GIC in group label inference and its flexibility in integration with various invariant learning algorithms. Interestingly, our analysis of misclassification cases reveals the semantic consistency phenomenon in GIC, which effectively disrupts spurious correlations and facilitates invariant learning.

Comparison data is essential for GIC and can be the labeled validation set, the subset of the unlabeled test set, or constructed non-uniformly from the training set, making GIC universally applicable. Additional experiments in Appendix C.4 demonstrate the feasibility of constructing comparison data non-uniformly from the training set, achieving comparable performance on worst-group accuracy as directly using an validation set as comparison data. Moreover, Appendix C.4 further emphasizes that while non-uniform sampling from training data can construct comparison data, considering larger and cheaper unlabeled data as comparison data is necessary since an increased sample size of comparison data improves GIC's performance. We also emphasize that the group distribution difference between comparison and training data can be subtle. Section 4.3 shows GIC's effectiveness on CelebA and Civilcomments, despite the high similarity in group distributions between the training and comparison data. In Appendix C.6, we further investigate the positive impact of group differences on GIC's performance. We propose readjusting the comparison data's group distribution based on GIC's inferred groups to further enhance the difference in group distribution and improve worst-group performance. This approach is supported by experiments detailed in Appendix C.6.

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Impact Statement

This paper presents work whose goal is to advance the field of Machine Learning. There are many potential societal consequences of our work, none which we feel must be specifically highlighted here.

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A. Proof Details

Given y^{tr} , the maximization of mutual information $I(y^{tr}; \hat{y}_{s,\mathbf{w}}^{tr})$ can be transformed into the minimization of cross-entropy $H(y^{tr}, \hat{y}_{s,\mathbf{w}}^{tr})$.

To demonstrate this assertion, we establish the following lemma:

Lemma A.1. Given y^{tr} , the correlation term is lower bounded by the difference between the entropy of y^{tr} and the cross-entropy between y^{tr} and $\hat{y}_{s,w}^{tr}$:

$$I(y^{tr}; \hat{y}_{s, \mathbf{w}}^{tr}) \ge H(y^{tr}) - H(y^{tr}, \hat{y}_{s, \mathbf{w}}^{tr})$$

Proof. For clearer expression, we omit the subscript w representing the training parameters in $\hat{y}_{s,w}$. We first expand the mutual information term:

$$I(y^{tr}; \hat{y}_{s}^{tr}) = H(y^{tr}) - H(y^{tr}|\hat{y}_{s}^{tr})$$

Since, the cross-entropy can be expanded as:

$$\begin{split} H(y^{tr}, \hat{y}_s^{tr}) &= -\sum \mathbb{P}(y^{tr}) \log \mathbb{P}(\hat{y}_s^{tr}) \\ &= \sum \mathbb{P}(y^{tr}) \log \frac{\mathbb{P}(y^{tr})}{\mathbb{P}(\hat{y}_s^{tr})} - \sum \mathbb{P}(y^{tr}) \log \mathbb{P}(y^{tr}) \\ &= \mathrm{KL}(y^{tr}||\hat{y}_s^{tr}) + H(y^{tr}) \\ &\geq \mathrm{KL}(y^{tr}||\hat{y}_s^{tr}) + H(y^{tr}|\hat{y}_s^{tr}) \\ &\geq H(y^{tr}|\hat{y}_s^{tr}). \end{split}$$

Then we have,

$$I(y^{tr}; \hat{y}_s^{tr}) = H(y^{tr}) - H(y|\hat{y}_s^{tr}) \ge H(y^{tr}) - H(y^{tr}, \hat{y}_s^{tr}).$$

According to Lemma A.1, when y^{tr} is given, maximizing the mutual information $I(y^{tr}; \hat{y}_{s,\mathbf{w}}^{tr})$ can be transformed into minimizing $H(y^{tr}, \hat{y}_{s,\mathbf{w}}^{tr})$, which is more computationally tractable in practice.

A.1. Proof of Theorem 3.1

To prove Theorem 3.1, we first demonstrate the causal structure between y_s , z, and y. Following the work (Li et al., 2022), we assume $y_s \leftarrow z \rightarrow y$. The fork causal structure (Lagnado & Sloman, 2019) between y_s , z and y exhibits the following properties:

Property A.2. The fork causal relationship $y_s \leftarrow z \rightarrow y$ adheres to the following properties:

- 1. $y_s \not\perp y$ means the true label y and the spurious label y_s are dependent.
- 2. $y \perp y_s \mid \mathbf{z}$ means given the representation \mathbf{z} , the true label y and the spurious label y_s are conditionally independent.

Naturally, the proxy $\hat{y}_{s,\mathbf{w}}$ for the true spurious attribute label y_s should also satisfy the aforementioned causal properties.

Then, we establish the following two lemmas:

Lemma A.3. Given representations \mathbf{z}^{tr} and \mathbf{z}^{c} , maximizing the spurious term is equivalent to maximizing the following expression:

$$\max_{\mathbf{w}} \operatorname{KL}(\mathbb{P}(y^{tr}|y^{tr}_{s,\mathbf{w}})||\mathbb{P}(y^{c}|y^{c}_{s,\mathbf{w}})) \Leftrightarrow \max_{\mathbf{w}} \operatorname{KL}(\mathbb{P}(y^{tr},\mathbf{z}^{tr}|y^{tr}_{s,\mathbf{w}})||\mathbb{P}(y^{c},\mathbf{z}^{c}|y^{c}_{s,\mathbf{w}}))$$
(14)

Proof. As stated in Section 3.2, different variable names are used to emphasize various data sources. In the proof section, we consider to a more formal expression for clarity. That is, we consider different distribution notations with the same variable names and also ignore the subscript w.

$$\mathbb{P}_{tr}(y|\hat{y}_s) := \mathbb{P}(y^{\text{tr}}|\hat{y}_s^{tr}) \\
\mathbb{P}_{c}(y|\hat{y}_s) := \mathbb{P}(y^c|\hat{y}_s^c).$$
(15)

According to the properties of KL divergence (Cover, 1999), we have the following:

$$\begin{aligned} \operatorname{KL}(\mathbb{P}_{tr}(y, \mathbf{z}|\hat{y}_{s})||\mathbb{P}_{c}(y, \mathbf{z}|\hat{y}_{s})) &- \operatorname{KL}(\mathbb{P}_{tr}(\mathbf{z}|y, \hat{y}_{s}))|\mathbb{P}_{c}(\mathbf{z}|y, \hat{y}_{s})) \\ &= \mathbb{E}_{(y, \mathbf{z}, \hat{y}_{s})} \left[\log \frac{\mathbb{P}_{tr}(y, \mathbf{z}|\hat{y}_{s})}{\mathbb{P}_{c}(y, \mathbf{z}|\hat{y}_{s})} \right] - \mathbb{E}_{(y, \mathbf{z}, \hat{y}_{s})} \left[\log \frac{\mathbb{P}_{tr}(\mathbf{z}|y, \hat{y}_{s})}{\mathbb{P}_{c}(\mathbf{z}|y, \hat{y}_{s})} \right] \\ &= \mathbb{E}_{(y, \mathbf{z}, \hat{y}_{s})} \left[\log \frac{\mathbb{P}_{tr}(y|\hat{y}_{s})}{\mathbb{P}_{c}(y|\hat{y}_{s})} \right] \\ &= \mathbb{E}_{(y, \hat{y}_{s})} \left[\log \frac{\mathbb{P}_{tr}(y|\hat{y}_{s})}{\mathbb{P}_{c}(y|\hat{y}_{s})} \right] \\ &= \operatorname{KL}(\mathbb{P}_{tr}(y|\hat{y}_{s}))|\mathbb{P}_{c}(y|\hat{y}_{s})). \end{aligned}$$
(16)

Since term $\operatorname{KL}(\mathbb{P}_{tr}(\mathbf{z}|y, \hat{y}_s)||\mathbb{P}_c(\mathbf{z}|y, \hat{y}_s))$ captures the similarity between the same group in the training and validation sets, i.e., $\mathbb{P}_{tr}(\mathbf{z}|y, \hat{y}_s) = \mathbb{P}_c(\mathbf{z}|y, y_s)$, we have

$$\mathrm{KL}(\mathbb{P}_{tr}(\mathbf{z}|y,\hat{y}_{s})||\mathbb{P}_{c}(\mathbf{z}|y,\hat{y}_{s})) = \sum_{g \in \mathcal{G}} \mathbb{P}_{tr}((y,\hat{y}_{s}) = g) \sum_{z} \mathbb{P}_{tr}(\mathbf{z} = z|(y,\hat{y}_{s}) = g) \log \frac{\mathbb{P}_{tr}(\mathbf{z} = z|(y,\hat{y}_{s}) = g)}{\mathbb{P}_{c}(\mathbf{z} = z|(y,y_{s}) = g)} = 0.$$
(17)

Therefore, maximizing the spurious term $\operatorname{KL}(\mathbb{P}_{tr}(y|\hat{y}_s)||\mathbb{P}_c(y|\hat{y}_s))$ is tantamount to maximizing $\operatorname{KL}(\mathbb{P}_{tr}(y,\mathbf{z}|\hat{y}_s))||\mathbb{P}_c(y,\mathbf{z}|\hat{y}_s))$.

Lemma A.4. Given representations \mathbf{z}^{tr} and \mathbf{z}^{c} , the equivalence of the spurious term is lower bounded by the following expression:

$$\mathrm{KL}(\mathbb{P}(y^{tr}, \mathbf{z}^{tr} | y^{tr}_{s, \mathbf{w}}) || \mathbb{P}(y^{c}, \mathbf{z}^{c} | y^{c}_{s, \mathbf{w}})) \ge \mathrm{KL}(\mathbb{P}(\mathbf{z}^{tr} | y^{tr}_{s, \mathbf{w}}) || \mathbb{P}(\mathbf{z}^{c} | y^{c}_{s, \mathbf{w}}))$$
(18)

Proof. We express our variables in the same manner as in Lemma A.3 and omit the subscript w.

$$\begin{aligned}
\operatorname{KL}(\mathbb{P}_{tr}(y, \mathbf{z} | \hat{y}_{s}) | | \mathbb{P}_{c}(y, \mathbf{z} | \hat{y}_{s})) \\
&= \mathbb{E}_{(y, \mathbf{z}, \hat{y}_{s})} \left[\log \frac{\mathbb{P}_{tr}(y, \mathbf{z} | \hat{y}_{s})}{\mathbb{P}_{c}(y, \mathbf{z} | \hat{y}_{s})} \right] \\
&= \mathbb{E}_{(y, \mathbf{z}, \hat{y}_{s})} \left[\log \frac{\mathbb{P}tr(y, \mathbf{z}, \hat{y}_{s})}{\mathbb{P}_{c}(y, \mathbf{z}, y_{s})} \right] - \mathbb{E}_{\hat{y}_{s}} \left[\log \frac{\mathbb{P}_{tr}(\hat{y}_{s})}{\mathbb{P}_{c}(\hat{y}_{s})} \right].
\end{aligned}$$
(19)

By the Property A.2, we derive:

$$\mathbb{P}(y, \mathbf{z}, \hat{y}_s) = \mathbb{P}(y|\mathbf{z})\mathbb{P}(\hat{y}_s|\mathbf{z})\mathbb{P}(\mathbf{z}) = \mathbb{P}(y|\mathbf{z})\mathbb{P}(\hat{y}_s, \mathbf{z}).$$
(20)

Hence, Equation (19) can be simplified as follows

$$\begin{aligned} \operatorname{KL}(\mathbb{P}_{tr}(y, \mathbf{z}|\hat{y}_{s})||\mathbb{P}_{c}(y, \mathbf{z}|\hat{y}_{s})) \\ &= \mathbb{E}_{(y, \mathbf{z}, \hat{y}_{s})} \left[\log \frac{\mathbb{P}_{tr}(y|\mathbf{z})\mathbb{P}_{tr}(\mathbf{z}, \hat{y}_{s})}{\mathbb{P}_{c}(y|\mathbf{z})\mathbb{P}_{c}(\mathbf{z}, \hat{y}_{s})} \right] - \operatorname{KL}(\mathbb{P}_{tr}(\hat{y}_{s})||\mathbb{P}_{c}(\hat{y}_{s})) \\ &= \mathbb{E}_{(y, \mathbf{z}, \hat{y}_{s})} \left[\log \frac{\mathbb{P}_{tr}(y|\mathbf{z})}{\mathbb{P}_{c}(y|\mathbf{z})} \right] + \mathbb{E}_{(y, \mathbf{z}, \hat{y}_{s})} \left[\log \frac{\mathbb{P}_{tr}(\mathbf{z}, \hat{y}_{s})}{\mathbb{P}_{c}(\mathbf{z}, \hat{y}_{s})} \right] - \operatorname{KL}(\mathbb{P}_{tr}(\mathbf{z}, \hat{y}_{s})) \\ &= \operatorname{KL}(\mathbb{P}_{tr}(y|\mathbf{z})||\mathbb{P}_{c}(y|\mathbf{z})) + \operatorname{KL}(\mathbb{P}_{tr}(\mathbf{z}|\hat{y}_{s})||\mathbb{P}_{c}(\mathbf{z}|\hat{y}_{s})) \\ &\geq \operatorname{KL}(\mathbb{P}_{tr}\left(\mathbf{z}|\hat{y}_{s})||\mathbb{P}_{c}(\mathbf{z}|\hat{y}_{s})\right). \end{aligned}$$
(21)

By Equation 21, we prove the lower bound of $\operatorname{KL}(\mathbb{P}_{tr}(y, \mathbf{z}|y_s))||\mathbb{P}_c(y, \mathbf{z}|y_s))$ is $\operatorname{KL}(\mathbb{P}_{tr}(\mathbf{z}|y_s))||\mathbb{P}_c(\mathbf{z}|y_{s,\mathbf{w}}))$. The proof is complete.

Theorem A.5. (*Restatement of Theorem 3.1*) Given representations \mathbf{z}^{tr} and \mathbf{z}^{c} , the spurious term is lower bounded by the following expression as:

$$\mathrm{KL}(\mathbb{P}(y^{tr}|\hat{y}^{tr}_{s,\mathbf{w}})||\mathbb{P}(y^{c}|\hat{y}^{c}_{s,\mathbf{w}})) \ge \mathrm{KL}(\mathbb{P}(\mathbf{z}^{tr}|\hat{y}^{tr}_{s,\mathbf{w}})||\mathbb{P}(\mathbf{z}^{c}|\hat{y}^{c}_{s,\mathbf{w}}))$$
(22)

Proof. Based on Lemma A.3 and Lemma A.4, we can directly deduce:

$$\mathrm{KL}(\mathbb{P}(y^{tr}|\hat{y}_{s,\mathbf{w}}^{tr})||\mathbb{P}(y^{c}|\hat{y}_{s,\mathbf{w}}^{c})) \ge \mathrm{KL}(\mathbb{P}(\mathbf{z}^{tr}|\hat{y}_{s,\mathbf{w}}^{tr})||\mathbb{P}(\mathbf{z}^{c}|\hat{y}_{s,\mathbf{w}}^{c})).$$
(23)

B. Experiments

B.1. Synthetic Toy Data

Synthetic data consists of three sets: training (\mathcal{D}^{tr}) , validation (\mathcal{D}^{c}) , and test (\mathcal{D}^{ts}) . These sets are created by blending four two-dimensional Gaussian distributions (representing four groups) with distinct means, equal variances, and zero correlation coefficients. Let's consider a 2D synthetic dataset with the following distribution:

Example B.1. (Synthetic 2D data) Let $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2) \in \mathbb{R}^2$ represent 2-dimensional features, with the spurious feature \mathbf{x}_1 and the invariant feature \mathbf{x}_2 , and $y \in \mathbb{R}^1$ denoting labels. The synthetic data comprises four groups, namely G_1, G_2, G_3 , and G_4 . The distributions and sample sizes in the training, validation, and test sets for each group are as follows:

$$\begin{cases} G_{1}: (\mathbf{x}_{1}, \mathbf{x}_{2}) \sim \mathcal{N} \begin{pmatrix} \begin{bmatrix} 4\\5\\5\\6\\\end{bmatrix}, \begin{bmatrix} 1 & 0\\0 & 1\\1\\0\\6\\\end{bmatrix} \end{pmatrix}; y = 0; (N^{tr}, N^{val}, N^{ts}) = (3900, 854, 3000) \\\\ G_{2}: (\mathbf{x}_{1}, \mathbf{x}_{2}) \sim \mathcal{N} \begin{pmatrix} \begin{bmatrix} 4\\8\\8\\8\\8\\8\\6\\5\\\end{bmatrix}, \begin{bmatrix} 1 & 0\\0 & 1\\1\\0\\6\\5\\\end{bmatrix}, y = 1; (N^{tr}, N^{val}, N^{ts}) = (100, 287, 3000) \\\\ (24) \\\\ G_{4}: (\mathbf{x}_{1}, \mathbf{x}_{2}) \sim \mathcal{N} \begin{pmatrix} \begin{bmatrix} 8\\8\\8\\8\\5\\\end{bmatrix}, \begin{bmatrix} 1 & 0\\0 & 1\\1\\1\\0\\6\\5\\\end{bmatrix}, y = 1; (N^{tr}, N^{val}, N^{ts}) = (3900, 18, 3000) \\\\ (y = 0; (N^{tr}, N^{c}, N^{ts}) = (100, 828, 3000) \\\\ (y = 0; (N^{tr}, N^{c}, N^{ts}) = (100, 828, 3000) \end{cases}$$

The varying sample sizes in groups G_1 , G_2 , G_3 , and G_4 indicate different group distributions across the training, validation, and test sets.

B.2. Real Data

B.2.1. DATASET DETAILS

CMNIST(Arjovsky et al., 2019) is a noisy digit recognition task. The binary feature (green and red), referred to as color, serves as a spurious feature, while the binary feature (digit contours) acts as the invariant feature. The CMNIST dataset involves two classes, where class 0 corresponds to the original digits (0,1,2,3,4), and class 1 represents digits (5,6,7,8,9). Following the approach recommended in (Yao et al., 2022), we construct a training set with a sample size of 30,000. In class 0, the ratio of red to green samples is set at 8:2, while in class 1, it is set at 2:8. For the validation set consisting of 10,000 samples, the proportion of green to red samples is equal at 1:1 for all classes. The test set, containing 20,000 samples, features a proportion of green to red samples at 1:9 in class 0 and 9:1 in class 1. Additionally, label flipping is applied with a probability of 0.25. In our experiments, we utilized the validation set as the comparison data and employed an unlabeled validation set to simulate scenarios where comparison data is unavailable. The four groups of CMNIST is $(g_1, g_2, g_3, g_4) = (\{0, green\}, \{0, red\}, \{1, green\}, \{1, red\})$ and the group distribution of the training data is $(g_1, g_2, g_3, g_4) = (0.1, 0.4, 0.4, 0.1)$, while the group distribution of the comparison data is $(g_1, g_2, g_3, g_4) = (0.26, 0.25, 0.25, 0.24)$.

Waterbirds aims to classify bird images as either waterbirds or landbirds, with each bird image falsely associated with either a water or land background. Waterbirds is a synthetic dataset where each image is generated by combining bird images sampled from the CUB dataset (Wah et al., 2011) with backgrounds selected from the Places dataset (Zhou et al., 2017). We directly load the Waterbirds dataset using the Wilds library in PyTorch (Koh et al., 2021). The dataset consists of a total of 4,795 training samples, with only 56 samples labeled as waterbirds on land and 184 samples labeled as landbirds on water. The remaining training data includes 3,498 samples from landbirds on land and 1,057 samples from waterbirds on water. We still directly use the validation set as comparison data. The waterbirds dataset can be divided into four groups, namely $(g_1, g_2, g_3, g_4) = (\{landbird, land\}, \{landbird, water\}, \{waterbird, land\}, \{waterbird, water\})$.

The class distribution of the training data is $(g_1, g_2, g_3, g_4) = (0.73, 0.04, 0.10, 0.13)$, while the class distribution of the comparison data is $(g_1, g_2, g_3, g_4) = (0.56, 0.22, 0.16, 0.16)$.

CelebA (Liu et al., 2015; Sagawa et al., 2019) is a hair-color prediction task, similar to the study conducted by (Yao et al., 2022), and follows the data preprocessing procedure outlined in (Sagawa et al., 2019). Given facial images of celebrities as input, the task is to identify their hair color as either blond or non-blond. This labeling is spuriously correlated with gender, which can be either male or female. In the training set, there are 71,629 instances (44%) of females with non-blond hair, 66,874 instances (41%) of non-blond males, 22,880 instances (14%) of blond females, and 1,387 instances (1%) of blond males. In the validation set, there are 8535 instances (43%) of females with non-blond hair, 8276 instances (42%) of non-blond males, 2874 instances (14%) of blond females, and 182 instances (1%) of blond males. The validation set is still regarded as the comparison data to infer group labels. We found that the group distribution of the training data and the comparison data in the CelebA dataset are very similar, which poses a challenge for GIC inference.

CivilComments-WILDS(Koh et al., 2021) used in our experiments is derived from the Jigsaw dataset (Borkan et al., 2019). The task of CivilComments is to determine whether a given online comment is toxic. The attribute of interest, denoted as a, is an 8-dimensional binary vector, where each entry is a binary indicator representing whether the online comment mentions one of the following 8 demographic identities: $a \in \{\text{male}, \text{female}, \text{LGBTQ}, \text{Christian}, \text{Muslim}, \text{other religion}, Black, White\}$. Comments that mention these identits tend to be more offensive and toxic. Similar to JTT (Liu et al., 2021), during the training of GIC, we binarize the spurious attribute labels, specifically using the dataset with "identity any" as the only identity attribute (Koh et al., 2021). And during the evaluation phase for worst-group accuracy, we evaluate over these 16 groups $\{(y, a_j)\}_{j=1}^8$ to calculate the wrost accuracy, where the true label y represents toxic or non-toxic comments. After binarizing the spurious attributes of the original data, there are 4 groups $(g_1, g_2, g_3, g_4) = \{\text{non-toxic no identities, non-toxic has identities}, toxic no identities, toxic has identities}\}$. However, the CivilComments dataset actually contains 16 subgroups , which can more finely characterize the group distribution differences between the training data and comparison data. Among these, the ratios of majority to minority groups in the training and validation data compared to the binarization groups.

B.2.2. BASELINE DETAILS

In this section, we main focus on baselines in this paper, categorizing them into two types based on the need for group labels: mitigating spurious correlations with group labels and mitigating spurious correlations without group labels.

Spurious correlations mitigation with group labels. GroupDRO (Sagawa et al., 2019) is a well-established method that enhances worst-group accuracy using group labels. Unlike standard ERM, which minimizes the average loss across all groups, GroupDRO partitions the data based on prior knowledge of groups and minimizes the worst-case loss over groups in the training data, thereby improving worst-group accuracy. DFR (Kirichenko et al., 2022) balances the training set by leveraging the Subsample strategy. This involves retaining all data from the smallest group and Subsample data from the other groups to equalize group sizes, followed by retraining the ERM model using this balanced dataset. LISA (Yao et al., 2022) addresses spurious correlation between the spurious attribute and true label through Mixup. It employs two mixup strategies: Intra-label, which interpolates samples with the same label but different spurious attributes, and intra-domain, which interpolates samples with the same spurious accuracy. It is important to emphasize that LISA utilizes different Mixup techniques for various experimental datasets. Specifically, for CMNIST and Waterbirds, the classic mixup (i.e., linear interpolation between two images) is considered. In the case of CelebA, CutMix, which involves replacing removed regions with a patch from another image, is employed. Meanwhile, for CivilComments, LISA resorts to using Manifold Mix. For all four datasets in the experiments, GIC adopts the same Mixup strategies as LISA.

Spurious correlations mitigation without group labels. JTT (Liu et al., 2021) initially treats misclassified points by a trained ERM as errors, which are then upsampled for improving model robustness. Similarly, CnC (Zhang et al., 2022) uses the outputs of an ERM model to identify samples with the same class but different spurious features, and trains a robust model with contrastive learning. EIIL (Creager et al., 2021) learns spurious attribute (group) labels using the EI method, which maximizes the loss of GroupDRO, and utilizes GroupDRO to learn invariant features. However, its performance is unstable and relatively poor in scenarios where learning spurious correlations is challenging (Lin et al., 2022). SSA (Nam et al., 2022) leverages semi-supervised learning with available group labels for some samples to train a spurious attribute predictor. ZIN (Lin et al., 2022) improves group inference with auxiliary information such as timestamps for time-series data

or meta-annotations for images, while DISC (Wu et al., 2023) constructs a concept bank with potential spurious attributes. However, acquiring such auxiliary information (human priors or partial group labels) may also pose difficulties, limiting the general applicability of these methods.

Downstream invariant learning methods. We considere four downstream invariant learning algorithms. Mixup (Yao et al., 2022) selectively mixes samples with the same label but different spurious features or samples with different labels but the same spurious feature, to achieve invariance. Subsample (Kirichenko et al., 2022) constructs balanced data by keeping the smallest sample size group and subsampling other groups to the same quantity. Upsample (Liu et al., 2021) oversamples samples in the misclassified sets using ERM, emphasizing difficult-to-predict groups, as well as the classic GrouDRO (Sagawa et al., 2019) algorithm.

B.2.3. TRAINING DETAILS

This section describes the experimental details, including hyperparameters and model architectures. We follow the stages mentioned in Algorithm 1 to describe the training details.

Stage 1: Extracting feature representations. First, we introduce the feature extractors $\Phi(\cdot)$ used for each dataset. We follow previous works (Kirichenko et al., 2022; Liu et al., 2021; Zhang et al., 2022; Yao et al., 2022) and consider architectures including LeNet-5 CNN (CMNIST), ResNet-50 (Waterbirds and CelebA), and BERT (CivilComments) as our feature extractors. We detail the feature extractors architecture and hyperparameters for each dataset below:

- 1. CMNIST: We use the LeNet-5 CNN architecture in the pytorch image classification tutorial. We train with SGD, epochs E = 5, learning rate 1e 3, batch size 32, default weight decay 1e 4, and momentum 0.9.
- 2. Waterbirds: We use the torchvision implementation of ResNet-50 with pretrained weights from ImageNet. Also as previous works, we train with SGD, default epochs E = 100, learning rate 1e 3, weight decay 1e 3, batch size 32, and momentum 0.9.
- 3. CelebA: We directly use the torchvision implementation of ResNet-50 with pretrained weights from ImageNet without any fine-tuning as the feature extractor.
- 4. CivilComments: We use the HuggingFace (pytorch-transformers) implementation of BERT with pre-trained weights and number of tokens capped at 220 without any fine-tuning.

The CelebA and CivilComments datasets directly use pretrained models as feature extractors without any fine-tuning, and CMNSIT trains the extractor from scratch. It is worth noting that the Waterbirds dataset utilizes pretrained weights from ImageNet and then fine-tunes them on the Waterbirds dataset. We adopt this strategy because previous work (Kirichenko et al., 2022) has observed that initializing the feature extractor with ImageNet trained weights and fine-tuning on the dataset can significantly improve the performance of feature extraction on the Waterbirds dataset. However, such improvements are not significant on datasets with larger sample sizes, such as CelebA.

Stage 2: Inferring group labels. In this section, we describe the model architectures and training hyperparameters used for training the spurious attribute classifier f_{GIC} . We also explain how we selected crucial hyperparameters, such as the weighting parameter γ and the training epochs K.

As the input to f_{GIC} are simple linear embeddings (similar to the input of the last layer of a neural network) after feature extraction, we only use a simple single-layer neural network as the model structure of f_{GIC} on all datasets. Specifically, we mapped the input to a 2-dimensional space and then used the Sigmoid function to convert it into a probability as the prediction of spurious attributes. The hyperparameters used for each dataset in Stage 2 are as follows:

- 1. CMNIST: We use training epochs K = 20, a weight of $\gamma = 10$, a learning rate of lr = 1e 5, and a momentum = 0.9.
- 2. Waterbirds: We use training epochs K = 10, a weight of $\gamma = 10$, a learning rate of lr = 1e 4, and a momentum = 0.9.
- 3. CelebA: We use training epochs K = 15, a weight of $\gamma = 10$, a learning rate of lr = 1e 5, and a momentum = 0.9.
- 4. CivilComments: We use training epochs K = 5, a weight of $\gamma = 5$, a learning rate of lr = 1e 5, and a momentum = 0.9.

In the above parameters, the most important ones are the weight parameter γ and the number of training epochs K. The weight parameter adjusts the balance of the correlated and spurious terms, and a large γ t can cause the GIC to overly focus on the spurious term, resulting in an increase in the correlated CE loss. On the other hand, a small γ may not facilitate the learning of spurious features. Additionally, when fixing the weight parameter, we observe the spurious loss of may decrease and the correlated term loss increases with too large training epochs K. Therefore, it is crucial to find a reasonable choices both for the weight parameter γ and training epochs K. We propose a grid search method for selecting γ and K by observing the trends of KL Loss and CE Loss. We start with $\gamma = 10$ and K = 20, and compute the corresponding KL loss (spurious term loss) and CE loss (relevant term loss). Our goal is to maximize the KL loss and minimize the CE loss. If we observe a decrease in the KL loss and an increase in the CE loss, we first decrease $K \in \{20, 15, 14, \dots, 2, 1\}$. Once K cannot be further reduced, we then decrease $\gamma \in \{10, 5, 4, 3, 2, 1\}$ and adjust K accordingly. We repeat this process until we no longer observe a decrease in the KL loss and an increase in the CE loss, and the corresponding values of γ and K at this point are the selected parameters. Taking the Waterbirds dataset as an example, Figure 6 visualizes the changes in KL loss and CE loss does not decrease significantly and even starts to increase around epoch = 10. This prompts us to reduce the number of training iterations K to 10.



Figure 6. The selection of important parameters γ and K in DIG on Waterbirds. The red circle indicates the inflection point where the CE Loss starts to increase. We observe that excessively large values of K and γ would cause the CE Loss to increase. Therefore, by observing the changing trends of the CE Loss and KL Loss, we determined the optimal parameters using grid search.

Stage 3: Invariant learning. After obtaining the inferred group labels using GIC, the final stage is the invariant learning stage. In the third stage, we train the robust model using the inferred group labels from the second stage for invariant learning. In our experiments, we consider four invariant learning algorithms: Mixup, GroupDRO, Subsample, and Upsample. During this stage, we use the parameters and model architecture corresponding to each specific invariant learning algorithm. For Mixup, we directly use the parameters from the original LISA paper (Yao et al., 2022). We only need to replace the spurious class labels of the original training set with the labels predicted by GIC. For GroupDRO and Subsample, we follow the parameters implemented in EIIL (Creager et al., 2021), CnC (Zhang et al., 2022), and DFR (Kirichenko et al., 2022). As for Upsample, we refer to the parameters selected by JTT (Liu et al., 2021).

In Phase 3, in line with baselines such as JTT, CnC, EIIL, and SSA, which tune all hyperparameters and also apply early stopping based on the highest worst-group accuracy on the validation set, we similarly use validation data with group labels for model selection. Specifically, GIC applies early stopping based on the highest worst-group accuracy on the validation set, thus establishing the final count of training epochs.

C. More Results

In this section, we provide additional experimental results as a supplement to Section 4. Firstly, we fully display the average-group accuracy and the worst-group accuracy as outlined in Section 4.4. Subsequently, we showcase the results of ablation experiments, illustrating the performance enhancement of GIC with the adoption of early stopping. Then, we present further error cases from the Waterbirds and CelebA datasets, underscoring the prevalent manifestation of semantic consistency in GIC.Following that, we discuss the various sources of comparison data and the impact of their sample sizes as mentioned in Section 3.4, to elucidate the effect of distinct origins and quantities of comparison data on the performance of GIC. Finally, we highlight the performance implications of the distribution discrepancy between the comparison data and training data on GIC, augmenting the insights in Section 5.

C.1. Complete Results of group inference method comparison

In this section, we present the experimental results that were not fully shown in Section 4.4 due to space limitations. These results include the average-group accuracy, where GIC outperforms baselines not only in the worst-performing group but also achieves higher accuracy in the average group. This further demonstrates that GIC has the ability to improve both the average and worst-group accuracy.

Method	Water	rbirds	Cel	ebA	Water	rbirds	CelebA	
Method	Avg.	Worst	Avg.	Worst	Avg.	Worst	Avg.	Worst
		+GroupDR	20	+Subsample				
ERM	94.6 ± 0.0	$75.6 {\pm} 0.4$	85.9 ± 0.1	77.2 ± 0.1	91.3±1.8	79.4 ± 0.3	88.9 ± 0.6	78.5 ± 0.1
EI	$96.5{\scriptstyle \pm 0.2}$	77.2 ± 1.0	85.7 ± 0.1	$81.7{\pm}_{0.8}$	88.1±0.3	$81.9{\pm}_{1.4}$	90.9 ± 0.1	$82.8 {\pm} 0.5$
$\operatorname{GIC}_{\mathcal{C}_{y}}$	$97.2{\pm}0.6$	80.2 ± 0.1	92.7 ± 1.0	82.1 ± 0.3	89.2 ± 0.9	$83.5{\scriptstyle\pm0.8}$	91.1 ± 0.1	86.1 ± 2.2
$\operatorname{GIC}_{\mathcal{C}}$	$97.6{\scriptstyle \pm 0.1}$	$79.2{\pm}_{0.4}$	$93.8{\pm}_{0.2}$	$79.7{\scriptstyle \pm 0.6}$	89.8±1.3	82.1 ± 1.1	90.3 ± 0.3	$83.1{\pm}0.3$
		+Upsampl	'e			+/	Mixup	
ERM	89.3 ± 0.7	83.8 ± 1.2	88.1±0.3	81.5 ± 1.7	94.0±0.4	82.1 ± 0.8	$90.5\pm_{0.3}$	80.6 ± 1.7
EI	88.8 ± 0.3	81.3 ± 0.7	$95.4{\pm}_{0.2}$	84.8 ± 0.2	90.1 ± 0.3	85.7 ± 0.4	90.7 ± 0.6	84.9 ± 3.7
$\operatorname{GIC}_{\mathcal{C}_{y}}$	$91.4{\scriptstyle \pm 0.3}$	84.1 ± 0.0	$88.5 {\pm} 0.7$	87.2 ± 0.0	89.6±1.3	86.3 ± 0.1	91.9 ± 0.1	89.4 ± 0.2
$\operatorname{GIC}_{\mathcal{C}}^{r_g}$	$90.8{\scriptstyle \pm 0.2}$	$82.1{\pm}0.7$	$89.7{\scriptstyle\pm0.0}$	$87.8{\scriptstyle\pm1.1}$	89.3±0.8	$85.4{\scriptstyle\pm0.1}$	92.1 ± 0.1	$89.5{\scriptstyle \pm 0.0}$

Table 3. Average and worst-group accuracy comparison (%).

C.2. Ablation Study

In this section, We present ablation experiments results. For each invariant learning algorithms, including Mixup, GroupDRO, Upsample, and Subsample, we followe previous research (Liu et al., 2021; Yao et al., 2022; Zhang et al., 2022; Creager et al., 2021), and us the group labels of the validation set and consider the worst-group accuracy to determine early stopping. Tables 4 and 5 show the average and worst-performing group performances obtained by combining GIC with different invariant learning algorithms, both with and without early stopping. We observe that the reference for early stopping does indeed improve performance, especially for the worst-group.

Table 4. Ablation experimental results. The results of combining GIC with Mixup, using early stopping based on validation set labels. Table 4 shows the performance improvement brought by early stopping.

Mathad	ES	CMN	NIST	Wate	rbirds	Cel	ebA	CivilCo	mments
Method	ES	Avg.	Worst	Avg.	Worst	Avg.	Worst	Avg.	Worst
$\operatorname{GIC}_{\mathcal{C}_{y}}$ -M	×	$70.3{\pm}_{0.4}$	65.1±1.1	92.6±0.6	80.1 ± 0.1	91.3±0.8	86.9 ± 1.4	90.8 ± 0.5	67.6±1.1
$\operatorname{GIC}_{\mathcal{C}}$ -M	×	$67.5{\scriptstyle \pm 1.5}$	63.1 ± 0.8	89.8 ± 0.5	$80.5{\scriptstyle \pm 0.0}$	92.1±0.0	$85.6{\scriptstyle\pm1.2}$	90.9 ± 0.2	$66.6{\scriptstyle \pm 0.3}$
$\operatorname{GIC}_{\mathcal{C}_u}$ -M	\checkmark	$73.2{\pm}0.2$	72.2 ± 0.5	89.6±1.3	86.3 ± 0.1	91.9 ± 0.1	$89.4{\scriptstyle\pm0.2}$	90.0 ± 0.2	72.5 ± 0.3
$\operatorname{GIC}_{\mathcal{C}}$ -M	\checkmark	$73.1{\pm}_{0.5}$	71.7 ± 0.3	89.3±0.8	85.4 ± 0.1	92.1±0.1	$89.5{\scriptstyle \pm 0.0}$	89.7±0.0	$72.3{\pm}_{0.2}$

Method	ES	Water	rbirds	Cel	ebA	Wate	rbirds	Cele	ebA
Method	ЕЭ	Avg.	Worst	Avg.	Worst	Avg.	Worst	Avg.	Worst
+GroupDRO							+Subs	ample	
$\operatorname{GIC}_{\mathcal{C}_{y}}$	×	98.0 ± 0.0	77.1±1.8	94.3±0.1	76.7 ± 0.6	88.9±0.4	80.0 ± 1.4	89.9 ± 0.2	84.1 ± 2.9
$\operatorname{GIC}_{\mathcal{C}}$	×	97.9 ± 0.0	70.1 ± 1.2	$93.9\pm_{0.0}$	71.7 ± 0.0	90.4 ± 0.4	79.6 ± 1.6	92.1 ± 0.5	77.6 ± 3.3
$\operatorname{GIC}_{\mathcal{C}_{y}}$	\checkmark	97.2 ± 0.6	80.2 ± 0.1	92.7 ± 1.0	82.1 ± 0.3	89.2 ± 0.9	$83.5 {\pm} 0.8$	91.1 ± 0.1	86.1 ± 2.2
$\operatorname{GIC}_{\mathcal{C}}$	\checkmark	$97.6{\scriptstyle \pm 0.1}$	$79.2{\pm}_{0.4}$	$93.8{\scriptstyle\pm0.2}$	$79.7{\scriptstyle\pm0.6}$	89.8±1.3	82.1 ± 1.1	90.3 ± 0.3	$83.1{\pm}0.3$
	+Upsample						+M	ixup	
$\operatorname{GIC}_{\mathcal{C}_y}$	×	85.8 ± 1.0	$77.7\pm_{0.1}$	86.9 ± 0.9	84.2 ± 1.4	92.6±0.6	$80.1\pm_{0.1}$	91.3 ± 0.8	86.9 ± 1.4
$\operatorname{GIC}_{\mathcal{C}_{y}}$	×	$83.3{\scriptstyle\pm2.9}$	70.9 ± 0.6	89.9 ± 0.1	87.5 ± 1.4	89.8 ± 0.5	80.5 ± 0.0	92.1 ± 0.0	85.6 ± 1.2
$\operatorname{GIC}_{\mathcal{C}_{y}}$	\checkmark	$91.4{\pm}_{0.3}$	$84.1{\pm}0.0$	88.5 ± 0.7	87.2 ± 0.0	89.6±1.3	$86.3{\pm}_{0.1}$	91.9 ± 0.1	89.4 ± 0.2
$\operatorname{GIC}_{\mathcal{C}}$	\checkmark	$90.8{\pm}_{0.2}$	$82.1{\pm}0.7$	89.7±0.0	87.8 ± 1.1	89.3 ± 0.8	85.4 ± 0.1	92.1 ± 0.1	89.5 ± 0.0

Table 5. Ablation experimental results. The results of combining GIC with GroupDRO, Subsample, Upsample and Mixup, using early stopping based on validation set labels. Table 5 displays the early stopping results of the experiments in Table 3, demonstrating the effectiveness of early stopping.

C.3. More Error Cases

In Section 4.5, we illustrate the semantic consistency of GIC using the celebA dataset, where images with similar semantics are considered as belonging to the same spurious feature category. This distinguishes GIC, which relies on semantic features for recognition, from human-based oracle group labels. We observe the same phenomenon on the waterbirds dataset, as shown in Figure 7. The misclassifications of GIC can be categorized into two types: (1) Land background with typical water features, such as extensive blue regions, often leads GIC to misclassify land as water. (2) Water background with typical land features, such as abundant tree branches, ponds with lush green vegetation, or large tree reflections, frequently results in GIC classifying them as land. We believe that such consistency precisely reflects GIC's accurate recognition of image semantics. As mentioned in the main text, such accurate recognition is crucial when it comes to invariant learning that requires leveraging different image semantics (e.g., using mixup to disrupt semantic features of spurious features). We present more examples of misclassifications by GIC from the Waterbirds and CelebA datasets in Figure 8, 9, and 10 to support the existence of semantic consistency in GIC.



Figure 7. Misclassified samples on Waterbirds. The semantic consistency in GIC leads to the misclassification of water with a large amount of land elements (such as twigs and greenery) as land (71.3%), and land with a large blue area (a typical characteristic of water) as water (28.7%).



Figure 8. More error cases on Waterbirds. Instances misclassified by GIC as land but are actually water. We find that most of these samples share common characteristics, such as having abundant green vegetation, striped patterns (tree trunks, branches, humans), or locations that combine land and water features (such as beaches, coastal cities). These typical land features are the reasons for GIC's misclassification.



Figure 9. More error cases on CelebA. Instances misclassified by GIC as woman but are actually man. We notice that most of them are males with long hair. The presence of long hair, a feature commonly associated with the female, may be the key factor leading to GIC's misclassification.



Figure 10. More error case on CelebA. Instances misclassified by GIC as male but are actually female. We find that most of these females have short hair or wear hats or headgear that obscures their long hair. The presence of short hair may be the reason for their misclassification by GIC, which aligns with the conclusion shown in Figure 9.

C.4. The Construction of Comparison Data

In this section, we discuss the methods for constructing comparison data. In Section 3.4, we proposed three methods for obtaining comparison data. In the experimental section (Section 4), we used labeled/unlabeled validation sets as labeled/unlabeled comparison data from non-training datasets. The significant improvement in worst-group accuracy indicates the effectiveness of these two methods of obtaining comparison data.

To support the effectiveness of the method of constructing comparison data by non-uniform sampling from the training set, we first conduct additional experiments on CMNIST. Following a similar approach to JTT, we train an ERM model on the training set and divide the samples into an error set (misclassified samples) and a non-error set (correctly classified samples). The error set is typically composed of samples from the minority group with spurious associations (Liu et al., 2021). We then sample an equal number of samples from both the error set and non-error set. For instance, when the sampling ratio is set to 1%, we sample 300 (1% of 30,000) samples from each set, resulting in a total of 600 samples as the comparison data. These comparison data samples are combined with the remaining 29,400 training samples for GIC training. After obtaining the spurious attribute classifier $f_{\rm GIC}$, we directly evaluate its prediction accuracy on the entire training dataset, as shown in Figure 11. We observe that as the sampling rate gradually increases, leading to a growth in the number of comparison data samples, GIC's capability to infer spurious features also enhances. Remarkably, on CMNIST, when the sampling rate is around 10%, the performance of GIC based on training data for inferring spurious features aligns with that of GIC using validation data directly.



Figure 11. Test accuracy on spurious attributes using non-uniform sampling from the training dataset. The dashed line represents the accuracy of GIC's spurious feature label inference using labeled validation data.

We also conduct additional experiments on CMNIST, Waterbirds, and CelebA to explore the strategy of non-uniform sampling from training data as comparison data. Notably, we observe that for Waterbirds and CelebA, relying solely on training data would significantly limit the sample size of comparison data. Therefore, we combine the training and validation data as a new dataset for constructing comparison data for the Waterbirds and CelebA datasets. Specifically, we mix the training and validation data, then split them into new training and validation sets at a 50% ratio. We train on the new training set using the ERM method and infer labels on the new validation set, resulting in an error set (misclassified samples) and a non-error set (correctly classified samples). Similarly, we train the model on the validation set and identified the error set and non-error set on the training set through group inference. We then combine the error and non-error sets and sample a fixed proportion (50%) from each set to serve as comparison data, with the remainder as training data. We then apply GIC to infer group labels and learn invariant features. To further enhance performance, we implement a boosting approach by repeating the aforementioned process twice. In the second iteration, we base it on the GIC model obtained from the first round of training to infer group labels and construct the error set and non-error set.

We further report the worst-group accuracy of GIC when the comparison data is generated by non-uniform sampling from the training dataset, using Mixup as the downstream algorithm. We refer to this variant of GIC as GIC_{C_t} -M. The experimental results in Table 6 demonstrates that constructing comparison data by non-uniform sampling from the training dataset is an effective strategy, as the worst-group accuracy is close to that achieved by the GIC approach using labeled/unlabeled validation data as the comparison dataset, particularly on CMNIST, where the performances are almost comparable.

Method	CMNIST	Waterbirds	CelebA
	valie	dation	
$\operatorname{GIC}_{\mathcal{C}_y}$ -M $\operatorname{GIC}_{\mathcal{C}}$ -M	72.2 ± 0.5 71.7 ± 0.3	86.3 ± 0.1 85.4 ± 0.1	$\begin{array}{c} 89.4{\pm}_{0.2} \\ 89.5{\pm}_{0.0} \end{array}$
	non-unifor	m sampling.	
$\operatorname{GIC}_{\mathcal{C}_t}$ -M	$72.2 \pm \scriptstyle 0.1$	85.7 ± 0.3	$87.5{\scriptstyle \pm 0.7}$

Table 6. Comparison of GIC's worst-group accuracy using different sources of comparison data.

C.5. The Necessity of Considering Unlabeled Datasets as Comparison Data.

Additionally, we want to emphasize the necessity of considering unlabeled comparison data, such as sampling from the test set. In the real world, unlabeled data is often more cost-effective and easier to obtain than labeled data. By utilizing a large amount of unlabeled data as comparison data, the applicability of GIC can be greatly expanded. Our results in Figure 12 demonstrate that when GIC trains a spurious feature classifier using labeled comparison data (with sample sizes ranging from 10 to 1000), its accuracy in predicting spurious features and improving the accuracy of the worst-performing group is significantly worse than when using unlabeled but larger comparison data (with sample sizes ranging from 3000 to 10000). This experiment highlights the importance of considering unlabeled comparison data.



Figure 12. The worst-group accuracy and spurious attributes accuracy on CMNIST. On the left side of the dashed line, labeled comparison data (ranging from 10 to 1000) is utilized, but due to the small sample size, GIC demonstrates poor performance in inferring groups and improving the worst-group accuracy. On the right side of the dashed line, a larger unlabeled validation set is used as comparison data, resulting in a noticeable improvement in GIC's performance.

C.6. Group Distribution Discrepancy Analysis

We then discuss the impact of differences in group distributions between the comparison data and training data on the effectiveness of GIC. As mentioned in Section 5, even slight differences in group distributions can force the spurious term to learn invariant features. Although GIC can still learn the spurious attributes and infer group labels in the presence of slight differences, we want to understand the relationship between the degree of differences and GIC's performance. To answer this question, we use the CelebA dataset as an example. As described in Appendix B.2.1, inferring spurious attributes on the CelebA dataset can be challenging because the training data and comparison data (validation set) have very similar group distributions. We keep the training set and test set fixed and adjust the group distribution of the comparison data, and their detailed group distributions are displayed in Figure 13. We then train GIC using the training data and these four different sets of comparison data while keeping the parameters and model consistent, and calculate the worst-group accuracy on the test set.

Table 7. The result after adjusting the group distribution using the group labels predicted by GIC.

Mathad	Deadlinet	Cel	ebA			
Method	Readjust	Avg.	Worst			
subsample						
$\overline{\operatorname{GIC}_{\mathcal{C}_y}}$	×	91.1±0.1	86.1±2.2			
$\overline{\operatorname{GIC}_{\mathcal{C}_y}}$	\checkmark	92.1±0.3	89.1±0.9			



Figure 13. Increasing differences in group distribution encourage GIC to better infer group labels, further improving the performance of the worst group.

In Figure 13, we observe that as the differences in group distributions between the comparison data and training data increase, the worst-group performance improves. Additionally, we calculate the KL Loss for each comparison data and find that as the differences in group distributions increase, the final KL Loss also increases. This suggests that GIC has the ability to accurately capture the differences in group distributions between the comparison data and training data.

It is worth noting that the group distribution of comparison data C1 is almost identical to the training data (KL loss close to 0), yet its worst-group accuracy still outperforms the worst-group accuracy of the ERM model. We believe that this is because when there is no group distribution difference, whether the spurious term forces GIC to learn invariant features or spurious features is a completely random event with equal probability. However, due to the presence of spurious correlations, GIC is more inclined to prioritize learning spurious features, thereby improving the worst-group accuracy. However, such events of prioritizing learning spurious features are not stable, which is why we observe larger variances in the results corresponding to the C1 data compared to other comparison datasets.

The phenomenon observed in Figure 13 (that larger differences can improve GIC performance) inspires us to attempt adjusting the group distribution of the comparison data again using the group label results predicted by GIC. Specifically, we use $f_{\rm GIC}$ trained on the celebA dataset to adjust the comparison data (validation set) again. This involves Upsample the two smallest groups to the same sample size as the second largest group, and then retraining GIC using the new comparison data and training data. Table 7 reports the GIC obtained after re-adjusting the comparison data, and we observe that the accuracy of the worst-group is further improved through this operation.

C.7. Compute Resources and Training Time of GIC

All experiments for CMNIST, Waterbirds, CelebA and CivilComments were run on a single NVIDIA GeForce RTX 4090 GPU.

Regarding the runtime of GIC, additional computational overhead compared to methods inferring spurious labels via ERM stems from inputting data representations z into the GIC model f_{GIC} for both training and predicting the spurious feature labels $\hat{y}_{s,\mathbf{w}}^c$. This supplementary step should not necessitate substantial computation cost. As the dimensionality of data representation z is reduced relative to the raw data, and the experiments have evidenced that a simple single-layer neural network for f_{GIC} suffices in delivering promising performance. Concurrently, it's noted in Appendix B.2.3 that the training epoch K can be contained within 20 epochs for all four experimental datasets. We further calculate the total time required for training the spurious feature classifier f_{GIC} and predicting the spurious feature labels $\hat{y}_{s,\mathbf{w}}^c$ across the four experimental datasets, manifesting that the computational cost introduced by GIC is rather minimal.

Table 8. The average runtime for training f_{GIC} and predicting $\hat{y}_{s,\mathbf{w}}^c$. The timing commences subsequent to obtaining the data representation \mathbf{z} and concludes upon acquiring the predicted $\hat{y}_{s,\mathbf{w}}^c$.

Dataset	Average Time
CMNIST	30.1s
Waterbirds	60.0s
CelebA	519.9s
CivilCommnets	901.0s