Pareto Invariant Risk Minimization

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Abstract

Despite the success of invariant risk minimization (IRM) in tackling the Out-of-Distribution generalization problem, IRM can compromise the optimality when applied in practice. The practical variants of IRM, e.g., IRMv1, have been shown to have significant gaps with IRM and thus could fail to capture the invariance even in simple problems. Moreover, the optimization procedure in IRMv1 involves two intrinsically conflicting objectives, and often requires careful tuning for the objective weights. To remedy the above issues, we reformulate IRM as a multi-objective optimization problem, and propose a new optimization scheme for IRM, called PAreto Invariant Risk Minimization (PAIR). PAIR can adaptively adjust the optimization direction under the objective conflicts. Furthermore, we show PAIR can empower the practical IRM variants to overcome the barriers with the original IRM when provided with proper guidance. We conduct experiments with ColoredMNIST to confirm our theory and the effectiveness of PAIR.

1. Introduction

There are surging evidences showing that machine learning models using empirical risk minimization (ERM) (Vapnik, 1991) are prone to exploit shortcuts, or spurious features, and thus can fail to generalize to out-of-distribution (OOD) data (Beery et al., 2018; DeGrave et al., 2021; Geirhos et al., 2020; Koh et al., 2021; Ji et al., 2022). To address the OOD failure, several strategies and algorithms were proposed (Peters et al., 2016; Rojas-Carulla et al., 2018; Bengio et al., 2020; Sagawa* et al., 2020; Koyama & Yamaguchi, 2020; Krueger et al., 2021; Creager et al., 2021; Liu et al., 2021; Ahuja et al., 2021a; Shi et al., 2022; Rame et al., 2021; Chen et al., 2022; Lin et al., 2022; Zhang et al., 2022). Among them, the Invariant Risk Minimization (IRM) (Arjovsky et al., 2019) framework has attracted much attention.

IRM assumes datasets are collected from multiple causally related environments, and tries to find an invariant data representation \( \varphi \). When a predictor \( w \) acting on \( \varphi \) minimizes the risks in all of the environments simultaneously, \( \varphi \) is expected to discard the spurious signals while keeping the causally invariant signals (Peters et al., 2016; Arjovsky et al., 2019). Although being powerful, recent works revealed that IRM can lead to suboptimal solutions when applied in the practice (Kamath et al., 2021; Rosenfeld et al., 2021; Ahuja et al., 2021b; Nagarajan et al., 2021; Aubin et al., 2022).

Specifically, to alleviate the difficulty in solving the challenging non-linear bi-level programming in the original IRM, Arjovsky et al. (2019) relax IRM into IRM\(_S\) by restricting the \( w \) to be linear, and further propose a more practical soft-constrained variant, IRMv1. However, Kamath et al. (2021) show the relaxed variants can have huge gap with the original IRM. In a simple example following the setting of IRM (Arjovsky et al., 2019), both IRM\(_S\) and IRMv1 could fail to capture the desired invariance even with infinite amounts of samples and environments. Moreover, since the optimization of IRMv1 involves two intrinsically conflicting objectives, the objective weights require careful tuning, otherwise IRMv1 may even underperform the vanilla empirical risk minimization (ERM) algorithm (Vapnik, 1991; Gulrajani & Lopez-Paz, 2021; Zhang et al., 2022).

Aiming to bridge the gap between the practical variants and the original IRM, we propose a new perspective with multi-objective optimization (MOO) for understanding the different behaviors between IRM\(_S\), IRMv1 and IRM, and develop a new optimization scheme for IRM, termed as PAreto Invariant Risk Minimization (PAIR). By reformulating IRM as a MOO problem, we find the failures of the practical variants are because of using the improper objectives for optimization. Therefore, we propose to pair IRM\(_S\) and IRMv1 with additional guidance from other robust objectives. More concretely, we show that, when guided by REx (Krueger et al., 2021), PAIR avoids the failure cases of IRM\(_S\) and IRMv1, and is capable of locating the desired invariant predictors using gradient-based methods such as the multiple-gradient descent algorithm (Désidéri, 2012). Hence, PAIR can resolve the theoretical drawbacks...
in IRM$_S$ and thus be more powerful than IRM$_S$. We conduct experiments on ColoredMNIST (Arjovsky et al., 2019) and its modified variants to verify the effectiveness of \textsc{Pair}.

## 2. Drawbacks of IRM in Practice

We begin by briefly introducing the basics of IRM and drawbacks of its practical variants. We refer readers to Kamath et al. (2021) for more theoretical details.

**Problem Setup.** The IRM (Arjovsky et al., 2019) framework typically considers a supervised learning setting based on the data $D = \{D_e\}_{e \in \mathcal{E}_{all}}$ collected from multiple causally related environments $\mathcal{E}_{all}$, where a subset of samples $D_e = \{X^e_i, Y^e_i\}$ from a single environment $e \in \mathcal{E}_{all}$ are drawn independently from an identical distribution $\mathbb{P}_e$. Given the data from training environments $\{D_e\}_{e \in \mathcal{E}_{tr}}$, the goal of OOD generalization is to find a predictor $f : \mathcal{X} \to \mathcal{Y}$ that generalizes well to all (unseen) environments, i.e., to minimize $\max_{e \in \mathcal{E}_{all}} R^c(f)$, where $R^c$ is the empirical risk under environment $e$. IRM approaches the problem by finding an invariant representation $\varphi : \mathcal{X} \to \mathcal{Z}$, such that there exists a predictor $w : \mathcal{Z} \to \mathcal{Y}$ acting on $\varphi$ that is simultaneously optimal among $\mathcal{E}_{all}$. Hence, IRM leads to a challenging bi-level optimization problem (Arjovsky et al., 2019) as

$$\begin{align*}
\min_{w, \varphi} & \sum_{e \in \mathcal{E}_{tr}} \mathcal{L}_e(w \circ \varphi), \\
\text{s.t.} & \ w = \arg \min_{\tilde{w} : \mathcal{Z} \to \mathcal{Y}} \mathcal{L}_e(\tilde{w} \circ \varphi), \ \forall e \in \mathcal{E}_{tr}. \quad (1)
\end{align*}$$

Given the training environments $\mathcal{E}_{tr}$, and functional spaces $\mathcal{W}$ for $w$ and $\Phi$ for $\varphi$, predictors $w \circ \varphi$ satisfying the constraint are called invariant predictors, denoted as $\mathcal{I}(\mathcal{E}_{tr})$. When solving Eq. 1, characterizing $\mathcal{I}(\mathcal{E}_{tr})$ is particularly difficult in practice, given the access only to finite samples from a small subset of environments. It is natural to introduce a restriction that $\mathcal{W}$ is the space of linear functions on $\mathcal{Z} = \mathbb{R}^d$ (Jacot et al., 2021). Furthermore, Arjovsky et al. (2019) argue that linear predictors actually do not provide additional representation power than *scalar* predictors, i.e.,

$$d = 1, \mathcal{W} = \mathcal{S} = \mathbb{R}^1.$$ 

The scalar restriction on $\mathcal{W}$ elicits a practical variant IRM$_S$ as

$$\begin{align*}
\min_{\varphi} & \sum_{e \in \mathcal{E}_{tr}} \mathcal{L}_e(\varphi), \text{ s.t. } \nabla_{w|w=1} \mathcal{L}_e(w \cdot \varphi) = 0, \ \forall e \in \mathcal{E}_{tr}. \quad (2)
\end{align*}$$

Let $\mathcal{I}(\mathcal{E}_{tr})$ denote the set of invariant predictors elicited by the relaxed constraint in IRM$_S$. It follows that $\mathcal{I}(\mathcal{E}_{tr}) \subseteq \mathcal{I}_S(\mathcal{E}_{tr})$ (Kamath et al., 2021). Yet, Eq. 2 remains a constrained programming. Hence, Arjovsky et al. (2019) introduce a soft-constrained variant IRMv1 as

$$\begin{align*}
\min_{\varphi} & \sum_{e \in \mathcal{E}_{tr}} \mathcal{L}_e(\varphi) + \lambda |\nabla_{w|w=1} \mathcal{L}_e(w \cdot \varphi)|^2. \quad (3)
\end{align*}$$

**Theoretical Failure of Practical IRM Variants.** Although the practical variants seem promising, Kamath et al. (2021) show there exists huge gaps between the variants and the original IRM such that both IRM$_S$ and IRMv1 can fail to capture the desired invariance, even being given the *population loss* and *infinite* amount of training environments. The failure case, called two-bit environment (Kamath et al., 2021), follows the setup of ColoredMNIST in IRM (Arjovsky et al., 2019), and defines environments with two parameters $\alpha, \beta \in [0, 1]$. Each $\mathcal{E}_e$ is defined as

$$Y := \text{Rad}(0.5), \ X_1 := Y \cdot \text{Rad}(\alpha), \ X_2 := Y \cdot \text{Rad}(\beta),$$

where $\text{Rad}(\sigma)$ is a random variable taking value $-1$ with probability $\sigma$ and $+1$ with probability $1 - \sigma$. We denote an environment $e$ with $(\alpha, \beta)$ for simplicity. The setup in IRM can be denoted as $\mathcal{E}_e = \{ (\alpha, \beta) : 0 < \beta < 1 \}$ where $X_1$ is the invariant feature as $\alpha$ is fixed for different $e$.

In the example given by Arjovsky et al. (2019), i.e., $\mathcal{E}_{tr} := \{ (0.25, 0.1), (0.25, 0.2) \}$, IRM$_S$ and IRMv1 are shown to be able to learn the invariant predictor $f_{\text{IRM}}$ as the original IRM despite of the relaxation. However, due to $\mathcal{I}(\mathcal{E}_{tr}) \not\subseteq \mathcal{I}_S(\mathcal{E}_{tr})$, Kamath et al. (2021) show that the set of “invariant predictors” produced by IRM$_S$ and IRMv1 is broader than our intuitive sense. For example, when
given $\mathcal{E}_\epsilon := \{(0.1, 0.11), (0.1, 0.4)\}$, the solutions satisfying the constraint in IRM$_S$ are those intersected points in Fig. 1 (The ellipsoids are the constraints). Although $f_0, f_1, f_2, f_{\text{IRM}} \in \mathcal{I}_S(\mathcal{E}_\epsilon)$, both IRM$_S$ and IRMv1 prefer $f_1$ instead of $f_{\text{IRM}}$ (the predictor elicited by the original IRM), as $f_1$ has the smallest ERM loss. In fact, Kamath et al. (2021) prove that, the failure can happen in a wide range of environments with $\alpha < 0.1464$ and $\alpha > 0.8356$, even being given infinite number of additional environments, under MSE loss. It follows that $\mathcal{I}(\mathcal{E}_\epsilon) \subseteq \mathcal{I}_S(\mathcal{E}_\epsilon)$. In other words, the relaxation in IRM$_S$ and IRMv1 will introduce additional “invariant predictors” which however do not satisfy the original IRM constraint. Both IRM$_S$ and IRMv1 will prefer those “invariant predictors” when they have lower ERM loss than $f_{\text{IRM}}$, demonstrating the significant theoretical gap between the practical variants and the original IRM.

**Practical Drawback of Practical IRM Variants.** In addition to the theoretical gap, the optimization of IRMv1 is also difficult due to the conflicts between the IRM penalty and ERM penalty in Eq. 3. It often requires significant efforts for choosing proper hyperparameters such as pretraining epochs and IRM penalty weights, i.e., $\lambda$. Otherwise, IRMv1 may not enforce the constraint in IRM$_S$, hence will lead to unsatisfactory performance, as shown in Fig. 2.

## 3. Pareto Optimization for IRM

As shown that both IRM$_S$ and IRMv1 have difficulties in handling the trade-off between ERM loss and IRM penalty, we introduce a new learning perspective for understanding the differences between the variants and the original IRM based on Multi-Objective Optimization (MOO).

**IRM as Multi-Objective Optimization.** MOO typically considers solving $m$ objectives, with $\{L_1, \ldots, L_m\}$ loss functions, i.e., $\min_{\theta} L(\theta) := (L_1(\theta), \ldots, L_m(\theta))^T$ (Kaisa, 1999). A solution $\theta$ dominates another $\tilde{\theta}$ if $L_i(\theta) \leq L_i(\tilde{\theta})$ for all $i$ and $L(\theta) \neq L(\tilde{\theta})$. A solution $\theta^*$ is called Pareto optimal if there exists no other solution that dominates $\theta^*$. The set of Pareto optimal solutions is called Pareto set and its image is called Pareto front, denoted as $\mathcal{P}$. In practice, it is usual that we cannot find a global optimal solution for all objectives, hence Pareto optimal solutions are of particular value. The paradigm proposed in multiple-gradient descent algorithm (MGDA) (Désidéri, 2012) can efficiently find the Pareto optimal solutions, and has been widely applied in multi-task learning (Sener & Koltun, 2018; Lin et al., 2019; Ma et al., 2020; Mahapatra & Rajan, 2020).

To understand the behaviors of IRM$_S$ and IRMv1, it is natural to introduce the following objectives as

$$\min_{\phi} (L_1, \ldots, L_{|\mathcal{E}_\epsilon|}, L_{\text{IRM}})^T,$$

where we denote $\sum_{e} |\nabla_w L_e(w, \phi)|^2$ as $L_{\text{IRM}}$ for short. We then visualize the Pareto front w.r.t. $L_1, L_2$ in Fig. 3, using the failure case in Fig. 1. Let $\mathcal{P}(L_1(\theta), \ldots, L_m(\theta))$ denote the set of Pareto optimal solutions w.r.t. the objectives $(L_1(\theta), \ldots, L_m(\theta))$. At first, we can find that $f_{\text{IRM}} \notin \mathcal{P}(L_1, L_2)$. In other words, any environment-reweighted ERM cannot find $f_{\text{IRM}}$ hence not capture the invariance. Moreover, combining Fig. 1, we can also find that $f_{\text{IRM}} \notin \mathcal{P}(L_1, L_2, L_{\text{IRM}})$, either, since $f_{\text{IRM}}$ is dominated by $f_1$. Therefore, the failures of IRM$_S$ and IRMv1 can be understood as because of using the improper objectives whose Pareto front does not contain the desired solution. Thus, choosing proper objectives is of great importance. The ideal objectives should constitute a Pareto front that contains the desired solutions.

**Pareto Robust Risk Minimization for IRM.** In pursuit of proper Pareto objectives, we resort to Distributionally Robust Optimization (Namkoong & Duchi, 2016) that aims to minimize the maximal error for any distribution in a convex hull formed under mixtures with positive weights of training distributions, or $\{\lambda_c D_c \mid \sum_{c \in \mathcal{E}_\epsilon} \lambda_c = 1, \lambda_c \geq 0, \forall c\}$ in our case. Bottou et al. (2019) argue that learning the invariance in IRM can extrapolate outside the convex hull by finding stationary points of $\sum_{c \in \mathcal{E}_\epsilon} \lambda_c L_c$ for some (possibly negative) $\{\lambda_c\}_{c \in \mathcal{E}_\epsilon} \subseteq \mathbb{R}$. However, IRM$_S$ and IRMv1 can fail to learn the invariant representations, weak-
minibatches tend to be noisy, leading to weaker signals. Let tends to vanish, while the signals from $\var$ tend to be smaller, the gradient signal of $\beta$ as the variation of spurious signals in two environments of REx (Krueger et al., 2021) (denoted as vrex) drops more between two environments getting closer, the performance $\beta$ different remain necessary? We find the answer is “Yes”. In Fig. 5, failure cases of IRM showing REx (Krueger et al., 2021) can help avoiding the failure of IRM. By resolving a large class of failure cases of IRM, we can adaptively find suitable gradient descent directions at each step, leading to the desired solutions in practice.

**Pareto Invariant Risk Minimization.** To summarize, by formulating IRM as a MOO problem in Eq. 5, we find that the failures of $\text{IRM}_S$ and IRMv1 are caused by using improper objectives for optimization. Nevertheless, we can introduce additional guidance from more robust objectives such as REx (Krueger et al., 2021) to narrow the gap between $\text{IRM}_S$ and IRM by resolving the failure cases of $\text{IRM}_S$. Moreover, leaving $\mathcal{L}_{\text{IRM}}$ in the objectives also keeps better gradient signals in practice where the signals from REx can vanish. Thus, it is natural to pair the objectives to enhance the extrapolation power and robustness against distribution shifts. Therefore, we propose the following MOO formulation, called Pareto Invariant Risk Minimization (PAIR),

$$\min_{\varphi} \left( \sum_{e} \mathcal{L}_{\varphi(e)}, \mathcal{L}_{\text{IRM}}, \var \left( \{ \mathcal{L}_{e} \} \in \mathcal{E}_e \right) \right)^T,$$  \hspace{1cm} (7)

where we merge $(\mathcal{L}_{1}, ..., \mathcal{L}_{|\mathcal{E}_e|})$ into the summation for reducing the search dimensions over the Pareto front. To guarantee the achievability of Pareto optimal solutions of Eq. 7, we can leverage the off-the-shelf MGDA algorithms. More concretely, in practice, $\mathcal{L}_{\text{IRM}}$ and $\var \left( \{ \mathcal{L}_{e} \} \in \mathcal{E}_e \right)$ often converge to some $\epsilon \geq 0$ due to the possible noises of invariant features (Ahuja et al., 2021b; Kamath et al., 2021). Using scalarization scheme to combine the objectives with scalars can lead to sub-optimal solutions when the desired solutions lie in the concave part of the Pareto front (Boyd & Vandenberghe, 2014; Lin et al., 2019). Moreover, in order to maximally satisfy the original constraints in IRM, i.e., $\mathcal{L}_{\text{IRM}} = 0$, we choose to use the EPO solver (Mahapatra & Rajan, 2020) and specify high preferences for $\mathcal{L}_{\text{IRM}}$ and $\var \left( \{ \mathcal{L}_{e} \} \in \mathcal{E}_e \right)$. Under the guidance of Eq. 7, EPO can adaptively find suitable gradient descent directions at each step, leading to the desired solutions in practice.

### 4. Experiments

**Datasets.** In experiments, we modify the ColoredMNIST dataset (Arjovsky et al., 2019) to verify our theoretical findings and the effectiveness of PAIR. Specifically, the label flipping probability and colored probability in ColoredMNIST essentially corresponds to $\alpha_e$ and $\beta_e$ in the two-bit environment (Eq. 4), respectively. Hence, we can construct the corresponding testbeds with different variants of ColoredMNIST. We mainly use the two variants, i.e., CMNIST-10: $(0.1, 0.25), (0.1, 0.2)$ which is the failure case used by Kamath et al. (2021), and CMNIST-25: $(0.25, 0.10), (0.25, 0.20)$ which is the same to the original IRM setting (Arjovsky et al., 2019).

**Baselines.** To show the effectiveness of PAIR in narrowing the gap between practical variants and the original formulation of IRM, we compare PAIR with ERM (Vapnik, 1991), IRMv1 (Arjovsky et al., 2019), V-REx (Krueger et al., 2021). To show the effectiveness of PAIR in approaching...
the Pareto optimal solutions, we also construct a strong baseline IRMx where the variance penalty and \( \mathcal{L}_{\text{IRM}} \) are simply added up with the same objective weights.

**Evaluation.** We follow the same evaluation settings as IRM (Arjovsky et al., 2019) and the test-domain selection as DomainBed (Gulrajani & Lopez-Paz, 2021) when conducting the experiments. Specifically, we use a 4-Layer MLP with a hidden dimension of 256. By default, we use Adam (Kingma & Ba, 2015) optimizer with a learning rate of \( 1e^{-3} \) and a weight decay of \( 1e^{-3} \) to train the model with 500 epochs and select the last epoch as the output model for each hyperparamter setting. We choose the final model as the one that maximizes the accuracy on the validation that shares the same distribution as test domain. We then do grid search for the other hyperparameters such as pretraining epochs and penalty weights. We evaluate each configuration of hyperparameters 10 times and report the mean and standard deviation of the performances. More details about the evaluation setting are given in Appendix C.1.

**Sufficiency of Enforcing the Invariance.** To begin with, we first conduct a probing experiments to show the sufficiency of objectives for guaranteed OOD performance. Specifically, we initialize all of the methods with a “perfect” weights that are learned from uncolored (gray-scale) ColoredMNIST, following Zhang et al. (2022). Besides the OOD methods used in the paper, we also include another OOD method IGA (Koyama & Yamaguchi, 2020) to give a more comprehensive overview of their performances with “perfect” initialization. Different from Zhang et al. (2022), we use SGD to continuously optimize the methods, as Adam would produce too large step sizes when the gradients stay within a small range under the “perfect” initialization. Fig. 6 shows the experimental results of “perfect” initialization on CMNIST-10. Results on other variants are given in Appendix C.2. It can be found that, as the optimization pursues, IRM, IRMx and IGA cannot maintain the performance, demonstrating the relatively low robustness of these objectives. In contrast, V-REx and \( \text{PAIR} \) maintain the performance, showing the sufficiency of both V-REx and \( \text{PAIR} \) in enforcing the invariance.

**Performances of Learning the Invariance.** Experimental results of different methods in learning the invariance from scratch are shown in Table 1. It can be found that \( \text{PAIR} \) significantly improves over IRMv1 and effectively captures the invariance across all environment settings, while the simple combination IRMx cannot yield satisfactory performance, confirming the drawbacks of linear scalarization (Boyd & Vandenberghe, 2014). Besides, \( \text{PAIR} \) achieves the best averaged performance over all methods, which further narrows the gap between practical variants and the original IRM in learning the invariance. More results and discussions in Appendix C.2. We will leave more comprehensive validation of effectiveness of \( \text{PAIR} \) in more difficult tasks (Gulrajani & Lopez-Paz, 2021; Koh et al., 2021) and more complex data (Chen et al., 2022; Ji et al., 2022) to future works.

5. Conclusion

In this work, we provided a new understanding of the different behaviors between IRMv1, IRMv1 and the original IRM through the lens of MOO. We revealed that using the improper optimization objectives in IRMv1 and IRMv1 is the main reason for their failures. Thus, we proposed \( \text{PAIR} \), that offers new capacity for incorporating additional guidance from more robust objectives. We showed that, with the additional guidance of REx, \( \text{PAIR} \) can effectively relocate and approach the desired invariant predictors onto the Pareto front. We will leave the pairing of other robust objectives with \( \text{PAIR} \) framework to future works. We hope \( \text{PAIR} \) can shed some light on understanding and improving the trade-off between ERM objective and OOD objective during the optimization. We provide an overview of related works and detailed discussions in Appendix A.

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A. Related Work

**Optimization Dilemma in OOD Algorithms.** Several recent works also notice the optimization dilemma in OOD algorithms, specifically, the trade-off between discovering the statistical correlations (i.e., ERM) and preventing the usage of spurious correlations (e.g., IRM). Empirically, Gulrajani & Lopez-Paz (2021) find that, with careful hyperparameter tuning and evaluation setting, many OOD algorithms cannot outperform ERM in domain generalization, demonstrating the difficulties in finding the desirable OOD solutions. Sagawa* et al. (2020); Zhai et al. (2022) find that, regularization on ERM, or sacrificing ERM performance, is usually needed for achieving satisfactory OOD performance, which aligns with our findings through Pareto front as Fig. 3 and Fig. 7(c). Zhang et al. (2022) find that, the performance of OOD algorithms largely relies on choosing proper pretraining epochs which aligns with our findings in Fig. 2, hence propose to construct a ready-to-use features for stable OOD generalization performance. Orthogonal to Zhang et al. (2022), we focus on developing better optimization scheme for OOD algorithms, including choosing the proper objectives and the achievability of the invariant predictors.

**MOO for Multi-Task Learning.** As it is usual that we cannot find a global optimal solution for all objectives in practice, hence Pareto optimal solutions are of particular value. The multiple-gradient descent algorithm (MGDA) is one of the commonly used approaches to efficiently find the Pareto optimal solutions (Désidéri, 2012) but limited to low-dimensional data. Sener & Koltun (2018) then resolve the issue and apply MGDA to high-dimensional multi-task learning scenarios, where the objective conflicts may degenerate the performance when using linear scalarization. As pure MGDA cannot find a Pareto optimal solution specified by certain objective preferences, Lin et al. (2019); Ma et al. (2020) propose efficient methods to explore the Pareto set. Mahapatra & Rajan (2020) propose EPO to find the exact Pareto optimal solution with the specified objective preferences. However, they are unable to solve OOD generalization, when without a suitable Pareto front. Besides, Lv et al. (2021) propose ParetoDA to use guidance of validation loss based on the data that has the identical distribution to test distribution, to trade-off the conflicts in domain adaption objectives. However, there can be multiple test domains and the data are usually unavailable in OOD generalization, limiting the adoption of ParetoDA.

B. More Details on Figures in Sections 2 and 3

We plot Fig. 1 and Fig. 4 based on the Mathematica code provided by Kamath et al. (2021), where we focus on the odd predictors due to the symmetry in two-bit environments, i.e., predictors satisfying $\varphi(1,-1) = -\varphi(-1,1)$ and $\varphi(1,1) = -\varphi(-1,-1)$. Besides, Fig. 1, Fig. 4 and Fig. 3 are implemented in MSE loss. Their Logistic loss counterparts are given as Fig. 7.

![Figure 7. Counterparts of Fig. 1, Fig. 4 and Fig. 3 implemented in Logistic loss.](image)

C. More Details on Experiments

C.1. Experimental Settings

We follow the evaluation settings as IRM (Arjovsky et al., 2019) and the test-domain selection as DomainBed (Gulrajani & Lopez-Paz, 2021) when conducting the experiments. Specifically, we use a 4-Layer MLP with a hidden dimension of 256. By default, we use Adam (Kingma & Ba, 2015) optimizer with a learning rate of $1e-3$ and a weight decay of $1e-3$ to train the model with 500 epochs and select the last epoch as the output model for each hyperparameter setting. We choose the final model as the one that maximizes the accuracy on the validation that share the same distribution as test domain. We then
do grid search for the other hyperparameters. For pretraining epochs, we search from \( \{0, 50, 100, 150, 200, 250\} \). For OOD penalty, we search from \( \{1e1, 1e2, 1e3, 1e4, 1e5\} \). We evaluate each configuration of hyperparameters 10 times and report the mean and standard deviation of the performances. Besides, we will refresh the history in Adam optimizer when the pretraining finishes, as suggested by Gulrajani & Lopez-Paz (2021). While for PAIR, we use SGD with a momentum of 0.9 (Sutskever et al., 2013) after pretraining to avoid the interference of Adam to the gradient direction and convergence of EPO (Mahapatra & Rajan, 2020) solver. Moreover, we empirically find that SGD requires larger learning rate (we use 0.1) for approaching the direction. This is because of the design in EPO solver that it first fits to the preference direction then does the “pure” gradient descent, while the intrinsically conflicting directions pointed by the objectives can make the loss surface more steep. We will leave in-depth understanding of the above phenomenon and more sophisticated optimizer design in more complex tasks and network architectures to future works (Zhou et al., 2020).

C.2. More Experimental Results and Discussions

We also conduct experiments with “perfect” initializations for different methods, to check whether the OOD constraints can enforce the invariance, following Zhang et al. (2022). Besides the OOD methods used in the paper, we also include another OOD method IGA (Koyama & Yamaguchi, 2020) to give a more comprehensive overview of their performances with “perfect” initialization. We also introduce another variant of ColoredMNIST, i.e., CMNIST-11: \( \{(0.25, 0.10), (0.25, 0.20)\} \) to complement more details. All methods are initialized with a ERM model learned on gray-scale ColoredMNIST data which is expected to learn to use digit shapes in the image to make predictions. The learning rate is \( 1e-3 \) and the penalty weight is \( 1e5 \). Different from Zhang et al. (2022), we use SGD to optimize the models, as Adam would generate larger step sizes when the gradients continue to be within a small range under the “perfect” initialization. Results are shown as in Fig. 8.

![Figure 8](image)

(a) “Perfect” initialization on CMNIST-10.  
(b) “Perfect” initialization on CMNIST-11.  
(c) “Perfect” initialization on CMNIST-25.

Figure 8. OOD performances with “Perfect” initializations.

It can be found that, in CMNIST-10, IRM, IRMx and IGA cannot enforce the invariance while V-REx and PAIR maintain the invariance, which is consistent to our previous findings. Moreover, IGA fails to maintain the invariance in CMNIST-11 and CMNIST-25, demonstrating the relatively low robustness of IGA objective. Besides, V-REx consistently maintain the invariance even in CMNIST-11, for the reason that the gradient signals of variance in “perfect” initialization tend to vanish. In contrast, PAIR improve over both IRM and IRMx to maintain the invariance, confirming the effectiveness of PAIR.