Meta-Learned Invariant Risk Minimization

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Abstract

Empirical Risk Minimization (ERM) based machine learning algorithms have suffered from weak generalization performance on data obtained from out-of-distribution (OOD). To address this problem, Invariant Risk Minimization (IRM) objective was suggested to find invariant optimal predictor which is less affected by the changes in data distribution. However, even with such progress, IRMv1, the practical formulation of IRM, still shows performance degradation when there are not enough training data, and even fails to generalize to OOD, if the number of spurious correlations is larger than the number of environments. In this paper, to address such problems, we propose a novel meta-learning based approach for IRM. In this method, we do not assume the linearity of classifier for the ease of optimization, and solve ideal bi-level IRM objective with Model-Agnostic Meta-Learning (MAML) framework. Our method is more robust to the data with spurious correlations and can provide an invariant optimal classifier even when data from each distribution are scarce. In experiments, we demonstrate that our algorithm not only has better OOD generalization performance than IRMv1 and all IRM variants, but also addresses the weakness of IRMv1 with improved stability.

1. Introduction

Conventional machine learning algorithms often fail to generalize, when training data include spurious correlations with strong correlations to a target label. With such data, they are more likely to learn spurious correlations, which does not correspond to the true causal relation that exists in data. Learning by minimizing empirical risks of data is reasonable choice for the generalization performance of model, if test data are sufficiently similar to a training distribution. However, if test data include strong spurious correlations, or sampled from the out-of-distribution (OOD), ERM based approach inevitably fails to provide reliable outcomes. This problem is known as OOD generalization problem and can be easily found in the real-world scenario for machine learning. (Beery et al., 2018; Ilyas et al., 2019; Geirhos et al., 2018; de Haan et al., 2019)

Invariant Risk Minimization (IRM) (Arjovsky et al., 2019) is a recently proposed learning paradigm to address OOD generalization problem with the theory of Invariant Causal Prediction (Peters et al., 2016; Heinze-Deml et al., 2018). It is based on the fundamental idea that true causal relations remain invariant while spurious correlations can vary across data distributions from different environments. Based on this idea, Arjovsky et al. (2019) introduce IRM objective which finds an invariant predictor that is also optimal for every available data environments. In its formulation, IRM enables finding invariant correlations that are robust to the changes in data distribution. However, because of its challenging bi-level optimization form, they instantiate the IRM objective into more practical version, with fixed linear classifier constraint called IRMv1. By assuming such classifier, they reformulate the hard constraints in IRM into the invariance penalty term, and in return, obtained reasonable OOD generalization performance.

However, despite the effectiveness of IRMv1 for OOD generalization, it lacks some formal guarantees which ideal IRM objective can provide (Kamath et al., 2021). IRMv1 and its variants inevitably fail when the number of training...
environments is smaller than the number of the spurious correlations existing in data (Rosenfeld et al., 2020). In addition, we find that OOD generalization performance of IRMv1 and its variant severely degrades when the training data in each training environment become too small.

In this paper, we propose a novel approach for IRM objective initiation which learns invariant optimal predictors with meta-learning based optimization. In this idea, instead of simplifying the challenging bi-level optimization objective of IRM, we keep the ideal objective form and solve it with Model-Agnostic Meta-Learning framework. Specifically, as in the conventional meta-learning approach, we treat each training environment as one of tasks in meta-learning. But, we apply disjoint training environments for each inner loop and outer loop (meta-loss) optimization, to introduce an invariance constraint to the classifier across different environments.

The main contribution of our work is providing a more effective initiation method of ideal IRM objective. While lifting the linear classifier assumption of IRMv1, our model still can find invariant representations existing across environments. We empirically show that the limitations of IRMv1 objective severely degrades OOD generalization performance even under simple conditions on data environment. Furthermore, we introduce a new auxiliary loss for non-linear invariant classifier which minimizes the standard deviation of meta-losses from all environments. In experiments, we show that our meta-IRM framework achieves better OOD generalization performance than IRMv1 and all other alternatives. Also it consistently provides invariant optimal predictor even when IRMv1 fails to generalize OOD.

2. Related Work

There are several works on practical variants of IRM (Ahuja et al., 2020a; Krueger et al., 2020). Invariant Risk Minimization Games (Ahuja et al., 2020a) expands IRM objective by adopting game theory that finds the Nash equilibrium of classifiers among training environments. Risk Extrapolation (MM-REx, V-REx) (Krueger et al., 2020) achieves OOD generalization with two objectives: minimizing average of empirical risks and maximizing similarity of empirical risks across training environments. As there is a trade-off between these two objective, MM-REx uses mini-max objective over training risks and V-REx uses the variance of empirical risks as a regularization loss. Our method has similarity to V-REx in terms of considering the variance of risks, but we regulate the meta-losses for each environment rather than empirical risks. Also, V-REx algorithm is mainly build upon regularization term to achieve OOD generalization when considering its large regularization coefficient. In contrast, we normally assign very small coefficient for the standard deviation of meta-losses since our algorithm mainly focuses on bi-level optimization with meta-learning approach. There are many research for IRM to understand its effect on OOD generalization (Rosenfeld et al., 2020; Ahuja et al., 2020b; Choe et al., 2020; Kamath et al., 2021). Analysis of Rosenfeld et al. (2020) demonstrates that IRMv1 and its alternatives are failed to generalize OOD not only in the linear regime but also in the non-linear case. We empirically show the limitation of IRMv1 in the linear regime and success of our meta-IRM in the same condition. In addition, there is no explicit assumption of the linear classifier in our proposed method, unlike IRMv1. Therefore, we expect our algorithm is able to provide OOD generalization even in nonlinear regimes.

Meta-learning (Schmidhuber, 1987; Bengio et al., 1990; Thrun & Pratt, 1998), also known as learning-to-learn, is a learning framework devised for fast adaptation for unseen tasks. While training with multiple tasks, it learns quick knowledge or meta-knowledge (Ravi & Larochelle, 2016) and applies the knowledge to a new task adaptation for enhanced generalization performance. Gradient-based meta-learning approaches (Ravi & Larochelle, 2016; Finn et al., 2017; Nichol et al., 2018) are widely researched methods and MAML (Finn et al., 2017) is one of such fundamental methods. MAML consists of two levels of optimization, inner and outer. Inner optimization updates parameters of the model adapting to a new task while outer or meta-optimization learns parameters which are needed for all other training tasks. Our method is built upon this two level optimization framework where training tasks corresponding to training environments. However, our algorithm adopts a new learning strategy which is applying different training environments for inner and meta-optimization loop to learn invariant features existing across different environments.

There are several meta-learning approaches targeting the OOD problem. However, their definition for OOD and the main purpose are different from ours. Jeong & Kim (2020) introduce OOD-MAML, an extension of MAML, to detect unseen classes by learning artificially generated fake samples which are considered to be OOD samples. They define OOD as samples from unseen classes and this definition is different from our goal of learning invariant correlations. Lee et al. (2019a) suggest Bayesian-TAML for imbalanced and OOD tasks. In Bayesian-TAML, the OOD generalization means relocating the initial parameters θ for adaptation to unseen OOD tasks, because meta-optimized θ may be less useful for the adaptation of OOD tasks. In our approach, we do not rely on inner optimization or adaptation for the test environment, because we are aimed to find θ that can achieve the best OOD generalization by itself.

For the bi-level optimization perspective, Jenni & Favaro (2018) have a similar idea with our method. They reformu-
late the training procedure based on the principles of cross-validation to reduce overfitting and set up a bi-level optimization problem which uses split mini-batches as validation and training sets. They structured bi-level optimization by assigning each level with validation data optimization and the training data optimization. In our algorithm, we also use different training environments for bi-level optimization, inner optimization and meta-optimization. However, their work is intended to generalize for test data which have similar data distribution with training data, whereas we are targeting an invariance of predictor even with the shift in data distribution.

3. Proposed Method

3.1. Problem Set-Up

We formalize our problem setting same as Arjovsky et al. (2019). We consider multiple $E$ training environments $E_{tr} = \{e_i\}_{i=1}^{E}$ and datasets $\{(x_{ik}^e, y_{ik}^e)\}_{k=1}^{n}$ collected from each environment $e$. The observational data $x_{ik}^e$ include invariant feature set $\Psi_e$ and spurious feature set $\Psi_s$ in which both have strong correlation with target variable. Each environment is related to one primary task but has a different data distribution. The risk under environment $e$ with a predictor $f$ is defined as $R_e(f) = \mathbb{E}_{x^e, y^e}[\ell(f(x^e), y^e)]$, where $\ell$ is a loss function, $f(x^e)$ is the output of the predictor and $y^e$ is the target variable. Each adapted parameter computes meta-loss from the training data from each environment are not sufficient. $E > \Psi_s$(Kamath et al., 2021). However, its translated form also introduces severe limitations on the capabilities of ideal IRM objective. The linear fixed classifier assumption of IRMv1 can guarantee to find optimal invariant classifier under the condition that the number of spurious correlations is smaller than the number of training environment, $E > |\Psi_s|$ (Rosenfeld et al., 2020). With simple violation of this condition, $E \leq |\Psi_s|$, IRMv1 can catastrophically fail to generalize for OOD. Furthermore, as the number of finite sample decreases, it is more likely to choose a fake invariant predictor which relies on environmental features, $\Psi_s$. (Rosenfeld et al., 2020). In addition, we find that IRMv1 does not appropriately approximate IRM, even when $E > |\Psi_s|$, if the training data from each environment are not sufficient. Despite its penalty term $\|\nabla_{\omega=\Phi} \cdot \Phi\|_{2}^{2}$ is close to zero, IRMv1 still cannot find an invariant predictions, as shown in Figure 6.

3.2. Invariant Risk Minimization

Invariant Risk Minimization is intended to estimate optimal invariant causal predictor $f$ by learning correlations invariant across all of the training environments. This also means to find a feature representation of data such that the optimal classifier is invariant across all environments. Based on this idea, IRM is formulated as the following constrained bi-level optimization problem:

$$\begin{align*}
\min_{\Phi: \mathcal{X} \rightarrow \mathcal{H}} & \sum_{e \in E_{tr}} R_e(\Phi) \\
\text{subject to} & \omega \in \arg \min_{\omega: \mathcal{H} \rightarrow \mathcal{Y}} R_e(\omega \circ \Phi), \forall e \in E_{tr}
\end{align*}$$

where $\omega$ is a classifier (or final layer for regression problems), $\Phi$ is a data representation and $\omega \circ \Phi$ is a predictor. However, it is difficult to solve such optimization problem directly since multiple constraints must be solved jointly. Arjovsky et al. (2019) introduce IRMv1, a practical version of IRM, with Lagrangian form to relax joint constraints such that the classifier $\omega$ is “approximately locally optimal”. IRMv1 also assumes linear classifier $\omega$ as fixed scalar. The learning objective of IRMv1 is as follows:

$$\min_{\Phi: \mathcal{X} \rightarrow \mathcal{H}} \sum_{e \in E_{tr}} R_e(\Phi) + \lambda \cdot \|\nabla_{\omega=1.0} R_e(\omega \cdot \Phi)\|_{2}^{2}$$

where $\lambda \in (0, \infty)$ controls the invariance of the predictor $\cdot \Phi(x)$. The gradient norm penalty $\|\nabla_{\omega=1.0} R_e(\omega \cdot \Phi)\|_{2}^{2}$ indicates the optimality of fixed linear $\omega = 1.0$.

Compared to an ideal IRM objective which possibly regards $\Psi_e$ with sampling noise as non-invariant features, IRMv1 with fixed $\lambda$ is more robust for the sampling noise of finite samples (Kamath et al., 2021). However, its translated form also introduces severe limitations on the capabilities of ideal IRM objective. The linear fixed classifier assumption of IRMv1 can guarantee to find optimal invariant classifier under the condition that the number of spurious correlations is smaller than the number of training environment, $E > |\Psi_s|$ (Rosenfeld et al., 2020). With simple violation of this condition, $E \leq |\Psi_s|$, IRMv1 can catastrophically fail to generalize for OOD. Furthermore, as the number of finite sample decreases, it is more likely to choose a fake invariant predictor which relies on environmental features, $\Psi_s$. (Rosenfeld et al., 2020). In addition, we find that IRMv1 does not appropriately approximate IRM, even when $E > |\Psi_s|$, if the training data from each environment are not sufficient. Despite its penalty term $\|\nabla_{\omega=1.0} R_e(\omega \cdot \Phi)\|_{2}^{2}$ is close to zero, IRMv1 still cannot find an invariant predictions, as shown in Figure 6.

3.3. Meta-learned Invariant Risk Minimization

We propose a novel learning framework for ideal IRM, meta-learned Invariant Risk Minimization (meta-IRM), which learns invariant optimal predictors with Model-Agnostic
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Meta-Learning framework. Contrary to IRMv1, we keep the ideal bi-level formulation of IRM and do not impose any linearity assumptions to the classifier $\omega$. Instead, our meta-IRM jointly optimizes inner and upper-level objectives with the meta-learning based optimization framework. Conventional meta-learning approaches are intended to find proper initial parameters for fast adaptation on new tasks. Our meta-IRM also finds optimal parameters that generalize well across not only for training environments but also for multiple unseen environments. To estimate optimal predictor, meta-IRM performs inner optimization to each training environment and utilizes the gradients of meta-losses derived from all other training environments except the one used for inner optimization. As shown in Figure 1, while ERM supposed to converge to the $\theta_{ERM}$ by learning spurious correlations, meta-IRM merges gradient obtained from $f_\theta$ and $f_{\theta_j^*}$ to reach $\theta_{optimal}$. Each gradient of meta-loss contributes to the converging path to $\theta_{optimal}$.

We consider multiple training tasks of meta-learning to be $\beta$ where $\alpha$ is a learning rate of the inner optimization. We only consider one gradient update of inner loop update for the simplicity of notation and it is possible to use multiple gradient updates generally.

With inner updated predictor $f_{\theta_j'}$, meta-optimization across training environments with stochastic gradient descent(SGD) can be expressed as follows:

$$
\theta' = \theta - \beta \nabla_{\theta} \sum_i R^{e_i}(f_{\theta_j'}) \; , \; e_j \sim E_{\text{tr}} \setminus e_i
$$  \hspace{1cm} (4)

where $\beta$ is the learning rate of the meta-optimization, $e_j$ is training environment for meta-optimization for the parameters $\theta_i$ and $R^{e_i}(f_{\theta_j'})$ is the risk for meta-optimization, or meta-loss. Note that the model $f_{\theta_j'}$ is evaluated with $e_j$ sampled from $E_{\text{tr}} \setminus e_i$ in the meta-optimization, whereas it is updated with $e_i$ in the inner optimization, as we want to use the information obtained from the discrepancy among different training environments. In addition, the meta-optimization is performed with the derivatives of $\theta' = \theta - \alpha \nabla R^{e_i}(f_\theta)$ through $\theta$ for all $i$, i.e., second-order derivatives of $\theta$. The first-order approximation of meta-IRM is also applicable, but we show that it degrades the performance, see Section 4.5. The schematic of learning process of meta-IRM is shown in Figure 2.

We introduce auxiliary loss, the standard deviation of meta-losses in meta-optimization process, for the invariance of predictor. The goal of IRM is learning invariant optimal predictor across environments. With such auxiliary loss, meta-IRM updates the parameter $\theta$ to achieve invariant predictions across multiple adapted predictors $f_{\theta_j'}$ in meta-optimization. In addition, the standard deviation loss makes meta-IRM enable more stable training and faster convergence. In our experiment, by adding auxiliary loss, it is enough to achieve invariant predictions with using less inner update steps for meta-IRM. Moreover, meta-IRM with auxiliary loss achieves the best results of OOD generalization in our experiment. The auxiliary loss is defined as follows:

$$
\sigma = \sqrt{\frac{1}{N} \sum_{k=1}^{N} \left( \frac{1}{N} \sum_{i=1}^{N} L_{\text{meta}}^k \right)^2}
$$  \hspace{1cm} (5)

where $N$ is the number of meta-losses and $L_{\text{meta}}^k$ indicates the $k$-th meta-loss. Applying the auxiliary loss, our meta-optimization update rule is changed from Equation 4 into as:

Algorithm 1 Meta-IRM

Require: $E_{\text{tr}}$: training environments
Require: $E_{\text{val}}$: validation environments divided from $E_{\text{tr}}$
Initialize: Randomly initialize $\theta$ while not done do
  for all $e_j \in E_{\text{tr}}$ do
    Evaluate $\nabla_{\theta} R^{e_i}(f_\theta)$ using $(x_k^{e_i}, y_k^{e_i})_{k=1}^n$
    Execute inner optimization: $\theta' = \theta - \alpha \nabla R^{e_i}(f_\theta)$
    Sample training environments $e_j$ from $E_{\text{tr}} \setminus e_i$
    for all $e_j$ do
      Compute meta-loss $R^{e_j}(f_{\theta_j'})$ using parameters $\theta_i$ and $(x_k^{e_j}, y_k^{e_j})_{k=1}^n$
    end for
  end for
  Compute standard deviation of $\{R^{e_j}(f_{\theta_j'})\}_{i,j}$
  Execute meta-optimization using Equation 6
end while
where \( \lambda \) is a hyperparameter enforcing meta-losses to have similar values and \( \sigma \) is a standard deviation of meta-losses. Without the auxiliary loss, meta-IRM still can achieve OOD as a consequence, the two-level optimization routines of \( \lambda \) more robust to sampling noise of empirical distributions. Furthermore, meta-IRM is also meta-IRM solves challenging bi-level optimization of IRM objective than IRMv1. Furthermore, meta-IRM is also minimizing sum of the meta-losses computed from \( \theta \) of IRM which updates the model parameters \( \omega \) to \( \theta \) by mini-

### 3.4. Connection between IRM and meta-IRM

In this section, we illustrate how ideal IRM formulation is translated and initiated with meta-IRM approach. In the formulation of IRMv1, each constraint of IRM is translated to squared norm of the gradients of the risk with respect to the fixed linear \( \omega \), for the simplification of problem. In our meta-IRM, which is built upon MAML, the challenging bi-level optimization of IRM is translated into two-level optimization scheme of meta-learning framework. In this framework, the inner loop optimization corresponds to \( \omega \in \arg \min_{\omega:H \rightarrow Y} R^{c}(\omega \circ \Phi) \) of IRM which updates the parameters \( \theta \) to \( \theta'_{i} \) for each training environment. Meta-optimization is regarded as the upper-level optimization of IRM which updates the model parameters \( \theta \) by minimizing sum of the meta-losses computed from \( \theta'_{i} \) for all \( i \). As a consequence, the two-level optimization routines of meta-IRM solves challenging bi-level optimization of IRM without simplification, and it is much closer to the original IRM objective than IRMv1. Furthermore, meta-IRM is also more robust to sampling noise of empirical distributions than IRMv1 in our experiment, see Figure 4.

Contrast to IRM, meta-IRM does not explicitly separate the data representation \( \Phi \) and the classifier \( \omega \) from predictor \( f \) for optimization. However, meta-IRM naturally follows IRM optimization structure, from the perspective of the classifier and data representation. As in the formulation of IRM, meta-IRM updates classifier in the inner loop optimization and learns data representation in the meta-optimization due to the property of MAML (Raghu et al., 2019).

### 4. Experiments and Results

#### 4.1. Colored MNIST

We evaluate meta-IRM with IRMv1 and its variants on Colored MNIST dataset from Arjovsky et al. (2019). It is modified MNIST images that are colored in either green or red. These colors have spurious correlations with the class labels which should be decided by the shape of each digit. Specifically, the digits from 0 to 4 have label \( \tilde{y} = 0 \) and 5 to 9 have label \( \tilde{y} = 1 \). We add noise to \( \tilde{y} \) to build final label \( y \) by flipping \( \tilde{y} \) with probability \( \eta_{c} = 0.25 \). To make spurious correlation, sample the color id \( z \) by flipping \( y \) with probability \( p_{c} \) varying across environments. Finally, color the digit with constructed color id as green if \( z = 0 \) or red if \( z = 1 \). There are two training environments and one test environment. We build validation set for early stopping by sampling from each training environments. For the training environments, we use \( p_{c} = 0.1 \) for the first environment and \( p_{c} = 0.2 \) for the second environment. The probability \( p_{c} = 0.9 \) is used for the test environment where the correlation between color and label is reversed. Each training environment has 25,000 images and test environment has 10,000 samples. The goal of this task is to classify digits based on the shape of digits without considering colors.

We use MLP with ReLU activation function and a hidden layer to evaluate meta-IRM and others. Table 1 shows the

| Algorithm                  | Test Accuracy |
|----------------------------|---------------|
|                           | \( p_{c} = 0.1 \) | \( p_{c} = 0.2 \) | \( p_{c} = 0.9 \) |
| ERM                       | 88.6 ± 0.3    | 79.7 ± 0.6     | 16.4 ± 0.8       |
| IRMv1                     | 71.4 ± 0.9    | 70.8 ± 1.0     | 66.9 ± 2.5       |
| MM-REx                    | 70.8 ± 1.5    | 70.4 ± 2.0     | 66.1 ± 4.9       |
| V-REx                     | 71.5 ± 0.8    | 71.1 ± 0.9     | 68.6 ± 1.2       |
| meta-IRM (Ours)           | 70.9 ± 0.9    | 70.8 ± 1.0     | 70.4 ± 0.9       |
| Random                    | 50            | 50             | 50               |
| ERM (grayscale)           | 72.6 ± 0.3    | 72.7 ± 0.3     | 73.0 ± 0.5       |
| Optimal                   | 75            | 75             | 75               |

We use MLP with ReLU activation function and a hidden layer to evaluate meta-IRM and others. Table 1 shows the
results of meta-IRM and other algorithms on test environments with $p_e$ as 0.1, 0.2 (similar to training environments), and 0.9 (out-of-distribution) on Colored MNIST task in 10 trials. The ideal accuracy for test environment is 75% due to the label noise $\eta_e = 0.25$. ERM achieves high test accuracy for test environment which has similar distribution to training environments as $p_e = 0.1$ and $p_e = 0.2$ respectively. However, it shows low accuracy for OOD worse than random selection. In result, it predicts labels based on the color, which is a spurious feature, failing to generalize in a test environment with contradictory correlation between color and target label. Our proposed meta-IRM achieves the highest mean accuracy of 70.4% and the lowest standard deviation of 0.9% compared with others. ERM grayscale images which do not include spurious features. As shown in Figure 3, we evaluated each algorithm by using test environment with diverse $p_e$ from 0.1 to 0.9 in steps of 0.1. The predictions of meta-IRM are invariant across multiple test environments while others show worse performance as the environment moves away from training environments.

### 4.2. Multi-Class Problem

Many real-world problems are multi-class. We compare meta-IRM with IRMv1 using 5-class and 10-class version of Colored MNIST (Choe et al., 2020). The number of colors is set to $k$ for $k$-class task and each color is assigned to a input channel of image. For $k = 5$, we consider two consecutive numbers as one class, such as 0-1, 2-3 etc. For $k = 10$, we consider each digit as one class. Instead flipping labels with fixed noise $\eta_e$, we increase label index by 1 as noise. For the label $\hat{y} = k$, the final label becomes $y = 0$.

The results of multi-class task is shown in Table 2. Though the test environment results of IRMv1 still shows better achievement than ERM for $k = 5$ and $k = 10$, the performance degrades as the number of classes increases. Also, IRMv1 absorbs small portion of spurious correlations as the number of classes increases. Our proposed meta-IRM achieves the best performance not only for $k = 5$ but also for $k = 10$ and shows invariant predictions across multiple environments despite having a slightly higher variance of test accuracy than $k = 2$.

### 4.3. Robustness to Sampling Noise

We also experiment meta-IRM on Colored MNIST to evaluate its robustness to empirical distributions, even if it targets the ideal IRM objective. In practice, finite samples cannot exactly represent the distribution, since they contain sampling noise. Kamath et al. (2021) regard a small difference of $\eta_e$ between training environments as sampling noise. We make a gap of $\eta_e$ between two training environments but still have the same average as 0.25 (Choe et al., 2020). Training environment with $p_e = 0.1$ has $\eta_e = 0.25 + \frac{0.05}{2}$ and the other with $p_e = 0.2$ has $\eta_e = 0.25 - \frac{0.05}{2}$. We increase the gap from 0 to 0.05 in steps of 0.01 and illustrate test environment accuracy of meta-IRM and IRMv1. As shown in Figure 4, meta-IRM shows robustness to noise while the

| Algorithm | # of class | Accuracy |
|-----------|------------|----------|
|           | Train      | Test     |
| ERM       | 95.2 ± 0.2 | 41.0 ± 0.6 |
| IRMv1     | 82.2 ± 0.4 | 62.0 ± 2.4 |
| meta-IRM (Ours) | 76.4 ± 1.4 | 74.0 ± 3.6 |
| Random    | 20         | 20       |
| ERM (grayscale) | 73.2 ± 0.2 | 71.7±0.4 |
| Optimal   | 75         | 75       |
| ERM       | 92.6 ± 0.2 | 39.2 ± 0.9 |
| IRMv1     | 83.4 ± 0.5 | 58.6 ± 2.5 |
| meta-IRM (Ours) | 79.5 ± 0.6 | 73.4 ± 3.2 |
| Random    | 10         | 10       |
| ERM (grayscale) | 73.2 ± 0.1 | 71.9 ± 0.5 |
| Optimal   | 75         | 75       |

Figure 3. Accuracy of different training algorithms for the test environment with various $p_e$ on Colored MNIST. Dots indicate means and error bars represent standard deviations of 10 trials. We slightly shifted the dots to prevent error bars from overlapping.

Figure 4. Accuracy of IRMv1 and meta-IRM for test environment with $\eta_e = 0.25, p_e = 0.9$ when the gap of $\eta_e$ between training environments increases. The line indicates mean and colored area indicates a standard deviation of 10 trials.
performance of IRMv1 is getting worse as the gap increases.

4.4. The limitations of IRMv1

From our experiments, we find that IRMv1 shows performance degradation with insufficient data in training environments. We experiment with two cases: 12,500 and 6,250 training samples per each environment which become half and quarter, respectively. IRMv1 shows worse test accuracy for OOD while meta-IRM shows comparable results as shown in Table 3. Figure 5 illustrates multiple test environments results of IRMv1 and meta-IRM in case of insufficient training data. IRMv1 and V-REx start to follow ERM as the number of data decreases while meta-IRM still achieves invariant predictions in changing $p_e$ despite having insufficient training data. As shown in Figure 6, even if the penalty term of IRMv1 is close to zero regardless of the number of data samples, it fails to approximate ideal IRM objective.

In a real-world scenario, there are many kinds of spurious correlations in the data distribution. However, IRMv1 can fail to achieve invariant predictor when the number of spurious correlations is greater than the number of training environments (Rosenfeld et al., 2020). Creating lots of training environments can be a solution for such problem, but the number of training samples per training environment will be decreased since available data in real-world scenario is always limited. Therefore, IRMv1 is going to fail to estimate invariant predictor in such condition. In our experiments, we show that our meta-IRM performs invariant predictions not only for the case that the data is insufficient but also for many spurious correlations in the data.

We design additional spurious correlation as (Ahuja et al., 2020a), by creating small patches of noise to the corner in the image where the locations of these patches are strongly correlated with the labels. Similar with the probability $p_e$ of Colored MNIST, we define patch id $z'$ by flipping $y$ with probability $p_{e2}$ also varying across environments. Based on the patch id, we add $(3 \times 3)$ patch in the top left corner of the image if $z' = 0$, or $(2 \times 2)$ patch in the bottom right corner of the image if $z' = 1$. There are two training environments: $p_e = 0.1, p_{e2} = 0.2$ for the first and $p_e = 0.2, p_{e2} = 0.1$ for the second and one test environment with $p_e = 0.9$ and $p_{e2} = 0.9$. The patches are independent with the colors of digits but have strong correlation with colors and target labels. Figure 7 illustrates the image samples of Colored MNIST task with additional spurious features. In this experiment, IRMv1 fails to generalize to OOD, following ERM. IRMv1 achieves high test accuracy for the test environments.
Figure 7. Image samples of Colored MNIST task with additional patch feature. These patches have strong but spurious correlation with target labels.

Figure 8. Test accuracy of different algorithms when the data include two spurious features, color and patch. Dots indicate means and error bars represent standard deviations of 10 trials. Analogous to the training environments but shows low accuracy for the test environments with \( p_e = 0.9 \) and \( p_{e2} = 0.9 \). Unlike IRMv1, meta-IRM achieves invariant predictions across multiple environments although the performance is slightly degraded as shown in see Table 4. Figure 8 illustrates results of meta-IRM and IRMv1. Since IRMv1 learns spurious features, the results of for test environments with \( p_e = 0.1 \) and \( 0.2 \) seem plausible. However, its test accuracy decreases for OOD.

### 4.5. Ablation Study

In this section, we show ablation experiments to demonstrate the importance of the standard deviation loss. Also, meta-IRM algorithm uses second-order derivatives of \( \theta \) and considers different training environments between inner optimization and meta-loss computation. We perform ablation study of meta-IRM in order to understand the effects. Without using the additional standard deviation loss, meta-IRM still shows comparable accuracy for OOD. However, it is recommended to use such auxiliary loss to stabilize the algorithm and achieve the best performance. We also show that it is important to use second-order derivatives of \( \theta \) in the objective of meta-IRM to achieve high-performance of OOD generalization. Furthermore, using different training environments for inner optimization and meta-loss computation is critical to learn invariant predictors as shown in Table 5.

### 5. Conclusion

In this work, we interpret IRM objective in meta-learning perspective and propose a novel meta-learning based method for ideal IRM initiation to obtain further enhanced OOD generalization. Our method maintains the bi-level optimization form of ideal IRM objective by efficiently relaxing the linearity restriction of classifier based on MAML. In experiments, meta-IRM shows superior OOD generalization performance than all other IRM variants and is able to provide invariant predictor even when IRMv1 and all its variants fail. Furthermore, our method shows more robustness to the noise in true causal features, although original IRM objective is susceptible to such condition. Our meta-IRM provides the most effective IRM initiation method for OOD generalization and also shows promising results for the non-linear regime by excluding the linearity assumption for predictor.

### References

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A. Additional Results

A.1. Representational Similarity Experiment

We show optimization characteristic of meta-IRM by measuring similarity between feature representations of each layer in the predictor before and after inner optimization (Raghu et al., 2019). We apply Projected Weighted Canonical Correlation Analysis (PWCCA) similarity (Morcos et al., 2018) to the feature representations. We experiment meta-IRM on Colored MNIST without using auxiliary loss in order to understand the effect of two-level optimization of meta-learning. We illustrate PWCCA similarities of representations just before the training is converged. As shown in Figure 9, feature representations of the first and second layers are highly similar, however, the classifier has a relatively low PWCCA similarity. The result demonstrates that the inner optimization mostly updates the classifier whereas the data representation has little functional changes. Consequently, meta-IRM can learn invariant optimal predictor under the original bi-level optimization of IRM objective.

Figure 9. PWCCA similarity between representations of each layer before and after inner optimization.

A.2. Invariant Data Representation

We already show the invariant predictions of meta-IRM as shown in Figure 3. The data representation which learns invariant correlations is invariant across environments. We experiment invariance of the data representation of IRMv1 and meta-IRM by using PWCCA similarity. The data representation of the predictor trained by each algorithm is obtained from the test environments with diverse \( p_e \) from 0.1 to 0.9 in steps of 0.1. We consider the data representation of the case of meta-IRM to be feature vectors which are the input of the classifier layer. For the case of IRMv1, the data representation is the output vector of the neural network due to its formulation. We compute the PWCCA similarity between the data representation obtained from the test environment with \( p_e = 0.1 \) and others. Figure 10 illustrates the results of the PWCCA similarity between the data representations across multiple test environments. The similarity between data representations of IRMv1 decreases as \( p_e \) of test environment increases. In contrast, meta-IRM shows more invariant data representations across entire test environments with higher similarity scores than IRMv1. Therefore, meta-IRM is better to learn invariant optimal predictor by learning invariant correlations across environments than IRMv1.

B. PunctuatedSST-2

We evaluate our meta-IRM on natural language processing (NLP) task using PunctuatedSST-2 dataset from Choe et al. (2020). PunctuatedSST-2 is a modified version of NLP benchmark dataset, Standford Sentiment Treebank (SST-2). Similar to the spurious feature ‘color’ in Colored MNIST task, we artificially make spurious features using punctuation marks. We add noise to target labels to construct final label \( y \) by flipping with probability \( \eta_e \). Punctuation mark id \( z \) is constructed by flipping \( y \) with probability \( p_e \). Finally, punctuate the input with an exclamation mark (!) if \( z = 0 \) or with a period (.) if \( z = 1 \). There are two training environments with \( p_e = 0.1 \) and \( p_e = 0.2 \), respectively, and one test environment \( p_e = 0.9 \).

Table 6. Test environment accuracy (%) on PunctuatedSST-2 task of different algorithms. ERM (grayscale) indicates the results of ERM with vanilla SST-2 dataset.

| Algorithm            | \( \eta_e \) | Test accuracy \((p_e = 0.9)\) |
|----------------------|-------------|-----------------------------|
| ERM                  |             | 30.7 ± 1.5                  |
| IRMv1                |             | 62.0 ± 1.9                  |
| meta-IRM (Ours)      | 0.25        | 62.2 ± 1.8                  |
| ERM (grayscale)      |             | 62.3 ± 0.5                  |
| Optimal              |             | 75                          |
| ERM                  |             | 56.2 ± 2.9                  |
| IRMv1                |             | 67.4 ± 1.4                  |
| meta-IRM (Ours)      | 0           | 73.0 ± 0.7                  |
| ERM (grayscale)      |             | 76.7 ± 2.7                  |
| Optimal              |             | 100                         |
We train the MLP with ReLU activation function and a hidden layer. The input data are embedded with GloVe (Pennington et al., 2014). As shown in Table 6, both IRMv1 and our meta-IRM show the results close to the optimal when the label noise \( \eta_e = 0.25 \). We also show the results when the label noise \( \eta_e = 0 \). Our meta-IRM shows much higher test accuracy than IRMv1 and ERM, close to ERM grayscale when \( \eta_e = 0 \).