Rich Feature Construction for the Optimization-Generalization Dilemma

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Abstract

There often is a dilemma between ease of optimization and robust out-of-distribution (OoD) generalization. For instance, many OoD methods rely on penalty terms whose optimization is challenging. They are either too strong to optimize reliably or too weak to achieve their goals.

In order to escape this dilemma, we propose to first construct a rich representation (RFC) containing a palette of potentially useful features, ready to be used by even simple models. On the one hand, a rich representation provides a good initialization for the optimizer. On the other hand, it also provides an inductive bias that helps OoD generalization. RFC is constructed in a succession of training episodes. During each step of the discovery phase, we craft a multi-objective optimization criterion and its associated datasets in a manner that prevents the network from using the features constructed in the previous iterations. During the synthesis phase, we use knowledge distillation to force the network to simultaneously develop all the features identified during the discovery phase.

RFC consistently helps six OoD methods achieve top performance on challenging invariant training benchmarks, ColoredMNIST (Arjovsky et al., 2020). Furthermore, on the realistic Camelyon17 task, our method helps both OoD and ERM methods outperform earlier compatable results by at least 5%, reduce standard deviation by at least 4.1%, and makes hyperparameter tuning and model selection more reliable.

1. Introduction

The interplay of optimization and generalization plays a crucial role in deep learning. It also changes nature when

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we focus on out-of-distribution (OoD) generalization, that is when training and testing sets are no longer assumed to follow the same distribution.

Simple optimization algorithms are surprisingly able to find uneventful descent paths in the non-convex cost landscape of deep learning networks (Gu et al., 2021; Sagun et al., 2017). However they also tend to construct features that capture spurious correlations (Szegedy et al., 2014; Beery et al., 2018; Arjovsky et al., 2020; Ilyas et al., 2019). Several recent papers propose to work around this problem by leveraging multiple training sets that illustrate the possible changes in distribution. The training algorithm must then satisfy certain constraints across training sets, usually enforced with additional penalty terms (Arjovsky et al., 2020; Koyama & Yamaguchi, 2020; Krueger et al., 2020; Pezeshki et al., 2020; Shi et al., 2021; Rame et al., 2021; Wald et al., 2021). The resulting optimization problem often turns substantially more challenging than the simple empirical risk minimization (ERM). In practice it is often necessary to schedule the penalty hyper-parameters in a manner that weakens them so much that they no longer enforce the intended constraints. As a result, when one initializes such a method with the correct solution, the training process deviates from the constraint set and finds inferior solutions (Figure 2).

We propose in this paper to work around the difficulties of the optimization problem by first obtaining a representation of the input patterns that contains a broad diversity of potentially useful features. Both the ERM and OoD methods can then easily pick the most useful features, according to the chosen training cost and constraints, in a much easier way. The Rich Feature Construction (RFC) method (Section 4) consists of a succession of training episodes, divided into two phases:

- 1. During each step of the *discovery phase*, we craft a multi-objective optimization criterion that prevents the network from using the features constructed in the previous steps.
- 2. During the *synthesis phase*, we force the final representation to simultaneously represents all the features identified during the *discovery phase*.

On the common out-of-distribution (OoD) COLOREDM-

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NIST task (Arjovsky et al., 2020), we show that RFC consistently helps six state-of-the-art OoD learning algorithms learn the robust feature and disregard the spurious one. We also show that RFC performs well on a modified task, RE-VERSECOLOREDMNIST, in which the robust feature is made more predictive than the spurious feature. Such a modification breaks all methods that aim for the 2nd easiestto-find features (Nam et al., 2020; Liu et al., 2021; Bao et al., 2021). Finally, we evaluate RFC on the real-world CAME-LYON17 task (Koh et al., 2021b) and show that RFC not only helps OoD and ERM methods match or exceed the best published results, but also facilitates the hyper-parameter tuning and model selection.¹

2. Related Work

2.1. Leveraging multiple training environments

In order to achieve a good performance on testing data that follows a different distribution from the training data, many OoD methods assume access to multiple training sets, or environments, whose different distributions illustrate a range of potential distribution changes. One possible direction consists of learning a representation such that the optimal classifier built on top is the same for all training environments: IRMv1/IRM (Arjovsky et al., 2020), MAML-IRM (Bae et al., 2021), CLOvE (Wald et al., 2021). Another line of work introduces gradient alignment constraints across training environments using dot-product (Fish (Shi et al., 2021)), squared distance of gradients (IGA (Koyama & Yamaguchi, 2020)), or squared distance of gradients variance (Fishr (Rame et al., 2021)). Methods such as vREx (Krueger et al., 2020) and GroupDRO (Sagawa et al., 2019) aim at finding a solution that performs equally well across training environments.

2.2. Facilitating the optimization

In contrast, the SD method (Pezeshki et al., 2020) relies on a single training set but fights the "gradient starvation" phenomenon that prevents the training algorithm from finding robust features even though they are assumed more predictive on the training set than easier-to-find spurious features.

2.3. Aiming for the second easiest representation

Closely related to the RFC *discovery phase*, several methods seek the *second easiest-to-find representation*, either by reweighting the dataset (Liu et al., 2021; Nam et al., 2020) or with distribution robust optimization, (Bao et al., 2021; Ahmed et al., 2020; Creager et al., 2021). The main drawback of these methods is the assumption that the secondeasiest representation is the correct one. This happens to be true in benchmarks such as COLOREDMNIST which are designed to frustrate ERM. However, these methods fail on simpler tasks that do not follow the assumption (Section 5.2).

2.4. Making use of diverse features

Closely related to the RFC *synthesis phase*, other methods attempt to steer the training process towards constructing a diversity of features: RSC (Huang et al., 2020) masks out features associated with large gradients to force the last layer to pick additional features; DiverseModel (Teney et al., 2021) constructs multiple classifiers on top of a given representation (e.g. ImageNet pre-trained) with a penalty that minimizes the alignment of gradients across classifiers. The drawback of these approaches is that they work best when starting from an existing portfolio of diverse features.

3. The optimization-generalization dilemma

This section presents experiments that illustrate the optimization-generalization dilemma that plagues OoD methods. All these experiments are carried out on the COL-ORMNIST task (Arjovsky et al., 2020). In this task, the relation between the robust feature (the digit class) and output label is invariant in all training and testing environments. In contrast, although the spurious feature (the digit color) is more predictive on the training environments, its relation with the output labels is not invariant across environments. We report results on a variety of published OoD algorithms: IRMv1 (Arjovsky et al., 2020), Fish (Shi et al., 2021), IGA (Koyama & Yamaguchi, 2020), vREx (Krueger et al., 2020), Spectral Decoupling (SD) (Pezeshki et al., 2020), Fishr (Rame et al., 2021), RSC (Huang et al., 2020), LfF (Nam et al., 2020), and CLOvE (Wald et al., 2021). We do not report results on MAML-IRM (Bae et al., 2021) because it is equivalent to Fish+vREx, and we do not report results on GroupDRO (Sagawa et al., 2019) because it performs like vREx (see Appendix A and B for details).

3.1. OoD penalties make the optimization challenging

Because their optimization is difficult, most authors recommend to pre-train the network with ERM before applying their OoD method. Figure 1 shows the final OoD test performance of models trained with each method as a function of the number $n_p \in \{0, 50, 100, 150, 200, 250\}$ of ERM pretraining epochs. During the execution of the OoD algorithm, we choose one of five penalty weights and select the best early-stopping epoch by directly peeking at the OoD test performance. All other hyper-parameters are copied from the COLORMNIST task (Arjovsky et al., 2020). Appendix C discusses these experiments with further details.

¹Code for these experiments is publically available at https: //github.com/TjuJianyu/RFC/.

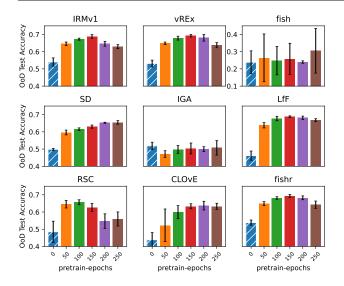


Figure 1. Test performance of nine penalized OoD methods as a function of the number of epochs used to pre-train the neural network with ERM. The final OoD testing performance is very dependent on choosing the right number of pretraining epochs, illustrating the challenges of these optimization problems.

Figure 1 shows that optimizing from a random initialization (blue bars, 0 pretraining epochs) fails for all nine algorithms and all five penalty weights. Although pretraining with ERM helps, the final performance of the competitive algorithms depends on the number of pretraining epochs in rather inconsistent. Too much pretraining can cause performance drops in excess of 20%. Even when one guesses the right amount of pretraining, the final performance comes short of the oracle performance (0.721 ± 0.002) achieved by a network that is trained only on the robust feature.

3.2. OoD penalties do not enforce the constraints

The previous section shows that the penalties introduced by these OoD methods are too strong to allow reliable optimization. We now show that they are also too weak to enforce the constraints they are meant to enforce.

To substantiate this assertion, we initialize a network with the correct solution, that is, the solution obtained by training the network on a variant of the COLORMNIST dataset in which the spurious color feature was removed. In order to keep the network from deviating from the target constraint, we use the largest penalty weight in the search space in each OoD method. We do not report results on the Fish method because it failed to learn the task. We do not report on RSC and LfF because their test accuracy drops too fast.

The top plot in figure 2 shows how the OoD testing performance of six algorithms deviates from the performance of our perfect initialization. This might happen because the

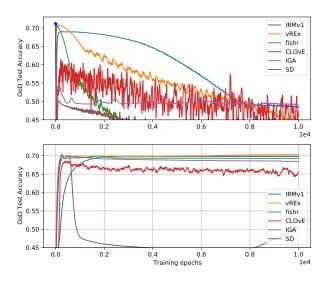


Figure 2. Test performance of OoD methods as a function of training epochs. Top: Six OoD methods are trained from a 'perfect' initialization where only the robust feature is well learned. The blue star indicates the initial test accuracy. Bottom: The OoD methods are trained from the proposed (frozen) RFC representation.

chosen constraints have spurious solutions (Kamath et al., 2021) or because the penalty terms are too weak to enforce the target constraints. Instead the training process pulls the perfect initialization in the direction of the spurious feature (the color) which happens to be more predictive on the training data.

4. Rich Feature Construction

This section presents tools for constructing rich representations. First we describe a mathematically sound approach to the problem of constructing a rich set of diverse features and we introduce the notions of *discovery phase* and *synthesis phase*. Then we show how to use distributionally robust optimization (DRO) to cut on the synthesis phases. Finally we present the practical RFC algorithm that we evaluate empirically in Section 5.

4.1. Feature discovery

Intuitively, constructing additional features is desirable when using these features increases the system performance on a pertinent subset of examples. Best would of course to achieve a large performance increase on large subsets of examples.

For the purposes of this section, let $\Phi_k(x)$ be a large vector containing all previously constructed k features for pattern x. Our first step consists of defining an ensemble $P = \{D^1 \dots D^i \dots\}$ of pertinent subsets D^i of the training set.

An effective way to choose a good ensemble of subsets is discussed at the end of this section. Having defined such subsets, we can define costs $C_i(\Phi, w)$ that measure the quality of a feature set Φ measured on subset D^i :

$$C_i(\Phi, w) = \frac{1}{|D^i|} \sum_{(x,y) \in D^i} \ell(y, w^\top \Phi(x)) \,.$$

where w represent the weights of a linear layer and $\ell(y, \hat{y})$ is a convex loss. In the context of deep learning, considering a linear layer operating a large feature vector is not an unreasonable way to investigate the effectiveness of a representation (Jacot et al., 2018). We can reweigh the training data in a manner that emphasizes the weaknesses of our current set of features, that is,

$$R_{rw} = \max_{\lambda} \min_{w} \sum_{i} \lambda_i C_i(\Phi_k, w) \tag{1}$$

where the λ_i coefficients are positive and sum to 1. Let λ_i^* be the pessimal mixture coefficients resulting from optimization problem (1). We can then learn a new set of features that help performance on this pessimal mixture,

$$R'_{rw} = \min_{w,\Phi} \sum_{i} \lambda_i^* C_i(\Phi, w) .$$
⁽²⁾

The main difference is that we are now training the features, yielding a new feature vectors $\Phi^*(x)$. If $R'_{rw}(2)$ is smaller than $R_{rw}(1)$, then we know that Φ^* contains *new useful features that were not present* in Φ_k . This is the *discovery phase*.

The next step consists in forming new feature vectors $\Phi_{k+1}(x)$ that contain the features present in both Φ_k and Φ^* , a synthesis phase. We can then iterate and obtain additional useful and diverse features at each iteration. The synthesis phase can be as simple as a vector concatenation. In the context of deep learning, however, one often has to use distillation, as discussed later in section 4.

The selection of a pertinent ensemble of subsets certainly affects which new features will be constructed at each iteration. In particular, it is desirable to make R_{rw} as high as possible using a minimal number of subsets. This goal can be easily achieved by forming subsets containing examples that were either correctly classified or misclassified by the learning systems constructed by problem (2).

4.2. Using DRO

We now show how a DRO reformulation of this process can cut the intermediate synthesis phase. Because the C_i are convex in w, we can first apply von Neumann's minimax theorem to problem (1) and obtain a DRO problem (Ben-Tal et al., 2009):

$$R_{rw} = \max_{\lambda} \min_{w} \sum_{i} \lambda_{i} C_{i}(\Phi_{k}, w)$$

$$= \min_{w} \max_{\lambda} \sum_{i} \lambda_{i} C_{i}(\Phi_{k}, w)$$

$$= \min_{w} \max_{i} C_{i}(\Phi_{k}, w) = R_{dro}.$$
 (3)

The next step is to run this same DRO optimization while also learning the features

$$R'_{dro} = \min_{w,\Phi} \max_{i} C_i(\Phi, w) .$$
(4)

To understand how quantity R'_{dro} relates to R'_{rw} , we can use the max-min inequality as follows:

$$\begin{aligned} R'_{dro} &= \min_{w,\Phi} \max_{\lambda} \sum_{i} \lambda_{i} C_{i}(\Phi, w) \\ &\geq \max_{\lambda} \min_{w,\Phi} \sum_{i} \lambda_{i} C_{i}(\Phi, w) \\ &\geq \min_{w,\Phi} \sum_{i} \lambda_{i}^{*} C_{i}(\Phi, w) = R'_{rw} . \end{aligned}$$

In other words, if R'_{dro} is smaller than R_{dro} , then R'_{rw} is smaller than $R_{rw} = R_{dro}$, and the new feature vector Φ contains new and useful features. The advantage of this approach is that problem (4) does not involve mixture coefficients λ^* . Therefore there is no need to solve (3) or (1), and no need for a synthesis phase at each iteration. The synthesis phase is only needed to construct the final rich representation after the last iteration.

4.3. Rich Feature Construction algorithm

We now describe a practical algorithm that implements the ideas discussed in the previous subsection in a manner that is usable with ordinary deep networks.

The workhorse of RFC is the Robust Empirical Risk Minimisation (RERM) algorithm (Algorithm 1) which takes an ensemble of datasets D^k representing multiple distributions and seeks neural network weights that simultaneously yields small errors for all these distributions. RERM is in fact a minimal form of DRO with overfitting control by cross-validation.

The RFC algorithm (Algorithm 2) first uses RERM to repeatedly solve an analogue of problem (4) that constructs a model f_k at each iteration, using an ensemble of subsets formed by selecting which examples were correctly or incorrectly recognized by the models $f_0 \dots f_{k-1}$ constructed during the previous iterations. This is the *discovery phase*.

After a predefined number of iterations, the RFC algorithm performs a distillation-based *synthesis phase*. The goal is to

Algorithm 1 Robust Empirical Risk Minimization (RERM)

- 1: **Required:** datasets $D^k = \{(x_i^k, y_i^k)\}_{i=1}^{n^k}$, for $k = 1, \ldots, K$; model f; learning rate α .
- 2: Randomly initialize f.
- 3: while no overfit do // By validation
- 4: Train on datasets D^1, \ldots, D^K by DRO: $f \leftarrow f \alpha \cdot \nabla_f \left[\max_k \left(\frac{1}{|D^k|} \sum_{(x_i^k, y_i^k) \in D^k} \ell(f(x_i^k), y_i^k) \right)_{k=1}^K \right]$ 5: return f

Algorithm 2 Rich Feature Construction (RFC)

- 1: **Input:** dataset D, the number of discovering rounds K
- 2: // Discovery phase
- 3: $f_1 \leftarrow \text{RERM}((D))$
- 4: Split D into groups A₁, B₁ according to f₁. (A₁ = examples correctly classified by f₁, B₁ = D\A₁)
- 5: Available groups $P = \{A_1, B_1\}$
- 6: for $k \in [2, ..., K]$ do
- 7: $f_k \leftarrow \text{RERM}(P)$
- 8: Split D into groups A_k, B_k according to f_k .
- 9: $P \leftarrow P \cup \{A_k, B_k\}$
- 10: // Synthesis phase
- 11: Pick a feature extractor function Φ , and K linear classifiers $\omega_1, \dots, \omega_k$ at random.
- 12: Create K groups of pseudo-labels y^k by applying each f_k on D.
- 13: $A = A_i \cap \ldots \cap A_k$
- 14: Update Φ, ω such that each pseudo-label y^k is well learned by the corresponding classifier ω_k and Φ: Σ_{k=1}^K 1/|A| Σ_{(xi,yi^k)∈A} ℓ(ω_k ∘ Φ(xi), yi^k) + 1/|D\A| Σ_{(xi,yi^k)∉A} ℓ(ω_k ∘ Φ(xi), yi^k)
 15: return Φ, {ω_k}^K_{k=1}
- learn a representation network $\Phi(x)$ such that we can emulate the functions f_k using a simple network with weights w_k on top of $\Phi(x)$. To that effect, we use the f_k models to compute pseudo-labels $y^k(x)$ for each example x. We then train a composite model with parameters Φ , w_1, \ldots, w_K

whose k outputs are trained to replicate the pseudo-labels.

5. Experiments

This section presents experimental results that illustrate how the rich representations constructed with RFC can help the OoD performance and reduce the performance variance of OoD methods. Subsection 5.1 extends the experiments of Section 3 with RFC constructed representations. Subsection 5.2 compares RFC-initialized OoD methods with recent methods that aim for the second easiest-to-find representation. Subsection 5.3 reports results obtained on the CAMELYON17 dataset (Bandi et al., 2018) that is part of

the WILDS benchmark suite (Koh et al., 2021a). The final subsection provides additional empirical observation that casts light on the hyper-parameter tuning process and on the feature construction process itself.

	Rand	ERM	RFC	RFC(cf)
IRMv1	54.0±2.4	68.9±1.1	66.5±1.5	69.9±0.6
vREx	53.1±2.0	69.3±0.7	70.3±0.4	69.9±0.4
SD	49.8±0.6	65.5 ± 1.1	$69.8 {\pm} 0.6$	70.4±0.4
IGA	51.8 ± 2.1	50.7 ± 4.2	$69.4 {\pm} 0.7$	70.0±0.8
fishr	53.9±1.5	$69.2 {\pm} 0.9$	70.2±0.4	$69.4 {\pm} 0.8$
cLOvE	43.9±4.2	$63.7 {\pm} 2.5$	67.1±3.8	68.4±0.8
ERM	27.3±0.4	27.3±0.4	43.4±2.8	35.6±1.2
oracle	72.1 ± 0.2			

Table 1. OoD testing accuracy achieved on the COLORMNIST. The first six rows of the table show the results achieved by six OoD methods using respectively random initialization (Rand), ERM initialization (ERM), RFC initialization (RFC). The last column, RFC(cf), reports the performance achieved by running the OoD algorithm on top of the frozen RFC representations. The seventh row reports the results achieved using ERM under the same conditions. The last row reminds us of the oracle performance achieved by a network using data from which the spurious feature (color) has been removed.

5.1. RFC helps all methods

All experiments reported in this section use the COLORM-NIST task (Arjovsky et al., 2020) which consists of predicting labels that indicate whether the class of a colored digit image is less than 5 or not. The target label is noisy and only matches the digit class with probability 0.75 (correlation coefficient 0.5). Two training sets are provided where a spurious feature, the color of the digit, correlates with the target label with respective probabilities 0.8 and 0.9 (correlation coefficients 0.6 and 0.8). However, in the OoD testing set, the digit color is negatively correlated with the label (correlation coefficient -0.8). This testing protocol hits algorithms that rely on the spurious color feature because it happens to be more predictive than the robust feature in both training environments.

We compare six OoD training methods (IRMv1, vREx, SD, IGA, Fishr, CLOvE) and ERM after four types of initialization: (a) a random initialization with the popular Xavier method (Glorot & Bengio, 2010), (b) random initialization followed by several epochs of ERM, and (c) initialization with RFC-computed representations, and (d) initialization with RFC-computed representations that are subsequently frozen: the training algorithm is not allowed to update them (referred as RFC(cf)). The ERM initialization essentially consists of switching off the penalty terms defined by the various OoD method. This is comparable to the delicate penalty annealing procedures that are used by most authors (Arjovsky et al., 2020; Krueger et al., 2020; Pezeshki et al., 2020; Rame et al., 2021). The RFC initialization was computed by two discovery phase iterations.

For all six OoD algorithms and four initialization strategies, we select one of five penalization weights, {10, 50, 100, 500, 1000} for the SD method, {1000, 5000, 10000, 50000, 100000} for the other methods. For ERM initialization, we also select among five numbers of pretraining epochs {50, 100, 150, 200, 250}. These hyper-parameters were selected by peeking at the test set performance.² All experiments use the same 2-hidden-layers MLP network architecture (390 hidden neurons), Adam optimizer, learning rate=0.0005, L_2 weights regularization=0.0011 and binary cross-entropy objective function as the COLOREDMNIST benchmark (Arjovsky et al., 2020). Further details are provided in Appendix C.

Table 1 reports the OoD testing accuracies obtained under these conditions. Both variants of RFC initialization help the OoD performance of most algorithms. Interestingly, the best results are achieved by freezing the RFC representation, which is consistent with the results of Section 3.2 showing that the OoD algorithm penalties are in fact insufficient to maintain the desired invariance constraints, even when initialized with the oracle weights. The bottom plot in Figure 2 shows that RFC helps most OoD methods in this scenario as well. However, this is not true of the SD algorithm which penalizes the L_2 norm of logits in a manner that drives away the network from the oracle weights. Freezing the RFC representation doesn't prevent this from happening.

5.2. Aiming for the second easiest-to-find feature

Recent work (Liu et al., 2021; Nam et al., 2020; Bao et al., 2021; Ahmed et al., 2020; Creager et al., 2021) claims to achieve OoD generalization by discovering and using only the second easiest-to-find features. Although this strategy often works on datasets that were constructed to showcase OoD problems, the assumption that the second easiest features are the robust ones is unreasonable.

To illustrate this claim we construct a variant of the COL-OREDMNIST dataset by changing the noise levels to make the robust feature (the digit shapes) more predictive than the spurious features (the digit color).

Table 2 compares the six OoD methods using the RFC(cf) initialization on both COLOREDMNIST and INVERSEC-OLOREDMNIST. All six methods achieve very compara-

Methods	ColoredMNIST	INVERSE ColoredMNIST
IRMv1(cf)	$69.9 {\pm} 0.6$	80.3±2.2
vREx(cf)	$69.9 {\pm} 0.4$	84.0±1.2
SD(cf)	$70.4{\pm}0.4$	81.9±1.3
IGA(cf)	$70.0{\pm}0.8$	78.5±3.6
fishr(cf)	$69.4 {\pm} 0.8$	82.6±1.4
CLOvE(cf)	$68.4{\pm}0.8$	71.9±0.7
ERM(cf)	35.6 ± 1.2	$71.7 {\pm} 0.7$
PI	70.9±0.3	51.0±4.7

Table 2. OoD test accuracy of PI and OOD/ERM methods on COL-OREDMNIST and INVERSECOLOREDMNIST. The OOD/ERM methods are trained on top of a frozen RFC representation.

ble OoD testing accuracies. The ERM method fails on COLOREDMNIST but performs quite well on INVERSE-COLOREDMNIST because relying in the most predictive features is a good strategy for this task. In contrast, the algorithm PI (Bao et al., 2021), which aims for the second easiest features, performs well on COLOREDMNIST but far worse on the easier INVERSECOLOREDMNIST task.

5.3. RFC on a real-world task

The CAMELYON17 dataset (Bandi et al., 2018) contains histopathological images accompanied by a label indicating whether the central region of the image contains a tumor. The images were collected from five different hospitals with potentially different imaging hardware and different procedures. The WILDS benchmark (Koh et al., 2021a) contains a task that uses this dataset with a very clear specification of which three hospitals are to be used as training data (302,436 images), which hospital is to be used for OoD generalization testing (85,054 images). The task also specifies multiple runs with different seeds in order to observe the result variability. Finally the task defines two ways to perform hyper-parameter selection: "IID tuning" selects hyper-parameters based on model performance on 33,560 images held out from the training data, "OOD tuning" selects hyper-parameters on the model performance observed on the fifth hospital (34,904 images).

We compare four different training methods, ERM, IRMv1, vREx, and CLOvE, using both ERM and RFC initialization with either two rounds (2-RFC) or three rounds (3-RFC) during the discovery phase. We also compare the effect of letting the training method tune the representation or freezing the representations obtained by the initialization procedure. We indicate the latter by adding a suffix "(cf)" to the method name.

We strictly follow these procedures as well as the experimental settings suggested in the WILDS task. The

²The small size of the COLOREDMNIST makes this hard to avoid. Tuning the hyper-parameters using the testing set favors in fact the ERM initialization because the test performance depends strongly on the number of pre-training epochs (Figure 1).

network is a Densenet121 model (Huang et al., 2017) trained by optimizing a cross-entropy loss with L_2 weight decay=0.01 using SGD with learning rate=0.001, momentum=0.9 and batch size=32. The penalty weights are selected from {0.5, 1, 5, 10, 50, 100, 500, 1000} for IRMv1 and vREx, {0.0005, 0.001, 0.005, 0.01, 0.05, 0.1, 0.5, 1} for CLOvE. In the case of ERM initialization, the number of ERM pre-training iterations is selected in set from {0, 500, 1000, 5000, 10000}. Further details are provided in Appendix D.

Table 3 reports the OoD testing accuracies obtained by using both the IID and OOD hyper-parameter tuning approach. Accuracies were averaged over five repetitions with different random seeds. The first block of rows reports accuracies obtained by all four methods using ERM initialization. These accuracies come with large error bars because they considerably vary across repetitions. As a consequence, the accuracies differences observed in this block are not significant. The second block of rows shows that freezing the representations does not significantly improve this situation. In contrast, using a RFC representation with two discovery rounds (2-RFC) consistently improves the accuracies obtained by all four methods using either the IID or OOD tuning approaches (third block of rows). Freezing the representation layers during training provides an additional improvement (fourth block of rows).

Using a RFC representation with three discovery rounds (3-RFC) does not work as well. In fact, the features extracted during the third discovery phase round are not as predictive as the first two rounds (Table 4). More discovery rounds also increase the difficulty of the synthesis phase, as we want to distillate more features (including poor ones) into the same fixed-size representation.

Much to our surprise, RFC consistently boosts the accuracies of both the ERM and OOD methods, using either the IID or OOD tuning method. The frozen RFC representations can even help ERM outperform earlier comparable results reported on the WILDS leaderboard³ by about 5%.

5.4. Further observations

5.4.1. Hyper-parameter tuning

Figure 1 and 2 illustrate how the OoD generalization performance of many OoD methods depends strongly on hyperparameters such as the number of pretraining epochs, the penalty weights, the learning epochs. This is in fact a consequence of the optimization-generalization dilemma itself. It is simply difficult to simultaneously ensure good OoD generalization performance and run a stable and efficient optimization process.

Network	Network Methods		Test Acc		
Initialization		IID Tune	OOD Tune		
×	ERM	66.6±9.8	70.2±8.7		
ERM	IRMv1	$68.6{\pm}6.8$	68.5 ± 6.2		
ERM	vREx	69.1 ± 8.1	69.1±13.2		
ERM	CLOvE	71.7±10.2	69.0±12.1		
ERM	ERM(cf)	×	×		
ERM	IRMv1(cf)	69.6 ± 10.5	70.7 ± 10.0		
ERM	vREx(cf)	69.6 ± 10.5	70.6 ± 10.0		
ERM	CLOvE(cf)	69.6±10.5	69.2 ± 9.5		
2-RFC	ERM	72.8±3.2	74.7±4.3		
2-RFC	IRMv1	71.6 ± 4.2	75.3 ± 4.8		
2-RFC	vREx	73.4 ± 3.3	76.4 ± 5.3		
2-RFC	CLOvE	$74.0{\pm}4.6$	76.6 ± 5.3		
2-RFC	ERM(cf)	78.2±2.6	78.6±2.6		
2-RFC	IRMv1(cf)	$78.0{\pm}2.1$	79.1±2.1		
2-RFC	vREx(cf)	77.9 ± 2.7	$79.5 {\pm} 2.7$		
2-RFC	CLOvE(cf)	77.8 ± 2.2	$78.6{\pm}2.6$		
3-RFC	ERM(cf)	72.9±5.3	73.3±5.3		
3-RFC	IRMv1(cf)	72.7 ± 5.5	$75.5 {\pm} 3.8$		
3-RFC	vREx(cf)	72.7±5.4	75.1±5.3		
3-RFC	vREx(cf)	$72.8 {\pm} 5.4$	73.2±7.1		

Table 3. Test Accuracy on the CAMELYON17 dataset. The hyperparameter tuning process is performed on either the iid validation or the OOD validation set ("IID/OOD Tune"). We test ERM pretrained initialization, 2-rounds, and 3-rounds RFC representation. As to the learning methods, we test ERM, IRMv1, vREx, and CLOvE. When freezing the representation and training the top-layer classifier only, we get "*(cf)" methods. The standard deviation is calculated on 5 random seeds [0-4].

The left half of Figure 3 show OoD testing accuracies for the CAMELYON17 task as a function of the penalty weights, with all other hyper-parameters chosen using either the IID or OOD tuning method. With ERM pretraining, the OoD testing performance of all three OoD methods (IRMv1, vREx, CLOvE) depends very chaotically on the penalty weight. In contrast, with RFC initialization and frozen representation, the OoD testing performance of OoD methods as a function of the penalty weight follows a much smoother curve.

The right half of Figure 3 shows the relation between the IID/OOD validation accuracies and the OoD testing accuracies for three OoD methods using both ERM and RFC initialization. RFC initialization reduces the variance of both the IID and OoD validation performances, making them far more reliable indicators of the actual OoD testing performance.

³https://wilds.stanford.edu/leaderboard

Rich Feature Construction for the Optimization-Generalization Dilemma

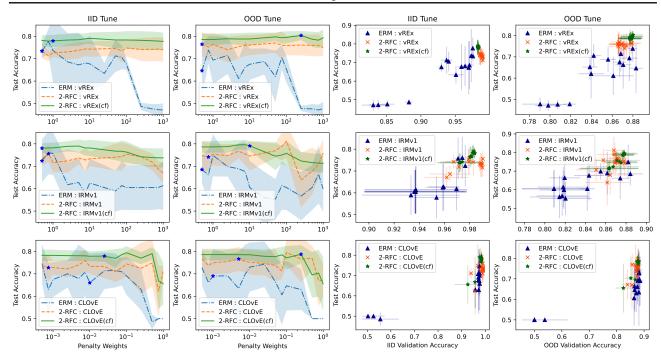


Figure 3. Left half: OoD testing accuracy as a function of the penalty weight. The six plots correspond to the IRMv1, vREx, and CLOvE algorithms with all other hyper-parameters selected using either the IID or OOD tuning method. RFC initialization makes these curves far more predictable than ERM initialization. Starts indicate the final penalty weight choice. **Right half**: OoD testing accuracy as a function of the validation accuracy. RFC initialization reduces the variance of both the IID and OOD validation performances, making them far more reliable indicators of the actual OoD testing performance.

5.4.2. The value of the RFC synthesis phase

The COLOREDMNIST and INVERSECOLOREDMNIST experiments (Table 2) show that the robust feature can be discovered during different rounds of the discovery phase. We can therefore wonder whether the discovery phase already produces the correct invariant representation during one of its successive rounds.

This is not the case in general. Table 4 reports the OoD testing accuracies of the classifiers constructed during the first three rounds of the discovery phase. All three accuracies are substantially worse than the accuracies achieved by any algorithm using a frozen 2-RFC representation (Table 3). This indicates that these higher accuracies are obtained by simultaneously exploiting features discovered by different rounds of the discovery phase. Making them all simultaneously available is indeed the role of the synthesis phase.

6. Conclusion

This work makes several contributions:

• We point out the severity of the optimizationgeneralization dilemma in the OoD setup, showing that the various penalties introduced by OoD methods are either too strong to optimize or too weak to achieve

Round 1	Round 2	Round 3
66.6±9.8	$73.2{\pm}5.7$	61.8±10.2

Table 4. OoD test accuracies for the models constructed by the first three rounds of the RFC discovery phase for the CAMELYON task. The first round amounts to performing ERM. The second round extracts a useful set of features. The third round extracts comparatively weaker features. All these accuracies remain substantially worse than those achieved by training a system on top of the combined representation computed during the RFC synthesis phase (see Table 3).

their goals.

- We propose to work around the problem by seeding the networks with a rich representation that contains a diversity of features readily exploitable by the algorithm. We formalize this objective, and we describe an algorithm, RFC, that constructs such rich representations.
- We show that RFC helps a variety of OoD methods achieve a better OoD testing performance. Interestingly, when we additionally prevent the learning algorithm from modifying the RFC features, we not only observe a further boost on the performance of OoD

methods, but we also raise the performance of ERM to the same level, substantially outperforming previous comparable results on the CAMELYON17 dataset for examples.

• Finally, we also show that RFC facilitates hyperparameter tuning and model selection.

Therefore, it appears that the inductive bias that comes with a broad set of diverse features brings more benefits to various penalties introduced by current OoD methods.

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A. MAML-IRM resembles vREx+Fish

We omit the MAML-IRM method in our experiments because we can show that minimizing its cost amounts to minimizing a mixture of the vREx and Fish costs.

Notations:

- E: indicates a set of environments.
- θ : indicates the model parameters.
- $L_i(\theta)$: indicates an ERM loss (e.g. MSE, cross-entropy) of a model parameterized by θ on environments *i*.
- $\bar{g}_i = L'_i(\theta)$: is the gradients of $L_i(\theta)$.
- $\bar{H}_i = L_i''(\theta)$: is the Hessian of $L_i(\theta)$.

Let $U_i(\theta) = \theta - \alpha L'_i(\theta)$ denote the updated parameters after performing a SGD iteration on environments *i*. The MAML-IRM loss can be expressed as:

$$L_{\text{maml-irm}} = \mathbb{E}_s[L_j(U_i(\theta))] + \lambda \sqrt{Var_s[L_j(U_i(\theta))]}$$
(5)

where the notation \mathbb{E}_s and Var_s respectively denote the average and the variance with respect to all pairs of distinct environment $s = \{i, j | i \in \mathcal{E}, j \in \mathcal{E}, i \neq j\}$, and where λ is a hyper-parameter.

According to (Nichol et al., 2018), the gradients of the first term is:

$$\frac{\partial (\mathbb{E}_s[L_j(U_i(\theta)))]}{\partial \theta} = \mathbb{E}_s[\bar{g}_j - 2\alpha \bar{H}_i \bar{g}_j] + O(\alpha^2)$$
(6)

Note that $\mathbb{E}_s[-2\bar{H}_i\bar{g}_j] = \mathbb{E}_s[-\frac{\partial \langle g_i, g_j \rangle}{\partial \theta}]$ is in fact the gradients of $-\langle g_i, g_j \rangle$, the Fish penalty.

We now turn out attention to the second term $\sqrt{Var_s[L_j(U_i(\theta))]}$. Expanding $L_j(U_i(\theta))$ with a Taylor series gives:

$$L_{j}(U_{i}(\theta)) = L_{j}(\theta) + \left\langle L_{j}^{'}(\theta), (U_{i}(\theta) - \theta) \right\rangle + O(\alpha^{2})$$

$$\tag{7}$$

$$= L_{j}(\theta) - \alpha \left\langle L_{i}^{'}(\theta), L_{j}^{'}(\theta) \right\rangle + O(\alpha^{2}) \qquad (\longleftarrow U_{i}(\theta) = \theta - \alpha L_{i}^{'}(\theta)) \tag{8}$$

$$= L_j(\theta) - \alpha \left\langle \bar{g}_i, \bar{g}_j \right\rangle + O(\alpha^2) \tag{9}$$

Therefore

$$Var_{s}(L_{j}(U_{i}(\theta))) = Var_{s}[L_{j}(\theta) - \alpha \langle \bar{g}_{i}, \bar{g}_{j} \rangle] + O(\alpha^{2})$$

$$= Var_{s}[L_{j}(\theta)] + \alpha^{2}Var_{s}[\langle \bar{g}_{i}, \bar{g}_{j} \rangle] - 2\alpha \text{Cov}_{s}[L_{j}(\theta), \langle \bar{g}_{i}, \bar{g}_{j} \rangle] + O(\alpha^{2})$$

$$= Var_{s}[L_{j}(\theta)] - 2\alpha \text{Cov}_{s}[L_{j}(\theta), \langle \bar{g}_{i}, \bar{g}_{j} \rangle] + O(\alpha^{2})$$

$$= Var_{s}[L_{j}(\theta)] - 2\alpha \{\mathbb{E}_{s}[L_{j}(\theta) \langle \bar{g}_{i}, \bar{g}_{j} \rangle] - \mathbb{E}_{s}[L_{j}(\theta)]\mathbb{E}_{s}[\langle \bar{g}_{i}, \bar{g}_{j} \rangle]\} + O(\alpha^{2})$$

$$= Var_{s}[L_{j}(\theta)] - 2\alpha \mathbb{E}_{s}[(\frac{L_{i}(\theta) + L_{j}(\theta)}{2} - \mathbb{E}[L(\theta)]) \langle \bar{g}_{i}, \bar{g}_{j} \rangle] + O(\alpha^{2})$$

The first term of this expression, $Var_s[L_j(\theta)]$, penalizes a high variance of the loss across environments. It is equal to the vREx penalty. The second term, $-2\alpha \mathbb{E}_s[(\frac{L_i(\theta)+L_j(\theta)}{2} - \mathbb{E}[L(\theta)])\langle \bar{g}_i, \bar{g}_j\rangle]$ is a weighted average of $\langle g_i, g_j\rangle$, that is a smoothed Fish penalty.

In conclusion, optimizing the MAML-IRM cost amounts to optimizing a λ controlled mixture of the vREx and Fish costs.

B. GroupDRO interpolates environments while vREx extrapolates.

The vREx objective function can be expressed as:

$$L_{\text{vrex}} = \mathbb{E}_{e \in \mathcal{E}}(L_e) + \lambda Var_{e \in \mathcal{E}}(L_e) \tag{11}$$

The GroupDRO objective function is a mixture of the per-environment costs L_e with positive coefficients:

$$L_{\text{groupDRO}} = \mathbb{E}_{e \in \mathcal{E}}(p_e L_e) \tag{12}$$

where the adjustable mixture coefficients $p_e \ge 0$, $\sum_{e \in \mathcal{E}} p_e = 1$, are treated as constaants for computing the gradients $\frac{\partial L_e}{\partial \theta}$. The gradient of these two cost functions are:

$$\frac{\partial L_{\text{vrex}}}{\theta} = \mathbb{E}_{e \in \mathcal{E}}([2\lambda(L_e - \mathbb{E}_i L_i) + 1]g_e)$$
(13)

$$\frac{\partial L_{\text{groupDRO}}}{\theta} = \mathbb{E}_{e \in \mathcal{E}}(p_e g_e) \tag{14}$$

where $g_e = \frac{\partial L_e}{\theta}$ is the gradients of network weights θ on environment e.

Because the p_e mixture coefficients are always positive, it is easy to see that GroupDRO follows a direction aligned with a convex combination of the per-environment gradients. In contrast, vREx can follow a direction that is outside this convex hull because the coefficients $\mathbb{E}_i L_i + 1$ can be positive or negative).

C. Experimental details for the ColoredMNIST experiments

We use the original COLOREDMNIST dataset (Arjovsky et al., 2020) with two training environments (0.25, 0.1), (0.25, 0.2). The target label correlates with the invariant feature (the digit shape) with a probability 0.75. The sirious feature (color) correlates with the target label with a probability 0.8 and 0.9, respectively. Each training environment contains 25000 images where the size of each image is $2 \times 14 \times 14$. For all COLOREDMNIST experiments, we use a fully connected neural network with 3 layers (392 (input dim) $\times 390 \times 390 \times 1$), trained with the Adam optimizer with learning rate 0.0005. We use a L2 weights regularization with parameter 0.0001 for INVERSECOLOREDMNIST tasks and 0.0001 in the regular COLOREDMNIST tasks. For the CLOVE method, we use a Laplacian kernel $k(r, r_0) = exp(\frac{-|r-r_0|}{0.4})$ (Kumar et al., 2018) with mini-batch size 512. All other methods train using full batches. For the ERM baseline and for computing the oracle performance, we search the L2 regularization parameter in $\{0.0001, 0.0005, 0.001, 0.005, 0.01\}$. We run each experiment 10 times to get the standard deviation.

C.1. Hyper-parameter searching space

Table C.1 shows the penalty weights searching space for all OoD methods in the COLOREDMNIST experiments. Table 6 shows the training epochs searching space for different OoD methods and network initialization/representation on the COLOREDMNIST dataset.

	COLOREDMNIST	INVERSECOLOREDMNIST
IRMv1	$10000 \times \{0.1, 0.5, 1, 5, 10\}$	$10000 \times \{0.1, 0.5, 1, 5, 10\}$
vREx	$10000 imes \{0.1, 0.5, 1, 5, 10\}$	$10000 \times \{0.1, 0.5, 1, 5, 10\}$
IGA	$10000 \times \{0.1, 0.5, 1, 5, 10\}$	$10000 \times \{0.1, 0.5, 1, 5, 10\}$
CLOvE	$10000 \times \{0.1, 0.5, 1, 5, 10\}$	$10 \times \{0.1, 0.5, 1, 5, 10\}$
Fishr	$10000 \times \{0.1, 0.5, 1, 5, 10\}$	$10000 \times \{0.1, 0.5, 1, 5, 10\}$
SD	$100 \times \{0.1, 0.5, 1, 5, 10\}$	$\{0.05, 0.1, 0.5, 1, 5\}$
RSC	$(0.995, 0.98) \times \{0.95, 0.97, 0.98, 0.99, 1\}$	-
LfF	$\{0.1, 0.2, 0.3, 0.4, 0.5\}$	-
Fish	$0.001\times\{0.1, 0.5, 1, 5, 10\}$	-

Table 5. Penalty weight search space for both the COLOREDMNIST and INVERSECOLOREDMNIST datasets.

C.2. RFC training

For all COLOREDMNIST experiments, we use a 2-rounds RFC *discovery phase* trained with respectively 50 and 500 epochs. Then we train 500 epochs for the distillation network of the RFC *synthesis phase*. For the INVERSECOLOREDMNIST experiments, we again use a 2-rounds RFC *discovery phase* trained with respectively 150 and 400 epochs. We choose these training epochs because they can maximize the IID validation performance during each round.

	Rand/ERM	RFC	RFC(cf)
IRMv1	$i \times 20$	$i \times 2$	$i \times 125$
vREx	$i \times 20$	$i \times 2$	$i \times 20$
IGA	$i \times 20$	$i \times 1$	$i \times 20$
CLOvE	$i \times 30$	$i \times 1$	$i \times 20$
Fishr	$i \times 20$	$i \times 1$	$i \times 20$
SD	$i \times 20$	$i \times 1$	$i \times 20$
RSC	$i \times 1$	-	-
LfF	$i \times 20$	-	-
Fish	$i \times 20$	-	-

Table 6. The number of training epochs search space for the COLOREDMNIST dataset, with $i \in [0, 24]$.

C.3. PI training

We use the original implementation from PI (Bao et al., 2021). Because the PI algorithm is closely related to the *discovery phase*, we use the same hyper-parameters and settings.

D. Experimental details for the CAMELYON17 experiments

We strictly follow the implementation of the CAMELYON17 task in the WILDS benchmark (Koh et al., 2021a). Betchmark (Koh et al., 2021b). For the results presented in section 5.4.1, we additionally search the penalty weights in the set {0.5, 0.75, 1, 2.5, 5, 7.5, 10, 25, 50, 75, 100, 250, 500, 750, 1000} for IRMv1 and vREx methods, and the set {0.5, 0.75, 1, 2.5, 5, 7.5, 10, 25, 50, 75, 100, 250, 500, 750, 1000} × 10⁻³. The CLOVE method require a kernel function, we choose the Laplacian kernel $k(r, r_0) = exp(\frac{-|r-r_0|}{l})$ (Kumar et al., 2018) where *l* is a positive scalar. For the CLOVE baseline with an ERM pretrained initialization (the fourth row of table 3), we test the scalar $l \in \{0.1, 0.2\}$ and choose the better one l = 0.2. For the other CLOVE experiments on CAMELYON17, we choose l = 0.1.

We train the synthesis phase 20 epochs and the other methods/phase 10 epochs. Hyper-paremeter tuning strictly follows the IID and OOD tuning process described in the WILDS task. We use a L2 weights regularization 1e - 6 during the synthesis phase to help it get a lower training loss on the pseudo-labels. During any further training that updates the weights of the learned representation, we keep the L2 weights regularization to be the same as 1e - 6. Otherwise, a stronger L2 weights regularization will destroy the learned representation. We also tried other L2 regularization weights in $\{1e - 2, 1e - 4, 1e - 6\}$. Table 8 shows the synthesis quality with different (synthesis phase) L2 weights decay. Two smaller L2 weights decay hyper-parameters $\{1e - 4, 1e - 6\}$ can arrive at a good synthesis quality. The corresponding "*(cf)" methods performances of these two hyper-parameters are good too in Table 7. Table 7 shows that the "*(cf)" methods can also reliability gain a good performance once the synthesis quality is good.

After K synthesis phase, RFC provides us a rich representation Φ and K linear classifiers $\omega_1, \ldots, \omega_K$. In the downstream tasks, such as OoD/ERM training, we will keep the representation Φ and initialize the top-layer classifier ω . There are at least two ways to initialize it: 1) initialize ω as the average of $\omega_1, \ldots, \omega_K$ with the hope that the initial top-layer classifier uses all discovered features. 2) randomly initialize ω . Table 9 shows the test performance of OOD/ERM methods with each top-layer initialization method. None of the two top-layer initialization methods significantly outperforms the other one. We choose the first top-layer initialization method in all main experiments because of the interpretation.

Synthesis phaseNetworkL2 weights decayInitialization		Methods	Tes IID Tune	t Acc OOD Tune
$ \begin{array}{r} 1e-6\\ 1e-6\\ 1e-6\\ 1e-6\\ \end{array} $	2-RFC 2-RFC 2-RFC	ERM(cf) IRMv1(cf) vREx(cf)	78.2±2.6 78.0±2.1 77.9±2.7	$\begin{array}{c} 78.6{\pm}2.6\\ 79.1{\pm}2.1\\ 79.5{\pm}2.7\end{array}$
1e - 4 $1e - 4$ $1e - 4$	2-RFC 2-RFC 2-RFC	ERM(cf) IRMv1(cf) vREx(cf)	77.8±1.7 77.7±1.7 77.9±1.7	$\begin{array}{c c} 78.8{\pm}2.3\\ 78.9{\pm}2.3\\ 79.7{\pm}1.7\end{array}$
$ \begin{array}{r} 1e-2\\ 1e-2\\ 1e-2\\ 1e-2 \end{array} $	2-RFC 2-RFC 2-RFC	ERM(cf) IRMv1(cf) vREx(cf)	75.2±7.8 75.0±7.9 75.4±7.7	75.5±7.4 75.4±7.5 75.8±7.3

Table 7. Test accuracy of OOD methods (IRMv1, vREx) and ERM methods. Three synthesis phase L2 weights decay $\{1e - 2, 1e - 4, 1e - 6\}$ are tested. All the other settings are the same as the main results in Table 3.

Table 8. The train and IID-validation performance of the *synthesis phase*. Note that it uses the pseudo-labels instead of the true labels as Y. Three *synthesis phase* L2 weights decay $\{1e - 2, 1e - 4, 1e - 6\}$ are tested.

(Synthesis phase) L2 weights decay	Train accuracy	IID-validation accuracy
1e-6	99.7±0.0	97.4±0.3
1e-4	99.6±0.1	$97.4{\pm}0.2$
1e-2	93.9±0.7	$94.9 {\pm} 0.5$

Table 9. Test performance of IRMv1, vREx, and ERM methods on a 2 rounds RFC representation. The top-layer classifier is initialized by the average of $\omega_1, \ldots, \omega_K$ (Average) or a random initialization (Random). When freezing the representation and training the top-layer classifier only, we get "*(cf)" methods.

Methods	Average		Random	
	IID Tune	OOD Tune	IID Tune	OOD Tune
ERM	72.8±3.2	74.7±4.3	73.0±3.7	75.9±6.7
IRMv1	71.6±4.2	75.3±4.8	74.5±2.3	$75.2{\pm}6.5$
vREx	73.4±3.3	76.4±5.3	73.0±3.9	77.1±5.0
ERM(cf)	78.2±2.6	78.6±2.6	77.8±2.4	78.6±2.6
IRMv1(cf)	78.0±2.1	79.1±2.1	78.0±2.1	79.1±2.1
vREx(cf)	77.9±2.7	79.5±2.7	78.0±2.6	79.7±2.4