

CGLearn: Consistent Gradient-Based Learning for Out-of-Distribution Generalization

Jawad Chowdhury¹, Gabriel Terejanu²

Department of Computer Science, University of North Carolina at Charlotte, Charlotte, NC, USA
mchowdh5@uncc.edu¹, gabriel.terejanu@uncc.edu²

Abstract

Improving generalization and achieving highly predictive, robust machine learning models necessitates learning the underlying causal structure of the variables of interest. A prominent and effective method for this is learning invariant predictors across multiple environments. In this work, we introduce a simple yet powerful approach, CGLearn, which relies on the agreement of gradients across various environments. This agreement serves as a powerful indication of reliable features, while disagreement suggests less reliability due to potential differences in underlying causal mechanisms. Our proposed method demonstrates superior performance compared to state-of-the-art methods in both linear and nonlinear settings across various regression and classification tasks. CGLearn shows robust applicability even in the absence of separate environments by exploiting invariance across different subsamples of observational data. Comprehensive experiments on both synthetic and real-world datasets highlight its effectiveness in diverse scenarios. Our findings underscore the importance of leveraging gradient agreement for learning causal invariance, providing a significant step forward in the field of robust machine learning. The source code of the linear and nonlinear implementation of CGLearn is open-source and available at: <https://github.com/hasanjawad001/CGLearn>.

Introduction

Machine learning models have achieved remarkable success in various domains driven by the recent availability of large datasets, sophisticated algorithms, and highly advanced complex models. However, these models perform well only when the test data follows the same distribution as the training data (i.i.d.), but they often suffer from overfitting due to overparametrization, learning spurious correlations from training data (Sagawa et al. 2020; Wang et al. 2021; Ming, Yin, and Li 2022). This issue arises because traditional models focus on predictive power without considering the causal relationships underlying the data. As a result, when the training and test distributions differ, models that rely on spurious correlations can perform very poorly, compromising their robustness, leading to poor generalization on out-of-distribution (OOD) test data (Arjovsky et al. 2019; He, Shen, and Cui 2021).

Learning causal relationships is the key to model explainability and enhancing generalization and robustness (Shin 2021; Wang et al. 2022; Santillan 2023). Although the ideal method for learning causal structures is through Randomized Control Trials (RCTs), these are often expensive, unethical, or impractical. Various methods have been developed for causal discovery. Constraint-based methods use conditional independence tests to identify causal directions (Spirtes, Glymour, and Scheines 2001; Pearl 2009; Colombo et al. 2012). This however often results in the Markov Equivalence Class (MEC) of causal structures. Score-based methods optimize causal graphs over Directed Acyclic Graphs (DAGs) (Chickering 2002; Ramsey et al. 2017; Huang et al. 2018), but the combinatorial nature of the search space can make it computationally expensive. Advances like NOTEARS (Zheng et al. 2018) transform this combinatorial challenge into continuous optimization, leading to various effective variants (Zheng et al. 2020; Yu et al. 2019; Lachapelle et al. 2019; Wei, Gao, and Yu 2020; Ng, Ghassami, and Zhang 2020; Ng et al. 2022). However, learning causal structures purely from observational data can be challenging due to issues like selection bias, measurement errors, and confounding factors (Zadrozny 2004; Torralba and Efros 2011). Moreover, relying solely on empirical risk optimization can result in models highly dependent on spurious relationships. To tackle this problem, researchers often use prior domain knowledge to improve causal discovery (O'Donnell et al. 2006; Gencoglu and Gruber 2020; Andrews, Spirtes, and Cooper 2020; Liu, Chen, and Zhao 2021; Chowdhury., Rashid., and Terejanu. 2023; Chowdhury and Terejanu 2023). Unfortunately, many causal discovery methods depend on specific assumptions (e.g., linearity, non-Gaussian noise) that do not always hold in real-world data. In addition to that some of these methods exploit variance scales e.g. var-sortability to identify causal orderings, performing well on unstandardized data but poorly after standardization (Reisach, Seiler, and Weichwald 2021; Kaiser and Sipos 2022; Reisach et al. 2024; Ormaniec et al. 2024).

A recent line of study focuses on exploiting the invariance property of causal relationships across different environments. Methods like Invariant Causal Prediction (ICP) (Peters, Bühlmann, and Meinshausen 2016) aim to identify causal predictors by ensuring the conditional distribution of the target given these predictors remains stable across envi-

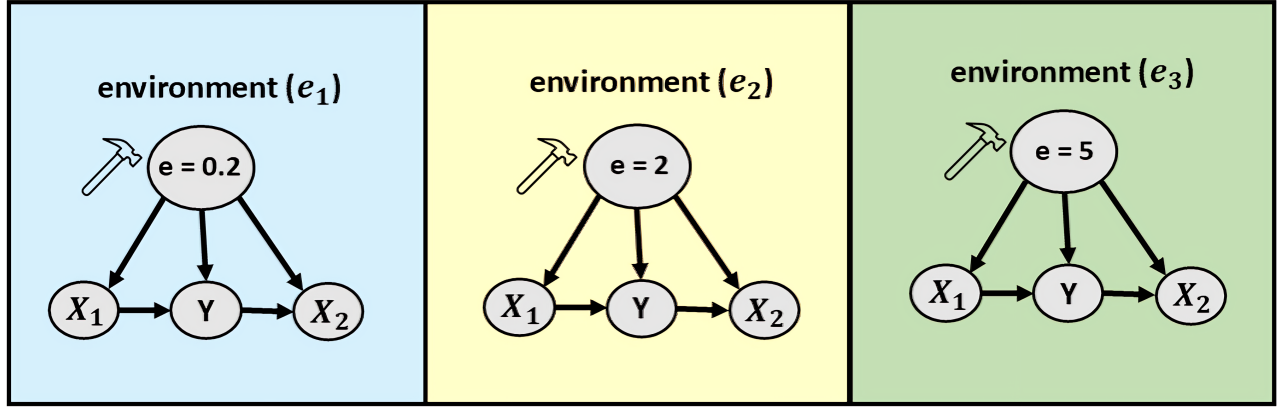


Figure 1: Illustration of three environments generated by intervening on the variable e , which takes distinct values $e = 0.2$, $e = 2$, and $e = 5$ in environments e_1 , e_2 , and e_3 , respectively. In each environment, X_1 acts as a causal factor for the target variable Y , while X_2 is a spurious (non-causal) factor with respect to Y . This figure exemplifies how different interventions on e create distinct environments.

ronments. This method leverages the invariance of causal relationships under different interventions, iterating over feature subsets to find those invariant across environments, considering them as potential causal parents of the target variable. Another study, IRM (Arjovsky et al. 2019) optimizes a penalty function to achieve OOD generalization for predictive models, ensuring robust performance across environments. These methods significantly reduce the absorption of spurious correlations by focusing on stable and invariant relationships. The invariant learning framework provides a promising approach to improve model robustness and generalization in the presence of distribution shifts, with various domains exploiting invariance to learn better predictors and robust models (Montavon et al. 2012; Wang et al. 2017; Chowdhury et al. 2024; Bose and Roy 2024). Some relevant works such as AND-mask (Parascandolo et al. 2020), Fishr (Rame, Dancette, and Cord 2022), Fish (Shi et al. 2021), IGA (Koyama and Yamaguchi 2020) use environment-specific gradients to improve generalization in diverse settings. Moreover, approaches examining the signal-to-noise ratio (GSRN) in gradients, such as the work by Liu et al. (Liu et al. 2020), measure the alignment of gradient directions across samples, while a similar strategy has been employed in large-batch training scenarios to improve model stability (Jiang et al. 2023).

Motivated by this line of work and the current drawbacks of existing methods in structure learning and OOD generalization, we introduce CGLearn, a general framework designed to improve the generalization of machine learning models by leveraging gradient consistency across different environments. CGLearn does not require extensive domain knowledge or assumptions over data linearity or noise, making it a versatile and practical approach for learning robust predictive models. By focusing on feature invariance, emphasizing on reliable features, and reducing dependence on spurious correlations, CGLearn enhances the reliability and robustness of the models. The main contributions of this study are stated as follows:

- We propose a novel general framework, CGLearn, which improves consistency in learning robust predictors by focusing on features that show consistent behavior across environments.
- We provide both linear and nonlinear implementations of CGLearn, demonstrating its versatility and applicability across different model architectures.
- We demonstrate that CGLearn achieves superior predictive power and generalization, even without multiple environments, unlike most state-of-the-art methods in this arena that require diverse environments for effective generalization.
- Our empirical evaluations on synthetic and real-world datasets, covering both linear and nonlinear settings, as well as regression and classification tasks, validate the effectiveness and robustness of the proposed method.

The remainder of this paper is organized as follows: First, we delve into the methodology of CGLearn, detailing its linear and nonlinear implementations. Next, we present our experimental settings and evaluations. Finally, we encapsulate our conclusions, highlight the significant takeaways, and discuss future directions.

Methodology

In this section, we present the methodology of CGLearn, detailing both its linear and nonlinear implementations. We start by explaining the regular Empirical Risk Minimization (ERM) approach and then introduce the concept of gradient consistency used in CGLearn. The primary concept of CGLearn is to enforce gradient consistency for each factor of our variable of interest across multiple environments to identify and utilize invariant features, thereby enhancing generalization and reducing dependence on spurious correlations.

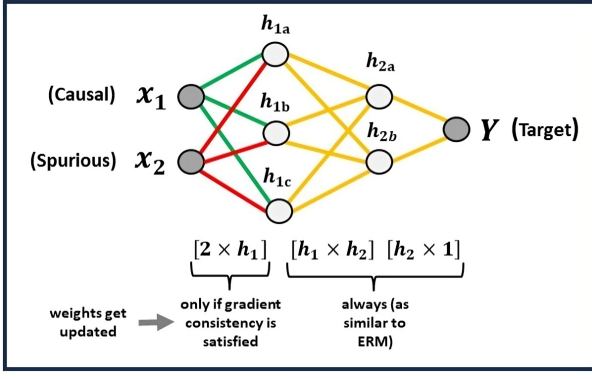


Figure 2: Nonlinear MLP implementation of CGLearn. X_1 (causal) and X_2 (spurious) feed into the first hidden layer h_1 . Weight updates in h_1 are performed based on gradient consistency (using L^2 -norm) for each feature across all training environments. The rest of the weights such as weights in h_2 , are updated similarly to ERM (without imposing any consistency constraints).

Empirical Risk Minimization (ERM)

Let's consider a simple linear problem where the goal is to predict the target variable Y using two features X_1 (causal) and X_2 (spurious) across multiple environments. Let e_1, e_2, \dots, e_m represent different environments. Environments can be considered as distinct distributions generated by different interventions, all of which share similar underlying causal mechanisms (see Fig. 1).

In the ERM framework, the weights for the features are updated by minimizing the empirical risk or the cost function (L), which is typically the mean squared error (MSE) between the predicted and actual values for a regression problem and cross-entropy loss for a classification task. Suppose the weights for the features at step t are w_1^t for X_1 and w_2^t for X_2 . The gradient of the loss (L) with respect to the weight associated with the j -th feature X_j in environment e_i is given by $\nabla L_j^{e_i}$, where $j \in \{1, 2\}$ and $i \in \{1, \dots, m\}$.

The aggregated gradient across all environments can be calculated as the mean of the gradients:

$$\mu_j^{\text{grad}} = \frac{1}{m} \sum_{i=1}^m \nabla L_j^{e_i} \quad \text{for } j \in \{1, 2\} \quad (1)$$

Using this aggregated gradient, the weights are updated as follows:

$$w_j^{t+1} = w_j^t - \eta \mu_j^{\text{grad}} \quad \text{for } j \in \{1, 2\} \quad (2)$$

where η is the learning rate. In this setup of a standard Empirical Risk Minimization, the weights for both X_1 and X_2 get updated in each step regardless of their consistency across environments.

Linear Implementation of CGLearn

CGLearn modifies this approach by introducing a consistency check for the gradients. The idea is to update the

weights only if the gradients are consistent across the available environments. This strategy focuses on invariant features and ignores spurious ones, expecting better generalization.

First, we calculate the gradient of each feature in every environment, as described in the previous section. The mean of the gradients can be calculated as described in Eq. 1. Next, we compute the standard deviation of the gradients for each feature across all environments as follows:

$$\sigma_j^{\text{grad}} = \sqrt{\frac{1}{m} \sum_{i=1}^m (\nabla L_j^{e_i} - \mu_j^{\text{grad}})^2} \quad (3)$$

We then calculate the consistency ratio, which is the absolute value of the ratio of the mean gradient to the standard deviation of the gradients:

$$C_j^{\text{ratio}} = \left| \frac{\mu_j^{\text{grad}}}{\sigma_j^{\text{grad}}} \right| \quad (4)$$

The consistency ratio, C_j^{ratio} defined in Eq. 4, is considered to be an indicator of the invariance of the gradient of variable X_j across all the training environments. A relatively larger mean compared to the standard deviation would indicate more similar or invariant gradients across the environments for the feature X_j , resulting in a higher value of C_j^{ratio} . On the other hand, a larger standard deviation indicates more diversity across the environments for X_j . Finally, we formulate a consistency mask based on a predefined threshold C^{thresh} :

$$C_j^{\text{mask}} = \begin{cases} 1 & \text{if } C_j^{\text{ratio}} \geq C^{\text{thresh}} \\ 0 & \text{otherwise} \end{cases} \quad (5)$$

The weights are updated only for the feature that has a nonzero mask and remains unchanged otherwise as per the following equation:

$$w_j^{t+1} = w_j^t - \eta (\mu_j^{\text{grad}} \cdot C_j^{\text{mask}}) \quad \text{for } j \in \{1, 2\} \quad (6)$$

Considering our motivating example, where X_1 is causal and expected to show more consistency across environments, C_1^{mask} is expected to be 1. Conversely, X_2 is spurious with respect to the target, expected to show inconsistency across environments, and C_2^{mask} is expected to be 0. Therefore, the weight for X_1 is mostly updated throughout the training steps while the weight for X_2 is not. The model thus focuses on the features that show consistency for learning the predictors of the target. This implementation strategy ensures to emphasis on reliable, invariant features while minimizing the impact of unreliable features by keeping their weights unchanged (or keeping the changes to a minimum). As a result, the contributions of the spurious features remain constant in the context of the model updates. In the next section, we extend the CGLearn method to a nonlinear setting using multilayer perceptron (MLP) as an instance.

Nonlinear Implementation

For the nonlinear implementation of CGLearn using a multilayer perceptron (MLP), we focus on the gradients in the

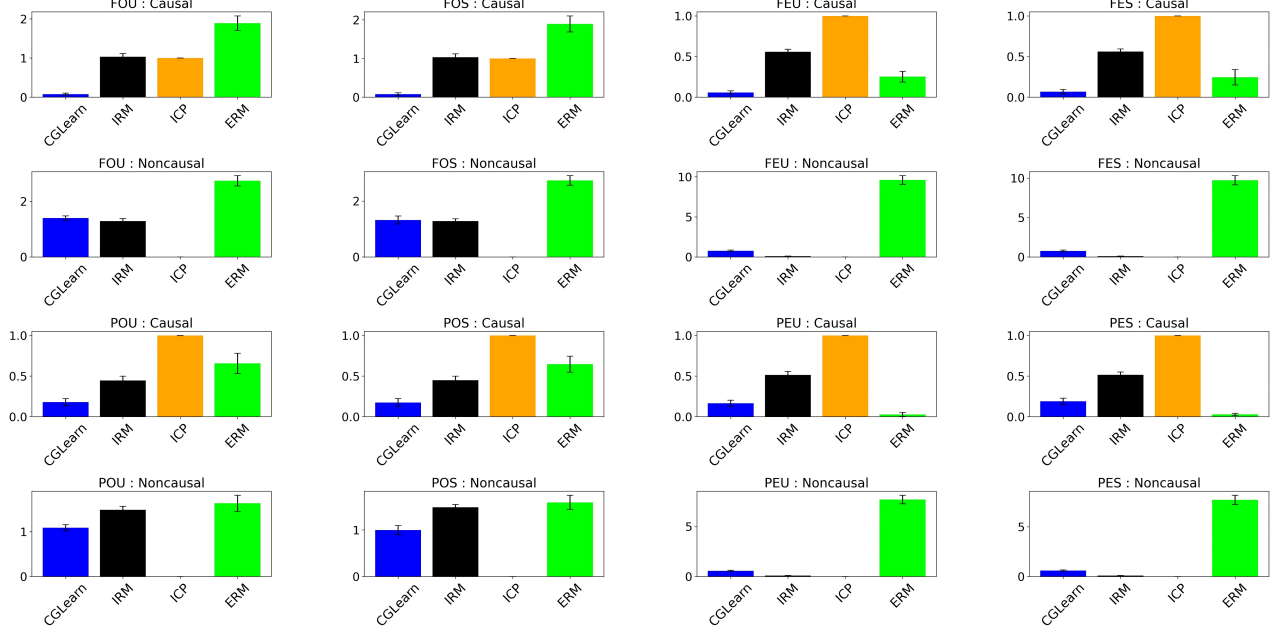


Figure 3: Performance comparison of CGLearn, IRM, ICP, and ERM across various linear multiple environment setups. Each subplot represents different configurations of the data, showing the mean squared error (MSE) for causal and noncausal variables over 50 trials.

first hidden layer (h_1), where feature contributions can be distinctly identified. By controlling the contribution of spurious features at the first hidden layer, we ensure they do not influence the final output. The process involves calculating the L^2 -norm of the gradients for each feature in each environment, followed by determining the consistency ratio and mask to impose the consistency constraint.

$\|\nabla L_{jh_1}^{e_i}\|_2$ denotes the L^2 -norm of the gradients of the j -th feature X_j in the i -th environment e_i at the first hidden layer h_1 . We compute the mean and standard deviation of the L^2 -norm of the gradients across all environments as follows:

$$\mu_j^{\text{grad}} = \frac{1}{m} \sum_{i=1}^m \|\nabla L_{jh_1}^{e_i}\|_2 \quad (7)$$

$$\sigma_j^{\text{grad}} = \sqrt{\frac{1}{m} \sum_{i=1}^m \left(\|\nabla L_{jh_1}^{e_i}\|_2 - \mu_j^{\text{grad}} \right)^2} \quad (8)$$

We then calculate the consistency ratio, C_j^{ratio} and the consistency mask, C_j^{mask} for feature X_j by following Eq. 4 and 5 respectively. All the weights that belong to a particular feature, X_j in the first hidden layer h_1 , are updated by following a similar strategy to Eq. 6. This updating strategy that depends on the consistency ratio, ensures that only the features that show consistency across the environments are considered to be updated. Otherwise, the weights remain unchanged, effectively treating them as constants similar to the linear implementation. For weights corresponding to the rest of the model other than the first hidden layer are updated as similar to ERM.

Fig. 2 illustrates a simple demonstration of the nonlinear MLP implementation of CGLearn. In this figure, X_1 and X_2 represent causal and spurious features, respectively, in accordance with our earlier motivating example. The gradient consistency is checked in the first hidden layer (h_1), and weights are updated only if the consistency ratio exceeds the threshold, ensuring that features that show invariance across environments are utilized.

In both implementations, the goal is to ensure that the model relies on features that show invariance across different environments. This leads to more robust and generalizable models by reducing dependency on spurious correlations.

Experiments and Results

We have considered three different major scenarios to assess the predictivity, robustness, and generalization capabilities of CGLearn. The first two scenarios are the ones where we considered linearly generated dataset-based experiments and in the last experimental case we have used the nonlinear implementation of CGLearn using multilayer perceptron (MLP) and applied it to different real world regression and classification tasks.

For all evaluations, we reported the mean and standard deviation of the performance metrics considered. For statistical significance tests, we used a t-test with $\alpha = 0.05$ as the significance level.

Cases	Causal Error (MSE)		Noncausal Error (MSE)	
	CGLearn	ERM	CGLearn	ERM
FOU	1.28 ± 0.40	1.57 ± 0.13	0.61 ± 0.19	0.54 ± 0.05
FOS	1.40 ± 0.43	1.61 ± 0.10	0.53 ± 0.17	0.52 ± 0.06
FEU	0.13 ± 0.05	0.20 ± 0.04	7.22 ± 2.15	8.28 ± 0.28
FES	0.16 ± 0.06	0.20 ± 0.04	7.47 ± 2.23	8.36 ± 0.30
POU	0.28 ± 0.11	0.37 ± 0.08	0.51 ± 0.18	0.48 ± 0.11
POS	0.34 ± 0.13	0.39 ± 0.07	0.46 ± 0.17	0.48 ± 0.10
PEU	0.24 ± 0.10	0.32 ± 0.07	5.11 ± 1.57	5.83 ± 0.43
PES	0.26 ± 0.10	0.31 ± 0.06	5.21 ± 1.58	5.81 ± 0.36

Table 1: Performance evaluation of CGLearn and ERM in linear single environmental setups. The table shows the Mean Squared Errors (MSE) for causal and noncausal variables across 50 trials for each configuration. Bold values indicate statistical significance.

Linear Multiple Environments

To evaluate the performance of our proposed CGLearn method, we generated synthetic linear datasets inspired by the approach used in the Invariant Risk Minimization (IRM) framework (Arjovsky et al. 2019). Our goal was to create diverse environments to test the robustness of our model under varying conditions.

We generated eight different experimental setups based on three key factors. Each setup included datasets with one target variable Y and ten feature variables X_1 to X_{10} . Features X_1 to X_5 acted as causal parents of Y , while X_6 to X_{10} were influenced by Y (non-causal). First, we distinguished between scrambled (S) and unscrambled (U) observations by applying an orthogonal transformation matrix S for scrambled data and using the identity matrix I for unscrambled data. This scrambling ensures that the features are not directly aligned with their original scales, making the learning task more challenging. Second, we designed fully-observed (F) scenarios where hidden confounders did not directly affect the features (i.e., no hidden confounder effects on features), and partially-observed (P) scenarios where hidden confounders influenced the features with Gaussian noise. Third, we incorporated two types of noise for the target variable Y : homoskedastic (O) noise, where the noise variance remained constant across different environments, and heteroskedastic (E) noise, where the noise variance varied depending on the environment, increasing with higher values of e . This distinction captures different real-world scenarios where noise may or may not depend on external factors. For each of these eight configurations (combinations of S/U, F/P, and O/E), we generated datasets corresponding to three distinct environments defined by the values $e \in \{0.2, 2, 5\}$. Each dataset consisted of 1000 samples. To ensure consistency with the IRM methodology and experimental setup, we used $e = 5$ as the validation environment and determined the optimal consistency threshold (C^{thresh}) for our CGLearn method using the performance based on this validation data. We selected the threshold C^{thresh} from the candidate values $\{0.25, 1, 4, 16, 64\}$ based on validation performance. This threshold is critical for identifying the invariant and most reliable features across different environments. For more details on the data generation process, we refer readers to the

IRM paper (Arjovsky et al. 2019).

We compared the performance of CGLearn with Empirical Risk Minimization (ERM), Invariant Causal Prediction (ICP) (Peters, Bühlmann, and Meinshausen 2016), and IRM (Arjovsky et al. 2019). We considered 50 random trials and reported the results in Fig. 3. In most cases, our proposed method CGLearn achieves the lowest mean squared error (MSE), demonstrating superior performance across various test cases to distinguish the causal and noncausal factors of the target by exploiting invariance across environments. IRM performs better than ERM but does not match the accuracy of CGLearn. ERM shows the highest errors in most cases, as it fails to differentiate between causal and non-causal features, relying on spurious correlations. Interestingly, ICP performs well in noncausal scenarios but poorly in causal ones. This observation aligns with the findings from the IRM study (Arjovsky et al. 2019), which noted that ICP’s conservative nature leads it to reject most covariates as direct causes, resulting in high causal errors.

Linear Single Environment

To evaluate the performance of our proposed CGLearn method in scenarios with only one environment, we generated synthetic linear datasets without relying on multiple environments as in previous experiments. For each of the eight cases, we used a single setting with $e = 2$. The data generation process was similar to the previous section, with each dataset consisting of 1000 samples and ten feature variables, X_1 to X_{10} . The first five features (X_1 to X_5) acted as causal parents of the target variable Y , while the remaining five features (X_6 to X_{10}) were influenced by Y . Given the single environment setup, we could not apply IRM and ICP methods, as they require multiple environments to distinguish between causal and noncausal factors. Therefore, we compared our results solely with Empirical Risk Minimization (ERM).

In the case of CGLearn, we created multiple batches, with $b = \{3, 5\}$ representing the number of batches created from the dataset. The last batch was used as the validation batch to determine the optimal consistency threshold parameter (C^{thresh}). We selected the threshold C^{thresh} from the candidate values $\{0.25, 1, 4, 16, 64\}$ based on validation performance. We imposed gradient consistency across different batches to learn consistent and reliable factors of the target.

Table 1 shows the results of our experiments in the single environment setup. Considering the causal error across all eight cases, CGLearn consistently achieves significantly lower mean squared errors (MSE) compared to ERM. For the noncausal error, CGLearn also outperforms ERM in most cases, suggesting the superiority of the proposed approach. Even in the absence of multiple environments, the optimization strategy based on gradient consistency across different batches enables CGLearn to achieve better predictive power than standard ERM.

Nonlinear Multiple Environments

For the nonlinear experimental setups, we considered two types of supervised learning tasks: regression and classification, both on real-world datasets. This approach allows us to evaluate the performance and robustness of our proposed CGLearn method in different real-world contexts. Recent work has highlighted limitations in the original Invariant Risk Minimization (IRM) framework, particularly in nonlinear settings where deep models tend to overfit (Rosenfeld, Ravikumar, and Risteski 2021). To address this, we included Bayesian Invariant Risk Minimization (BIRM) as a baseline, which has been shown to alleviate overfitting issues by incorporating Bayesian inference and thereby improving generalization in nonlinear scenarios (Lin et al. 2022).

Regression Tasks. In the nonlinear implementation of CGLearn, we used a multilayer perceptron (MLP) to evaluate its performance on real-world regression tasks, comparing it with other baselines. For the regression tasks, we used the Boston Housing dataset (Harrison and Rubinfeld 1978) and the Yacht Hydrodynamics dataset (Gerritsma, Onink, and Versluis 2013). The Boston Housing dataset consists of 506 instances and 13 continuous attributes. It concerns housing values in suburbs of Boston, with the task being to predict the median value of owner-occupied homes (MEDV) based on attributes such as per capita crime rate (CRIM), proportion of residential land zoned for large lots (ZN), average number of rooms per dwelling, and etc. The Yacht Hydrodynamics dataset consists of 308 instances and 6 attributes. The task is to predict the residuary resistance per unit weight of displacement of a yacht based on various hull geometry coefficients and the Froude number, such as the longitudinal position of the center of buoyancy, prismatic coefficient, and beam-draught ratio.

Since real-world datasets do not naturally come with different environments, we followed a similar approach to the study by Ge et al. (2022). We used the K-Means (Lloyd 1982) clustering algorithm to generate diverse environments and determined the optimal number of environments (between 3 to 10) using the Silhouette (Rousseeuw 1987) method. For each dataset, we created all possible test cases where each environment was considered as the test environment once, and the rest were used as training environments. We averaged the results over all possible test cases and repeated the process for 10 random trials. We evaluated the models based on RMSE, with the results shown in Table 2. For the Boston Housing dataset, we found the optimal number of environments was 7, while for the Yacht Hydrodynamics dataset, it was 5. From Table 2, we observe that all

four methods perform better on the training environments than the test environments, as expected. However, CGLearn shows significantly lower error in the testing or unseen environments compared to the other methods, demonstrating that imposing gradient consistency leads to less dependence on spurious features and thus better generalization.

Classification Tasks. For the classification tasks, we evaluated the performance on two real-world classification datasets: the Wine Quality dataset for red and white wines from the UCI repository (Cortez et al. 2009). The Wine Quality dataset for red wine has 1599 instances and 11 attributes, while the dataset for white wine has 4898 instances and 11 attributes. The goal is to model wine quality based on physicochemical tests, such as fixed acidity, volatile acidity, citric acid, residual sugar, pH, and etc. Similar to the regression tasks, we used K-means clustering to generate diverse environments and determined the optimal number of environments using the Silhouette method, finding 4 as the optimal number of environments for both classification datasets. We then generated all possible test cases where each environment was considered the test environment once, and the rest were used as training environments (as we did with the regression tasks). We averaged the performance over all possible test cases and conducted the process for 10 random trials. We used accuracy and F1-score as evaluation metrics, with the results shown in Table 3. As expected, all methods performed better in training environments compared to test environments. However, we found that CGLearn achieved higher accuracy and F1-scores, which are desirable, and the superior performance was statistically significant for the F1-score on the Wine Quality Red dataset. It also had significantly better accuracy on the Wine Quality White dataset. Similar to the regression tasks, CGLearn demonstrated better predictive power and generalization over ERM, IRM, and BIRM for the classification tasks.

Limitations of CGLearn with Invariant Spurious Features. We evaluated CGLearn on the Colored MNIST dataset, a synthetic binary classification task derived from MNIST (LeCun et al. 1995) and proposed in the IRM study (Arjovsky et al. 2019). This dataset introduces color as a spurious feature that strongly correlates with the label in the training environments but has the correlation reversed in the test environment. We applied the nonlinear implementation of CGLearn and compared it with the results of ERM and IRM as reported in the IRM study (Arjovsky et al. 2019). Over 10 trials, ERM achieved a training accuracy of 87.4 ± 0.2 and a test accuracy of 17.1 ± 0.6 , while IRM achieved a training accuracy of 70.8 ± 0.9 and a test accuracy of 66.9 ± 2.5 . In our experimental study, CGLearn achieved a training accuracy of 93.1 ± 0.8 and a test accuracy of 29.1 ± 0.8 . While CGLearn slightly outperformed ERM in the test environment, it still struggled to generalize. This limitation arises because CGLearn imposes gradient consistency on the training environments to distinguish invariant features from spurious ones. However, in the Colored MNIST setup, the spurious feature (color) is consistent across both training environments, leading CGLearn to erroneously treat it as an invariant feature. Consequently, CGLearn relies on color and performs poorly in the test environment. To im-

Dataset	# Optimal Envs.	Method	RMSE (Train)	RMSE (Test)
Boston	7	ERM	3.57 ± 0.11	6.43 ± 0.45
		IRM	3.79 ± 0.33	6.99 ± 0.74
		BIRM	3.77 ± 0.50	7.70 ± 0.52
		CGLearn	1.91 ± 0.26	5.49 ± 0.28
Yacht	5	ERM	0.21 ± 0.04	3.47 ± 1.15
		IRM	2.90 ± 0.03	4.36 ± 0.38
		BIRM	0.71 ± 0.19	3.15 ± 0.75
		CGLearn	0.48 ± 0.23	2.29 ± 0.42

Table 2: Performance comparison in nonlinear experimental setups for regression tasks. The table shows the RMSE for training and test environments across 10 trials. In test cases, we mark the statistically significant values in bold.

Dataset	# Optimal Envs.	Method	Accuracy (Train)	Accuracy (Test)	F1-score (Train)	F1-score (Test)
WQ Red	4	ERM	62.07 ± 0.34	58.08 ± 1.72	0.692 ± 0.004	0.535 ± 0.010
		IRM	63.68 ± 0.19	58.70 ± 1.54	0.644 ± 0.003	0.542 ± 0.014
		BIRM	64.94 ± 0.37	57.97 ± 0.93	0.626 ± 0.004	0.536 ± 0.011
		CGLearn	61.59 ± 0.44	59.60 ± 0.46	0.638 ± 0.008	0.553 ± 0.007
WQ White	4	ERM	58.73 ± 0.22	51.15 ± 0.34	0.590 ± 0.002	0.447 ± 0.008
		IRM	58.82 ± 0.26	51.60 ± 0.40	0.566 ± 0.003	0.450 ± 0.013
		BIRM	58.04 ± 0.18	51.87 ± 0.32	0.530 ± 0.006	0.460 ± 0.026
		CGLearn	58.23 ± 0.38	52.33 ± 0.32	0.555 ± 0.005	0.460 ± 0.007

Table 3: Performance comparison in nonlinear setups for classification tasks. The table shows accuracy and F1-score for training and test environments across 10 trials. The statistically significant values are in bold for the test cases. WQ Red and WQ White represent the Wine Quality Red and Wine Quality White datasets respectively.

prove CGLearn’s generalization, future work should focus on adapting the method to account for the varying nature of spurious features, even when they appear consistent across training environments.

Conclusions

In this study, we presented CGLearn, a novel approach for developing robust and predictive machine learning models by leveraging gradient consistency across multiple environments. By focusing on the agreement of gradients, CGLearn effectively identifies and utilizes invariant features, leading to superior generalization and reduced reliance on spurious correlations. Our extensive experiments on both synthetic and real-world datasets, including regression and classification tasks, demonstrated that CGLearn outperforms traditional ERM and state-of-the-art invariant learners like ICP, IRM, and BIRM, achieving lower errors and better generalization in diverse scenarios. Notably, even in the absence of predefined environments, we demonstrated that CGLearn can be effectively applied to different subsamples of data, leading to better predictive models than regular ERM. This flexibility enhances the applicability of CGLearn in a wide range of real-world scenarios where many state-of-the-art methods require diverse and defined environments for OOD generalization.

Despite its strengths, CGLearn has limitations, particularly in scenarios where spurious features are invariant across environments, as observed in the Colored MNIST experiments. Such cases violate our assumption as generally we expect and observe causal features to be stable and invariant in nature whereas spurious features do not (Wood-

ward 2005; Wang et al. 2022). CGLearn erroneously considers these invariant but spurious features as reliable, impacting its generalization performance. Addressing this limitation and adapting CGLearn to better handle such cases is a promising direction for future research.

Overall, CGLearn provides a significant step forward in the field of robust machine learning by effectively harnessing causal invariance. Our work opens new avenues for developing models that are not only highly predictive but also resilient to distribution shifts, paving the way for more reliable applications in real-world settings.

Acknowledgments

This research was supported by the Army Research Office under Grant W911NF-22-1-0035 and by the National Science Foundation under grant no. CBET 2218841. The views expressed are those of the authors and do not necessarily reflect the official policies of the Army Research Office or the U.S. Government. The U.S. Government retains the right to reproduce and distribute reprints for governmental purposes.

References

- Andrews, B.; Spirtes, P.; and Cooper, G. F. 2020. On the completeness of causal discovery in the presence of latent confounding with tiered background knowledge. In *International Conference on Artificial Intelligence and Statistics*, 4002–4011. PMLR.
- Arjovsky, M.; Bottou, L.; Gulrajani, I.; and Lopez-Paz, D. 2019. Invariant risk minimization. *arXiv preprint arXiv:1907.02893*.

- Bose, R.; and Roy, A. M. 2024. Invariance embedded physics-infused deep neural network-based sub-grid scale models for turbulent flows. *Engineering Applications of Artificial Intelligence*, 128: 107483.
- Chickering, D. M. 2002. Optimal structure identification with greedy search. *Journal of Machine Learning Research*, 3(Nov): 507–554.
- Chowdhury, J.; Fricke, C.; Bamidele, O.; Bello, M.; Yang, W.; Heyden, A.; and Terejanu, G. 2024. Invariant Molecular Representations for Heterogeneous Catalysis. *Journal of Chemical Information and Modeling*, 64(2): 327–339.
- Chowdhury, J.; Rashid, R.; and Terejanu, G. 2023. Evaluation of Induced Expert Knowledge in Causal Structure Learning by NOTEARS. In *Proceedings of the 12th International Conference on Pattern Recognition Applications and Methods - ICPRAM*, 136–146. INSTICC, SciTePress. ISBN 978-989-758-626-2.
- Chowdhury, J.; and Terejanu, G. 2023. CD-NOTEARS: Concept Driven Causal Structure Learning Using NOTEARS. In *2023 International Conference on Machine Learning and Applications (ICMLA)*, 808–813. IEEE.
- Colombo, D.; Maathuis, M. H.; Kalisch, M.; and Richardson, T. S. 2012. Learning high-dimensional directed acyclic graphs with latent and selection variables. *The Annals of Statistics*, 294–321.
- Cortez, P.; Cerdeira, A.; Almeida, F.; Matos, T.; and Reis, J. 2009. Wine Quality. UCI Machine Learning Repository. DOI: <https://doi.org/10.24432/C56S3T>.
- Ge, Y.; Arik, S. Ö.; Yoon, J.; Xu, A.; Itti, L.; and Pfister, T. 2022. Invariant Structure Learning for Better Generalization and Causal Explainability. *arXiv preprint arXiv:2206.06469*.
- Gencoglu, O.; and Gruber, M. 2020. Causal modeling of twitter activity during covid-19. *Computation*, 8(4): 85.
- Gerritsma, J.; Onnink, R.; and Versluis, A. 2013. Yacht Hydrodynamics. UCI Machine Learning Repository. DOI: <https://doi.org/10.24432/C5XG7R>.
- Harrison, D.; and Rubinfeld, D. L. 1978. Hedonic prices and the demand for clean air. *J. Environ. Econ. and Management*. UCI Machine Learning Repository, <http://lib.stat.cmu.edu/datasets/boston>.
- He, Y.; Shen, Z.; and Cui, P. 2021. Towards non-iid image classification: A dataset and baselines. *Pattern Recognition*, 110: 107383.
- Huang, B.; Zhang, K.; Lin, Y.; Schölkopf, B.; and Glymour, C. 2018. Generalized score functions for causal discovery. In *Proceedings of the 24th ACM SIGKDD international conference on knowledge discovery & data mining*, 1551–1560.
- Jiang, G.-q.; Liu, J.; Ding, Z.; Guo, L.; and Lin, W. 2023. Accelerating Large Batch Training via Gradient Signal to Noise Ratio (GSNR). *arXiv preprint arXiv:2309.13681*.
- Kaiser, M.; and Sipos, M. 2022. Unsuitability of NOTEARS for causal graph discovery when dealing with dimensional quantities. *Neural Processing Letters*, 54(3): 1587–1595.
- Koyama, M.; and Yamaguchi, S. 2020. Out-of-distribution generalization with maximal invariant predictor.
- Lachapelle, S.; Brouillard, P.; Deleu, T.; and Lacoste-Julien, S. 2019. Gradient-based neural dag learning. *arXiv preprint arXiv:1906.02226*.
- LeCun, Y.; Jackel, L. D.; Bottou, L.; Cortes, C.; Denker, J. S.; Drucker, H.; Guyon, I.; Muller, U. A.; Sackinger, E.; Simard, P.; et al. 1995. Learning algorithms for classification: A comparison on handwritten digit recognition. *Neural networks: the statistical mechanics perspective*, 261(276): 2.
- Lin, Y.; Dong, H.; Wang, H.; and Zhang, T. 2022. Bayesian invariant risk minimization. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, 16021–16030.
- Liu, J.; Chen, Y.; and Zhao, J. 2021. Knowledge enhanced event causality identification with mention masking generalizations. In *Proceedings of the twenty-ninth international conference on international joint conferences on artificial intelligence*, 3608–3614.
- Liu, J.; Jiang, G.; Bai, Y.; Chen, T.; and Wang, H. 2020. Understanding why neural networks generalize well through gsnr of parameters. *arXiv preprint arXiv:2001.07384*.
- Lloyd, S. 1982. Least squares quantization in PCM. *IEEE transactions on information theory*, 28(2): 129–137.
- Ming, Y.; Yin, H.; and Li, Y. 2022. On the impact of spurious correlation for out-of-distribution detection. In *Proceedings of the AAAI conference on artificial intelligence*, volume 36, 10051–10059.
- Montavon, G.; Hansen, K.; Fazli, S.; Rupp, M.; Biegler, F.; Ziehe, A.; Tkatchenko, A.; Lilienfeld, A.; and Müller, K.-R. 2012. Learning invariant representations of molecules for atomization energy prediction. *Advances in neural information processing systems*, 25.
- Ng, I.; Ghassami, A.; and Zhang, K. 2020. On the role of sparsity and dag constraints for learning linear dags. *Advances in Neural Information Processing Systems*, 33: 17943–17954.
- Ng, I.; Zhu, S.; Fang, Z.; Li, H.; Chen, Z.; and Wang, J. 2022. Masked gradient-based causal structure learning. In *Proceedings of the 2022 SIAM International Conference on Data Mining (SDM)*, 424–432. SIAM.
- Ormaniec, W.; Sussex, S.; Lorch, L.; Schölkopf, B.; and Krause, A. 2024. Standardizing Structural Causal Models. *arXiv preprint arXiv:2406.11601*.
- O'Donnell, R. T.; Nicholson, A. E.; Han, B.; Korb, K. B.; Alam, M. J.; and Hope, L. R. 2006. Causal discovery with prior information. In *AI 2006: Advances in Artificial Intelligence: 19th Australian Joint Conference on Artificial Intelligence, Hobart, Australia, December 4-8, 2006. Proceedings 19*, 1162–1167. Springer.
- Parascandolo, G.; Neitz, A.; Orvieto, A.; Gresele, L.; and Schölkopf, B. 2020. Learning explanations that are hard to vary. *arXiv preprint arXiv:2009.00329*.
- Pearl, J. 2009. *Causality*. Cambridge university press.
- Peters, J.; Bühlmann, P.; and Meinshausen, N. 2016. Causal inference by using invariant prediction: identification and

- confidence intervals. *Journal of the Royal Statistical Society Series B: Statistical Methodology*, 78(5): 947–1012.
- Rame, A.; Dancette, C.; and Cord, M. 2022. Fishr: Invariant gradient variances for out-of-distribution generalization. In *International Conference on Machine Learning*, 18347–18377. PMLR.
- Ramsey, J.; Glymour, M.; Sanchez-Romero, R.; and Glymour, C. 2017. A million variables and more: the fast greedy equivalence search algorithm for learning high-dimensional graphical causal models, with an application to functional magnetic resonance images. *International Journal of Data Science and Analytics*, 3: 121–129.
- Reisach, A.; Seiler, C.; and Weichwald, S. 2021. Beware of the simulated dag! causal discovery benchmarks may be easy to game. *Advances in Neural Information Processing Systems*, 34: 27772–27784.
- Reisach, A.; Tami, M.; Seiler, C.; Chambaz, A.; and Weichwald, S. 2024. A scale-invariant sorting criterion to find a causal order in additive noise models. *Advances in Neural Information Processing Systems*, 36.
- Rosenfeld, E.; Ravikumar, P. K.; and Risteski, A. 2021. The Risks of Invariant Risk Minimization. In *International Conference on Learning Representations*.
- Rousseeuw, P. J. 1987. Silhouettes: a graphical aid to the interpretation and validation of cluster analysis. *Journal of computational and applied mathematics*, 20: 53–65.
- Sagawa, S.; Raghunathan, A.; Koh, P. W.; and Liang, P. 2020. An investigation of why overparameterization exacerbates spurious correlations. In *International Conference on Machine Learning*, 8346–8356. PMLR.
- Santillan, B. G. 2023. A step towards the applicability of algorithms based on invariant causal learning on observational data. *arXiv preprint arXiv:2304.02286*.
- Shi, Y.; Seely, J.; Torr, P. H.; Siddharth, N.; Hannun, A.; Usunier, N.; and Synnaeve, G. 2021. Gradient matching for domain generalization. *arXiv preprint arXiv:2104.09937*.
- Shin, D. 2021. The effects of explainability and causability on perception, trust, and acceptance: Implications for explainable AI. *International journal of human-computer studies*, 146: 102551.
- Spirites, P.; Glymour, C.; and Scheines, R. 2001. *Causation, prediction, and search*. MIT press.
- Torralba, A.; and Efros, A. A. 2011. Unbiased look at dataset bias. In *CVPR 2011*, 1521–1528. IEEE.
- Wang, J.; Lan, C.; Liu, C.; Ouyang, Y.; Qin, T.; Lu, W.; Chen, Y.; Zeng, W.; and Philip, S. Y. 2022. Generalizing to unseen domains: A survey on domain generalization. *IEEE transactions on knowledge and data engineering*, 35(8): 8052–8072.
- Wang, Q.; Zheng, Y.; Yang, G.; Jin, W.; Chen, X.; and Yin, Y. 2017. Multiscale rotation-invariant convolutional neural networks for lung texture classification. *IEEE journal of biomedical and health informatics*, 22(1): 184–195.
- Wang, T.; Sridhar, R.; Yang, D.; and Wang, X. 2021. Identifying and mitigating spurious correlations for improving robustness in nlp models. *arXiv preprint arXiv:2110.07736*.
- Wei, D.; Gao, T.; and Yu, Y. 2020. DAGs with No Fears: A closer look at continuous optimization for learning Bayesian networks. *Advances in Neural Information Processing Systems*, 33: 3895–3906.
- Woodward, J. 2005. *Making things happen: A theory of causal explanation*. Oxford university press.
- Yu, Y.; Chen, J.; Gao, T.; and Yu, M. 2019. DAG-GNN: DAG structure learning with graph neural networks. In *International conference on machine learning*, 7154–7163. PMLR.
- Zadrozny, B. 2004. Learning and evaluating classifiers under sample selection bias. In *Proceedings of the twenty-first international conference on Machine learning*, 114.
- Zheng, X.; Aragam, B.; Ravikumar, P. K.; and Xing, E. P. 2018. Dags with no tears: Continuous optimization for structure learning. *Advances in neural information processing systems*, 31.
- Zheng, X.; Dan, C.; Aragam, B.; Ravikumar, P.; and Xing, E. 2020. Learning sparse nonparametric dags. In *International Conference on Artificial Intelligence and Statistics*, 3414–3425. Pmlr.