Abstract

Machine learning models trained with purely observational data and the principle of empirical risk minimization (Vapnik, 1992) can fail to generalize to unseen domains. In this paper, we focus on the case where the problem arises through spurious correlation between the observed domains and the actual task labels. We find that many domain generalization methods do not explicitly take this spurious correlation into account. Instead, especially in more application-oriented research areas like medical imaging or robotics, data augmentation techniques that are based on heuristics are used to learn domain invariant features. To bridge the gap between theory and practice, we develop a causal perspective on the problem of domain generalization. We argue that causal concepts can be used to explain the success of data augmentation by describing how they can weaken the spurious correlation between the observed domains and the task labels. We demonstrate that data augmentation can serve as a tool for simulating interventional data. Lastly, but unsurprisingly, we show that augmenting data improperly can cause a significant decrease in performance.

1 Introduction

Despite recent advancements in machine learning fueled by deep learning, studies like Azulay & Weiss (2019) have shown that those methods may not generalize to inputs from outside of their training distribution. In safety-critical fields like medical imaging, robotics and, self-driving cars, however, it is essential that machine learning models are robust to changes in the environment. Without the ability to generalize, machine learning models cannot be safely deployed in the real world.

In the field of domain generalization, one tries to find a representation that generalizes across different environments, called domains, each with a different shift of the input. This problem is especially challenging when changes in the domain are spuriously associated with changes in the actual task labels. This can, for instance, happen when the data gathering process is biased. An example is given by Arjovsky et al. (2019): If we consider a dataset of images of cows and camels in their natural habitat, then there is a strong correlation between the type of animal and the landscape in the photo, e.g., a camel standing in a savanna. If we now train a machine learning model to predict the animal in a given image, the model is prone to exploit the spurious correlation between the type of animal and the type of landscape. As a result, the model can fail to recognize a camel standing in a green pasture or a cow standing in a savanna.

In recent years, a large corpus of methods designed to representations that will generalize across domains has been formulated. While the proposed methods are able to achieve good results on a variety of domain generalization benchmarks, the majority of them lack a theoretical foundation. In the worst-case scenario, these methods enforce the wrong type of invariance, see Section 2.2.

Interestingly, we find that especially in more applied fields, like medical imaging and robotics, researchers have found a practical way of dealing with the spurious correlation between domains and the actual task. Data augmentation in combination with Empirical Risk Minimization (ERM) (Vapnik, 1992) is used to enforce invariance of the machine learning model with respect to changes in the domain. Hereby, prior knowledge is used to guide the selection of appropriate data augmentation. In Section 4.2.1 and 4.2.2 we give a detailed summary of two successful applications of data augmentation in the context of domain generalization.
However, the success of data augmentation is often described in vague terms like ‘artificially expanding labeled training datasets’ (Li, 2020) and ‘reduce overfitting’ (Krizhevsky et al., 2012). In this paper, we present a causal perspective on data augmentation in the context of domain generalization and contribute to the field in the following manner:

- First, we use a Structural Causal Model (SCM) to describe what we believe reflects the underlying causal model of the majority of domain generalization problems. We show that the spurious correlation between domains and the actual task can be modeled by a hidden confounder.

- Second, we show that prior knowledge can be used to guide the design of data augmentation techniques that exploits a form of intervention-augmentation equivariance of the true underlying causal model that generated the data. As a result, such augmented data samples can be used to simulate data that would come from a distribution where one intervened on the domain.

- Last, we compare the performance of different data augmentation techniques on a synthetic dataset and three domain generalization benchmarks. We show that accurately designed data augmentation techniques lead to machine learning models with good generalization properties.

2 Background

2.1 Domain generalization

We first formalize the problem of domain generalization following the notations used in Muandet et al. (2013). We assume that during training we have access to samples $S$ from $N$ different domains, where $S = \{S^{d=1}\}_{i=1}^{N}$. From each domain $n_i$ samples $S^{d=i} = \{(x_k^{d=i}, y_k^{d=i})\}_{k=1}^{n_i}$ are included in the training set. The training data is represented as tuples of the form $(x, y, d)$ sampled from the observational distribution $p(x, y, d)$. The goal of domain generalization is to develop machine learning methods that generalize well to unseen domains. In order to test the ability of a machine learning model to generalize, we use samples $S^{d=N+1}$ from a previously unseen test domain $d = N + 1$.

In this paper, we are interested in the general case where the observed domains $d$ and targets $y$ are spuriously correlated in the training dataset, i.e., where we might have $p(y|d = i) \neq p(y|d = j)$, $i, j \in \{1, \ldots, N\}$. Since the correlation between $d$ and $y$ is assumed to be spurious, it does not necessarily hold for the test domain $d = N + 1$.

2.2 Domain generalization via invariant feature representation

Arguably, the most commonly used approach in domain generalization relies on learning domain invariant features. The learning of invariant features can be achieved by mapping an input $x$ to intermediate features $z$ that are uninformative of the domain $d$, i.e., $p(z|d = i) = p(z|d = j)$. At the same time, the intermediate features $z$ are optimized for a low prediction error on all training domains. This results in finding a saddle point for the setting commonly referred to as domain adversarial learning (Ganin et al., 2016). It is assumed that such $z$ will generalize well to the test domain and, thus, result in a low test error.

Recent work of Zhao et al. (2019), Johansson et al. (2019) and Arjovsky et al. (2019), in the context of domain adaptation, shows that enforcing $p(z|d = i) = p(z|d = j)$ is not necessarily leading to a low test error if the domains $d$ and targets $y$ are spuriously correlated, i.e., $p(y|d = i) \neq p(y|d = j)$. This leads us to investigate this general case as already indicated in section 2.1.

We now extend the findings of Zhao et al. (2019) to domain generalization. The full derivation can be found in the Appendix, here we will only present the main result. Assuming there exists an intermediate representation $z$ satisfying $p(z|d = i) = p(z|d = j)$, then the joint empirical risk (rhs) across all domains (training and test) is lower bounded by the pairwise divergence of the marginal label distribution of all domains (lhs):

$$\sum_{1 \leq i < j \leq N+1} \text{JSD}(p(y|d = i)||p(y|d = j)) \leq 2 \sum_{i}^{N+1} \sqrt{\epsilon^{d=i}},$$

where JSD is the Jensen-Shannon divergence between two distributions and $\epsilon^{d=i}$ is the empirical risk on domain $d = i$. The bound in Equation 1 shows that if indeed the domains $d$ and targets $y$ are spuriously correlated, i.e., $p(y|d = i) \neq p(y|d = j)$, then the joint empirical risk can be become large.

To the best of our knowledge, there are currently very few methods that address the issue of spuriously correlated domains $d$ and targets $y$ (Arjovsky et al., 2019; Heinze-Deml & Meinshausen, 2019; Li et al., 2018; Krueger et al., 2020), where Li et al. (2018) extends the idea of domain adversarial learning to enforce conditional domain invariance, i.e., $p(z|y, d = i) = p(z|y, d = j)$. However, we find that especially in more application-oriented research areas, such as medical imaging and robotics, researchers have found a practical solution to
deal with domain generalization. A variety of data augmentation techniques in combination with Empirical Risk Minimization (ERM) (Vapnik, 1992) is used. In Section 3 we will develop a causal perspective that helps to explain the success of data augmentation for domain generalization.

2.3 Data augmentation

Before we discuss data augmentation from a causal point of view, we will briefly summarize how it is currently viewed in the computer vision community (Shorten & Khoshgoftaar, 2019). In computer vision data augmentation is seen as an effective technique for improving the performance on a variety of tasks such as image classification, object detection, and image segmentation. In the image domain, data augmentation techniques can be roughly divided into two categories:

1. Augmenting the geometry of an image: Commonly used transformations are rotations, horizontal and vertical flips, scaling, cropping, occlusion, and elastic deformations.

2. Augmenting the color of an image: Random values are added or subtracted from the color channels of an image. Instead of applying this transformation directly in the RGB colorspace, other color spaces like CIELAB and HSL are commonly used (Tellez et al., 2019).

Data augmentation is a combination of the transformation listed above that are randomly applied to all images during training. Its success is commonly attributed to reducing overfitting by increasing the amount of training data. Below, we develop a novel causal perspective on data augmentation to explain its success.

3 Domain generalization and data augmentation from a causal perspective

For readers unfamiliar with the concepts of causality, a brief introduction of the causal concepts that are used throughout this paper can be found in the Appendix. For an in-depth introduction please see Pearl (2009) or Peters et al. (2017).

First, we introduce a Structural Causal Model (SCM) in order to describe what we believe in many cases reflects the underlying "true" causal structure of domain generalization problems. We assume the following SCM

\[
\begin{align*}
    d &:= f_D(c) \\
    y &:= f_Y(c) \\
    h_d &:= f_{h_d}(d) \\
    h_y &:= f_{h_y}(y) \\
    x &:= f_X(h_d, h_y),
\end{align*}
\]

where \( c \) is a hidden confounder (and an exogenous variable), \( d \) the domain, \( y \) the target, \( h_d \) high-level features, e.g., color and orientation, caused by \( d \), \( h_y \) high-level features, e.g., shape and texture, caused by \( y \), and \( x \) the input. We omit including noise variables for clarity.

The corresponding Directed Acyclic Graph (DAG) is shown in Figure 1, where a grey node means the variable is observed and a white node corresponds to a latent (unobserved) variable. The presented DAG is similar to the ones constructed in Subbaswamy & Saria (2019); Castro et al. (2019); Heinze-Deml & Meinshausen (2019).

In Figure 1 the node \( c \) is a hidden confounder. The hidden confounder \( c \) opens up a backdoor path (a non-causal path) \( d \leftarrow c \rightarrow y \) (Pearl, 2009). This path allows \( d \) to enter \( y \) through the back door. As a result, the domain \( d \) and the target \( y \) are in general no longer independent, \( p(y, d) \neq p(y)p(d) \). Since the high-level features, \( h_d \) are children of \( d \), they are spuriously correlated with \( y \) as well, i.e., \( h_d \) becomes predictive of \( y \).

Now we assume that we train a machine learning model using ERM (Vapnik, 1992) and observational data generated from the DAG in Figure 1. The task is to predict \( y \) from \( x \), which itself is anti-causal. Since \( d \) and \( y \) are correlated, it is likely that the machine learning model will rely on all high-level features \( h_d \) and \( h_y \) to predict \( y \). Furthermore, we assume that the correlation of \( d \) and \( y \) is spurious. Therefore, it will not hold in general and will break under intervention. A machine learning model...
relying on high-level features $h_d$ that are caused by $d$ is thus likely to generalize poorly to unseen domains.

Returning to our introductory example of classifying animals in images, the hidden confounder can be used to model the fact that there is a common cause for the type of animal and the landscape in an image. For example, the confounder could be the country in which a particular image was taken, e.g., in Switzerland we are more likely to see a cow standing in a green pasture than a camel or a savanna.

### 3.1 Simulating interventions

One possible approach to deal with the spurious correlations between $d$ and $y$, is to perform an intervention on $d$. Such an intervention would render $d$ and $y$ independent, i.e., $p(y|do(d)) = p(y)$. In Figure 2 (left), we see the same DAG as in Figure 1 but after we intervened on $d$. We find that in Figure 2 (left) there is no more arrow connecting the hidden confounder $c$ and the domain $d$. The backdoor path $d \leftarrow c \rightarrow y$ has vanished.

In the examples of animals and landscapes, to intervene on the domain $d$, here the landscape, we would have to physically move a cow to a savanna. It becomes apparent that the interventions have to happen in the real world and are not operations on the already gathered observational data. In the majority of domain generalization problems, it will not be feasible to collect new data with specific interventions.

In Figure 2 (center) we present a second way of addressing the problem of correlated variables $d$ and $y$. In theory one could perform an intervention on all high-level features $h_d$, i.e., $do(h_d)$, since $d$ affects $x$ only indirectly via $h_d$, where $h_d$ could represent the colors of the landscapes, e.g., green and beige. Again, an intervention like this would need to happen during the data collection process in the real world.

However, we argue that in certain cases we can simulate data from the interventional distribution $p(x, y|do(h_d))$ using data augmentation in combination with observational data. For example, we could randomly perturb the colors in the animal images. This type of augmentation simulates a noise intervention on $h_d$; i.e., $do(h_d = \xi)$, where $\xi$ is sampled from a noise distribution $N_\xi$ (Peters et al., 2016). By augmenting only high-level features $h_d$ that are caused by $d$ we guarantee that the target $y$ is unchanged. After data augmentation the pairs $(x_{\text{aug}}, y)$ should closely resemble samples from the interventional distribution $p(x, y|do(h_d))$. In Figure 2 (right) we see that we only require observational data from the SCM without any interventions. We argue that for correctly designed data augmentation we cannot distinguish the data generated by any of the three models in Figure 2.

In theory, we could intervene on $h_d$ by setting $h_d$ to a fixed value, instead of performing a noise intervention. However, in order to simulate data from such an interventional distribution using data augmentation, we would require $h_d$ to be observed, which we argue is generally not the case. In Section 4.2.1 we describe that there exist data augmentation methods that try to infer $h_d$ for each sample $x$ before setting $h_d$ to a fixed value for all samples, yet these augmentations seem to perform worse than random augmentations.

If we want to design data augmentation $x_{\text{aug}} = \text{aug}(x)$, as a transformation $\text{aug}(\cdot)$ applied to observed data $x$, such that it simulates an intervention on the high-level features $h_d$ caused by $d$, one needs to make assumption about the causal data generating process. Formally, we require that augmenting the data $x$ to $x_{\text{aug}} = \text{aug}(x)$ commutes with an intervention $do(h_d)$ prior to the data generation. We call this intervention-augmentation equivariance. In more formal detail, assume that we have the causal process from Equation 2:

$$x := f_X(h_d, h_y).$$

Then augmenting $x$ via $\text{aug}(\cdot)$ does:

$$x_{\text{aug}} = \text{aug}(x) = \text{aug}(f_X(h_d, h_y)).$$

We then say that the causal process $f_X : \mathcal{H}_d \times \mathcal{H}_y \rightarrow \mathcal{X}$, is intervention-augmentation equivariant if for every considered stochastic data augmentation transformation $\text{aug}(\cdot)$ on $x \in \mathcal{X}$ we have a corresponding noise intervention $do(\cdot)$ on $h_d \in \mathcal{H}_d$ such that:

$$\text{aug}(f_X(h_d, h_y)) = f_X(do(h_d), h_y).$$

The intervention-augmentation equivariance is expressed as a commutative diagram in Figure 3. We argue that by making strong assumptions about the true causal process we need to first identify the high-level features $h_d$ caused by $d$. Second, we have to design data augmentation $\text{aug}(x)$ that commutes with a corresponding intervention $do(h_d)$ under the causal process $f_X(h_d, h_y)$.

![Diagram](image3.png)

**Figure 3:** Intervention-augmentation equivariance expressed in a commutative diagram.
Figure 2: Left: DAG with hidden confounder after intervention on $d$. Center: DAG with hidden confounder after intervention on $h_d$. Interventional nodes are squared. Right: DAG with hidden confounder plus data augmentation. Note that in the latter case we do not have to intervene on the system that generates the data. Data augmentation should be designed in a way such that the augmented data simulates data from the center or left DAG.

3.1.1 Linear example

We now consider the case where $f_X(\cdot)$ is a linear transformation

$$x = f_X(h_d, h_y) = Ch_d + Dh_y + e,$$

where $x, h_d, h_y, e$ are vectors and $C, D$ are matrices correspondingly sized. We further assume that the data augmentation can be expressed as a linear transformation of the form

$$x_{aug} = \text{aug}_A(x) = Ax,$$

where $A$ is a correspondingly sized matrix. Combining Equation 5 and 6, we obtain

$$x_{aug} = Ax = ACh_d + ADh_y + Ae = C(C^{-1}ACH_d) + ADh_y + Ae = f_X(\text{do}_A(h_d), h_y).$$

We find that if $A$ is sampled from the set of all matrices so that $AD = D$ and $Ae = e$ the transformation $Ax$ successfully simulates the noise intervention $\text{do}_A(h_d) := C^{-1}ACH_d$ (with slight abuse of notation), i.e., we find that it satisfy the intervention-augmentation equivariance condition. To illustrate the result of Equation 7 we consider the concrete example where the domain $d$ causes a specific ordering in $h_d$ that is spuriously correlated with the label $y$. If we choose $A$ to be a stochastic permutation matrix and assume $D$ and $e$ to be permutation invariant ($AD = D$ and $Ae = e$), it can be easily seen that the augmentation $Ax$ satisfies Equation 7.

There is one caveat though. In this section, we assume that we are successfully augmenting all high-level features $h_d$ caused by $d$. In a real-world application, we usually have no means to validate this assumption, i.e., we might only augment a subset of $h_d$. Furthermore, we might even augmenting high-level features $h_y$ that are caused by the target node $y$. Nonetheless, we argue there are cases where we still obtain better generalization performance than a machine learning model trained without data augmentation. This may happen in cases where weakening the spurious confounding influence of $h_d$ on $y$ recovers more of the anti-causal signal for $y$ than the data augmentation on the features $h_y$ destroys. We evaluate this hypothesis empirically in Section 5.

4 Related work

4.1 Learning invariant representations

As described in Section 2.2 there exists a multitude of domain generalization methods that do not explicitly address the problem of hidden confounders (Balaji et al., 2018; Carlucci et al., 2018, 2019; Ding & Fu, 2018; Ghifary et al., 2015; Ilse et al., 2019; Li et al., 2017b; Mancini et al., 2018; Motian et al., 2017; Shankar et al., 2018; Tzeng et al., 2014; Wang et al., 2018). However,
the majority of these methods are evaluate on benchmark datasets, e.g., VLCS (Khosla et al., 2012) or PACS (Li et al., 2017a), where the domain \( d \) and the target \( y \) are confounded. As shown in Equation 1 this can result in a poor generalization performance. Nonetheless, we cannot rule out the possibility that some of these methods are implicitly able to deal with confounders, thus achieving good generalization performance.

4.2 Data augmentation in application-focused research areas

In the following, we give a summary of two examples of the successful application of data augmentation for domain generalization in medical imaging and robotics. We want to highlight that in both examples the actual task and the domains are spuriously correlated.

4.2.1 Histopathology

The high variability of the appearance of histopathology images is a major obstacle for the deployment of automatic image analysis systems. The variability of appearance is the result of a multitude of preparation steps that are applied to the specimen: cutting, fixating, staining, and scanning. Each step introduces its own artifacts. This leads to different color distributions among histopathology laboratories. Tellez et al. (2019) perform a detailed comparison of commonly used data augmentation, see Appendix Figure 9. The augmentation techniques consist of random rotation and flipping, random color perturbation, and color normalization. These augmentation techniques are compared on a dataset composed of histopathology images from nine different laboratories. We argue that there exists a hidden confounder that spuriously correlates the staining and scanner artifacts (caused by the laboratories) and the abnormalities in the tissue (caused by the diseases). By augmenting the color of the histopathology images Tellez et al. (2019) are able to learn features that are invariant to the laboratories. Furthermore, Tellez et al. (2019) find that random color perturbation outperforms color normalization. We argue that random color perturbation simulates noise interventions, whereas color normalization tries to simulate interventions where the color of a histopathology image is set to a fixed value. As described in Section 3.1 this requires to first estimate the color distribution of the original histopathology image which is a challenging problem. As a result, data augmentation in the form of random color perturbation is better suited to simulate interventional data.

4.2.2 Robotics

Performing robotic learning on physical hardware is often not feasible due to: (i) the large number of training samples that are required, and (ii) potential damage to the hardware if the learning relies on random exploration. Therefore, learning in a physics simulator is of great interest. While learning in a simulator is cheap and safe, we are facing a new problem, namely, how to overcome the so-called reality gap, i.e., the differences between simulation and the real world. In Tobin et al. (2017) they focus on a robotic manipulation task that involves a robotic arm and eight 3D objects that are placed on a table. In this scenario, a neural network is used to detect the location of an object. In order to be able to generalize from the simulation to the real world, Tobin et al. (2017) apply a variety of data augmentation techniques to the simulator, e.g., randomization of position and texture of all objects on the table, textures of the table, floor, skybox, and robot, and the addition of random noise. We argue that there exists a hidden confounder that introduces a spurious correlation between, e.g., the lighting conditions and the location of the objects on the table. By applying heavy data augmentation during the training process they are able to generalize to unseen lighting conditions in the real world.

4.3 Advanced data augmentation techniques

In addition to the techniques described in Section 2.3 there exist more advanced methods. Zhang et al. (2018) introduced a method called mixup that constructs new training examples by linearly interpolating between two existing examples \((x_i, y_i)\) and \((x_j, y_j)\). In Gowal et al. (2019); Perez & Wang (2017) a Generative Adversarial Network (GAN) is used to perform so-called `adversarial mixing’. The GAN is able to generate new training examples that belong to the same class \(y\) but have different styles. Furthermore, Perez & Wang (2017) propose a novel method called ‘neural augmentation’ where they train the first part of their model to generate an augmented image from two training examples with the same class \(y\).

4.4 Causality

Another research area that is concerned with finding invariant features across different domains is causal discovery. In Peters et al. (2016) a method for Invariant Causal Prediction (ICP) is developed. It is built on the assumption that causal features are stable given different experimental settings. Given the complete set of causal features, the conditional distribution of the target variable \(y\) must remain the same under interventions, e.g.,
change of the domain. Whereas, predictions made by a machine learning model relying on non-causal features are in general not stable under interventions.

Recently, Arjovsky et al. (2019) proposed a framework called Invariant Risk Minimization (IRM), that shares the same goal as ICP. In IRM a soft penalty in combination with an ERM term is used to balance the invariance and predictive power of the learned machine learning model. In contrast to ICP, IRM can be used for tasks on unstructured data, e.g., images. However, while both methods (ICP and IRM) try to learn features that are parents of y, we argue that for the majority of domain generalization problems the task of predicting y from x is anti-causal. Therefore we are interested in augmenting only features caused by d, i.e., the descendants of d, assuming that the remaining features are caused by y.

In Arjovsky et al. (2019), they argue that there exists a discrepancy between the true label (part of the true causal mechanism) that caused x and the annotation produced by human labelers. Learning this 'labeler function' will lead to a good generalization performance, even though it might rely on patterns that are anti-causal or non-causal. In this situation, the IRM objective becomes ineffective.

Last, Heinze-Deml & Meinshausen (2019) introduced the Conditional variance Regularization (CoRe). CoRe uses grouped observations (e.g., training samples with the same class y but different styles) to learn invariant representations. Samples are grouped by an additional ID variable, which is different from the label y. We find that in most cases it is difficult to obtain an additional ID variable, e.g., none of the datasets in Section 5 feature such a variable. If no such ID variable exists, CoRe can use pairs of original images and augmented images to learn invariant representations. Furthermore, they assume that the domain is an unobserved parent node of y. In their case, an intervention on d would not resolve the issue of the spurious correlation between y and d.

5 Experiments

We evaluate the performance of data augmentation in combination with Empirical Risk Minimization (ERM) (Vapnik 1992) on four datasets. While the first is a synthetic dataset, the other three are domain generalization benchmark image datasets (rotated MNIST, colored MNIST and PACS) where the domain d and target y are confounded. Code to replicate the experiments can be found under https://github.com/AMLab-Amsterdam/DataAugmentationInterventions.

5.1 Synthetic data

For the first experiment we simulate data from the following linear Gaussian SCM:

\begin{align}
    c & := \mathcal{N}(0, \sigma_c^2) \\
    d & := c \cdot W_{c \rightarrow d} + \mathcal{N}(0, \sigma_d^2) \\
    y & := c \cdot W_{c \rightarrow y} + \mathcal{N}(0, \sigma_y^2) \\
    h_d & := d \cdot W_{d \rightarrow h_d} + \mathcal{N}(0, \sigma_{h_d}^2) \\
    h_y & := y \cdot W_{y \rightarrow h_y} + \mathcal{N}(0, \sigma_{h_y}^2),
\end{align}

where the corresponding DAG can be seen in Figure 4.

![Figure 4: DAG of linear Gaussian SCM.](https://example.com/dag.png)

We choose c, d, y, h_d and h_y to be five dimensional vectors. Furthermore, we sample the elements of the square matrices W_{c \rightarrow d}, W_{c \rightarrow y}, W_{d \rightarrow h_d} and W_{y \rightarrow h_y} from \mathcal{N}(0, I). In all of our experiments \sigma_c = I and \sigma = 0.1 \cdot I.

The task is to regress \sum_i y_i from x, where x = [h_d, h_y], a 10 dimensional feature vector. During training the data is generated using the DAG in Figure 4 where due the confounder c the features h_d and y are spuriously correlated. During testing we set d := \mathcal{N}(0, I), keeping W_{c \rightarrow d}, W_{c \rightarrow y}, W_{d \rightarrow h_d} and W_{y \rightarrow h_y} the same as during training. As a result, features h_d and y are no longer correlated. A model relying on features h_d will not be able to generalize well to the test data. In all experiments, we use linear regression to minimize the empirical risk. We choose to add noise sampled from a uniform distribution U[−10, 10] as our data augmentation technique. We vary the number of dimensions of h_d as well as of h_y that are augmented. Each experiment is repeated 50 times, in Figure 5 we plot the mean of the mean square error (MSE) together with the standard error.

In Figure 5 we see that ERM using only features h_y (pink line) achieves the lowest MSE. Next, we apply data augmentation to one, two, three, four, and five dimensions of h_d while keeping h_y unchanged (orange line). We find that if data augmentation is applied to all five
dimensions of \( h_d \) we can match the MSE of ERM with only features \( h_y \). In this case, we are satisfying the condition in Equation 4. Furthermore, we find that unsurprisingly the MSE of models trained with data augmentation applied to features \( h_y \) increases (green, red, purple, and brown line). However, we can see that as long as we apply data augmentation to at least three dimensions of \( h_d \) the resulting MSE is lower than ERM using all features \( h_d \) and \( h_y \) (blue line). Perhaps the most surprising result of this experiment is that there exist conditions under which applying data augmentation to features caused by \( d \) and \( y \) will result in better generalization performance compared to ERM using all features.

5.2 Rotated MNIST

We construct the rotated MNIST dataset following Li et al. (2018). This dataset consists of four different domains \( d \) and ten different classes \( y \), each domain corresponds to a different rotation angle: \( d = \{0^\circ, 30^\circ, 60^\circ, 90^\circ\} \). We first randomly select a subset of images \( x \) from the MNIST training dataset and afterward apply the rotation to each image of the subset. For the next domain, we randomly select a new subset. To guarantee the variance of \( p(y) \) among the domains, the number of training examples for each digit class \( y \) is randomly chosen from a uniform distribution \( U[80, 160] \). For each experiment three of the domains are selected for training and one domain is selected for testing. For the test domain, the corresponding rotation is applied to the 10000 examples of the MNIST testset.

In Table 1 we compare data augmentation in combination with ERM to ERM, a Domain Adversarial Neural Network (DANN) (Ganin et al., 2016) and a Conditional Domain Adversarial Neural Network (CDANN) (Li et al., 2018). All methods use a LeNet (LeCun et al., 1998) type architecture and we repeat each experiment 10 times.

We select two types of data augmentation for this dataset. First, we apply random rotations between \( 0^\circ \) and \( 359^\circ \) to the images \( x \) during training, denoted by DA+. Randomly rotating the images \( x \) can be interpreted as a way to simulate a noise intervention on \( d \). The result is a training dataset where \( d \) and \( y \) are independent. We argue that such a transformation satisfies the condition in Equation 4. If we assume \( h_d \) to be equal to the rotation angle of the MNIST digit in a given image \( x \), applying random rotations to \( x \) is equal to a noise intervention on \( h_d \).

\[
x_{aug} = R(u)x = f_X(do(h_d = u), h_y)
\]

where \( u \) is uniformly sampled from \([0^\circ, 359^\circ]\) and \( R(u) \) is a rotation matrix acting on the coordinate grid of \( x \), which itself is a form of permutation, see Section 3.1.1.

In Table 1 we see that the results of DA+ are similar for all test domains. Furthermore, we find that DA+ outperforms ERM, DANN, and CDANN, where CDANN is especially designed for the case where \( d \) and \( y \) are spurious correlated. Second, we apply random horizontal and vertical flips to the images \( x \) during training, denoted by DA-. We argue that such a transformation is not satisfying the condition in Equation 4. For some classes, this transformation is augmenting features that are caused by \( y \). We find that for the classes ‘2’, ‘4’, ‘5’ the classification accuracy is especially low. As a result, DA- is the worst performing method in Table 1.

5.3 Colored MNIST

Following Arjovsky et al. (2019), we create a version of the MNIST dataset where the color of each digit is spuriously correlated with a binary label \( y \). We construct two training domains and one test domain where the digits of the original MNIST classes ‘0’ to ‘4’ are labeled \( y = 0 \) and the digits of the classes ‘5’ to ‘9’ are labeled \( y = 1 \). Subsequently, for 25% of the digits we flip the label \( y \). We now color digits which are labeled \( y = 0 \) red and digits which are labeled \( y = 1 \) green.
Last, we flip the color of a digit with a probability of 0.2 for the first training domain and with a probability of 0.1 for the second training domain. In the case of the test domain, the color of a digit is flipped with a probability of 0.9. By design, the original MNIST class of each digit (‘0’ to ‘9’) is a direct cause of the new label $y$ whereas the color of each digit is a descendant of the new label $y$. In Table 2 we see that while ERM is performing well on the training domains it fails to generalize to the test domain since it is using the color information to predict $y$. In contrast, IRM (Arjovsky et al., 2019) and REx (Krueger et al., 2020) generalizes well to the test domain. Again, we can use data augmentation to simulate a noise intervention on the data generating process. We use random color perturbations consisting of randomly changing: brightness, contrast, saturation, and hue denoted by DA. We use the same network architecture and training procedure as described in Arjovsky et al. (2019). Each experiment is repeated 10 times. We find that DA can successfully weaken the spurious confounding influence of the domain $d$ on $y$, see Table 2.

| Acc  | ERM   | IRM   | REx   | DA    |
|------|-------|-------|-------|-------|
| train | 87.4 ± 0.2 | 70.8 ± 0.9 | 71.5 ± 1.0 | 81.6 ± 1.1 |
| test  | 17.1 ± 0.6 | 66.9 ± 2.5 | 68.7 ± 0.9 | 68.8 ± 0.7 |

5.4 PACS

The PACS dataset (Li et al., 2017a) was introduced as a strong benchmark dataset for domain generalization methods that features large domain shifts. The dataset consists of four domains: $d = \{\text{‘photo’ (P), ‘art-painting’ (A), ‘cartoon’ (C), ‘sketch’ (S)}\}$, i.e., each image style is viewed as a domain. The numbers of images in each domain are 1670, 2048, 2344, 3929 respectively. There are seven classes: $y = \{\text{dog, elephant, giraffe, guitar, horse, house, person}\}$. In the case of the PACS dataset, it is very challenging to design a data augmentation technique that satisfies the condition in Equation 4. Eventually, we use the same data augmentation technique as Carlucci et al. (2019): During training, each image is transformed to greyscale with a probability of 10%, denoted by DA. We argue that this data augmentation technique partially satisfies the condition in Equation 4 since, as shown in Figure 6, the colors in each domain seem to be spuriously correlated with the object class $y$. We fine-tune an AlexNet-model (Krizhevsky et al., 2012), that was pre-trained on ImageNet, using ERM in combination with data augmentation.

In Table 3 we compare DA to various domain generalization methods: CDANN (Li et al., 2018), L2G (Li et al., 2017b), GLCM (Wang et al., 2018), SSN (Mancini et al., 2018), IRM (Arjovsky et al., 2019), REx (Krueger et al., 2020), MetaReg (Balaji et al., 2018), JigSaw (Carlucci et al., 2019), where all methods use the same pre-trained AlexNet-model. We repeat each experiment 5 times and report the average accuracy. We find that DA obtains a high average accuracy. Only two other methods, MetaReg and JigSaw, are able to achieve higher average accuracy.

The biggest performance gains of DA compared to ERM are on the test domains ‘art painting’ and ‘sketch’. The domain ‘sketch’ consists of black sketches of the seven object classes on white background, see Figure 6. In contrast to all other domains, here the color of the object is not correlated with the class. A model relying on color features will, therefore, generalize poorly to the ‘sketch’ domain. However, by randomly transforming the images of the training domains (‘art painting’, ‘cartoon’, ‘photo’) to greyscale with a probability of 10% during training, we find that DA is able to generalize much better. It seems reasonable to assume that some of the performance of Carlucci et al. (2019) can be attributed to the data augmentation.

6 Conclusion

In this paper, we present a causal perspective on the effectiveness of domain augmentation in the context of
Table 3: Results on PACS dataset. Ordered by average accuracy.

| Target | ERM | CDANN | L2G | GLCM | SSN | IRM | REx | DA | MetaReg | JigSaw |
|--------|-----|-------|-----|------|-----|-----|-----|----|---------|-------|
| A      | 63.30 | 62.70 | 66.23 | 66.8 | 64.1 | 67.05 | 67.04 | 67.77 | 69.82 | 67.63 |
| C      | 63.13 | 69.73 | 66.88 | 69.7 | 66.8 | 68.49 | 67.97 | 66.11 | 70.35 | 71.71 |
| P      | 87.70 | 78.65 | 88.00 | 87.9 | 90.2 | 89.39 | 89.74 | 86.74 | 91.07 | 89.00 |
| S      | 54.07 | 64.45 | 58.96 | 56.3 | 60.1 | 70.69 | 59.81 | 64.69 | 59.26 | 65.18 |
| Ave    | 67.05 | 68.88 | 70.01 | 70.2 | 70.3 | 70.69 | 71.14 | 71.33 | 72.62 | 73.38 |

domain generalization. By using an SCM we address a core problem of domain generalization: the spurious correlation of the domain variable $d$ and the target variable $y$. From a causal perspective, one solution for this problem is to intervene on the domain variable $d$. Unfortunately, this solution is impractical since we assume that we only have access to observational data. However, we show that data augmentation can serve as a surrogate tool for simulating interventions on the domain variable $d$. Hereby, prior knowledge needs to be used to design data augmentation techniques that only act on the non-descendants of the target variable $y$. We evaluated this approach on three different datasets and were able to show that empirical risk minimization in combination with accurately designed data augmentation results in good generalization performance. Furthermore, we summarized two studies that show the effectiveness of data augmentation for real-world applications, where the ability to generalize is crucial.

Last, we want to summarize what we believe is the current state of domain generalization. Currently, there are three approaches to address the problem of domain generalization, each with their limitations:

1. Computer vision methods, see Section 4.1, that are lacking a theoretical foundation, and in the worst-case scenario optimizing for the wrong type of invariance, see Section 2.2.
2. Causal methods, see Section 4.4, that in their current form rely on strong assumptions and are difficult to scale.
3. Data augmentation methods, see Section 2.3, that need to be designed by hand and are mostly limited to the visual domain.

The analysis in this paper could be further used to design data augmentation to simulate interventional datasets for domain generalization methods by exploiting intervention-augmentation equivariance.

Acknowledgements

The authors want to thank Leon Bottou and Ishaan Gulrajani for their help with IRM.

Maximilian Ilse was funded by the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (Grant DLMedia: Deep Learning for Medical Image Analysis).

References

Martin Arjovsky, Ilya Sutskever, and Yoshua Bengio. Invariant Risk Minimization. *arXiv*, 2019.

Aharon Azulay and Yair Weiss. Why do deep convolutional networks generalize so poorly to small image transformations? *arXiv*, 2019.

Yogesh Balaji, Swami Sankaranarayanan, and Rama Chellappa. MetaReg: Towards Domain Generalization using Meta-regularization. In *NeurIPS*, 2018.

Fabio M. Carlucci, Paolo Russo, Tatiana Tommasi, and Barbara Caputo. Hallucinating Agnostic Images to Generalize Across Domains. *arXiv*, 2018.

Fabio Maria Carlucci, Antonio D’Innocente, Silvia Bucci, Barbara Caputo, and Tatiana Tommasi. Domain Generalization by Solving Jigsaw Puzzles. *arXiv*, 2019.

Daniel C. Castro, Ian Walker, and Ben Glocker. Causality matters in medical imaging. *arXiv*, 2019.

Zhengming Ding and Yun Fu. Deep Domain Generalization With Structured Low-Rank Constraint. *IEEE Transactions on Image Processing*, 27(1):304–313, 2018.

Yaroslav Ganin, Evgeniya Ustinova, Hana Ajakan, Pascal Germain, Hugo Larochelle, Fran ois Laviolette, Mario Marchand, and Victor Lempitsky. Domain-Adversarial Training of Neural Networks. *arXiv*, 2016.

Muhammad Ghifary, W. Bastiaan Kleijn, Mengjie Zhang, and David Balduzzi. Domain Generalization for Object Recognition with Multi-task Autoencoders. In *ICCV*, 2015.

Sven Gowal, Chongli Qin, Po-Sen Huang, Taylan Cemgil, Krishnamurthy Dvijotham, Timothy Mann, and Pushmeet Kohli. Achieving Robustness in the Wild via Adversarial Mixing with Disentangled Representations. *arXiv*, 2019.
Christina Heinze-Deml and Nicolai Meinshausen. Conditional Variance Penalties and Domain Shift Robustness. arXiv, 2019.

Maximilian Ilse, Jakub M. Tomczak, Christos Louizos, and Max Welling. DIVA: Domain Invariant Variational Autoencoders. arXiv, 2019.

Fredrik D. Johansson, David Sontag, and Rajesh Ranjanath. Support and Invertibility in Domain-Invariant Representations. arXiv, 2019.

Aditya Khosla, Tinghui Zhou, Tomas Malisiewicz, Alexei A. Efros, and Antonio Torralba. Undoing the Damage of Dataset Bias. In ECCV. Berlin, Heidelberg, 2012.

Alex Krizhevsky, Ilya Sutskever, and Geoffrey E. Hinton. ImageNet Classification with Deep Convolutional Neural Networks. In NIPS. 2012.

David Krueger, Ethan Caballero, Joern-Henrik Jacobsen, Amy Zhang, Jonathan Binas, Remi Le Priol, and Antonio Torralba. Out-of-Distribution Generalization via Risk Extrapolation (REx). arXiv:2003.00688 [cs, stat], March 2020. arXiv: 2003.00688.

Yann LeCun, Leon Bottou, Yoshua Bengio, and Patrick Ha. Gradient-Based Learning Applied to Document Recognition. 1998.

Da Li, Yongxin Yang, Yi-Zhe Song, and Timothy M. Hospedales. Deeper, Broader and Artier Domain Generalization. In ICCV, October 2017a.

Da Li, Yongxin Yang, Yi-Zhe Song, and Timothy M. Hospedales. Learning to Generalize: Meta-Learning for Domain Generalization. arXiv, 2017b.

Sharon Y. Li. Automating Data Augmentation: Practice, Theory and New Direction, April 2020. Library Catalog: ai.stanford.edu.

Ya Li, Xinmei Tian, Mingming Gong, Yajing Liu, Tongliang Liu, Kun Zhang, and Dacheng Tao. Deep Domain Generalization via Conditional Invariant Adversarial Networks. In ECCV. 2018.

Massimiliano Mancini, Samuel Rota Bul, Barbara Caputo, and Elisa Ricci. Best sources forward: domain generalization through source-specific nets. arXiv, 2018.

Saeid Motiian, Marco Piccirilli, Donald A. Adjeroh, and Gianfranco Doretto. Unified Deep Supervised Domain Adaptation and Generalization. arXiv, 2017.

Krikamol Muandet, David Balduzzi, and Bernhard Scholkopf. Domain Generalization via Invariant Feature Representation. arXiv:1301.2115 [cs, stat], January 2013.

Judea Pearl. Causal inference in statistics: An overview. Statistics Surveys, 3:96–146, 2009.

Luis Perez and Jason Wang. The Effectiveness of Data Augmentation in Image Classification using Deep Learning. arXiv, 2017.

J. Peters, D. Janzing, and B. Schölkopf. Elements of Causal Inference: Foundations and Learning Algorithms. MIT Press, Cambridge, MA, USA, 2017.

Jonas Peters, Peter Bhlmann, and Nicolai Meinshausen. Causal inference by using invariant prediction: identification and confidence intervals. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 78(5):947–1012, 2016.

Shiv Shankar, Vihari Piratla, Soumen Chakrabarti, Siddhartha Chaudhuri, Preethi Jyothi, and Sunita Sarawagi. Generalizing Across Domains via Cross-Gradient Training. arXiv, 2018.

Connor Shorten and Taghi M Khoshgoftaar. A survey on image data augmentation for deep learning. Journal of Big Data, 6(1):60, 2019.

Adarsh Subbaswamy and Suchi Saria. From development to deployment: dataset shift, causality, and shift-stable models in health AI. BioStatistics, 2019.

David Tellez, Geert Litjens, Peter Bandi, Wouter Bulten, John-Melle Bokhorst, Francesco Ciompi, and Jeroen van der Laak. Quantifying the effects of data augmentation and stain color normalization in convolutional neural networks for computational pathology. arXiv, 2019.

Josh Tobin, Rachel Fong, Alex Ray, Jonas Schneider, Wojciech Zaremba, and Pieter Abbeel. Domain Randomization for Transferring Deep Neural Networks from Simulation to the Real World. arXiv, 2017.

Eric Tzeng, Judy Hoffman, Ning Zhang, Kate Saenko, and Trevor Darrell. Deep Domain Confusion: Maximizing for Domain Invariance. arXiv, 2014.

V. Vapnik. Principles of Risk Minimization for Learning Theory. In NIPS. 1992.

Haohan Wang, Zexue He, Zachary C. Lipton, and Eric P. Xing. Learning Robust Representations by Projecting Superfluous Statistics Out. In ICLR, 2018.

Hongyi Zhang, Moustapha Cisse, Yann N. Dauphin, and David Lopez-Paz. mixup: Beyond Empirical Risk Minimization. arXiv, 2018.

Han Zhao, Remi Tachet des Combes, Kun Zhang, and Geoffrey J. Gordon. On Learning Invariant Representation for Domain Adaptation. arXiv, 2019.
7 Appendix

7.1 Causality

What follows is a brief introduction of causal concepts that are used throughout this paper. It hopefully makes the paper more self-contained, as well as more accessible for readers that encounter these concepts for the first time. For an in-depth introduction please see (Pearl 2009) or (Peters et al. 2017).

7.1.1 Structural causal models

We say that a set of variables \(x_1, \ldots, x_l\) causes a variable \(y\) if intervening on any of the \(x_m\) changes the distribution of \(y\). This is usually different from (conditional) observational dependence between the \(x_m\) and \(y\). Structural Causal Models (SCMs) are used to formalize those causal interactions between variables. We need to distinguish between two types of variables: exogenous and endogenous variables. Exogenous variables can be seen as an entry point to our SCM (and are usually unobserved independent random variables). The endogenous variables \(x_m\) are then determined by the causal mechanisms, which are formalized via functional relations: \(x_m = f_m(x_{pa_m})\), where \(x_{pa_m}\) is the tuple of the so-called parent variables of \(x_m\). These relations of an SCM induce a corresponding graphical model. In this paper, we only deal with acyclic relationships, leading to Directed Acyclic Graphs (DAGs) as part of a Bayesian network. In Figure 7 we see three SCMs and their corresponding DAGs. Note that the direction of the arrows indicates the causal direction.

The SCMs in Figure 7 are considered to be the three main building blocks of every causal model: chain, confounder, and collider. Where each of them introduces a different (conditional in-)dependence structure. First row: In case of a chain the variables \(x\) and \(z\) become conditionally independent if we condition on the center variable \(y\), i.e., \(p(z|x, y) = p(z|y)\). Second row: An observed confounder \(y\) can introduce spurious correlation between its two children variables \(x\) and \(z\), i.e., we may have \(p(x, z) \neq p(x)p(z)\). If we condition on the confounding variable \(y\) they become conditionally independent again, i.e., \(p(z|x, y) = p(z|y)\) and \(p(x|z, y) = p(x|y)\). Third row: In case of an unobserved collider \(y\) the two parent variables are independent, \(p(x, z) = p(x)p(z)\). However, if we condition on \(y\) they may become conditionally dependent, i.e., \(p(x, z|y) \neq p(x|y)p(z|y)\).

DAG

SCM

Figure 7: Top to bottom: chain, confounder, collider, chain with intervention on \(y\).

7.1.2 Interventions

In its simplest form an intervention can be described as setting a variable \(y\) to a constant value, e.g., \(y = y_0\) irrespective of its parent variables. The result of such an intervention on the SCM of a chain and the corresponding DAG can be seen in the bottom row of Figure 7. In this example, the variable \(y\) becomes independent of its parent variable \(x\), i.e., we are replacing the function assignment \(y = f(x)\) with \(y = y_0\), effectively deleting the function \(f(\cdot)\) and the corresponding arrow in the DAG. Using the do-operator (Pearl 2009) we can write the resulting interventional distribution as follows: \(p(z|x, do(y = y_0)) = p(z|do(y = y_0))\). In this paper, we use a special form of interventions, so-called noise or stochastic interventions (Peters et al. 2016). Instead of setting the intervened variable to a fixed value, we randomize the values of \(y\), i.e., \(do(y = \xi)\), where \(\xi\) is sampled from a noise distribution \(N_\xi\).

7.2 Bound for non-conditional DG methods

As shown in Zhao et al. (2019) an information-theoretic lower bound can be derived for the domain adaptation case. The bound "demonstrates that learning invariant representations could lead to a feature space where the joint error on both domains is large." We provide a straightforward expression of this bound for the domain generalization case.

Introduction of notation:
\begin{itemize}
  \item \(x\): input
  \item \(z\): intermediate representation
  \item \(\hat{y}\): output
  \item \(h\): function mapping \(x\) to \(z\)
  \item \(g\): function mapping \(z\) to \(\hat{y}\)
  \item JSD: Jensen-Shannon divergence
  \item \(\epsilon^{d=i}\): empirical risk on domain \(d = i\)
\end{itemize}

In addition, we need the following two lemmas from \cite{Zhao2019}. Proofs can be found in \cite{Zhao2019}.

\textbf{Lemma 4.6:}

\begin{equation}
\text{JSD}(p(\hat{y}|d = i)||p(\hat{y}|d = j)) \leq \text{JSD}(p(z|d = i)||p(z|d = j)),
\end{equation}

where \(p(\hat{y}|d = i)\) are the marginal distributions of the output in domain \(d = i\) and \(p(z|d = i)\) are the marginal distributions of the intermediate representation in domain \(d = i\).

\textbf{Lemma 4.7:}

\begin{equation}
\text{JSD}(p(y|d = i)||p(\hat{y}|d = i)) \leq \sqrt{\epsilon_i(h \circ g)},
\end{equation}

i.e., how well is my output distribution matching the true labels distribution.

We start with the pairwise sum of Jensen-Shannon divergence between all \(N\) training domains and the \(N+1\) test domain

\begin{equation}
\sum_{1 \leq i < j \leq N+1} \text{JSD}(p(y|d = i)||p(y|d = j)).
\end{equation}

Since JSD is a metric we can write

\begin{equation}
\sum_{1 \leq i < j \leq N+1} \text{JSD}(p(y|d = i)||p(y|d = j)) \leq \sum_{1 \leq i < j \leq N+1} \text{JSD}(p(\hat{y}|d = i)||p(\hat{y}|d = j))
\end{equation}

\begin{equation}
+ 2 \sum_{k}^N \text{JSD}(p(y|d = k)||p(\hat{y}|d = k)).
\end{equation}

Using Lemma 4.6 we get

\begin{equation}
\sum_{1 \leq i < j \leq N+1} \text{JSD}(p(y|d = i)||p(y|d = j)) \leq \sum_{1 \leq i < j \leq N+1} \text{JSD}(p(z|d = i)||p(z|d = j))
\end{equation}

\begin{equation}
+ 2 \sum_{k}^N \text{JSD}(p(y|d = k)||p(\hat{y}|d = k)).
\end{equation}

Using Lemma 4.7 we get

\begin{equation}
\sum_{1 \leq i < j \leq N+1} \text{JSD}(p(y|d = i)||p(y|d = j)) \leq \sum_{1 \leq i < j \leq N+1} \text{JSD}(p(z|d = i)||p(z|d = j))
\end{equation}

\begin{equation}
+ 2 \sum_{k}^N \sqrt{\epsilon^{d=k}(h \circ g)}.\tag{27}
\end{equation}

Extracting terms that belong to the test domain \(d = N+1\) leads to

\begin{equation}
\sum_{l=1}^N \text{JSD}(p(y|d = l)||p(y|d = N+1))
\end{equation}

\begin{equation}
+ \sum_{1 \leq i < j \leq N} \text{JSD}(p(y|d = i)||p(y|d = j))
\end{equation}

\begin{equation}\leq \sum_{l=1}^N \text{JSD}(p(z|d = l)||p(z|d = N+1))
\end{equation}

\begin{equation}\leq \sum_{1 \leq i < j \leq N} \text{JSD}(p(z|d = i)||p(z|d = j))
\end{equation}

\begin{equation}
+ 2 \sum_{k}^N \sqrt{\epsilon^{d=k}(h \circ g)}.
\end{equation}

Assuming we find a perfect intermediate representation \(z\) for all \(N\) training domains and the test domain \(d = N+1\) (assuming such an \(z\) exists) we are left with

\begin{equation}
\sum_{l=1}^N \text{JSD}(p(y|d = l)||p(y|d = N+1))
\end{equation}

\begin{equation}\leq 2 \sqrt{\epsilon^{d=N+1}(h \circ g)} + 2 \sum_{k}^N \sqrt{\epsilon^{d=k}(h \circ g)}.
\end{equation}

We see that, as it was the case for domain adaptation, that the joint risk across all domains (training and test) is lower bounded by the pairwise divergence of the
marginal label distribution of all domains. Given the existence of an unobserved confounder as seen in Figure 1 the marginal label distribution are unlikely to match.

From this result, we can derive a design principle for learning invariant representations for domain generalization with confounders. Instead of enforcing

\[ p(z|d = i) = p(z|d = j), \]  
(31)

we have to enforce

\[ p(z|y, d = i) = p(z|y, d = j), \]  
(32)

as seen in, e.g., Li et al. (2018).

### 7.3 Example images

Example images of data augmentation for Section 4.2.1, see Figure 9 and for Section 4.2.2, see Figure 10. Example images of data augmentation for Section 5.3, see Figure 8.

![Figure 8: Data augmentation for Colored MNIST.](image)

Figure 8: Data augmentation for Colored MNIST.

![Figure 9: Domain randomization histo, taken from Tellez et al. (2019).](image)

Figure 9: Domain randomization histo, taken from Tellez et al. (2019).

![Figure 10: Domain randomization robots, taken from Torchbin et al. (2017).](image)

Figure 10: Domain randomization robots, taken from Torchbin et al. (2017).