LEARNING ROBUST MODELS USING THE PRINCIPLE OF INDEPENDENT CAUSAL MECHANISMS

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ABSTRACT

Standard supervised learning breaks down under data distribution shift. However, the principle of independent causal mechanisms (ICM, Peters et al. [2017]) can turn this weakness into an opportunity: one can take advantage of distribution shift between different environments during training in order to obtain more robust models. We propose a new gradient-based learning framework whose objective function is derived from the ICM principle. We show theoretically and experimentally that neural networks trained in this framework focus on relations remaining invariant across environments and ignore unstable ones. Moreover, we prove that the recovered stable relations correspond to the true causal mechanisms under certain conditions. In both regression and classification, the resulting models generalize well to unseen scenarios where traditionally trained models fail.

1 INTRODUCTION

Standard supervised learning has shown impressive results when training and test samples follow the same distribution. However, many real world applications do not conform to this setting, so that research successes do not readily translate into practice (Lake et al., 2017). The task of Domain Generalization (DG) addresses this problem: it aims at training models that generalize well under domain shift. In contrast to domain adaption, where a few labeled and/or many unlabeled examples are provided for each target test domain, in DG absolutely no data is available from the test domains’ distributions making the problem unsolvable in general.

In this work, we view the problem of DG specifically using ideas from causal discovery. To make the problem of DG well-posed from this viewpoint, we assume that there exists a certain feature $h^* (X)$ whose relation to the target variable $Y$ is invariant across all environments. Consequently, the conditional probability $p(Y | h^*(X))$ has predictive power in each environment. From a causal perspective, changes between domains or environments can be described as interventions; and causal relationships – unlike purely statistical ones – remain invariant across environments unless explicitly changed under intervention. This is due to the fundamental principle of “Independent Causal Mechanisms” which will be discussed in Section 3. From a causal standpoint, finding robust models is therefore a causal discovery task (Bareinboim & Pearl, 2016; Meinshausen, 2018). Taking a causal perspective on DG, we aim at identifying features which (i) have an invariant relationship to the target variable $Y$ and (ii) are maximally informative about $Y$.

This problem has already been addressed with some simplifying assumptions and a discrete combinatorical search in Magliacane et al. (2018); Rojas-Carulla et al. (2018), but we make weaker assumption and use gradient based optimization. Gradient based optimization is attractive because it combines the well-founded approach of causal discovery with the potential of learning suitable features, instead of merely selecting among predefined ones. Similar definitions of invariant relations as in this work are considered by Arjovsky et al. (2019); Ghassami et al. (2017). A differentiably learnable algorithm that deals with problems (i) and (ii) for a weaker notion of invariant relations has been put forward by Arjovsky et al. (2019).

Problems (i) and (ii) are quite intricate because the search space has combinatorial complexity and comparison of conditional probabilities or testing for conditional independence are notoriously dif-
ficult. Our main contribution to this problem is the following. Firstly, we propose a two-part loss function of the form $L(Y; h(X)) + \lambda I f$, where $I$ is the mutual information and $L f$ enforces the invariance of the relation between $h(X)$ and $Y$ across all environments. This loss operationalizes the ICM principle and $\lambda I f$ determines a trade-off between feature informativeness and invariance. Secondly, we show how this objective can be optimized using normalizing flows, as well as how it simplifies in special cases such as softmax classification and least squares regression. Based on experiments we show that models trained with this loss are able to perform DG. We further discuss relations to causality. We show theoretically as well as experimentally that under certain conditions our method is able to find the direct causes of $Y$.

2 RELATED WORK

Different types of invariances have been considered in the field of DG. One type is defined on the feature level, i.e. features $h(X)$ are invariant across environments if they follow the same distribution in all environments (e.g. [Pan et al., 2010]; [Ganin et al., 2016]; [Ben-David et al., 2007]). However, this form of invariance is problematic since for instance the distribution of the target variable might change between environments. In this case we might expect that the distribution $h(X)$ changes as well. A more plausible and theoretically justified type of invariance is the invariance of relations (Peters et al., 2016; Magliacane et al., 2018; Rojas-Carulla et al., 2018). A relation between a target $Y$ and some features is invariant across environments, if the conditional distribution of $Y$ given the features is the same for all environments. Existing approaches model a conditional distribution for each feature selection and check for the invariance property (Peters et al., 2016; Rojas-Carulla et al., 2018; Magliacane et al., 2018). However, this does not scale well. We provide a theoretical result connecting normalizing flows and invariant relations which in turn allows for gradient-based learning of the problem. In order to exploit our formulation, we also use the Hilbert-Schmidt-Independence Criterion that has been used for robust learning by [Greenfeld & Shalit, 2019] in the one environment setting. [Arjovsky et al., 2019] propose a gradient-based learning framework which exploits a weaker notion of invariance. Their definition is only a necessary condition, but does not guarantee the more causal definition of invariance we treat in this work. The connection between DG, invariances and causality has been pointed out for instance by [Meinshausen, 2018]; [Rojas-Carulla et al., 2018]; [Zhang et al., 2015]. From a causal perspective, DG is a causal discovery task (Meinshausen, 2018). For studies on causal discovery in the purely observational setting see e.g. [Spirtes & Glymour, 1991]; [Pearl, 2009]; [Chickering, 2002]; [Peters & Bühlmann, 2014]; [Hoyer et al., 2009]; [Peters et al., 2014]. The case of different environments has been studied by [Tian & Pearl, 2013]; [Mooij et al., 2016]; [Peters et al., 2016]; [Bareinboim & Pearl, 2016]; [Magliacane et al., 2018]. The importance of invariant relations for causal discovery was emphasized by Peters et al., 2016. Their estimator – Invariant Causal Prediction (ICP) – returns the intersection of all subsets of variables that have an invariant relation w.r.t. $Y$. The output is shown to be the set of the direct causes of $Y$ under suitable conditions. However, their method assumes an underlying linear model and must perform an exhaustive search over all possible variable sets $X_T$, which does not scale. Extensions to time series and non-linear additive noise models were studied in [Heinze-Deml et al., 2018]; [Pfister et al., 2019]. Our treatment of invariance is inspired by these papers and also discusses identifiability results, i.e. conditions when the identified variables are indeed the direct causes. Key differences between ICP and our approach are the following: Firstly, we propose a formulation that allows for a gradient-based learning without strong assumptions on the underlying causal model such as linearity. Second, while ICP tends to exclude features from the parent set when in doubt, our algorithm prefers to err in the direction of best prediction performance in this case.

3 PRELIMINARIES

In the following we introduce the basics of this article as well as the connection between DG and causality. Basics on causality are presented in Appendix A. We first define our notation as follows:

We denote the set of all variables describing the system under study as $X = \{X_1, \ldots, X_D\}$. One of these variables will be singled out as our prediction target, whereas the remaining ones are observed and may serve as predictors. To clarify notation, we call the target variable $Y \equiv X_i$ for some $i \in \{1, \ldots, D\}$, and the remaining observations are $X = X \setminus \{Y\}$. Realizations of a random variable are denoted with lower case letters, e.g. $x_i$. We assume that observations can be obtained in different environments $e \in \mathcal{E}$. Symbols with superscript, e.g. $Y^e$, refer to a specific environment, whereas symbols without refer to data pooled over all environments. We distinguish known environments
e ∈ \mathcal{E}_{\text{seen}}$, where training data are available, from unknown ones \(e \in \mathcal{E}_{\text{unseen}}\), where we wish our models to generalize to. The set of all environments is \(\mathcal{E} = \mathcal{E}_{\text{seen}} \cup \mathcal{E}_{\text{unseen}}\). We assume that all random variables have a density \(p_A\) with probability distribution \(P_A\) (for some variable or set \(A\)). We consider the environment to be a random variable \(E\) and therefore a system variable similar to \(\text{Mooij et al.} [2016]\). This gives an additional view on causal discovery and the DG problem.

Independence and dependence of two variables \(A\) and \(B\) is written as \(A \perp B\) and \(A \not\perp B\) respectively. Two random variables \(A, B\) are conditionally independent given \(C\) if \(p(A, B \mid C) = p(A \mid C)p(B \mid C)\). This is denoted with \(A \perp B \mid C\). Intuitively, it means \(A\) does not contain any information about \(B\) if \(C\) is known (for details see e.g. \text{Peters et al.} [2017]). Similarly, one can define independence and conditional independence for sets of random variables.

### 3.1 Invariance and the Principle of ICM

DG is in general unsolvable because distributions between seen and unseen environments could differ arbitrarily. In order to transfer knowledge from \(\mathcal{E}_{\text{seen}}\) to \(\mathcal{E}_{\text{unseen}}\), we have to make assumptions on how seen and unseen environments relate. These assumptions have a close link to causality.

We assume certain relations between variables remain invariant across all environments. A subset \(X_S \subset X\) of variables elicits an invariant relation or satisfies the invariance property w.r.t. \(Y\) over a subset \(W \subset \mathcal{E}\) of environments if

\[
\forall e, e' \in W: \quad P(Y^e \mid X_S = u) = P(Y^{e'} \mid X_S = u) \tag{1}
\]

for all \(u\) where both conditional distributions are well-defined. Equivalently, we can define the invariance property by \(Y \perp E \mid X_S\) and \(I(Y; E \mid X_S) = 0\) for \(E\) restricted to \(W\). The invariance property for computed features \(h(X)\) is defined analogously by the relation \(Y \perp E \mid h(X)\).

Although we can only test for (equation 1) in \(\mathcal{E}_{\text{seen}}\), taking a causal perspective allows us to derive plausible conditions – expressed by Assumptions 1 and 2 – for an invariance to remain valid in all environments \(\mathcal{E}\). In brief, we assume that environments correspond to interventions in the system and invariance arises from the principle of independent causal mechanisms (Peters et al., 2017 ICM).

At first, consider the joint density \(p_X(\bar{X})\). The chain rule offers a combinatorial number of ways to decompose this distribution into a product of conditionals. Among those, the causal factorization

\[
p_X(x_1, \ldots, x_D) = \prod_{i=1}^{D} p_i(x_i \mid x_{\text{pa}(i)}) \tag{2}
\]

is singled out by conditioning each \(X_i\) onto its causal parents or direct causes \(x_{\text{pa}(i)}\), where \(\text{pa}(i)\) denotes the appropriate index set. The special properties of this factorization are discussed in Peters et al. (2017). The conditionals \(p_i\) of the causal factorization are called causal mechanisms. An intervention onto the system is defined by replacing one or several factors in the decomposition with different (conditional) densities \(\pi\). Here, we distinguish soft-interventions where \(\bar{p}_j(x_j \mid x_{\text{pa}(j)}) \neq p_j(x_j \mid x_{\text{pa}(j)})\) and do-interventions where \(\bar{p}_j(x_j \mid x_{\text{pa}(j)}) = \bar{p}_j(x_j)\) is a density which does not depend on \(x_{\text{pa}(j)}\) (e.g. a hard intervention where \(x_j\) is forced to take a specific value \(\pi\)). The resulting joint distribution for a single intervention is

\[
\bar{p}_X(x_1, \ldots, x_D) = \bar{p}_j(x_j \mid x_{\text{pa}(j)}) \prod_{i=1, i \neq j}^{D} p_i(x_i \mid x_{\text{pa}(i)}) \tag{3}
\]

and extends to multiple simultaneous interventions in the obvious way. The principle of independent causal mechanisms (ICM) states that every mechanism acts independently of the others (Peters et al., 2017). Consequently, an intervention replacing \(p_j\) with \(\bar{p}_j\) has no effect on the other factors \(p_i \neq j\), as indicated by equation 3. This is a crucial property of the causal decomposition – alternative factorizations do not exhibit this behavior. Instead, a coordinated modification of several factors is generally required to model the effect of an intervention in a non-causal decomposition.

We utilize this principle as a tool to train robust models. To do so, we make two additional assumptions, similar to Peters et al. (2016) and Heinze-Deml et al. (2018):

**Assumption 1.** Any differences in the joint distributions \(p_X^e\) from one environment to the other are fully explainable as interventions: replacing factors \(p_i^e(x_i \mid x_{\text{pa}(i)})\) in environment \(e\) with factors \(\bar{p}_i^e(x_i \mid x_{\text{pa}(i)})\) in environment \(e'\) (for some subset of the variables) is the only admissible change.
Assumption 2. The mechanism \( p(y \mid x_{pa(Y)}) \) for the target variable is invariant under changes of environment. In other words, we require conditional independence \( Y \perp E \mid X_{pa(Y)} \).

If we knew the causal decomposition, we could use these assumptions directly to train a robust model for \( Y \) – we would simply regress \( Y \) on its parents \( X_{pa(Y)} \). However, we only require that a causal decomposition with these properties exists, but do not assume that it is known. Instead, our method uses the assumptions indirectly – by simultaneously considering data from different environments – to identify a stable regressor for \( Y \).

We call a regressor stable if it solely relies on predictors whose relationship to \( Y \) remains invariant across environments, i.e. is not influenced by any intervention. By assumption \( \square \) such a regressor always exists. However, predictor variables beyond \( X_{pa(Y)} \) may be used as well, e.g. children of \( Y \) or parents of children, provided their relationships to \( Y \) do not depend on the environment. The case of children is especially interesting: Suppose \( X_j \) is a noisy measurement of \( Y \), described by the causal mechanism \( p_j(X_j \mid Y) \). As long as the measurement device works identically in all environments, including \( X_j \) as a predictor of \( Y \) is desirable, despite it being a child. We illustrate Assumption \( \square \) for prediction in Appendix \( \Box \). In general, prediction accuracy will be maximized when all suitable predictor variables are included into the model. Accordingly, our algorithm will asymptotically identify the full set of stable predictors for \( Y \). In addition, we will prove under which conditions this set contains exactly the parents of \( Y \). Note that there are different ideas on whether most supervised learning tasks conform to this setting (Schölkopf et al., 2012; Arjovsky et al., 2019).

3.2 Normalizing Flows

Normalizing flows are a specific type of neural network architecture which are by construction invertible and have a tractable Jacobian. They are used for density estimation and sampling of a target density (see Papamakarios et al., 2019 for an overview). This in turn allows optimizing information theoretic objectives in a convenient and mathematically sound way.

We denote with \( \mathcal{H} \) the set of feature extractors \( h : \mathbb{R}^D \to \mathbb{R}^m \) where \( m \) is chosen a priori. In this work, we consider 1-dimensional conditional normalizing flows \( T : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R} \). \( T \) is a diffeomorphism in the first dimension and differentiable in all other dimensions. The set of all \( T \) representable by a particular model family is denoted by \( T \). The negative log-likelihood (NLL) for conditional normalizing flows with a standard normal base distribution in latent space is

\[
\mathcal{L}_{\text{NLL}}(T, h) := \mathbb{E}_{h(X), y} \left[ \| T(Y; h(X)) \|^2 / 2 - \log |\nabla_y T(Y; h(X))| \right] + C
\]

where \( C = \dim(Y) \log(\sqrt{2\pi}) \) is a constant.

**Lemma 1.** (proof in Appendix \( \Box \)) If the function space \( \mathcal{T} \) is sufficiently rich, the following relevant properties are guaranteed at the minimum of the NLL: \( h^*, T^* = \arg\min_{h \in \mathcal{H}, T \in \mathcal{T}} \mathcal{L}_{\text{NLL}}(T, h) \)

\[
\begin{align*}
(a) \quad h^* &\text{ maximizes the mutual information: } h^* = \arg\max_{h \in \mathcal{H}} I(h(X); Y) \\
(b) \quad h^* &\text{ is independent of the flow’s latent variable: } T^*(Y; h^*(X)) \perp h^*(X).
\end{align*}
\]

Statement (a) shows that a normalizing flow can identify features which share maximal information with the target variable \( Y \). Due to statement (b), it is possible to draw samples from the conditional distribution \( P(Y \mid h^*(X)) \). Statement (b) holds in an even stronger form: If we keep \( h \) fixed and select the argmin over \( T \) in the NLL, we obtain the same statement as in (b). A more formal and detailed introduction into normalizing flows can be found in Appendix \( \Box \).

4 Method

In order to exploits the principle of ICM for DG, we formulate the DG problem as follows

\[
h^* := \arg\max_{h \in \mathcal{H}} \left\{ \min_{e \in \mathcal{E}} I(Y^e; h(X^e)) \right\} \quad \text{s.t.} \quad Y \perp E \mid h(X)
\]

(4)

As it stands, problem equation[4] is hard to solve, because conditional independence testing is notoriously difficult, especially when conditioning on functions from the potentially infinitely large space \( \mathcal{H} \). We now introduce a reformulation in terms of normalizing flows that is much easier to optimize.
4.1 Learning the Invariance Property

The following theorem establishes a connection between invariant relations, prediction residuals and normalizing flows.

**Theorem 1.** Let \( h \) be a differentiable function and \( Y, X, E \) be random variables. Furthermore, let \( R = T(Y; h(X)) \) be a continuous, differentiable function that is a diffeomorphism in \( Y \). Suppose that \( R \perp E, h(X) \). Then, it holds that \( Y \perp E \mid h(X) \).

**Proof.** The decomposition rule for the assumption \( R \perp E, h(X) \) (1) implies \( R \perp h(X) \) (2). To simplify notation, we define \( Z := h(X) \). Because \( T \) is invertible in \( Y \) and due to the change of variables (c.o.v.) formula, we obtain

\[
p_{Y \mid Z, E}(y \mid z, e) = p_{R \mid Z, E}(T(y, z) \mid z, e) \left| \det \frac{\partial T}{\partial y}(y, z) \right| \overset{(1)}{=} p_R(r) \left| \det \frac{\partial T}{\partial y}(y, z) \right| \overset{(2)}{=} p_{R \mid Z}(r \mid z) \left| \det \frac{\partial T}{\partial y}(y, z) \right| \overset{\text{(c.o.v.)}}{=} p_Y(y \mid z).
\]

This implies \( Y \perp E \mid Z \). \( \square \)

The theorem states in particular that if there exists a suitable diffeomorphism \( T \) such that \( R \perp E, h(X) \), then \( h(X) \) satisfies the invariance property w.r.t. \( Y \). We exploit Theorem 1 in order to learn features \( h \) that meet this requirement. In the following, we denote a conditional normalizing flow parameterized via \( \theta \) with \( T_\theta \). Furthermore, \( h_\phi \) denotes a feature extractor implemented as a neural network parameterized via \( \phi \). We can relax condition \( R \perp h_\phi(X), E \) by means of the Hilbert Schmidt Independence Criterion, a kernel-based independence measure (see Appendix D for details). This loss, denoted as \( \mathcal{L}_I \), penalizes dependence between the distributions of \( R \) and \( h_\phi(X), E \). The HSIC guarantees that

\[
\mathcal{L}_I(P_R, P_{h_\phi(X), E}) = 0 \iff R \perp h_\phi(X), E
\]

where \( R = T_\theta(Y; h_\phi(X)) \) and \( P_R, P_{h_\phi(X), E} \) are the distributions implied by the parameter choices \( \phi \) and \( \theta \). Due to Theorem 1, minimizing of \( \mathcal{L}_I(P_R, P_{h_\phi(X), E}) \) w.r.t. \( \phi \) and \( \theta \) will thus approximate the desired invariance property \( Y \perp E \mid h_\phi(X) \), with exact validity upon perfect convergence.

When \( R \perp h_\phi(X), E \) is fulfilled, the decomposition rule implies \( R \perp E \) as well. However, if the differences between environments are small, empirical convergence is accelerated by adding a Wasserstein loss which explicitly enforces the latter, see Appendix D and section 5.2 for details.

4.2 Exploiting Invariances for Prediction

Equation 4 can be re-formulated as a differentiable loss using a Lagrange multiplier \( \lambda_I \) on the HSIC loss. \( \lambda_I \) acts as a hyperparameter to adjust the trade-off between the invariance property of \( h_\phi(X) \) w.r.t. \( Y \) and the mutual information between \( h_\phi(X) \) and \( Y \). See Appendix E for algorithm details.

**Normalizing Flows** Using Lemma 1(a), we maximize \( \min_{e \in E} I(Y^e; h_\phi(X^e)) \) by minimizing \( \max_{e \in E} \{ \mathcal{L}_{\text{NLL}}(T_\theta, h_\phi) \} \) w.r.t. \( \phi, \theta \). To achieve the described trade-off between goodness-of-fit and invariance, we therefore optimize

\[
\arg \min_{\phi, \theta} \left( \max_{e \in E} \{ \mathcal{L}_{\text{NLL}}(T_\theta, h_\phi) \} + \lambda_I \mathcal{L}_I(P_R, P_{h_\phi(X), E}) \right)
\]

where \( R^e = T_\theta(Y^e, h_\phi(X^e)) \) and \( \lambda_I > 0 \). The first term maximizes the mutual information between \( h_\phi(X) \) and \( Y \) in the environment where the features are least informative about \( Y \) and the last term aims to achieve an invariant relation.

**Additive Noise** Let \( f_\theta \) be a regression function. Solving for the noise term gives \( R = Y - f_\theta(X) \) which corresponds to a diffeomorphism in \( Y \), namely \( T_\theta(Y; X) = Y - f_\theta(X) \). If we make two simplified assumptions: (i) the noise is gaussian with zero mean and (ii) \( R \perp f_\theta(X) \), then we obtain

\[
I(Y; f_\theta(X)) = H(Y) - H(R \mid f_\theta(X)) = H(Y) - H(R \mid f_\theta(X)) \overset{(ii)}{=} H(Y) - H(R) \overset{(i)}{=} H(Y) - 1/2 \log(2\pi e \sigma^2)
\]
where \( \sigma^2 = \mathbb{E}[(Y - f_\theta(X))^2] \). In this case maximizing the mutual information \( I(Y; f_\theta(X)) \) amounts to minimizing \( \mathbb{E}[(Y - f_\theta(X))^2] \) w.r.t. \( \theta \), i.e. the standard L2-loss. From this, we obtain a simplified version of equation \( \text{4} \) via

\[
\arg\min_\theta \left( \max_{c \in \mathbb{L}_{\text{seen}}} \left\{ \mathbb{E}[(Y^c - f_\theta(X^c))^2] \right\} + \lambda_1 \mathcal{L}_1(P_R; P_{f_\theta(X), E}) \right)
\]

(6)

where \( R^c = Y - f_\theta(X^c) \) and \( \lambda_1 > 0 \). Under the conditions stated above, the objective achieves the mentioned trade-off between information and invariance.

Alternatively we can view the problem as to find features \( h_\phi : \mathbb{R}^D \to \mathbb{R}^m \) such that \( I(h_\phi(X), Y) \) gets maximized under the assumption that there exists a model \( f_\theta(h_\phi(X)) + R = Y \) where \( R \) is independent of \( h(X) \) and \( R \) is gaussian. In this case we obtain similarly as above the learning objective

\[
\arg\min_{\theta, \phi} \left( \max_{c \in \mathbb{L}_{\text{seen}}} \left\{ \mathbb{E}[(Y^c - f_\theta(h_\phi(X^c)))^2] \right\} + \lambda_1 \mathcal{L}_1(P_R; P_{h_\phi(X), E}) \right)
\]

(7)

\section*{Classification}

The expected cross-entropy loss is given through

\[
-\mathbb{E}_{X,Y} \left[ f(X)_Y - \log \left( \sum_c \exp(f(X)_c) \right) \right]
\]

where \( f : \mathcal{X} \to \mathbb{R}^m \) returns the logits. Minimizing the expected cross-entropy loss amounts to maximizing the mutual information between \( f(X) \) and \( Y \) (Qin & Kim, 2019; Barber & Agakov, 2003, eq. 3). Let \( T(Y; f(X)) = Y \cdot \text{softmax}(f(X)) \) with component-wise multiplication, then \( T \) is invertible in \( Y \) conditioned on the softmax output. Now we can apply the same invariance loss as above in order to obtain a solution to equation \( \text{4} \).

\subsection{Relation to Causal Discovery}

Under certain conditions, solving equation \( \text{4} \) leads to features which correspond to the direct causes of \( Y \) (identifiability). In this case, we obtain the causal mechanism by computing the conditional distribution of \( Y \) given the direct causes. Therefore equation \( \text{4} \) can also be seen as approximation of the causal mechanism when the identifiability conditions are met. The following Proposition states under which assumptions the direct causes of \( Y \) can be recovered by exploiting Theorem \( \text{1} \).

\begin{proposition}
Assume that the underlying causal graph \( G \) is faithful with respect to \( P_{X,E} \). We further assume that every child of \( Y \) in \( G \) is also a child of \( E \) in \( G \). A variable selection \( h(X) = X_T \) corresponds to the direct causes if the following conditions are met: (i) \( T(Y; X) \perp\!
\!
\!
\perp E, h(X) \) is satisfied for a diffeomorphism \( T(\cdot; h(X)) \), (ii) \( h(X) \) is maximally informative about \( Y \) and (iii) \( h(X) \) contains only variables from the Markov blanket of \( Y \).
\end{proposition}

The Markov blanket of \( Y \) is the only set of vertices which are necessary to predict \( Y \) (see Appendix \( \text{A} \)). We give a proof of Proposition \( \text{1} \) as well as a discussion in Appendix \( \text{E} \).

For reasons of explainability and for the task of causal discovery, we employ a gating function \( h_a \) in order to obtain a variable selection. We use the same gating function as in Kalainathan et al. (2018). The gating function \( h_a \) represents a \( 0 \)-1 mask of the input. A complexity loss \( \mathcal{L}(\phi) \) represents how many variables are selected and therefore penalizes to include variables. Intuitively speaking, if we search for a variable selection that conforms to the conditions in Proposition \( \text{1} \) the complexity loss would exclude all non-task relevant variables. Therefore, if \( \mathcal{H} \) is the set of gating functions, then \( h^* \) in equation \( \text{4} \) would correspond to the direct causes of \( Y \) under the conditions listed in Proposition \( \text{1} \).

The complexity loss as well as the gating function can be optimized by gradient descent.

\section{Experiments}

\subsection{Synthetic Causal Graphs}

To evaluate our methods for the regression case, we follow the experimental design of Heinze-Deml et al. (2018). It rests on the causal graph in Figure \( \text{1} \). Each variable \( X_1, \ldots, X_6 \) is chosen as the regression target \( Y \) in turn, so that a rich variety of local configurations around \( Y \) is tested. The corresponding structural equations are selected among four model types of the form \( f(X_{pa(i)}, N_i) = \sum_{j \in pa(i)} \text{mech}(a_j X_j) + N_i \), where ‘mech’ is either the identity (hence we get a linear SCM), Tanhshrink, Softplus or ReLU, and one multiplicative noise mechanism of the form
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To demonstrate that our method is able to perform DG in the classification case, we use the colored
more robust in this respect. A detailed analysis of our experiments can be found in Appendix G.

to identify the invariant mechanism or the unseen environment requires extrapolation beyond the training data boundaries. Models without gating (Flow, ANM) seem to be slightly
poor detection of the direct causes. ICP wins for linear SCMs, but otherwise has largest errors, since
it cannot accurately account for non-linear mechanisms. ERM gives reasonable test errors (it even
provides the expected behavior: it clearly outperforms the baselines, with a slight edge for ANMG, as long as its assumption of additive noise is fulfilled.

Figure 1 and Table 1 report regression errors for seen and unseen environments, with CERM indicating the theoretical lower bound. The PC algorithm is excluded from this experiment due to its poor detection of the direct causes. ICP wins for linear SCMs, but otherwise has largest errors, since it cannot accurately account for non-linear mechanisms. ERM gives reasonable test errors (it even
overfits the training data), but generalizes poorly to unseen environments, as expected. Our models perform quite similarly to CERM. We again find a slight edge for ANMG, except under multiplicative noise, where ANMG’s additive noise assumption is violated and Flow is superior. All methods (including CERM) occasionally fail in the domain generalization task, indicating that some DG problems are more difficult than others, e.g. when the differences between seen environments are too small to reliably identify the invariant mechanism or the unseen environment requires extrapolation beyond the training data boundaries. Models without gating (Flow, ANM) seem to be slightly
more robust in this respect. A detailed analysis of our experiments can be found in Appendix G.

5.2 Colored MNIST

To demonstrate that our method is able to perform DG in the classification case, we use the colored
variant of the MNIST-dataset established by Arjovsky et al. (2019). The response is reduced to two
labels – 0 for all images with digit \{0, \ldots, 4\} and 1 for digits \{5, \ldots, 9\} – with deliberate label noise that limits the achievable shape-based classification accuracy to 75%. To confuse the classifier, digits are additionally colored such that colors are spuriously associated with the true labels at accuracies of 90% resp. 80% in the first two environments, whereas the association is only 10% correct in the third environment. A classifier naively trained on the first two environments will identify color as the best predictor, but will perform terribly when tested on the third environment. In contrast, a robust model will ignore the unstable relation between colors and labels and use the invariant relation, namely the one between digit shapes and labels, for prediction. We supplement the HSIC loss with a Wasserstein term to explicitly enforce $R \perp E$, i.e. $\mathcal{L}_I = \text{HSIC} + \text{L2(sort}(R^1), \text{sort}(R^2))$ (see Appendix D). This gives a better training signal as the HSIC alone, as the difference in label-color association between environments 1 and 2 (90% vs. 80%) is deliberately chosen very small to make the task hard to learn. Experimental details can be found in Appendix [I]. Figure [I] shows the results for our model: Naive training ($\lambda_1 = 0$, i.e. invariance of residuals is not enforced) gives accuracies corresponding to the association between colors and labels and thus completely fails in test environment 3. In contrast, our model performs at the best possible rate for invariant classifiers in environments 1 and 2 and still achieves 67% in environment 3. Figure [I] demonstrates the trade-off between goodness of fit in the training environments 1 and 2 and the robustness of the resulting classifier: the model’s ability to perform DG to the unseen environment 3 improves as $\lambda_I$ increases. If $\lambda_I$ is too large, it dominates the classification training signal and performance breaks down in all environments. However, the choice of $\lambda_I$ is not critical, as good results are obtained over a wide range of settings.
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APPENDIX

A  CAUSALITY: BASICS

A causal factorization as in equation [3] allows to model causal relations. With Structural Causal Models (SCM), we are able to express causal relations on a functional level. Following Peters et al. (2017) we define a SCM in the following way:

**Definition 1.** A Structural Causal Model (SCM) is a collection of a set of variables denoted as $\mathcal{X}$ which corresponds to vertices in a graph and the structural assignments are denoted as $\mathcal{A}$. An SCM defined as above produces an acyclic graph $G$ and induces a probability distribution over $P_x$.

The random variables in an SCM correspond to vertices in a graph and the structural assignments $\mathcal{S}$ define the edges of this graph. Two sets of vertices $\mathcal{A}, \mathcal{B}$ are said to be d-separated if there exists a set of vertices $\mathcal{C}$ such that every path between $\mathcal{A}$ and $\mathcal{B}$ is blocked. For details see e.g. Peters et al. (2017). The subscript $\perp_d$ denotes d-separability which in this case is denoted by $\mathcal{A} \perp_d \mathcal{B}$. An SCM generates a probability distribution $P_x$ which satisfies the Causal Markov Condition, that is $\mathcal{A} \perp_d \mathcal{B} | \mathcal{C}$ for all $\mathcal{A}, \mathcal{B}, \mathcal{C} \subseteq \mathcal{X}$. The Causal Markov Condition can be seen as an inherent property of a causal system which leaves marks in the data distribution.

A distribution $P_x$ is said to be faithful to the graph $G$ if $\mathcal{A} \perp \mathcal{B} | \mathcal{C}$ results in $\mathcal{A} \perp_d \mathcal{B} | \mathcal{C}$ for all $\mathcal{A}, \mathcal{B}, \mathcal{C} \subseteq \mathcal{X}$. This means from the distribution $P_x$ statements about the underlying graph $G$ can be made.

Assuming both, faithfulness and the Causal Markov condition, we obtain that the d-separation statements in $G$ are equivalent to the conditional independence statements in $P_x$. These two assumptions allow for a whole class of causal discovery algorithms like the PC- or IC-algorithm (Spirtes & Glymour, 1991; Pearl, 2009).

The smallest set $\mathcal{M}$ such that $Y \perp_d \mathcal{X} \setminus \{\mathcal{Y} \cup \mathcal{M}\}$ is called Markov Blanket. It is given by $\mathcal{M} = \mathcal{X}_{pa(Y)} \cup \mathcal{X}_{ch(Y)} \cup \mathcal{X}_{pa(ch(Y))} \setminus \{Y\}$. The Markov Blanket of $Y$ is the only set of vertices which are necessary to predict $Y$.

B  ILLUSTRATION OF ASSUMPTIONS

To illustrate the impact of causality on robustness, consider the following example: Suppose we would like to estimate the gas consumption of a car. In a sufficiently narrow setting, the total amount of money spent on gas might be a simple and accurate predictor. However, gas prices vary dramatically between countries and over time, so statistical models relying on it will not be robust, even if they fit the training data very well. Gas costs are an effect of gas consumption, and this relationship is unstable due to external influences. In contrast, predictions on the basis of the causes of gas consumption (e.g. car model, local speed limits and geography, owner’s driving habits) tend to be much more robust, because these causal relations are intrinsic to the system and not subjected to external influences. Note that there is a trade-off here: Including gas costs in the model will improve estimation accuracy when gas prices remain sufficiently stable, but will impair results otherwise. By considering the same phenomenon in several environments simultaneously, we hope to gain enough information to adjust this trade-off properly.

In the gas example, countries can be considered as environments that “intervene” on the relation between consumed gas and money spent, e.g. by applying different tax policies. In contrast, interventions changing the impact of motor properties or geography on gas consumption are much less plausible – powerful motors and steep roads will always lead to higher consumption. From a causal standpoint, finding robust models is therefore a causal discovery task (Meinshausen, 2018).
\textbf{C \ NORMALIZING FLOWS}

Normalizing flows are a specific type of neural network architecture which are by construction invertible and have a tractable Jacobian. They are used for density estimation and sampling of a target density (for an overview see Papamakarios et al. (2019)). This in turn allows optimizing information theoretic objectives in a convenient and mathematically sound way.

Similarly as in the paper, we denote with $H$ the set of feature extractors $h : \mathbb{R}^D \to \mathbb{R}^m$ where $m$ is chosen a priori. The set of all one-dimensional (conditional) normalizing flows is denoted by $\mathcal{T}$.

Together with a reference distribution $p_{\text{ref}}, T$ defines a new distribution $p_{\nu_T} = (T(\cdot ; h(x)))_{\ref}^{-1} p_{\text{ref}}$ which is called the push-forward of the reference distribution $p_{\text{ref}}$ (Marzouk et al. 2016). By drawing samples from $p_{\text{ref}}$ and applying $T$ on these samples we obtain samples from this new distribution. The density of this so-obtained distribution $p_{\nu_T}$ can be derived from the change of variables formula:

\[
p_{\nu_T}(y \mid h(x)) = p_{\text{ref}}(T(y; h(x)))|\nabla_y T(y; h(x))|.
\] (9)

The KL-divergence between the target distribution $p_Y|h(X)$ and the flow-based model $p_{\nu_T}$ can be written as follows:

\[
E_{h(X)}[D_{\text{KL}}(p_Y|h(X) \parallel p_{\nu_T})] = E_{h(X)} \left[ E_{Y|h(X)} \left[ \log \frac{p_Y|h(X)}{p_{\nu_T}} \right] \right]
\]

\[
= -H(Y \mid h(X)) - E_{h(X),Y}[\log p_{\nu_T}(Y \mid h(X))]
\]

\[
= -H(Y | h(X)) + E_{h(X),Y}[- \log p_{\nu_T}(T(y; h(x)) - \log |\nabla_y T(y; h(x))|]
\] (10)

The last two terms in equation (10) correspond to the negative log-likelihood (NLL) for conditional flows with distribution $p_{\text{ref}}$ in latent space. The NLL in Section 3 is given in case we assume the reference distribution is the standard normal distribution.

We restate Lemma 1 with a more general notation:

\textbf{Lemma 1}. Let $X, Y$ be random variables. We furthermore assume that for each $h \in H$ there exists one $T \in T$ with $H_{h(X)}[D_{\text{KL}}(p_Y|h(X) \parallel p_{\nu_T})] = 0$. Then, the following two statements are true

(a) Let

\[
h^{*}, T^{*} = \arg \min_{h \in H, T \in T} \left[ -H(h(X),Y) \right]
\]

then it holds $h^{*} = \arg \max_{h \in H} I(h(X); Y)$

(b) Let

\[
T^{*} = \arg \min_{T \in T} \left[ E_{h(X)}[D_{\text{KL}}(p_Y|h(X) \parallel p_{\nu_T})] \right]
\]

then it holds $T^{*}(Y; h(X)) \perp h(X)$

\textbf{Proof}. (a) From equation equation (10) we obtain $-E_{h(X),Y}|\log p_{\nu_T}(Y \mid h(X))| \geq H(Y \mid h(X))$ for all $h \in H, T \in T$. We furthermore have $\min_{T \in T} -E_{h(X),Y}|\log p_{\nu_T}(Y \mid h(X))| = H(Y \mid h(X))$ due to our assumptions on $T$. Therefore, $\min_{h \in H} H(Y \mid h(X)) = \min_{h \in H} H(Y \mid h(X))$. Since we have $I(Y; h(X)) = H(Y) - H(Y \mid h(X))$ and only the second term depends on $h$, statement (a) holds true.

(b) For convenience, we denote $T(Y; h(X)) = R$ and $h(X) = Z$. We have $E_Z[D_{\text{KL}}(p_Y|Z \parallel p_{\nu_T})] = 0$ and therefore $p_{Y|Z}(y \mid z) = p_{\text{ref}}(T(y; z))|\nabla_y T^{-1}(y; z)|$.

Then it holds

\[
p_{R|Z}(r \mid z) = p_{Y|Z}(T^{-1}(r; z) | z) \cdot |\nabla_y T^{-1}(r; z)|
\]

\[
= p_{\text{ref}}(T(T^{-1}(r; z); z)) \cdot |\nabla_y T(y; z)| \cdot |\nabla_y T^{-1}(r; z)|
\]

\[
= p_{\text{ref}}(r) \cdot 1
\]

Since the density $p_{\text{ref}}$ is independent of $Z$, we obtain $R \perp Z$ which concludes the proof of (b) \qed
Statement (a) describes an optimization problem that allows to find features which share maximal information with the target variable $Y$. Due to statement (b) it is possible to draw samples from the conditional distribution $P(Y \mid h(X))$ via the reference distribution.

### D HSIC AND WASSERSTEIN

The Hilbert-Schmidt Independence Criterion (HSIC) is a kernel based measure for independence which is in expectation 0 if and only if the compared random variables are independent \cite{Gretton2005}. An empirical estimate of $\text{HSIC}(A, B)$ for two random variables $A, B$ is given by

$$\text{HSIC}((\{a_j\}_{j=1}^n, \{b_j\}_{j=1}^n) = \frac{1}{(n-1)^2} \text{tr}(KHK')$$

(11)

where tr is the trace operator. $K_{ij} = k(a_i, a_j)$ and $K'_{ij} = k'(b_i, b_j)$ are kernel matrices for given kernels $k$ and $k'$. The matrix $H$ is a centering matrix $H_{i,j} = \delta_{i,j} - 1/n$.

The one dimensional Wasserstein loss compares the similarity of two distributions \cite{Kolouri2018}. This loss has expectation 0 if both distributions are equal. An empirical estimate of the one dimensional Wasserstein loss for two random variables $A, B$ is given by

$$\mathcal{L}_W = \|\text{sort}(\{a_j\}_{j=1}^n) - \text{sort}(\{b_j\}_{j=1}^n)\|_2$$

Here, the two batches are sorted in ascending order and then compared in the L2-Norm. We assume that both batches have the same size.

### E ALGORITHM

In order to optimize the DG problem in equation 4 we optimize a normalizing flow $T_\theta$ and a feed forward neural network $h_\phi$ as described in Algorithm 1. There is an inherent trade-off between robustness and goodness-of-fit. The hyperparameter $\lambda_I$ describes this trade-off and is chosen a priori.

**Data:** Samples from $P_{X^e, Y^e}$ in different environments $e \in \mathcal{E}_{\text{seen}}$.

**Initialize** $\theta, \phi$.

**for number of training iterations do**

**for** $e \in \mathcal{E}_{\text{seen}}$ **do**

Sample minibatch $\{(y^e_1, x^e_1), \ldots, (y^e_m, x^e_m)\}$ from $P_{Y^e \mid X^e = e}$ for $e \in \mathcal{E}_{\text{seen}}$.

Compute: $r^e_j = T_\theta(y^e_j; h_\phi(x^e_j))$;

**end**

Update $\theta, \phi$ by descending alongside the stochastic gradient

$$\nabla_{\theta, \phi} \left( \max_{e \in \mathcal{E}_{\text{seen}}} \left\{ \sum_{i=1}^m \frac{1}{2} \| T_\theta(y^e_i; h_\phi(x^e_i)) \|^2 - \log \nabla_y T_\theta(y^e_i; h_\phi(x^e_i)) \right\} \right)$$

$$+ \lambda_I \mathcal{L}_I(\{r^e_j \}_{j,e}, \{h_\phi(x^e_j), e \}_{j,e})$$

**end**

**Result:** In case of convergence, we obtain $T_{\theta^*}, h_{\phi^*}$ with

$$\theta^*, \phi^* = \arg \min_{\theta, \phi} \left\{ \max_{e \in \mathcal{E}_{\text{seen}}} \left\{ \frac{1}{2} \| T_\theta(Y^e \mid X^e; h_\phi(X^e)) \|^2 - \log \nabla_y T_\theta(Y^e \mid X^e; h_\phi(X^e)) \right\} \right\}$$

$$+ \lambda_I \mathcal{L}_I(P_R, P_{h_\phi(X^e)})$$

**Algorithm 1:** DG training with normalizing flows

If we choose a gating mechanisms $h_\phi$ as feature extractor similar to \cite{Kalainathan2018}, then a complexity loss is added to the loss in the gradient update step.
In case we assume that the underlying mechanisms elaborates the noise in an additive manner, we could replace the normalizing flow $T_\theta$ with a feed forward neural network $f_\theta$ and execute Algorithm 2.

**Data:** Samples from $P_{X^e, Y^e}$ in different environments $e \in \mathcal{E}_{\text{seen}}$.

**Initialize:** $\theta$;

**for number of training iterations do**

**for $e \in \mathcal{E}_{\text{seen}}$ do**

- Sample minibatch $\{(y^e_{j1}, x^e_{j1}), \ldots, (y^e_{jm}, x^e_{jm})\}$ from $P_{Y|X|E=e}$ for $e \in \mathcal{E}_{\text{seen}}$;
- Compute: $r^e_j = y^e_j - f_\theta(x^e_j)$;

**end**

Update $\theta$ by descending alongside the stochastic gradient

$$\nabla_\theta \left( \max_{e \in \mathcal{E}_{\text{seen}}} \left\{ \sum_{i=1}^m |r^e_j|^2 \right\} + \lambda_I L_I(\{r^e_j\}_{j,e}, \{f_\theta(x^e_j), e\}_{j,e}) \right)$$

**end**

**Result:** In case of convergence, we obtain $f_{\theta^*}$ with

$$\theta^* = \arg\min_\theta \left( \max_{e \in \mathcal{E}_{\text{seen}}} \left\{ E_{X^e, Y^e} \left[ |Y^e - f_\theta(X^e)|^2 \right] \right\} + \lambda_I L_I(P_R, P_{f_\theta(X^e), E}) \right)$$

**Algorithm 2:** DG training under the assumption of additive noise

If we choose a gating mechanism, minor adjustments have to be made to Algorithm 2 such that we optimize. The classification case can be obtained similarly as described in.

### F Identifiability Result

Under certain conditions on the environment and the underlying causal graph, the direct causes of $Y$ become identifiable:

**Proposition 1.** We assume that the underlying causal graph $G$ is faithful with respect to $P_{X^e, E}$. We further assume that every child of $Y$ in $G$ is also a child of $E$ in $G$. A variable selection $h(X) = X_T$ corresponds to the direct causes if the following conditions are met: (i) $T(Y; h(X)) \perp\!\!\!\perp E$, $h(X)$ are satisfied for a diffeomorphism $T(\cdot; h(X))$, (ii) $h(X)$ is maximally informative about $Y$ and (iii) $h(X)$ contains only variables from the Markov blanket of $Y$.

**Proof.** Let $S(\mathcal{E}_{\text{seen}})$ denote a subset of $X$ which corresponds to the variable selection due to $h$. Without loss of generality, we assume $S(\mathcal{E}_{\text{seen}}) \subset M$ where $M$ is the Markov Blanket. This assumption is reasonable since we have $Y \perp X \setminus M \mid M$ in the asymptotic limit.

Since $pa(Y)$ cannot contain colliders between $Y$ and $E$, we obtain that $Y \perp E \mid S(\mathcal{E}_{\text{seen}})$ implies $Y \perp E \mid (S(\mathcal{E}_{\text{seen}}) \cup pa(Y))$. This means using $pa(Y)$ as predictors does not harm the constraint in the optimization problem. Due to faithfulness and since the parents of $Y$ are directly connected to $Y$, we obtain that $pa(Y) \subset S(\mathcal{E}_{\text{seen}})$.

For each subset $X_T \subset X$ for which there exists an $X_i \in X_T \cap X_{ch(Y)}$, we have $X_T \not\perp\!\!\!\perp Y \mid E$. This follows from the fact that $X_i$ is a collider, in particular $E \rightarrow X_i \leftarrow Y$. Conditioning on $X_i$ leads to the result that $Y$ and $E$ are not $d$-separated anymore. Hence, we obtain $Y \not\perp\!\!\!\perp X_T \mid E$ due to the faithfulness assumption. Hence, for each $X_T$ with $Y \perp E \mid X_T$ we have $X_T \cap X_{ch(Y)} = \emptyset$ and therefore $X_{ch(Y)} \cap S(\mathcal{E}_{\text{seen}}) = \emptyset$.

Since $X_{pa(Y)} \subset S(\mathcal{E}_{\text{seen}})$, we obtain that $Y \perp X_{pa(ch(Y))} \mid X_{pa(Y)}$ and therefore the parents of $ch(Y)$ are not in $S(\mathcal{E}_{\text{seen}})$ except when they are parents of $Y$.

Therefore, we obtain that $S(\mathcal{E}_{\text{seen}}) = X_{pa(Y)}$.

One might argue that the conditions are very strict in order to obtain the true direct causes. But the conditions set in Proposition 1 are necessary if we do not impose additional constraints on the
true underlying causal mechanisms, e.g. linearity as done by Peters et al. (2016). For instance if $E \rightarrow X_1 \rightarrow Y \rightarrow X_2$, a model including $X_1$ and $X_2$ as predictor might be a better predictor than the one using only $X_1$. From the Causal Markov Condition we obtain $E \perp Y \mid X_1, X_2$ which results in $X_1, X_2 \in S(c_{\text{scen}})$. Under certain conditions however, the relation $Y \rightarrow X_2$ might be invariant across $E$. This is for instance the case when $X_2$ is a measurement of $Y$. In this cases it might be useful to use $X_2$ for a good prediction.

### G Experimental Setting for Synthetic Dataset

#### G.1 Data Generation

In Section 4 we described how we choose different Structural Causal Models (SCM). In the following we describe details of this process.

We simulate the datasets in a way that the conditions in Proposition 1 are met. We choose different variables in the graph shown in Figure 1 as target variable. Hence, we consider different “topological” scenarios. We assume the data is generated by some underlying SCM. We define the structural assignments in the SCM as follows

(a) $f_i^{(1)}(X_{pa(i)}, N_i) = \sum_{j \in \text{pa}(i)} a_j X_j + N_i$ [Linear]

(b) $f_i^{(2)}(X_{pa(i)}, N_i) = \sum_{j \in \text{pa}(i)} a_j X_j - \tanh(a_j X_j) + N_i$ [Tanhshrink]

(c) $f_i^{(3)}(X_{pa(i)}, N_i) = \sum_{j \in \text{pa}(i)} \log(1 + \exp(a_j X_j)) + N_i$ [Softplus]

(d) $f_i^{(4)}(X_{pa(i)}, N_i) = \sum_{j \in \text{pa}(i)} \max\{0, a_j X_j\} + N_i$ [ReLU]

(e) $f_i^{(5)}(X_{pa(i)}, N_i) = \left( \sum_{j \in \text{pa}(i)} a_j X_j \right) \cdot (1 + (1/4)N_i) + N_i$ [Mult. Noise]

with $N_i \sim \mathcal{N}(0, c_i^2)$ where $c_i \sim \mathcal{U}(0.8, 1.2)$, $i \in \{0, \ldots, 5\}$ and $a_i \in \{-1, 1\}$ according to Figure 6. Note that the mechanisms in (b), (c) and (d) are non-linear with additive noise and (e) elaborates the noise in a non-linear manner.

We consider do- and soft-interventions on the assignments $f_i$. We either intervene on all variables except the target variable at once or on all parents and children of the target variable (Intervention Location). We consider three types of interventions:

- **Do-Intervention** on $X_i$: Force $X_i \sim e_1 + e_2 \mathcal{N}(0, 1)$ where we sample for each environment $e_2 \sim \mathcal{U}([1.5, 2.5])$ and $e_1 \sim \mathcal{U}([-1.5, -0.5])$.

- **Soft-Intervention I** on $X_i$: Add $e_1 + e_2 \mathcal{N}(0, 1)$ to $X_i$ where we sample for each environment $e_2 \sim \mathcal{U}([1.5, 2.5])$ and $e_1 \sim \mathcal{U}([-0.5, 0.5])$.

- **Soft-Intervention II** on $X_i$: Set the noise distribution $N_i$ to $\mathcal{N}(0, 2^2)$ for $E = 3$.

Per run, we consider one environment without intervention ($E = 1$) and two environments with either both soft- or do-interventions ($E = 2, 3$). We also create a fourth environment to measure a models’ ability for out-of-distribution generalization:

- **Do-Intervention**: Force $X_i \sim e + \mathcal{N}(0, 4^2)$ where $e = e_1 \pm 1$ with $e_1$ from environment $E = 1$. The sign $\{\pm\}$ is chosen once for each $i$ with equal probability.

- **Soft-Intervention I**: Add $e + \mathcal{N}(0, 4^2)$ to $X_i$ where $e = e_1 \pm 1$ with $e_1$ from environment $E = 1$. The sign $\{\pm\}$ is chosen once for each $i$ with equal probability as for the do-intervention case.
We randomly sample causal graphs as described above. Per environment, we consider the conditional data found in Papamakarios et al. (2019). For each layer of the flow, a conditioner network $C$ maps developed by us. An overview of different architectures for one-dimensional normalizing flows can be found in Papamakarios et al. (2019).

More-Than-Affine-Flow (MTA-Flow)

We use as one-dimension normalizing flow the $T$-izing flow we use $\lambda$ to decay the learning rate every 400 epochs by 0.5. For each model we use $\lambda_i = 1$ and the HSIC $\mathcal{L}_I$ employs a Gaussian kernel with $\sigma = 1$. The gating architecture was trained without the complexity loss for 200 epochs and then with complexity loss weighted by 5. For the Flow model without gating architecture we use a feed forward neural network $h_\phi$ with two internal layers of size 256 mapping to an one dimensional vector. In total, we evaluated our models on 1365 created datasets as described in [G.1]

Once the normalizing flow $T$ is learned, we predict $y$ given features $h(x)$ using 512 normally distributed samples $u_i$ which are mapped to samples from $p(y|h(x))$ by the trained normalizing flow $T(u_i, h(x))$. As prediction we use the mean of these samples.

G.2 Training Details

All used feed forward neural networks have two internal layers of size 256. For the normalizing flows we use a 2 layer MTA-Flow described in Appendix [G.3] with $K=32$. As optimizer we use Adam with a learning rate of $10^{-3}$ and a L2-Regularizer weighted by $10^{-3}$ for all models. Each model is trained with a batch size of 256. We train each model for 1000 epochs and decay the learning rate every 400 epochs by 0.5.

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G.3 One-Dimensional Normalizing Flow

We use as one-dimension normalizing flow the More-Than-Affine-Flow (MTA-Flow), which was developed by us. An overview of different architectures for one-dimensional normalizing flows can be found in Papamakarios et al. (2019). For each layer of the flow, a conditioner network $C$ maps the conditional data $h(X)$ to a set of parameters $a, b \in \mathbb{R}$ and $w, v, r \in \mathbb{R}^K$ for a chosen $K \in \mathbb{N}$. It builds the transformer $\tau$ for each layer as

$$ z = \tau(y \mid h(X)) := a \left( y + \frac{1}{N(w, v)} \sum_{i=1}^{K} w_i f(v_i y + r_i) \right) + b, \quad (12) $$

where $f$ is any almost everywhere smooth function with a derivative bounded by 1. In this work we used a gaussian function with normalized derivative for $f$. The division by

$$ N(w, v) := \varepsilon^{-1} \left( \sum_{i=1}^{K} |w_i v_i| + \delta \right), \quad (13) $$

with numeric stabilizers $\varepsilon < 1$ and $\delta > 0$, assures the strict monotonicity of $\tau$ and thus its invertibility $\forall x \in \mathbb{R}$. We also used a slightly different version of the MTA-Flow which uses the ELU activation function and – because of its monotonicity – can use a relaxed normalizing expression $N(w, v)$.

G.4 PC-VARIANT

Since we are interested in the direct causes of $Y$, the widely applied PC-Algorithm gives not the complete answer to the query for the parents of $Y$. This is due to the fact that it is not able to orient all edges. To compare the PC-Algorithm we include the environment as system-intern variable and use a conservative assignment scheme where non-oriented edges are thrown away. This assignment scheme corresponds to the conservative nature of the ICP.

For further interest going beyond this work, we consider diverse variants of the PC-Algorithm. We consider two orientation schemes: A conservative one, where non-oriented edges are thrown away
and a non-conservative one where non-oriented edges from a node $X_i$ to $Y$ are considered parents of $Y$.

We furthermore consider three scenarios: (1) the samples across all environments are pooled, (2) only the observational data (from the first environment) is given, and (3) the environment variable is considered as system-intern variable and is seen by the PC-Algorithm (similar as in Mooij et al. (2016)). Results are shown in Figure 7. In order to obtain these results, we sampled 1500 graphs as described above and applied on each of these datasets a PC-Variant. Best accuracies are achieved if we consider the environment variable as system-intern variable and use the non-conservative orientation scheme (EnvIn).

G.5 VARIABLE SELECTION

We consider the task of finding the direct causes of a target variable $Y$. Our models based on the gating mechanism perform a variable selection and are therefore compared to the PC-Algorithm and ICP. In the following we show the accuracies of this variable selection according to different scenarios.

Figure 8 shows the accuracies of ICP, the PC-Algorithm and our models pooled over all scenarios. Our models perform comparably well and better than the baseline in the causal discovery task.

In the following we show results due to different mechanisms, target variables, intervention types and intervention locations.

Figure 9b shows the accuracies of all models across different target variables. Parentless target variables, i.e. $Y = X_4$ or $Y = X_0$ are easy to solve for ICP due to its conservative nature. All our models solve the parentless case quite well. Performance of the PC-variant depends strongly on the position of the target variable in the SCM indicating that its conservative assignment scheme has a strong influence on its performance. As expected, the PC-variant deals well with with $Y = X_6$ which is a childless collider. The causal discovery task seems to be particularly hard for variable $Y = X_6$ for all other models. This is the variable which has the most parents.

The type of intervention and its location seem to play a minor role as shown in Figure 9a and Figure 9d.

Figure 9b shows that ICP performs well if the underlying causal model is linear, but degrades if the mechanism become non-linear. The PC-Algorithm performs under all mechanisms comparably, but not well. ANMG performs quite well in all cases and even slightly better than FlowG in the cases of additive noise. However in the case of non-additive noise FlowG performs quite well whereas ANMG perform slightly worse – probably because their requirements on the underlying mechanisms are not met.
Figure 8: Accuracies for different models across all scenarios. FlowG and ANMG are our models.

(a) Accuracies of different models for different intervention types and locations. 1 stands for intervention on all variables except Y and 2 stands for interventions on parents and children only.

(b) Accuracies of different models according to target variables and mechanisms of the underlying SCM.

Figure 9: Comparison of models across different scenarios in the causal discovery task.
Figure 10: Logarithmic plot of L2 errors, normalized by CERM test error. For each method (ours in bold) from left to right: training error, test error on seen environments, domain generalization error on unseen environments. Scenarios for different mechanisms are shown.

G.6 Transfer Study

In the following we show the performance of different models on the training set, a test set of the same distribution and a set drawn from an unseen environment for different scenarios. As in Section 5, we use the L2-Loss on samples of an unseen environment to measure out-of-distribution generalization. Figure 10, 11 and 12 show results according to the underlying mechanisms, target variable or type of intervention respectively.
Figure 11: Logarithmic plot of L2 errors, normalized by CERM test error. For each method (ours in bold) from left to right: training error, test error on seen environments, domain generalization error on unseen environments. Scenarios for different target variables are shown.
Figure 12: Logarithmic plot of L2 errors, normalized by CERM test error. For each method (ours in bold) from left to right: training error, test error on seen environments, domain generalization error on unseen environments. Scenarios for different intervention types are shown.
H EXPERIMENTAL DETAILS COLORED MNIST

For the training, we use a feed forward neural network consisting of a feature selector followed by a classificator. The feature selector consists of two convolutional layers with a kernel size of 3 with 16 respectively 32 channels followed by a max pooling layer with kernel size 2, one dropout layer and a fully connected layer mapping to 16 feature dimensions. After the first convolutional layer and after the pooling layer a ReLU activation function is applied. For the classification we use a ReLU activation function followed by a linear layer which maps the 16 features onto the two classes corresponding to the labels.

We use the dataset from [Arjovsky et al. (2019)]. 50 000 samples are used for training and 10 000 samples as test set. For training, we choose a batch size of 2048 and train our models for 300 epochs. We choose a starting learning rate of $6 \cdot 10^{-3}$. The learning rate is decayed by 0.33 after 100 epochs. We use an L2-Regularization loss weighted by $10^{-5}$. After each epoch we randomly reassign the colors and the labels with the corresponding probabilities. The one-dimensional Wasserstein loss is applied dimension-wise and the maximum over dimensions is computed in order to compare residuals. Since the output of the Wasserstein is very small, we multiplied it by a factor of 10. For the HSIC we use a gaussian kernel with $\sigma = 1$. For Figure 4 we trained our model with $\lambda_I \approx 1.585$. 

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