NEURAL NETWORK EXTRAPOLATIONS WITH G-INVARIANCES FROM A SINGLE ENVIRONMENT

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ABSTRACT

Despite —or maybe because of— their astonishing capacity to fit data, neural networks are widely believed to be unable to extrapolate beyond training data distribution. This work shows that, for extrapolations based on transformation groups, a model's inability to extrapolate is unrelated to its capacity. Rather, the shortcoming is inherited from a classical statistical learning hypothesis: *Examples not explicitly observed with infinitely many training examples cannot be likely outcomes in the learner's model.* In order to endow neural networks with the ability to extrapolate over group transformations, we introduce a learning framework guided by a new learning hypothesis: *Any invariance to transformation groups is mandatory even without evidence, unless the learner deems it inconsistent with the training data*. Unlike existing invariance-driven methods for counterfactual inference, this framework allows extrapolations from a single environment. Finally, we introduce sequence and image extrapolation tasks that validate our framework and showcase the shortcomings of traditional approaches.

1 INTRODUCTION

Neural networks are widely praised for their ability to interpolate the training data. However, they are also simultaneously criticized for their inability to learn patterns that can extrapolate beyond the training data (see Section 6, Arjovsky et al. (2019), Schölkopf (2019), and de Haan et al. (2019) for examples). Designing learning frameworks (optimization & neural architectures) that allow them to learn patterns that extrapolate beyond the training data is an aspiration of machine learning today.

Because extrapolation error is not the same as generalization error (Marcus, 1998) —we will refer to generalization error as the interpolation error to avoid confusion—, standard learning frameworks fail to address the extrapolation shortcoming of neural networks. Recent counterfactual-based learning frameworks for extrapolation tasks —such as ICM, IRM, and CDC (Arjovsky et al., 2019; Besserve et al., 2018; Johansson et al., 2016; Louizos et al., 2017; Schölkopf, 2019) detailed in Section 2— assume the learner is given data from multiple environmental conditions (say environments E1 and E2) and is expected to learn patterns that work well over an unseen environment E3. That is, the learner imagines what would have happened if the environment were E3 instead of E1 or E2. Their key idea is to force the neural network to learn an internal representation of the input data that is invariant to environmental changes between E1 and E2, and, hence, hopefully also invariant to E3. While successful for a class of extrapolation tasks, these frameworks will fail if the learner is given a single environment or is unable to distinguish the different environments in the training data. *But, are we asking the impossible? Can humans even perform single-environment extrapolation?*

Young children, unlike monkeys and baboons, assume that a conditional stimulus F given another stimulus D extrapolates to a symmetric relation D given F without ever seeing any such examples (Sidman et al., 1982). E.g., if given D, action F produces a treat, the child assumes that given F, action D also produces a treat. Young children differ from primates (and pigeons) in their ability to use symmetries to build conceptual relations beyond visual patterns (Hollard and Delius, 1982; Sidman et al., 1982; Westphal-Fitch et al., 2012) and hypothesize equivalence classes (Sidman and Tailby, 1982), allowing extrapolations from intelligent reasoning. However, forcing symmetries against data evidence is not how intelligence works, since symmetries provide valuable evidence when they are broken. For instance, syntax antisymmetry is thought to encode fundamental relationships between words in sentences (Kayne et al., 1994).

Unfortunately, a prevailing learning hypothesis is blocking progress for single-environment extrapolation: *Examples not explicitly observed with infinitely many independent training examples are forbidden from happening in the learner's statistical model*, which is shared by both objective (frequentist) and subjective (Bayesian) learner's frameworks. To illustrate its effect on symmetry-based extrapolations, consider a supervised learning task where the training data contains infinitely many sequences $x^{(\text{tr})}$=(A,B) associated with label $y^{(\text{tr})}$=C, but no examples of a sequence $x^{(\text{tr})}$=(B,A). If given a test example $x^{(\text{te})}$=(B,A), the hypothesis considers it to be out of distribution (forbidden) and the prediction $P(Y^{(\text{te})}=\text{C}|X^{(\text{te})}=(\text{B,A}))$ is undefined, since $P(X^{(\text{tr})}=(\text{B,A}))=0$. This happens regardless of the prior over $P(X^{(\text{tr})})$. This *unseen-is-forbidden* learning hypothesis is currently preventing neural networks from assuming symmetric extrapolations without evidence.

Contributions. Since symmetries are intrinsically tied to human single-environment extrapolation capabilities, *this work explores a novel learning framework that modifies the learner's hypothesis space to allow symmetric extrapolation without evidence, while not losing valuable antisymmetric information if observed to predict the target variable in the training data.* Formally, a symmetry is an invariance to transformations of a group, known as a group transformation invariance or simply *G-invariance*. In Theorem 1 we show that the counterfactual invariances needed for symmetry extrapolation —denoted Counterfactual G-invariances (CG-invariances)— are stronger than traditional G-invariances. Theorem 2, then, introduces a condition in the structural causal model where G-invariances of linear automorphism groups are safe to use as CG-invariances. With that, Theorem 3 defines a partial order over the invariant subspaces of the Reynolds operators of all overgroups of these groups, which we use in a novel learning framework capable of learning the correct G-invariances from a single environment without evidence, while retaining the ability to be sensitive to antisymmetries shown to be relevant in the training data. Finally, we introduce sequence and image extrapolation tasks with experiments that validate the theoretical results and showcase the shortcomings of traditional approaches.

2 Related Work

Counterfactual inference and invariances. Recent efforts have brought counterfactual inference to machine learning models. *Independence of causal mechanism (ICM)* methods (Bengio et al., 2019; Besserve et al., 2018; Johansson et al., 2016; Louizos et al., 2017; Raj et al., 2020; Schölkopf, 2019), *Causal Discovery from Change (CDC)* methods (Tian and Pearl, 2001), and *representation disentanglement* methods (Bengio et al., 2019; Goudet et al., 2017; Locatello et al., 2019). Invariant risk minimization (IRM) (Arjovsky et al., 2019) is a type of ICM (Schölkopf, 2019). Broadly, these efforts look for representations (or mechanism descriptions) that are invariant across multiple environments observed in the training data. These can be categorized as *unseen-is-forbidden* methods, since they rely on multiple environment samples in order to learn to reason over new environments.

Counterfactual inference from a single environment cannot rely on *unseen-is-forbidden* methods. To the best of our knowledge there is no clear effort for extrapolations from a single environment. The key similarity between the ICM framework and our framework is the assumption of independently sampled mechanisms (transformations) and causes (raw inputs). Besides the challenge of defining the new task, we also develop a learning framework for our new learning hypothesis.

Domain adaptation and domain generalization. Domain adaptation and domain generalization (e.g. (Long et al., 2017; Muandet et al., 2013; Quionero-Candela et al., 2009; Rojas-Carulla et al., 2018; Shimodaira, 2000; Zhang et al., 2015) and others) ask questions about specific —observed or known— changes in the data distribution rather than counterfactual questions. A key difference is that counterfactual inference accounts for hypothetical interventions, not known ones.

Forced G-invariances. *Forcing a G-invariance may contradict the training data, where the target variable is actually influenced by the transformation of the input.* For instance, handwritten digits are not invariant to 180° rotations, since digits 6 and 9 would get confused. Data augmentation is a type of forced G-invariance (Chen et al., 2019; Lyle et al., 2020) and hence, will fail to extrapolate. Other works forcing G-invariances that will also fail include (not an extensive list): Ravanbakhsh et al. (2017) proposes a parameter-sharing technique for incorporating invariances to finite permutation subgroups in a neural network layer. Yarotsky (2018) is a great read, showing that any G-invariant map can be approximated to arbitrary precision by neural networks through a polynomial layer for some given groups. Zaheer et al. (2017) considers a neural network architecture for set representations; Murphy et al. (2019a;b) consider symmetrization approaches for permutation groups for sets and

graph representations; Maron et al. (2019) describes linear G-equivariant/G-invariant also for graphs. Maron et al. (2020) applies these ideas to multiple sets. Cohen et al. (2016; 2019) describes representations for the dihedral group D_4 and spherical transformation groups; Kicki et al. (2020) proposes an architecture that is invariant to general subgroups via symmetrization. Zweig and Bruna (2020) considers permutation and input-size invariance in representation learning.

3 Extrapolations from a Single Environment

Geometrically, extrapolation can be thought as reasoning beyond a convex hull of a set of training points (Hastie et al., 2012; Haffner, 2002; King and Zeng, 2006). However, for neural networks —with their arbitrary representation mappings— this geometric interpretation is insufficient. Rather, extrapolations should be described through counterfactual reasoning (Neyman, 1923; Rubin, 1974; Pearl, 2009; Schölkopf, 2019). Specifically in our task, we ask: *After seeing training data from environment A, the learner wants to extrapolate and predict what would have been the output if the training environment were B.* Extrapolations differ from traditional domain adaptation due to its counterfactual nature —a *what-if* question of an intervention that can only be imagined given offline data (Bareinboim et al., 2020; Pearl and Mackenzie, 2018), rather than a known distributional change.

Transformation groups. We focus on extrapolations tied to finite linear automorphism groups acting on the input data. We start with an example. Consider an input $\boldsymbol{x} \in \mathcal{X} = \mathbb{R}^{3n^2}$ representing a vectorized $n \times n$ pixel RGB image. We can define at least three linear automorphism groups: (1) $\mathcal{G}_{\text{rot}} \equiv \{T^{(k)}\}_{k\in\{0^\circ,90^\circ,180^\circ,270^\circ\}}$, which rotates the image by k degrees, (2) $\mathcal{G}_{\text{color}} \equiv \{T^{(\alpha)}\}_{\alpha\in\mathbb{S}_3}$, which permutes the RGB channels of the image, and (3) $\mathcal{G}_{\text{vflip}} \equiv \{T^{(v)}, T^{(0)}\}$, which flips the image vertically. More generally, a linear automorphism group $\mathcal{G}$ satisfies six properties: (automorphism) $\forall T \in \mathcal{G}$, $T : \mathcal{X} \to \mathcal{X}$;(identity) $I(x) = x$, $I \in \mathcal{G}$; (is closed under composition) $\forall T, T' \in G$, $T \circ T' \in G$, where $T \circ T'(x) = T(T'(x))$; (associative) $\forall T, T', T^\dagger \in \mathcal{G}, T \circ (T' \circ T^\dagger) = (T \circ T') \circ T^\dagger$; (has inverses) $\forall T \in \mathcal{G}$, $\exists T^{-1} \in \mathcal{G}$ s.t. $T^{-1} \circ T = I$; and (is linear) $T \in \mathcal{G}$ is a linear function.

Besides images, sequences $\boldsymbol{x} = (x_1, x_2, \ldots)$ are another input of interest, where $\boldsymbol{x} \in \mathcal{X}$ for some appropriately defined set $\mathcal{X}$. Here, the symmetric group (permutation group) $\mathbb{S}_n$, is the set of all permutations $\mathbb{S}_n = \{\pi \mid \pi : \{1, \ldots, n\} \to \{1, \ldots, n\}$ is a bijection$\}$ equipped with the composition operator. Attributed graphs $(\mathbf{A}, \boldsymbol{X}) \in \mathcal{X}$, where $\mathbf{A}$ is tensor of edge properties and $\boldsymbol{X}$ is a matrix of node attributes, are also of interest for the permutation group $\mathbb{S}_n$.

Subgroups and overgroups. Just as we can compose image transformations to make new image transformations, we can also compose automorphism groups into larger automorphism groups (overgroups). For instance, we can compose rotations and image flips to form a linear automorphism group $\mathcal{G}_{\{\text{rot,vflip}\}} = \langle \mathcal{G}_{\text{rot}} \cup \mathcal{G}_{\text{vflip}} \rangle$ containing all such compositions, where $\langle \cdot \rangle$ is the group join operator. Following standard notation, we say $\mathcal{G}_{\text{rot}} \leq \mathcal{G}_{\{\text{rot,vflip}\}}$ to indicate that $\mathcal{G}_{\text{rot}}$ is a subgroup of $\mathcal{G}_{\{\text{rot,vflip}\}}$, or, equivalently, $\mathcal{G}_{\{\text{rot,vflip}\}}$ is an overgroup of $\mathcal{G}_{\text{rot}}$. Henceforth, we use $\mathcal{G}_{\{1,\ldots,m\}} \equiv \langle \cup_{i=1}^m \mathcal{G}_i \rangle$ to denote the group generated by the groups $\mathcal{G}_1, \ldots, \mathcal{G}_m$.

The causal mechanism as an *economical data generation process*. We assume that a fundamentally economical process created the training data, where the focus was on sampling diverse environments in a way that mattered to the task. For instance, image datasets will contain mostly upright pictures, rather than images over all possible orientations, but we will assume the dataset curators strive for a somewhat a diverse set of subjects for each label (e.g., a good representation of different types of subjects and environmental conditions). *Hence, the absence of variation over image orientations in the dataset can be counted as evidence against its effect on the image labels.*

We describe the data generation with the help of a structural causal model (SCM) (Pearl, 2009, Definition 7.1.1). Consider a supervised task over inputs $X^{(\text{obs})}$ and their corresponding outputs Y, which are random variables defined over a suitable space. The training data consists of a set $\mathcal{D}^{(\text{tr})} = \{(Y_i^{(\text{tr})}, X_i^{(\text{tr,obs})})\}_{i=1}^N$ of independent and identically distributed samples drawn from a joint distribution $P(Y, X^{(\text{obs})})$. The hidden random variable

$$X^{(\text{hid})} := g(U_u), \tag{1}$$

where $g : \mathcal{U} \to \mathcal{X}$ is a measurable map (deterministic function) that describes the input $X^{(\text{obs})}$ in some unknown canonical form, where U_u is a random variable (e.g., $U_u \sim \text{Uniform}(0, 1)$). Next, we define how $X^{(\text{hid})}$ is modified by transformations into the observed input $X^{(\text{obs})}$.

Transformation of $X^{(hid)}$ into $X^{(obs)}$. Consider a collection of finite linear automorphism groups $\mathcal{G}_1, \ldots, \mathcal{G}_m$. Let $\mathcal{I} \subseteq \{1, \ldots, m\}$ be a subset and $\mathcal{D} \subseteq \{1, \ldots, m\} \backslash \mathcal{I}$ be a subset of its complement. Consider independent and identically distributed random variables $U_{\mathcal{D}}$ and $U_{\mathcal{I}}$ that select transformations in the respective overgroups $\mathcal{G}_{\mathcal{D}} = \langle \cup_{i \in \mathcal{D}} \mathcal{G}_i \rangle$ and $\mathcal{G}_{\mathcal{I}} = \langle \cup_{j \in \mathcal{I}} \mathcal{G}_j \rangle$. We note in passing that we allow $\mathcal{G}_{\mathcal{D}} \cap \mathcal{G}_{\mathcal{I}} \neq \emptyset$, but $\mathcal{G}_{\mathcal{D}} \cap \mathcal{G}_{\mathcal{I}} = \emptyset$ makes the counterfactual task easier. The reader can roughly interpret $U_{\mathcal{D}}$ (or $U_{\mathcal{I}}$) as the random seed of a random number generator that gives an ordered sequence of transformations of $\mathcal{G}_{\mathcal{D}}$ (or $\mathcal{G}_{\mathcal{I}}$). The observed input is defined as

$$X^{(\text{obs})} := T_{U_{\mathcal{D}}, U_{\mathcal{I}}} \circ X^{(\text{hid})}, \tag{2}$$

where $T_{U_{\mathcal{D}}, U_{\mathcal{I}}}$ is a transformation in $\mathcal{G}_{\mathcal{D} \cup \mathcal{I}}$ indexed by two independent *hidden* environment background random variables $U_{\mathcal{D}}, U_{\mathcal{I}}$. Such a surjective indexing is always possible, with an example given in the Supplementary Material (Appendix B).

Target variable and transformation groups. The output Y associated with $X^{(\text{obs})}$ is given by

$$Y := h(X^{(\text{hid})}, U_{\mathcal{D}}, U_Y), \tag{3}$$

where h is a deterministic function and U_Y is an independent random variable. Since the outputs Y do not depend on $U_{\mathcal{I}}$, the training data may contain only a few (or just one) sample of the variable $U_{\mathcal{I}}$. *The low diversity of samples of $U_{\mathcal{I}}$ in the training data is due to an economical data generation process*. For instance, if the environment is the camera orientation, and the image label Y does not depend on image rotation, then the images are all upright since the sampling is economical. Other examples include sequences $X^{(\text{obs})} = (X_1^{(\text{obs})}, \ldots, X_n^{(\text{obs})})$ that are presented in lexicographical order when their order is irrelevant to Y.

Extrapolation as counterfactual reasoning. Our training data is described through the set of background random variables $\mathcal{U}_{\text{all}} = \{U_u, U_Y, U_{\mathcal{D}}, U_{\mathcal{I}}\}$ and Equations (2) and (3) transformations

$$(Y^{(\text{tr})}, X^{(\text{tr,obs})}) \sim \mathbb{E}_{\mathcal{U}_{\text{all}}} \left[\mathbf{1}\{Y = h(g(U_u), U_{\mathcal{D}}, U_Y)\} \cdot \mathbf{1}\{X = T_{U_{\mathcal{D}}, U_{\mathcal{I}}} \circ g(U_u)\} \right], \tag{4}$$

where $\mathbf{1}\{\cdot\}$ is the indicator function (or Dirac delta for continuous variables).

We can now ask "what would have happened to Y in the training data (Equation (4)) if we had given specific values of $U_{\mathcal{I}}$ to the data generation process in Equations (2) and (3), rather than sampling them from $P(U_{\mathcal{I}})$". For instance, would the class of an image change if we had flipped the image along the vertical axis? Would we re-classify outlier events if we changed the order of events in a stationary time series? These are counterfactual queries over environment background variables $U_{\mathcal{I}}$.

The existing counterfactual notation in the literature (see Definition 7 of Bareinboim et al. (2020)) could be ambiguous in our setting. Hence, we choose to repurpose the powerful concept of random variable coupling from Markov chains (Pitman, 1976; Propp and Wilson, 1996) to describe our counterfactual inference problem:

Definition 1 (Counterfactual coupling (CFC))**.** *The counterfactual coupling of Equation* (4) *is*

$$\begin{aligned} P(Y = y, X^{(obs)} = x^{(obs)}, X^{(cf)} = x^{(cf)}) = \mathbb{E}_{\mathcal{U}_{all} \cup \{\tilde{U}_{\mathcal{I}}\}} \Big[& \mathbf{1}\{y = h(g(U_u), U_{\mathcal{D}}, U_Y)\} \\ & \cdot \mathbf{1}\{x^{(obs)} = T_{U_{\mathcal{D}}, U_{\mathcal{I}}} \circ g(U_u)\} \cdot \mathbf{1}\{x^{(cf)} = T_{U_{\mathcal{D}}, \tilde{U}_{\mathcal{I}}} \circ g(U_u)\} \Big], \end{aligned} \tag{5}$$

and $\tilde{U}_{\mathcal{I}}$ and $U_{\mathcal{I}}$ are independent random variables with possibly different distributions. The counterfactual coupled variable $X^{(cf)}$ asks what would have happened to $X^{(obs)}$ if we had used $\tilde{U}_{\mathcal{I}}$ in place of $U_{\mathcal{I}}$ in Equation (4)*.*

Armed with Definition 1, we are now ready to describe our task.

Extrapolation model. We start defining counterfactual G-invariant (CG-invariant) representations.

Definition 2 (Representations that are CG-invariant to $U_{\mathcal{I}}$)**.** *Let $X^{(obs)}$ and $X^{(cf)}$ be* ***coupled random variables*** *with respect to the background environment variable $U_{\mathcal{I}}$ as in Definition 1. A representation function $\Gamma : \mathcal{X} \to \mathbb{R}^d$, $d \geq 1$, is deemed CG-invariant to $U_{\mathcal{I}}$ if*

$$\Gamma(X^{(obs)}) \overset{a.s.}{=} \Gamma(X^{(cf)}), \tag{6}$$

where a.s. means almost surely (i.e., the equality is true for any sample of $X^{(cf)}$ and $X^{(obs)}$).

Extrapolated model: Our task is to find a representation $\Gamma_{\text{true}} : \mathcal{X} \to \mathbb{R}^d$, $d \geq 1$, and a link function $g_{\text{true}} : \mathbb{R}^d \to \text{Im}\, P(Y = y|X^{(\text{cf})})$ —where $\text{Im}\, P(\cdot)$ is the image of $P(\cdot)$— such that

$$Y|X^{(\text{cf})} \stackrel{d}{=} \hat{Y}|X^{(\text{cf})}, \text{ with } \hat{Y}|X^{(\text{cf})} \sim g_{\text{true}}(\Gamma_{\text{true}}(X^{(\text{cf})})) \stackrel{a.s.}{=} g_{\text{true}}(\Gamma_{\text{true}}(X^{(\text{obs})})), \tag{7}$$

where $\stackrel{d}{=}$ means the random variables have the same distribution. Hence, Equation (7) shows that **if** $\Gamma_{\text{true}}(X^{(\text{cf})}) \stackrel{a.s.}{=} \Gamma_{\text{true}}(X^{(\text{obs})})$ (Equation (6)), **then** we could approximate g_{true} by training an expressive-enough feedforward network on samples of $\hat{Y}|X^{(\text{obs})}$ (i.e., the training data).

Alas, learning Γ_{true} is the real challenge. We cannot find Γ_{true} by augmenting the training data (i.e., counterfactually replacing $X^{(\text{obs})}$ by $X^{(\text{cf})}$ in the data) since: (i) We do not know $\mathcal{I}$ (the group $\mathcal{G}_{\mathcal{I}}$ which is related to the CG-invariance); (ii) this would also require knowing $P(\tilde{U}_{\mathcal{I}})$, which we don't. Without an observed $X^{(\text{cf})}$, the statistical assumption that *examples not explicitly observed with infinitely large training data are forbidden from happening in the learner's statistical model* will prevent us from learning Γ_{true}. We must change this assumption.

4 CG-INVARIANCES FOR EXTRAPOLATION

In this section we introduce our learning framework, which seeks to use the training data (samples of $\hat{Y}|X^{(\text{obs})}$) to approximate Γ_{true} and g_{true} of Equation (7). Our framework regularizes neural network weights towards representations that are invariant to groups that negligibly impact training data accuracy. Our framework overcomes some key challenges:
(a) Theorem 1 below shows that CG-invariances (Definition 2) are stronger than $G_{\mathcal{I}}$-invariances. After that, Theorem 2 defines conditions under which $G_{\mathcal{I}}$-invariances suffice as CG-invariances.
(b) We need to derive an optimization objective where *all G-invariances are mandatory, except the ones deemed inconsistent with the training data*, replacing the traditional *unseen-is-forbidden* learning hypothesis. The challenge is not knowing $\mathcal{I}$. Here, the neural network weights are regularized to find the largest transformation overgroup to be G-invariant without hurting training accuracy.

Our first question is whether CG-invariances are just G-invariances. Theorem 1 shows they are not.

Theorem 1 (CG-invariance is stronger than G-invariance)**.** *Let $X^{(obs)}$ and $X^{(cf)}$ be coupled random variables per Definition 1. For a representation $\Gamma : \mathcal{X} \to \mathbb{R}^d$, $d \geq 1$, let*

$$\textit{G-inv}: \ \forall T_{\mathcal{I}} \in \mathcal{G}_{\mathcal{I}}, \ \ \Gamma(X^{(obs)}) = \Gamma(T_{\mathcal{I}} \circ X^{(obs)}),$$
$$\textit{CG-inv}: \ \Gamma(X^{(obs)}) = \Gamma(X^{(cf)}),$$

denote the conditions on Γ for $\mathcal{G}_{\mathcal{I}}$-invariance and CG-invariance respectively. Then, CG-inv $\Longrightarrow$ G-inv, but G-inv $\not\Longrightarrow$ CG-inv.

However, the following condition ensures that a $G_{\mathcal{I}}$-invariance is also a CG-invariance.

Theorem 2. *If $\mathcal{G}_{\mathcal{I}}$ is a normal subgroup of $\mathcal{G}_{\mathcal{D}\cup\mathcal{I}}$, then CG-inv $\iff$ G-inv.*

A subgroup H of a group G is called normal (denoted $H \trianglelefteq G$) if for all $h \in H$ and $g \in G$, $ghg^{-1} \in H$. In our context, $\mathcal{G}_{\mathcal{I}} \trianglelefteq \mathcal{G}_{\mathcal{D}\cup\mathcal{I}}$ ensures that any $T \in \mathcal{G}_{\mathcal{D}\cup\mathcal{I}}$ can be written as $T = T_{\mathcal{I}} \circ T_{\mathcal{D}}$ for some $T_{\mathcal{I}} \in \mathcal{G}_{\mathcal{I}}, T_{\mathcal{D}} \in \mathcal{G}_{\mathcal{D}}$. Throughout the rest of the paper, we will assume that $\mathcal{G}_{\mathcal{I}}$ is a normal subgroup of $\mathcal{G}_{\mathcal{D}\cup\mathcal{I}}$ in the SCM Equation (2).

Learning CG-invariant representations without knowledge of $\mathcal{G}_{\mathcal{I}}$. We start by restating the Reynolds operator, which has been extensively used in the literature of G-invariant representations without attribution:

Lemma 1 (Reynolds operator (Billik and Rota, 1960))**.** *Let $\mathcal{G}$ be a finite linear automorphism group over vec$(\mathcal{X})$. Then,*

$$\overline{T} = \frac{1}{|\mathcal{G}|} \sum_{T \in \mathcal{G}} T \tag{8}$$

is a $\mathcal{G}$-invariant linear automorphism, i.e., $\forall T_\dagger \in \mathcal{G}$ and $\forall \boldsymbol{x} \in$ vec$(\mathcal{X})$, it must be that $\overline{T}(T_\dagger \boldsymbol{x}) = \overline{T}\boldsymbol{x}$.

Since $\overline{T}$ is a projection operator (i.e., $\overline{T}^2 = \overline{T}$), all the eigenvalues of $\overline{T}$ are either 0 or 1. Using this fact, we now describe G-invariant neurons using the left eigenspace of $\overline{T}$ corresponding to the eigenvalue 1.

Lemma 2. *If $\mathcal{W}$ denotes the left eigenspace corresponding to the eigenvalue 1 of the Reynolds operator $\overline{T}$ for the group $\mathcal{G}$,* **then** *$\forall b \in \mathbb{R}$, the linear transformation $\gamma(\boldsymbol{x}; \boldsymbol{w}, b) = \boldsymbol{w}^T \boldsymbol{x} + b$ is invariant to any transformation $T \in \mathcal{G}$* **if and only if** *$\boldsymbol{w} \in \mathcal{W}$.*

The above property of the Reynolds operator can be leveraged to build neural networks that adhere to particular group symmetries, as done by Yarotsky (2018) and van der Pol et al. (2020). If we knew $\mathcal{G}_\mathcal{I}$, restricting the parameters of each neuron to the left 1-eigenspace of the Reynolds operator of $\mathcal{G}_\mathcal{I}$ would give us a way to build a $\mathcal{G}_\mathcal{I}$-invariant neural network.

Alas, we do not know $\mathcal{G}_\mathcal{I}$. Instead, we want to construct bases for the complete space $\text{vec}(\mathcal{X})$ such that they are partially ordered by their invariance strength: From most invariant bases to least (a precise definition comes after Theorem 3). Later, we will use this partial order to define a regularization term for our method. Theorem 3 shows how these bases can be constructed inductively, where we start with the most invariant subspace and judiciously work our way over increasingly less invariant subspaces, where each step of our inductive method performs a Gram-Schmidt orthogonalization.

Theorem 3 (Invariant subspace bases can be partially ordered by invariance strength)**.** *Let $\mathcal{W}_i \subseteq \text{vec}(\mathcal{X})$ be the left eigenspace corresponding to the eigenvalue 1 of the Reynolds operator $\overline{T}_i$ for group $\mathcal{G}_i$, $i = 1, \ldots, m$. We construct the invariant subspace partitions*

$$\widetilde{\mathcal{B}}_M = \bigcap_{i \in M} \mathcal{W}_i \,; \quad \mathcal{B}_M = \widetilde{\mathcal{B}}_M - \text{proj}_{\mathcal{B}_{\supsetneq M}}(\widetilde{\mathcal{B}}_M) \,, \quad \forall M \in \wp(\{1, \ldots, m\}) \setminus \emptyset, \tag{9}$$

where $\wp$ is the power set, $\mathcal{B}_{\supsetneq M} = \bigoplus_{N \supsetneq M} \mathcal{B}_N$, $\text{proj}_{\mathcal{A}_1}(\mathcal{A}_2)$ finds the orthogonal projection of a subspace $\mathcal{A}_2$ onto the subspace $\mathcal{A}_1$, and $\bigoplus$ is the direct sum operator. **Then***, the linear transformation $\gamma(\boldsymbol{x}; \boldsymbol{w}, b) = \boldsymbol{w}^T \boldsymbol{x} + b,\ b \in \mathbb{R}, \forall \boldsymbol{w} \in \mathcal{B}_M \setminus \{\boldsymbol{0}\}$, is $\mathcal{G}_M$-invariant but not $\mathcal{G}_j$-invariant $\forall j \in \overline{M}$.*

In addition, if needed, we obtain the basis for the rest of the space through $\mathcal{B}_\emptyset = \text{vec}(\mathcal{X}) - \text{proj}_{\mathcal{B}_{\supsetneq \emptyset}}(\text{vec}(\mathcal{X}))$. Note that if $\boldsymbol{w} \in \mathcal{B}_N$, then $\boldsymbol{w}$ is never $\mathcal{G}_H$-invariant for $H \supsetneq N$ as we remove all such $\boldsymbol{w}$ from $\mathcal{B}_N$. Hence, the partial order of nested subsets in $\wp(\{1, \ldots, m\})$ induces a partial order of invariance strengths in the bases of the input domain $\text{vec}(\mathcal{X})$.

Practical aspects. The algorithm in Theorem 3 needs to run only once for groups $\mathcal{G}_1, \ldots, \mathcal{G}_m$, and the results reused in all experiments. Moreover, for any $M \subsetneq \{1, \ldots, m\}$, as soon as $\cup_{N \supsetneq M} \mathcal{B}_N$ has already covered the entire space $\text{vec}(\mathcal{X})$, $\mathcal{B}_M$ will be the zero subspace and the algorithm can stop. All of our experimental runtimes of this algorithm are less than one minute in commodity machines.

Learning framework. We are now ready to learn an approximate CG-invariant representation using neural networks Γ and g, which we use to approximate the distribution of $\widehat{Y}$ in Equation (7) with the training data. Let $\mathcal{G}_1, \ldots, \mathcal{G}_m$ be known linear automorphism groups. It is important to remember that, under the assumption of Theorem 2, we just need Γ to be $\mathcal{G}_\mathcal{I}$-invariant, with $\mathcal{G}_\mathcal{I} \equiv \langle \cup_{i \in \mathcal{I}} \mathcal{G}_i \rangle$, but $\mathcal{I} \subseteq \{1, \ldots, m\}$ is unknown to us. We achieve the correct $\mathcal{G}_\mathcal{I}$-invariance by redefining the neuron weights of Γ using the subspaces of Theorem 3 and proposing a regularized objective that pushes Γ towards the strongest overgroup G-invariance that does not *significantly* hurt the training data, where *significantly* is controlled by a regularization strength $\lambda > 0$.

More formally, let $\Gamma : \text{vec}(\mathcal{X}) \times \mathbb{R}^{d_\mathcal{X} \times H} \times \mathbb{R}^H \to \mathbb{R}^d$, $H \geq 1, d \geq 1$, be a neural network with H neurons, parameterized by free parameters $\boldsymbol{\Omega} \in \mathbb{R}^{d_\mathcal{X} \times H}$ and $\boldsymbol{b} \in \mathbb{R}^H$. The H neurons are arranged in an appropriate architecture as described in Section 5, but reader can imagine a feedforward network for now. Let $g : \mathbb{R}^d \to \text{Im} P(Y|X)$ be a link function. The training data $\mathcal{D}^{(\text{tr})} = \{(y_i^{(\text{tr})}, \boldsymbol{x}_i^{(\text{tr,obs})})\}_{i=1}^N$, $N > 1$, is assumed to be sampled according to the SCM data generation process in Equations (1) to (3), with the hidden $\mathcal{G}_\mathcal{I}$ satisfying the conditions in Theorem 2.

Let $\boldsymbol{B}_M \in \mathbb{R}^{d_\mathcal{X} \times d_M}$ be a matrix whose columns are the orthogonal basis of subspace $\mathcal{B}_M \neq \{\boldsymbol{0}\}$ (Theorem 3) with dimension d_M. Our neuron weights $\boldsymbol{\Omega}$ have a correspondence to $\boldsymbol{B}_{M_1}, \boldsymbol{B}_{M_2}, \ldots$:

$$\boldsymbol{\Omega} = \begin{bmatrix} \boldsymbol{\omega}_{M_1,1} & \cdots & \boldsymbol{\omega}_{M_1,H} \\ \boldsymbol{\omega}_{M_2,1} & \cdots & \boldsymbol{\omega}_{M_2,H} \\ \vdots & \cdots & \vdots \end{bmatrix} \tag{10}$$

where $\boldsymbol{\omega}_{M,h} \in \mathbb{R}^{d_M \times 1}$ and the h-th neuron in Γ, $h \in \{1, \ldots, H\}$, has the form

$$\Gamma^{(h)}(\boldsymbol{x}) = \sigma\Bigg(\boldsymbol{x}^\top \Bigg(\sum_{M : \mathcal{B}_M \neq \{\boldsymbol{0}\}} \boldsymbol{B}_M \boldsymbol{\omega}_{M,h} \Bigg) + b_h \Bigg), \tag{11}$$

and $\sigma(\cdot)$ is a nonpolynomial activation function. Our optimization objective is then

$$\widehat{\boldsymbol{\Omega}}, \widehat{\boldsymbol{b}}, \widehat{\boldsymbol{W}}_g = \underset{\boldsymbol{\Omega}, \boldsymbol{b}, \boldsymbol{W}_g}{\arg\min} \sum_{(y^{(\text{tr})}, \boldsymbol{x}^{(\text{tr,obs})}) \in \mathcal{D}^{(\text{tr})}} \mathcal{L}\left(y^{(\text{tr})}, g(\Gamma(\boldsymbol{x}^{(\text{tr,obs})}; \boldsymbol{\Omega}, \boldsymbol{b}); \boldsymbol{W}_g)\right) + \lambda R(\boldsymbol{\Omega}) \tag{12}$$

where $\mathcal{L} : \mathcal{Y} \times \text{Im}P(Y|X) \to \mathbb{R}_{\geq 0}$ is a nonnegative loss function, and $\lambda > 0$ is a regularization strength. The regularization penalty $R(\boldsymbol{\Omega})$ is given by,

$$R(\boldsymbol{\Omega}) = f_l(\boldsymbol{\Omega}) := \sum_{\substack{M:|M|=l \\ \mathcal{B}_M \neq \{\mathbf{0}\}}} \mathbf{1}\{\|\boldsymbol{\omega}_{M,\cdot}\|_2^2 > 0\} \; + \; |\{M : |M| > l, \mathcal{B}_M \neq \{\mathbf{0}\}\}| \,, \tag{13}$$

where $l = \min\{|M|\mathbf{1}\{\|\boldsymbol{\omega}_{M,\cdot}\|_2^2 > 0\}, \forall M \in \wp(\{1, \ldots, m\}) \setminus \{1, \ldots, m\}\}$. That is, if M' is the least-invariant basis with non-zero weights $\boldsymbol{\omega}_{M',\cdot}$ then $l = |M'|$ and the penalty is the sum of (i) the total number of bases with non-zero corresponding weights and the same level of invariance as M', and (ii) the number of bases with greater invariance than M' (regardless of the corresponding weights). The regularization term $R(\boldsymbol{\Omega})$ in Equation (13) is discrete but can be approximated by a differentiable formula. First, we replace the indicator function $\mathbf{1}\{z > 0\}$ in Equation (13) with the approximation $\tilde{\mathbf{1}}\{z > 0\} = \tau z/(\tau z + 1)$, where $\tau \geq 1$ is a temperature hyperparameter. We then use the following recursion: $R(\boldsymbol{\Omega}) = R_m(\boldsymbol{\Omega})$, where $R_l(\boldsymbol{\Omega}) = (1 - \beta_l(\boldsymbol{\Omega})) \cdot R_{l-1}(\boldsymbol{\Omega}) + f_l(\boldsymbol{\Omega})\beta_l(\boldsymbol{\Omega})$ for $l = 1, \ldots, m$, $R_0(\boldsymbol{\Omega}) = 0$, and $\beta_l(\boldsymbol{\Omega}) = \tilde{\mathbf{1}}\{\sum_{N:|N|=l, \mathcal{B}_N \neq \{\mathbf{0}\}} \|\boldsymbol{\omega}_{N,\cdot}\|_2^2 > 0\}$, where $\beta_l(\boldsymbol{\Omega})$ is approximately one if at least one neuron h has nonzero $\boldsymbol{\omega}_{N,h}$ parameters for a partition $N \in \wp(\{1, \ldots, m\}) \setminus \{1, \ldots, m\}\}$ of size l (i.e., with l groups). In all our experiments, we choose the maximum value of regularization strength λ that is within a 5% threshold of the maximum *non-extrapolated validation accuracy* obtained from any value of λ.

5 CG-INVARIANT NEURAL ARCHITECTURES

We should be mindful when creating CG-invariant neural network architectures, so that all the potential $\mathcal{G}_{\mathcal{I}}$-invariances can be realized, since we do not know the true $\mathcal{G}_{\mathcal{I}}$. For instance, for **image tasks** with the rotation transformation group: We can apply the CG-regularization of Equations (11) and (12) in the convolutional layers of a CNN architecture like VGG (Simonyan and Zisserman, 2014), but need each channel of the last convolution to output a single neuron, ensuring it can be rotation-invariant if needed. Residual connections need to be applied with care, since they can undo the G-invariance of the neurons they skip. See our Supplementary Material for architecture examples.

For **sequence and array tasks** (graph & tensor tasks), the architecture is more direct: One can simply apply a feedforward network. For permutation groups on sequences, the neuron weight bases $\boldsymbol{B}_M$ of Equation (11) are interesting. For a sequence $\boldsymbol{X} = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n] \in \mathbb{R}^{p \times n}$, we can consider $m = \binom{n}{2}$ permutation groups for all the pair-wise permutations: $\mathcal{G}_{1,2}, \mathcal{G}_{2,3}, \mathcal{G}_{1,3}, \ldots, \mathcal{G}_{n-1,n}$. With the bases of Theorem 3, the h-th neuron is $\sigma(\boldsymbol{x}_1^T \boldsymbol{\omega}_{\{1,\ldots,m\},h} + \sum_{i=2}^n \boldsymbol{x}_i^T (\boldsymbol{\omega}_{\{1,\ldots,m\},h} + \boldsymbol{\omega}_{\{1,\ldots,m\}\setminus\{i\},h}) + b_h)$, with $\boldsymbol{\omega}_{\{1,\ldots,m\}\setminus\cdot,h} \in \mathbb{R}^{p \times 1}$. Equation (12) will regularize, $\forall i, h$, $\|\boldsymbol{\omega}_{\{1,\ldots,m\}\setminus\{i\},h}\|_2^2 \to \mathbf{0}$ if the training data accuracy is not hurt by permutation invariance. To obtain full permutation sensitivity, Equation (12) pushes $\boldsymbol{\omega}_{\{1,\ldots,m\}\setminus\{i\},h}$ to be all nonzero and different, for all i. Equation (12) finds G-invariances to subgroup permutations (e.g., G-invariant only to $\mathcal{G}_{\mathcal{I}} = \langle \mathcal{G}_{1,2} \cup \mathcal{G}_{2,3} \cup \mathcal{G}_{1,3} \rangle$) by pushing the respective $\boldsymbol{\omega}_{\{1,\ldots,m\}\setminus\{i\},h}$ to share the same value. See our Supplementary Material for architecture examples.

For permutation groups on tensor and matrices (attributed graphs), some of the bases automatically obtained by Theorem 3 coincide with the bases described by the forced G-invariance of Maron et al. (2019), with the added benefit that: (a) Theorem 3 automatically finds them; (b) Theorem 3 automatically finds bases for permutation groups combined with other transformation groups (Maron et al. (2019) only considers permutations), (c) and, most importantly, Equation (12) decides if permutation sensitivity is important for the task, unlike a forced G-invariance which assumes it is not.

6 EMPIRICAL RESULTS

We now provide empirical results of 12 different tasks to showcase the properties and advantages of our framework. Due to space limitations, our results are only briefly summarized here, with most of the details described in the Supplementary Material (Appendix D). Appendix A also shows a task where CG-invariance is stronger than G-invariance, showing the practical relevance of Theorem 1.

Table 1: Extrapolation accuracy ($\pm$ 95% confidence interval, **bold** means $p < 0.05$ significant)

Image transformation groups $\{\mathcal{G}_{\text{rot}}, \mathcal{G}_{\text{vertical-flip}}, \mathcal{G}_{\text{colors}}\}$
Task: Predict digit & which transformations of $\mathcal{G}_{\mathcal{D}}$ was applied to image

MNIST $\{3,4\}$ images				MNIST all images		
$\mathcal{I}$	VGG	+G-inv	**+CGreg**	VGG	+G-inv	**+CGreg**
$\emptyset$	**96.06±0.63**	15.96±2.17	94.49±01.49	89.35±0.52	15.64±1.55	**90.89±0.93**
color	15.06±6.70	50.05±2.17	**94.16±06.43**	4.51±1.36	47.61±0.45	**88.69±2.11**
rot,vflip	54.87±0.90	32.05±1.16	**95.78±07.11**	25.91±0.95	44.41±3.28	**62.68±6.02**
rot,col,vflip	49.52±2.37	**97.19±1.02**	**94.89±07.49**	11.27±0.34	**68.46±2.83**	64.99±2.76

Sequences $\{\mathcal{G}_{1,2}, \ldots, \mathcal{G}_{n-1,n}\}$
Tasks depend on $\mathcal{I}$ (see Supplementary Material)

Sequence Tasks			
$\mathcal{I}$	Transformer	Best FF+G-inv	**FF+CGreg**
$\emptyset$	**100.00±0.00**	23.38±1.88	95.70±03.05
$\{(i,i{+}2k)\}_{i,k}$	0.85±0.37	0.97±0.60	**71.85±26.61**
$\{(i,j)\}_{j>i\geq 2}$	12.15±16.05	10.68±1.49	**42.08±18.99**
$\{(i,j)\}_{j>i\geq 1}$	20.26±32.08	**100.00±0.00**	**100.00±00.00**

Validation of our learning framework (CGreg): In 12 different image and sequence tasks, we confirmed that our CG-regularization of Equation (12) is able to selectively learn to be invariant to the largest overgroup that doesn't contradict the training data, all of this *without* any evidence in the data supporting the invariance. The results are summarized in Table 1, which also shows that both standard neural networks and forced G-invariant networks —Cohen et al. (2016) for images and Lee et al. (2019); Murphy et al. (2019a); Zaheer et al. (2017) for sequences and images (color)— do not extrapolate to new environments when $\mathcal{I} \neq \emptyset$ and $\mathcal{I} \subsetneq \{1, \ldots, m\}$, respectively.

Transformation groups: Our task considers m linear automorphism groups $\mathcal{G}_1, \ldots, \mathcal{G}_m$. We generate $\mathcal{G}_{\mathcal{I}}$ from a subset $\mathcal{I} \subseteq \{1, \ldots, m\}$ of the groups, i.e., $\mathcal{G}_{\mathcal{I}} = \langle \mathcal{G}_{i \in \mathcal{I}} \rangle$. We construct $\mathcal{G}_{\mathcal{D}}$ using a subset of $\{1, \ldots, m\} \setminus \mathcal{I}$, while ensuring that $\mathcal{G}_{\mathcal{I}} \trianglelefteq \mathcal{G}_{\mathcal{D} \cup \mathcal{I}}$ in order to fulfill the conditions in Theorem 2.

Training data: $X^{(\text{hid})}$ is the canonically ordered input (e.g., upright images, sorted sequences). The training data is sampled via Equation (4) using an economical data generation process, which means obtaining the observed input $X^{(\text{tr, obs})}$ through the decomposition[1]: $X^{(\text{tr,obs})} = T_{U_{\mathcal{I}}, U_{\mathcal{D}}} \circ X^{(\text{hid})} = T_{U'_{\mathcal{I}}|U_{\mathcal{D}}} \circ T_{U_{\mathcal{D}}} \circ X^{(\text{hid})}$, where $U_{\mathcal{I}}$ and $U'_{\mathcal{I}}|U_{\mathcal{D}}$ are appropriately defined such that $P(T_{U'_{\mathcal{I}}|U_{\mathcal{D}}} = T_{\mathcal{I}}) = 1$, for some transformation $T_{\mathcal{I}} \in \mathcal{G}_{\mathcal{I}}$, and the random transformations $T_{U_{\mathcal{D}}}$ have full support $\mathcal{G}_{\mathcal{D}}$. Following Equation (3), the label Y of $X^{(\text{obs})}$ is a combination of the original label of $X^{(\text{hid})}$ and the transformation $T_{U_{\mathcal{D}}}$ applied to $X^{(\text{hid})}$.

Extrapolation task: The extrapolation test data consists of samples from the coupled random variable $X^{(\text{te, cf})}$ (Definition 1) obtained by defining $\tilde{U}_{\mathcal{I}}$ such that the support of the random transformation $T_{\tilde{U}_{\mathcal{I}}, U_{\mathcal{D}}}$ is the entire group $\mathcal{G}_{\mathcal{D} \cup \mathcal{I}}$, hence $X^{(\text{te, cf})} = T_{\tilde{U}_{\mathcal{I}}, U_{\mathcal{D}}} \circ X^{(\text{hid})}$, and Y is as before.

For *image* tasks, we consider $m = 3$ groups: $\mathcal{G}_{\text{rot}}, \mathcal{G}_{\text{color}}, \mathcal{G}_{\text{vertical-flip}}$, and sample from the MNIST dataset (with its mostly upright images) to obtain $X^{(\text{hid})}$ and its original label. For *sequence* tasks, we sample $X^{(\text{hid})}$ as a sequence of n sorted integers from a fixed vocabulary, and consider $m = \binom{n}{2}$ pairwise permutation groups: $\{\mathcal{G}_{i,j}\}_{1 \leq i < j \leq n}$. The original label for the sequence $X^{(\text{hid})}$ is obtained by applying an arithmetic function to $X^{(\text{hid})}$ that is invariant to the chosen group $\mathcal{G}_{\mathcal{I}}$.

Results: Standard neural networks such as CNNs (e.g., VGG (Simonyan and Zisserman, 2014)) (for images) and GRUs/Transformers (Cho et al., 2014; Vaswani et al., 2017) (for sequences) fail whenever the extrapolation task requires some invariance ($\mathcal{I} \neq \emptyset$), but excel at the *interpolation task* ($\mathcal{I} = \emptyset$). Adding forced $\mathcal{G}_{\mathcal{D} \cup \mathcal{I}}$-invariances via G-CNNs (Cohen et al., 2016) (for images) and permutation-invariant models (Lee et al., 2019; Murphy et al., 2019a; Zaheer et al., 2017) (for sequences) clearly fails when $\mathcal{D} \neq \emptyset$ but succeed when $\mathcal{D} = \emptyset$. Our CG-regularized neural network representations, on the other hand, achieve high extrapolation accuracy across all tasks for all choices of $\mathcal{I} \subseteq \{1, \ldots, m\}$ and $\mathcal{D} \subseteq \{1, \ldots, m\} \setminus \mathcal{I}$. These results plainly show that our approach is able to selectively learn to be invariant only to the appropriate groups. Furthermore, this $\mathcal{G}_{\mathcal{I}}$-invariance is achieved without any evidence in the training data, thanks to our novel learning paradigm that considers all G-invariances mandatory unless contradicted by the training data.

7 Conclusion

This work studied the task of learning representations that can extrapolate beyond the training data, even when presented with a single training environment. We considered the case of extrapolation from linear automorphism groups and described a framework where all G-invariances (and CG-invariances via Theorem 2) are mandatory, except the ones deemed inconsistent with the training data. Our framework replaces the classical *unseen-is-forbidden* statistical hypothesis, with our empirical results showing strong support for the proposed approach. Finally, this learning paradigm offers a promising novel research direction for neural networks to go beyond their current interpolation capabilities.

[1]Since by Theorem 2, $\mathcal{G}_{\mathcal{I}} \trianglelefteq \mathcal{G}_{\mathcal{D} \cup \mathcal{I}}$, any $T \in \mathcal{G}_{\mathcal{D} \cup \mathcal{I}}$ can be written as $T_{\mathcal{I}} \circ T_{\mathcal{D}}$.

REFERENCES

Martin Arjovsky, Léon Bottou, Ishaan Gulrajani, and David Lopez-Paz. Invariant risk minimization. *arXiv preprint arXiv:1907.02893*, 2019.

Elias Bareinboim, Juan Correa, Duligur Ibeling, and Thomas Icard. On Pearl's hierarchy and the foundations of causal inference. *ACM special volume in honor of Judea Pearl*, 2020.

Yoshua Bengio, Tristan Deleu, Nasim Rahaman, Rosemary Ke, Sébastien Lachapelle, Olexa Bilaniuk, Anirudh Goyal, and Christopher Pal. A meta-transfer objective for learning to disentangle causal mechanisms. *arXiv preprint arXiv:1901.10912*, 2019.

Michel Besserve, Naji Shajarisales, Bernhard Schölkopf, and Dominik Janzing. Group invariance principles for causal generative models. In *International Conference on Artificial Intelligence and Statistics*, pages 557–565, 2018.

Martin Billik and Gian-Carlo Rota. On reynolds operators in finite-dimensional algebras. *Journal of Mathematics and Mechanics*, 9(6):927–932, 1960.

Shuxiao Chen, Edgar Dobriban, and Jane H Lee. Invariance reduces variance: Understanding data augmentation in deep learning and beyond. *stat*, 1050:25, 2019.

Kyunghyun Cho, Bart Van Merriënboer, Dzmitry Bahdanau, and Yoshua Bengio. On the properties of neural machine translation: Encoder-decoder approaches. *arXiv preprint arXiv:1409.1259*, 2014.

Taco S Cohen, T S Cohen, and Uva Nl. Group Equivariant Convolutional Networks. page 10, 2016.

Taco S Cohen, Mario Geiger, and Maurice Weiler. A general theory of equivariant cnns on homogeneous spaces. In *Advances in Neural Information Processing Systems*, pages 9145–9156, 2019.

Pim de Haan, Dinesh Jayaraman, and Sergey Levine. Causal confusion in imitation learning. In *Advances in Neural Information Processing Systems*, pages 11698–11709, 2019.

Olivier Goudet, Diviyan Kalainathan, Philippe Caillou, Isabelle Guyon, David Lopez-Paz, and Michèle Sebag. Causal generative neural networks. *arXiv preprint arXiv:1711.08936*, 2017.

Patrick Haffner. Escaping the convex hull with extrapolated vector machines. In *Advances in Neural Information Processing Systems*, pages 753–760, 2002.

Trevor Hastie, Robert Tibshirani, and Jerome Friedman. *The elements of statistical learning*, volume 1. Springer series in statistics, 2012.

Valerie D Hollard and Juan D Delius. Rotational invariance in visual pattern recognition by pigeons and humans. *Science*, 218(4574):804–806, 1982.

Fredrik Johansson, Uri Shalit, and David Sontag. Learning representations for counterfactual inference. In *International conference on machine learning*, pages 3020–3029, 2016.

Richard S Kayne, Richard S Kayne, et al. *The antisymmetry of syntax*, volume 25. MIT press, 1994.

Piotr Kicki, Mete Ozay, and Piotr Skrzypczyński. A Computationally Efficient Neural Network Invariant to the Action of Symmetry Subgroups. *arXiv:2002.07528 [cs, stat]*, February 2020.

Gary King and Langche Zeng. The dangers of extreme counterfactuals. *Political Analysis*, 14(2): 131–159, 2006.

Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.

Juho Lee, Yoonho Lee, Jungtaek Kim, Adam R. Kosiorek, Seungjin Choi, and Yee Whye Teh. Set Transformer: A Framework for Attention-based Permutation-Invariant Neural Networks. In *Proceedings of the 36th International Conference on Machine Learning*, 2019.

Francesco Locatello, Stefan Bauer, Mario Lucic, Gunnar Raetsch, Sylvain Gelly, Bernhard Schölkopf, and Olivier Bachem. Challenging common assumptions in the unsupervised learning of disentangled representations. In *international conference on machine learning*, pages 4114–4124, 2019.

Mingsheng Long, Han Zhu, Jianmin Wang, and Michael I Jordan. Deep transfer learning with joint adaptation networks. In *International conference on machine learning*, pages 2208–2217. PMLR, 2017.

Christos Louizos, Uri Shalit, Joris M Mooij, David Sontag, Richard Zemel, and Max Welling. Causal effect inference with deep latent-variable models. In *Advances in Neural Information Processing Systems*, pages 6446–6456, 2017.

Clare Lyle, Mark van der Wilk, Marta Kwiatkowska, Yarin Gal, and Benjamin Bloem-Reddy. On the benefits of invariance in neural networks. *arXiv preprint arXiv:2005.00178*, 2020.

Gary F Marcus. Rethinking eliminative connectionism. *Cognitive psychology*, 37(3):243–282, 1998.

Haggai Maron, Ethan Fetaya, Nimrod Segol, and Yaron Lipman. On the Universality of Invariant Networks. *arXiv:1901.09342 [cs, stat]*, May 2019.

Haggai Maron, Or Litany, Gal Chechik, and Ethan Fetaya. On Learning Sets of Symmetric Elements. *arXiv:2002.08599 [cs, stat]*, February 2020.

Krikamol Muandet, David Balduzzi, and Bernhard Schölkopf. Domain generalization via invariant feature representation. In *International Conference on Machine Learning*, pages 10–18, 2013.

R. Murphy, B. Srinivasan, V. Rao, and B. Ribeiro. Janossy pooling: Learning deep permutation-invariant functions for variable-size inputs. In *International Conference on Learning Representations*, 2019a.

Ryan Murphy, Balasubramaniam Srinivasan, Vinayak Rao, and Bruno Ribeiro. Relational pooling for graph representations. In *Proceedings of the 36th International Conference on Machine Learning*, 2019b.

Ryan L. Murphy, Balasubramaniam Srinivasan, Vinayak Rao, and Bruno Ribeiro. Janossy Pooling: Learning Deep Permutation-Invariant Functions for Variable-Size Inputs. In *International Conference on Learning Representations*, September 2018.

J Neyman. Sur les applications de la theorie des probabilites aux experiences agricoles: essai des principes (masters thesis); justification of applications of the calculus of probabilities to the solutions of certain questions in agricultural experimentation. excerpts english translation (reprinted). *Stat Sci*, 5:463–472, 1923.

J Pearl and D Mackenzie. The ladder of causation. *The book of why: the new science of cause and effect. New York (NY): Basic Books*, pages 23–52, 2018.

Judea Pearl. *Causality*. Cambridge university press, 2009.

JW Pitman. On coupling of markov chains. *Zeitschrift für Wahrscheinlichkeitstheorie und verwandte Gebiete*, 35(4):315–322, 1976.

James Gary Propp and David Bruce Wilson. Exact sampling with coupled markov chains and applications to statistical mechanics. *Random Structures & Algorithms*, 9(1-2):223–252, 1996.

Joaquin Quionero-Candela, Masashi Sugiyama, Anton Schwaighofer, and Neil D Lawrence. *Dataset shift in machine learning*. The MIT Press, 2009.

Anant Raj, Stefan Bauer, Ashkan Soleymani, Michel Besserve, and Bernhard Schölkopf. Causal feature selection via orthogonal search. *arXiv preprint arXiv:2007.02938*, 2020.

Siamak Ravanbakhsh, Jeff Schneider, and Barnabás Póczos. Equivariance through parameter-sharing. In *Proceedings of the 34th International Conference on Machine Learning - Volume 70*, ICML'17, pages 2892–2901, Sydney, NSW, Australia, August 2017. JMLR.

Mateo Rojas-Carulla, Bernhard Schölkopf, Richard Turner, and Jonas Peters. Invariant models for causal transfer learning. *The Journal of Machine Learning Research*, 19(1):1309–1342, 2018.

Donald B Rubin. Estimating causal effects of treatments in randomized and nonrandomized studies. *Journal of educational Psychology*, 66(5):688, 1974.

Bernhard Schölkopf. Causality for machine learning. *arXiv preprint arXiv:1911.10500*, 2019.

Hidetoshi Shimodaira. Improving predictive inference under covariate shift by weighting the log-likelihood function. *Journal of statistical planning and inference*, 90(2):227–244, 2000.

Murray Sidman and William Tailby. Conditional discrimination vs. matching to sample: An expansion of the testing paradigm. *Journal of the Experimental Analysis of behavior*, 37(1):5–22, 1982.

Murray Sidman, Ricki Rauzin, Ronald Lazar, Sharon Cunningham, William Tailby, and Philip Carrigan. A search for symmetry in the conditional discriminations of rhesus monkeys, baboons, and children. *Journal of the experimental analysis of behavior*, 37(1):23–44, 1982.

Karen Simonyan and Andrew Zisserman. Very deep convolutional networks for large-scale image recognition. *arXiv preprint arXiv:1409.1556*, 2014.

Jin Tian and Judea Pearl. Causal discovery from changes. *UAI*, 2001.

Elise van der Pol, Daniel E Worrall, Herke van Hoof, Frans A Oliehoek, and Max Welling. Mdp homomorphic networks: Group symmetries in reinforcement learning. *arXiv preprint arXiv:2006.16908*, 2020.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, and Illia Polosukhin. Attention Is All You Need. June 2017.

Gesche Westphal-Fitch, Ludwig Huber, Juan Carlos Gomez, and W Tecumseh Fitch. Production and perception rules underlying visual patterns: effects of symmetry and hierarchy. *Philosophical Transactions of the Royal Society B: Biological Sciences*, 367(1598):2007–2022, 2012.

Dmitry Yarotsky. Universal approximations of invariant maps by neural networks. *arXiv:1804.10306 [cs]*, April 2018.

Manzil Zaheer, Satwik Kottur, Siamak Ravanbakhsh, Barnabas Poczos, Russ R Salakhutdinov, and Alexander J Smola. Deep Sets. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems 30*, pages 3391–3401. Curran Associates, Inc., 2017.

Kun Zhang, Mingming Gong, and Bernhard Schölkopf. Multi-source domain adaptation: A causal view. In *AAAI*, volume 1, pages 3150–3157, 2015.

Aaron Zweig and Joan Bruna. A functional perspective on learning symmetric functions with neural networks. *arXiv preprint arXiv:2008.06952*, 2020.

Supplementary Material of "Neural Network Extrapolations with G-invariances from a Single Environment"

A THE PRACTICAL IMPORTANCE OF THEOREM 1

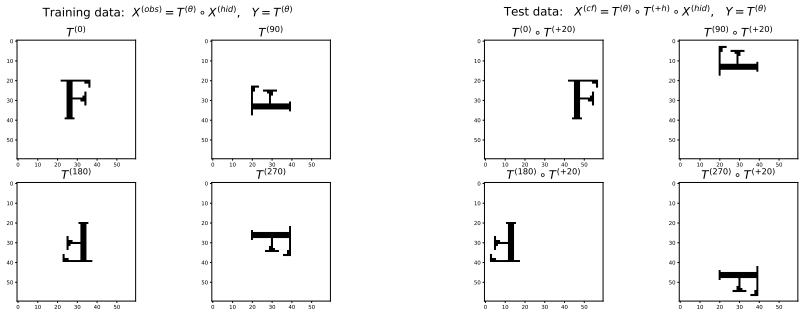

Figure 1: An example task where CG-invariance is stronger than G-invariance. The task is to predict the orientation of the image while being CG-invariant to horizontal translations.

There are real tasks where CG-invariance is stronger than G-invariance. We consider a task with 60×60 image shown in Figure 1 and two transformation groups: the rotation group $\mathcal{G}_{\text{rot}}$ and the cyclic horizontal-translation group $\mathcal{G}_{\text{h-translate}} \cong \mathbb{Z}_{60}$. Each transformation $T^{(\theta^\circ)}$ in $\mathcal{G}_{\text{rot}}$ rotates the image along its center by θ°, whereas every transformation $T^{(+h)}$ in $\mathcal{G}_{\text{h-translate}}$ translates the image horizontally by h pixels while wrapping around the edges. Let $\mathcal{G}_{\mathcal{I}} = \mathcal{G}_{\text{rot}}$ and $\mathcal{G}_{\mathcal{D}} = \mathcal{G}_{\text{h-translate}}$. The training data consists of images $X^{(\text{tr, obs})} = T^{(\theta^\circ)} \circ X^{(\text{hid})}$ for all $T^{(\theta^\circ)} \in \mathcal{G}_{\text{rot}}$, whereas the test data consists of images $X^{(\text{te, cf})} = T^{(\theta^\circ)} \circ T^{(+20)} \circ X^{(\text{hid})}$ for all $T^{(\theta^\circ)} \in \mathcal{G}_{\text{rot}}$ The task is to predict the orientation of the image, i.e., degrees of rotation. It is easy to see that the label requires CG-invariance to $\mathcal{G}_{\text{h-translate}}$ but sensitivity to $\mathcal{G}_{\text{rot}}$. We train a *strictly* $\mathcal{G}_{\text{h-translate}}$-invariant model on this dataset; whereas the model is able to achieve a 100% accuracy on training, it does poorly with 75% on test dataset, showing that it is not enough to be $\mathcal{G}_{\mathcal{I}}$-invariant to achieve CG-invariance.

B PROOFS

B.1 GENERATING ANY $T \in \mathcal{G}_{\mathcal{D} \cup \mathcal{I}}$ USING NOISES $U_{\mathcal{I}}$ AND $U_{\mathcal{D}}$

The structural causal model for $X^{(\text{obs})}$ in Equation (2) requires that any $T \in \mathcal{G}_{\mathcal{D} \cup \mathcal{I}}$ can be indexed by the hidden background variables $U_{\mathcal{I}}$ and $U_{\mathcal{D}}$. We first interpret $U_{\mathcal{D}}$ (or $U_{\mathcal{I}}$) as the random seed of a random number generator that gives an ordered sequence of transformations of $\mathcal{G}_{\mathcal{D}}$ (or $\mathcal{G}_{\mathcal{I}}$). Let $T_{\mathcal{D}}^{(1)}, \ldots, T_{\mathcal{D}}^{(a)}$ and $T_{\mathcal{I}}^{(1)}, \ldots, T_{\mathcal{I}}^{(b)}$ be those ordered sequences respectively generated by $U_{\mathcal{D}}$ and $U_{\mathcal{I}}$. Then we can obtain a transformation in $\mathcal{G}_{\mathcal{D} \cup \mathcal{I}}$ by interleaving these two sequences (in order): $T_{U_{\mathcal{D}}, U_{\mathcal{I}}} = T_{\mathcal{D}}^{(1)} \circ T_{\mathcal{I}}^{(1)} \circ T_{\mathcal{D}}^{(2)} \circ \ldots$. Since $U_{\mathcal{I}}$ and $U_{\mathcal{D}}$ can always choose the identity transformation from the respective groups, all possible transformations from the $\mathcal{G}_{\mathcal{D} \cup \mathcal{I}}$ can be generated. Note that for the same reason, it does not matter that we began interleaving the sequences from $T_{\mathcal{D}}^{(1)}$. This property of the noises to appropriately index any $T \in \mathcal{G}_{\mathcal{D} \cup \mathcal{I}}$ will be used in the proof of Theorems 1 and 2.

B.2 PROOF OF THEOREMS 1 AND 2

Theorem 1 (CG-invariance is stronger than G-invariance)**.** *Let $X^{(obs)}$ and $X^{(cf)}$ be coupled random variables per Definition 1. For a representation $\Gamma : \mathcal{X} \to \mathbb{R}^d$, $d \geq 1$, let*

$$\textit{G-inv}: \ \forall T_{\mathcal{I}} \in \mathcal{G}_{\mathcal{I}}, \ \ \Gamma(X^{(obs)}) = \Gamma(T_{\mathcal{I}} \circ X^{(obs)}),$$
$$\textit{CG-inv}: \ \Gamma(X^{(obs)}) = \Gamma(X^{(cf)}),$$

denote the conditions on Γ for $\mathcal{G}_{\mathcal{I}}$-invariance and CG-invariance respectively. Then, CG-inv $\implies$ G-inv, but G-inv $\not\Longrightarrow$ CG-inv.

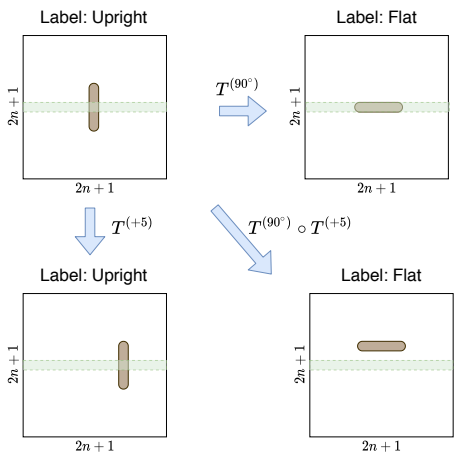

Figure 2: Counterexample to show that $\mathcal{G}_{\mathcal{I}}$-invariance does not imply CG-invariance. Given images of a rod (shown in brown), we wish to predict the orientation of the rod, i.e., whether the rod is upright or flat. In this example, we have $\mathcal{G}_{\mathcal{D}} = \mathcal{G}_{\text{rot}}$ and $\mathcal{G}_{\mathcal{I}} = \mathcal{G}_{\text{h-translate}}$ as any horizontal translation does not affect the orientation of the rod. $\Gamma : \mathcal{X} \to \mathbb{R}$ sums the pixel values across the green shaded region, and is clearly G-invariant to horizontal translations. However, Γ is not CG-invariant.

Proof. First, we will show that CG-invariance $\implies$ G-invariance. Given $\Gamma : \mathcal{X} \to \mathbb{R}^d$ is CG-invariant and $X^{(\text{obs})} = T_{U_{\mathcal{D}},U_{\mathcal{I}}} \circ X^{(\text{hid})}$, we wish to show that $\Gamma(T_{\mathcal{I}}^{\dagger} \circ X^{(\text{obs})}) = \Gamma(X^{(\text{obs})})$ for any $T_{\mathcal{I}}^{\dagger} \in \mathcal{G}_{\mathcal{I}}$. Construct a variable $X^{(\text{cf})} = T_{\mathcal{I}}^{\dagger} \circ T_{U_{\mathcal{D}},U_{\mathcal{I}}} \circ X^{(\text{hid})}$. Recall that $T_{U_{\mathcal{D}},U_{\mathcal{I}}}$ was generated using two separate sequences of transformations obtained from the background variables $U_{\mathcal{D}}$ and $U_{\mathcal{I}}$ respectively. Then, we can always find a $\widetilde{U}_{\mathcal{I}}$ such that $T_{U_{\mathcal{D}},\widetilde{U}_{\mathcal{I}}} = T_{\mathcal{I}}^{\dagger} \circ T_{U_{\mathcal{D}},U_{\mathcal{I}}} \circ X^{(\text{hid})}$ such that $X^{(\text{cf})} = T_{U_{\mathcal{D}},\widetilde{U}_{\mathcal{I}}} \circ X^{(\text{hid})}$ is actually coupled with $X^{(\text{obs})}$. Now since Γ is CG-invariant, we have that $\Gamma(T_{\mathcal{I}}^{\dagger} \circ X^{(\text{obs})}) = \Gamma(X^{(\text{cf})}) = \Gamma(X^{(\text{obs})})$, thus proving that Γ is $\mathcal{G}_{\mathcal{I}}$-invariant.

Next, we will show G-invariance $\not\Longrightarrow$ CG-invariance by constructing a counterexample. Let $X^{(\text{hid})} \in \mathbb{R}^{(2n+1)\times(2n+1)}$ be the $(2n+1) \times (2n+1)$ grayscale image of an upright rod as shown in Figure 2. Consider two groups that act on this image: the rotation group $\mathcal{G}_{\text{rot}} = \{T^{(k)}\}_{k\in\{0^\circ,90^\circ,180^\circ,270^\circ\}}$ and the cyclic horizontal-translation group $\mathcal{G}_{\text{h-translate}} = \{T^{(+u)}\}_{u\in\mathbb{Z}_n}$. Let $\mathcal{G}_{\mathcal{D}} = \mathcal{G}_{\text{rot}}$ and $\mathcal{G}_{\mathcal{I}} = \mathcal{G}_{\text{h-translate}}$ and the label of the image Y deterministically given by the orientation of the rod: upright ($Y = 0$) or flat ($Y = 1$).

Now consider a representation $\Gamma : \mathbb{R}^{(2n+1)\times(2n+1)} \to \mathbb{R}$ such that $\Gamma(X) = \sum_{i=1}^{2n+1} X_{n,i}$ finds the sum of the middle row of the image. Note that a) Γ is able to distinguish between the labels for the training data (that is transformed by $\mathcal{G}_{\text{h-translate}}$ only via the identity $T^{(+0)}$; see top row of Figure 1), and b) Γ is $\mathcal{G}_{\text{h-translate}}$-invariant.

We can define the random variables $X^{(\text{obs})} = T^{(90^\circ)} \circ X^{(\text{hid})}$ and $X^{(\text{cf})} = T^{(90^\circ)} \circ T^{(+5)} \circ X^{(\text{hid})}$ coupled with respect to the transformation $T^{(90^\circ)}$ in $\mathcal{G}_{\mathcal{D}}$. Then, as shown in Figure 2, $\Gamma(X^{(\text{cf})}) = \Gamma(T^{(90^\circ)} \circ T^{(+5)} \circ X) \neq \Gamma(T^{(90^\circ)} \circ X) = \Gamma(X^{(\text{obs})})$, thus showing that Γ is not CG-invariant.

□

Theorem 2. *If $\mathcal{G}_{\mathcal{I}}$ is a normal subgroup of $\mathcal{G}_{\mathcal{D}\cup\mathcal{I}}$, then CG-inv $\iff$ G-inv.*

Proof. We only need to prove that G-invariance $\implies$ CG-invariance when $\mathcal{G}_{\mathcal{I}}$ is a normal subgroup of $\mathcal{G}_{\mathcal{D}\cup\mathcal{I}}$. We begin with a representation Γ that is $\mathcal{G}_{\mathcal{I}}$-invariant and consider the simpler case when $X^{(\text{obs})}$ is obtained by applying only $r = 2$ transformations to $X^{(\text{hid})}$, and is given by: $X^{(\text{obs})} = T_{\mathcal{D}} \circ T_{\mathcal{I}} \circ X^{(\text{hid})}$ for arbitrary transformations $T_{\mathcal{D}} \in \mathcal{G}_{\mathcal{D}}$ and $T_{\mathcal{I}} \in \mathcal{G}_{\mathcal{I}}$. Then the coupled variable

is $X^{(\text{cf})} = T_{\mathcal{D}} \circ \widetilde{T}_{\mathcal{I}} \circ X^{(\text{hid})}$ for another arbitrary transformation $\widetilde{T}_{\mathcal{I}} \in \mathcal{G}_{\mathcal{I}}$. The condition for CG-invariance with respect to $\mathcal{G}_{\mathcal{I}}$ requires that

$$\text{(requirement:)} \quad \Gamma(X^{(\text{obs})}) = \Gamma(T_{\mathcal{D}} \circ T_{\mathcal{I}} \circ X^{(\text{hid})}) = \Gamma(T_{\mathcal{D}} \circ X^{(\text{hid})}) = \Gamma(T_{\mathcal{D}} \circ \widetilde{T}_{\mathcal{I}} \circ X^{(\text{hid})}) = \Gamma(X^{(\text{cf})}) \tag{14}$$

Since $\mathcal{G}_{\mathcal{I}}$ is a normal subgroup of $\mathcal{G}_{\mathcal{D}\cup\mathcal{I}}$ and $\mathcal{G}_{\mathcal{D}} \leq \mathcal{G}_{\mathcal{D}\cup\mathcal{I}}$, we have

$$\forall T_{\mathcal{D}} \in \mathcal{G}_{\mathcal{D}}, \ \ \forall T_{\mathcal{I}} \in \mathcal{G}_{\mathcal{I}}, \ \ T_{\mathcal{D}} \circ T_{\mathcal{I}} \circ T_{\mathcal{D}}^{-1} \in \mathcal{G}_{\mathcal{I}},$$

or equivalently,

$$\begin{aligned} &\forall T_{\mathcal{D}} \in \mathcal{G}_{\mathcal{D}}, \ \ \forall T_{\mathcal{I}} \in \mathcal{G}_{\mathcal{I}}, \ \exists T'_{\mathcal{I}}, \ \text{ s.t.,} \\ &\quad T_{\mathcal{D}} \circ T_{\mathcal{I}} \circ T_{\mathcal{D}}^{-1} = T'_{\mathcal{I}} \\ &\implies \quad T_{\mathcal{D}} \circ T_{\mathcal{I}} = T'_{\mathcal{I}} \circ T_{\mathcal{D}} \end{aligned} \tag{15}$$

(A special case is when the groups $\mathcal{G}_{\mathcal{D}}$ and $\mathcal{G}_{\mathcal{I}}$ commute, as then $T_{\mathcal{D}} \circ T_{\mathcal{I}} = T_{\mathcal{I}} \circ T_{\mathcal{D}}$.)

Then,

$$\begin{aligned} \Gamma(X^{(\text{obs})}) &= \Gamma(T_{\mathcal{D}} \circ T_{\mathcal{I}} \circ X^{(\text{hid})}) \\ &= \Gamma(T'_{\mathcal{I}} \circ T_{\mathcal{D}} \circ X^{(\text{hid})}) && \text{(there exists such a } T'_{\mathcal{I}} \in \mathcal{G}_{\mathcal{I}}) \\ &= \Gamma(T_{\mathcal{D}} \circ X^{(\text{hid})}) && (\Gamma \text{ is invariant to } \mathcal{G}_{\mathcal{I}}) \end{aligned}$$

Similarly, we can prove that $\Gamma(X^{(\text{cf})}) = \Gamma(T_{\mathcal{D}} \circ \tilde{T}_{\mathcal{I}} \circ X^{(\text{hid})}) = \Gamma(T_{\mathcal{D}} \circ X^{(\text{hid})})$, thus satisfying the requirement of CG-invariance for $r = 2$ transformations in Equation (14).

Extension to the case when $r > 2$ transformations are applied to $X^{(\text{hid})}$ is trivial as any transformation $T_{U_{\mathcal{D}},U_{\mathcal{I}}} = \cdots \circ T_{\mathcal{D}}^{(i)} \circ T_{\mathcal{I}}^{(k)} \circ T_{\mathcal{D}}^{(i+1)} \circ \cdots$ can be written in the form $T_{\mathcal{I}}^{\dagger} \circ T_{\mathcal{D}}^{(1)} \circ T_{\mathcal{D}}^{(2)} \circ \cdots$ by repeatedly applying the normal subgroup property in Equation (15). Then $\Gamma(T_{U_{\mathcal{D}},U_{\mathcal{I}}} \circ X^{(\text{hid})}) = \Gamma(T_{\mathcal{I}}^{\dagger} \circ T_{\mathcal{D}}^{(1)} \circ T_{\mathcal{D}}^{(2)} \circ \cdots \circ X^{(\text{hid})}) = \Gamma(T_{\mathcal{D}}^{(1)} \circ T_{\mathcal{D}}^{(2)} \circ \cdots \circ X^{(\text{hid})})$ as Γ is $\mathcal{G}_{\mathcal{I}}$-invariant. Clearly, the same holds for $\Gamma(T_{U_{\mathcal{D}},\tilde{U}_{\mathcal{I}}} \circ X^{(\text{hid})})$, thus proving that Γ is CG-invariant. □

B.3 Proofs of Lemma 1, Lemma 2 and Theorem 3

Lemma 1 (Reynolds operator (Billik and Rota, 1960))**.** *Let $\mathcal{G}$ be a finite linear automorphism group over vec$(\mathcal{X})$. Then,*

$$\overline{T} = \frac{1}{|\mathcal{G}|} \sum_{T \in \mathcal{G}} T \tag{8}$$

is a $\mathcal{G}$-invariant linear automorphism, i.e., $\forall T_{\dagger} \in \mathcal{G}$ and $\forall \boldsymbol{x} \in$ vec$(\mathcal{X})$, it must be that $\overline{T}(T_{\dagger}\boldsymbol{x}) = \overline{T}\boldsymbol{x}$.

Proof. Note that because $\exists T_{\dagger}^{-1} \in \mathcal{G}$, we can define $\mathcal{G}_{\dagger} = \{TT_{\dagger}^{-1} : \forall T \in \mathcal{G}\}$. Since $\forall T \in \mathcal{G}$, $TT_{\dagger}^{-1} \in \mathcal{G}$, we have $\mathcal{G}_{\dagger} \subseteq \mathcal{G}$. Because $T_{\dagger}^{-1}$ is a bijection it must be that $|\mathcal{G}_{\dagger}| = |\mathcal{G}|$. Hence, $\mathcal{G}_{\dagger} = \mathcal{G}$. □

Lemma 2. *If $\mathcal{W}$ denotes the left eigenspace corresponding to the eigenvalue 1 of the Reynolds operator $\overline{T}$ for the group $\mathcal{G}$,* **then** *$\forall b \in \mathbb{R}$, the linear transformation $\gamma(\boldsymbol{x}; \boldsymbol{w}, b) = \boldsymbol{w}^T\boldsymbol{x} + b$ is invariant to any transformation $T \in \mathcal{G}$* **if and only if** *$\boldsymbol{w} \in \mathcal{W}$.*

Proof. Sufficiency: Let $\{\boldsymbol{w}_i^T\}_{i=1}^{d_W}$ be the set of left eigenvectors of $\overline{T}$ with eigenvalue 1 and constitute the orthogonal basis for $\mathcal{W}$. Consider any non-zero $\boldsymbol{w} \in \mathcal{W}$, then

$$\boldsymbol{w}^T = \sum_{i=1}^{d_W} \alpha_i \boldsymbol{w}_i^T = \sum_{i=1}^{d_W} \alpha_i \boldsymbol{w}_i^T \overline{T} \tag{16}$$

for some coefficients $\{\alpha_i\}_{i=1}^{d_W}$. For any $\boldsymbol{x} \in \text{vec}(\mathcal{X})$ and any $T \in \mathcal{G}$ we have,

$$\begin{aligned}
\gamma(T\boldsymbol{x}; \boldsymbol{w}, b) &= \boldsymbol{w}^T(T\boldsymbol{x}) + b \\
&= \sum_{i=1}^{d_W} \alpha_i \boldsymbol{w}_i^T \overline{T}(T\boldsymbol{x}) + b && \text{(using Equation (16))} \\
&= \sum_{i=1}^{d_W} \alpha_i \boldsymbol{w}_i^T \overline{T}\boldsymbol{x} + b && \text{(from Lemma 1)} \\
&= \gamma(\boldsymbol{x}; \boldsymbol{w}, b)
\end{aligned}$$

Necessity: Given a non-zero $\boldsymbol{w} \in \mathcal{W}$ and $b \in \mathbb{R}$, let $\gamma(T\boldsymbol{x}; \boldsymbol{w}, b) = \gamma(\boldsymbol{x}; \boldsymbol{w}, b)$ for all $\boldsymbol{x} \in \text{vec}(\mathcal{X})$ and all $T \in \mathcal{G}$. Then,

$$\begin{aligned}
& \boldsymbol{w}^T T\boldsymbol{x} = \boldsymbol{w}^T\boldsymbol{x}\ , \quad \forall \boldsymbol{x}, \forall T \\
\implies & \boldsymbol{w}^T T = \boldsymbol{w}^T\ , \quad \forall T \\
\implies & \boldsymbol{w}^T \sum_{T \in \mathcal{G}} T = |\mathcal{G}| \boldsymbol{w}^T && \text{(summing over all } T \in \mathcal{G}) \\
\implies & \boldsymbol{w}^T \overline{T} = \boldsymbol{w}^T\ .
\end{aligned}$$

Hence proved that $\boldsymbol{w}^T$ is a left eigenvector of $\overline{T}$ with eigenvalue 1.

□

Theorem 3 (Invariant subspace bases can be partially ordered by invariance strength)**.** *Let $\mathcal{W}_i \subseteq vec(\mathcal{X})$ be the left eigenspace corresponding to the eigenvalue 1 of the Reynolds operator $\overline{T}_i$ for group $\mathcal{G}_i$, $i = 1, \ldots, m$. We construct the invariant subspace partitions*

$$\widetilde{\mathcal{B}}_M = \bigcap_{i \in M} \mathcal{W}_i\ ; \quad \mathcal{B}_M = \widetilde{\mathcal{B}}_M - proj_{\mathcal{B}_{\supsetneq M}}(\widetilde{\mathcal{B}}_M)\ , \quad \forall M \in \wp(\{1, \ldots, m\}) \setminus \emptyset, \tag{9}$$

where $\wp$ is the power set, $\mathcal{B}_{\supsetneq M} = \bigoplus_{N \supsetneq M} \mathcal{B}_N$, $proj_{\mathcal{A}_1}(\mathcal{A}_2)$ finds the orthogonal projection of a subspace $\mathcal{A}_2$ onto the subspace $\mathcal{A}_1$, and $\bigoplus$ is the direct sum operator. **Then***, the linear transformation $\gamma(\boldsymbol{x}; \boldsymbol{w}, b) = \boldsymbol{w}^T\boldsymbol{x} + b,\ b \in \mathbb{R}, \forall \boldsymbol{w} \in \mathcal{B}_M \setminus \{\boldsymbol{0}\}$, is $\mathcal{G}_M$-invariant but not $\mathcal{G}_j$-invariant $\forall j \in \overline{M}$.*

Proof. Throughout this proof, we will slightly abuse notation by calling a $\boldsymbol{w} \in \text{vec}(\mathcal{X})$ as $\mathcal{G}$-invariant for some group $\mathcal{G}$, where we mean the transformation $\gamma(\cdot; \boldsymbol{w}, b), b \in \mathbb{R}$ is $\mathcal{G}$-invariant.

We begin our proof by showing that any non-zero $\boldsymbol{w} \in \text{vec}(\mathcal{X})$ is $\mathcal{G}_M$-invariant where $\mathcal{G}_M = \langle \cup_{i \in M} \mathcal{G}_i \rangle$ iff $\boldsymbol{w} \in \widetilde{\mathcal{B}}_M$. Since $\boldsymbol{w} \in \widetilde{\mathcal{B}}_M \iff \boldsymbol{w} \in \mathcal{W}_i,\ \forall i \in M$, we have from Lemma 2 that $\boldsymbol{w}$ is $\mathcal{G}_i$-invariant for all $i \in M$. It is easy to see that any non-zero $\boldsymbol{w}$ is $\mathcal{G}_M$-invariant iff it is $\mathcal{G}_i$-invariant for all $i \in M$. Note that it is possible to have $\widetilde{\mathcal{B}}_M = \{\boldsymbol{0}\}$ implying that there is no non-zero $\boldsymbol{w} \in \text{vec}(\mathcal{X})$ that is $\mathcal{G}_M$-invariant.

Now consider the subspace $\mathcal{B}_{\supsetneq M} = \bigoplus_{N \supsetneq M} \mathcal{B}_N$, where $\bigoplus$ is the direct sum operator. Using induction on the size of M, we first show that $\mathcal{B}_{\supsetneq M} = \bigoplus_{N \supsetneq M} \widetilde{\mathcal{B}}_N$. The statement trivially holds for $\mathcal{B}_{\supsetneq \{1, \ldots, m\}}$. Then the induction hypothesis is that for all sets M such that $|M| > k$,

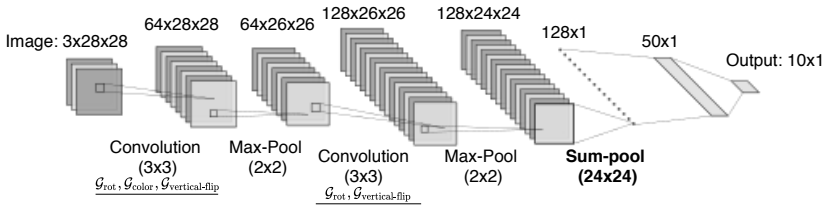

Figure 3: An example architecture of CG-invariant CNN architecture.

$\mathcal{B}_{\supsetneq M} = \bigoplus_{N \supsetneq M} \widetilde{\mathcal{B}}_N$. We prove that the statement holds for all sets M with $|M| = k$ as follows,

$$
\begin{aligned}
\mathcal{B}_{\supsetneq M} &= \bigoplus_{N \supsetneq M} \mathcal{B}_N \\
&= \bigoplus_{\substack{N \supsetneq M \\ |N| = \lceil |M| + 1}} (\mathcal{B}_N \oplus \mathcal{B}_{\supsetneq N}) \\
&= \bigoplus_{\substack{N \supsetneq M \\ |N| = \lceil |M| + 1}} \left(\left(\widetilde{\mathcal{B}}_N - \text{proj}_{\mathcal{B}_{\supsetneq N}}(\widetilde{\mathcal{B}}_N) \right) \oplus \mathcal{B}_{\supsetneq N} \right) && \text{(Definition of } \mathcal{B}_N\text{)} \\
&= \bigoplus_{\substack{N \supsetneq M \\ |N| = \lceil |M| + 1}} \left(\widetilde{\mathcal{B}}_N \oplus \mathcal{B}_{\supsetneq N} \right) \\
& && \text{(For vector subspaces } V \text{ and } W\text{, } (V - \text{proj}_W(V)) \oplus W = V \oplus W\text{)} \\
&= \bigoplus_{\substack{N \supsetneq M \\ |N| = \lceil |M| + 1}} \left(\widetilde{\mathcal{B}}_N \oplus \widetilde{\mathcal{B}}_{\supsetneq N} \right) && \text{(Inductive hypothesis holds for sets } N \text{ as } |N| > k\text{)} \\
&= \bigoplus_{N \supsetneq M} \widetilde{\mathcal{B}}_N \,.
\end{aligned}
$$

This proves our claim that $\mathcal{B}_{\supsetneq M} = \bigoplus_{N \supsetneq M} \widetilde{\mathcal{B}}_N$. Now letting $P \supsetneq M$, it is clear that $\mathcal{B}_{\supsetneq M} \supseteq \widetilde{\mathcal{B}}_P$, which implies from Lemma 2 that any $\boldsymbol{w} \in \text{vec}(\mathcal{X})$ that is $\mathcal{G}_P$-invariant lies inside $\mathcal{B}_{\supsetneq M}$. Now, the orthogonalization step ensures that $\mathcal{B}_M \perp \mathcal{B}_{\supsetneq M}$ and thus, $\mathcal{B}_M \perp \widetilde{\mathcal{B}}_P$ and $\mathcal{B}_M \cap \widetilde{\mathcal{B}}_P = \{\mathbf{0}\}$. Hence there is no non-zero $\boldsymbol{w} \in \mathcal{B}_M$ such that $\boldsymbol{w}$ is $\mathcal{G}_P$-invariant. This applies for all $P \supsetneq M$.

Finally, we consider supersets of M of the form $P' = M \cup \{j\}$ for $j \in \overline{M}$. If a nonzero $\boldsymbol{w} \in \mathcal{B}_M$ is invariant to $\mathcal{G}_j$, then it will hold that $\boldsymbol{w}$ is invariant to $\mathcal{G}_{P'}$ resulting in a contradiction. Hence, we have that if $\mathcal{B}_M \neq \{\mathbf{0}\}$, then any $\boldsymbol{w} \in \mathcal{B}_M \setminus \{\mathbf{0}\}$ is $\mathcal{G}_M$-invariant but not $\mathcal{G}_j$-invariant for any $j \in \overline{M}$.

□

C ARCHITECTURES

C.1 IMAGES

An example CG-invariant CNN architecture is depicted in Figure 3. Majority of the CNN architecture remains the same with the exception that the filters are obtained using the bases of the subspaces obtained in Theorem 3 for the given set of groups. We use the three groups $\mathcal{G}_{\text{rot}}$, $\mathcal{G}_{\text{color}}$ and $\mathcal{G}_{\text{vertical-flip}}$ for the first convolutional layer, but remove $\mathcal{G}_{\text{color}}$ in the further layers as we do not wish to be invariant to channel permutation after the first layer. Once the filter is obtained as a linear combination of the bases, it is convolved with the image or the feature maps. After all the convolutional and max-pooling layers, we use a sum-pooling layer over the entire channel to ensure that the model can be invariant to the transformations (e.g., rotations) on the whole image if needed.

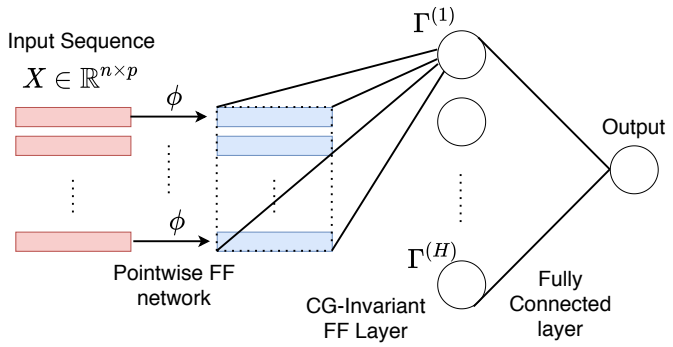

Figure 4: An example architecture of CG-invariant feedforward network.

C.2 Sequences

A CG-invariant architecture for sequences is depicted in Figure 4. We begin by constructing the bases according to Theorem 3 given the $m = \binom{n}{2}$ groups pairwise permutation groups: $\{\mathcal{G}_{i,j}\}_{i<j}$. Then, each element of the sequence is passed through a shared feedforward network ϕ that returns a representation $\boldsymbol{Z} \in \mathbb{R}^{n \times p'}$. Each neuron in the CG-invariant layer shares the constructed bases, we compute the weight matrix for the neuron h using the bases and $\boldsymbol{\omega}_{\cdot,h}$ in Equation (10). Finally, any number of fully connected layers can be stacked after the CG-invariant layer for the final output.

D Datasets and Empirical Results

D.1 Images

Datasets. We consider the standard MNIST dataset and its subset MNIST-34 that contains only the digits 3 & 4 alone. We chose to experiment on the MNIST-34 dataset since it does not have digits that can be confused with a rotation transformation (e.g., 6 and 9) or are invariant to some rotations (e.g., 0, 1 and 8), thus avoiding any confounding factors while testing our hypothesis. We also experiment on the full MNIST dataset to depict the scenario when the data does contain these contradictions. First, we modify all the images in the dataset to have three RGB color channels and color each digit *red* initially, i.e., all active pixels in the digit are set to (255, 0, 0). We sample $X^{(\text{hid})}$ from this dataset with the target digit as its original label.

Groups. We consider $m = 3$ linear automorphism groups on images: the rotation group $\mathcal{G}_{\text{rot}} = \{T^{(0^\circ)}, T^{(90^\circ)}, T^{(180^\circ)}, T^{(270^\circ)}\}$ that rotates the entire image by multiples of 90°, the channel-permutation group $\mathcal{G}_{\text{color}} \cong \mathbb{S}_3$ that permutes the three RGB channels of the image, and the vertical flip group $\mathcal{G}_{\text{vertical-flip}} = \{T^{(0)}, T^{(v)}\}$ that vertically flips the image.

Tasks. For both MNIST and MNIST-34 datasets, we consider 4 classification tasks where each task represents the case when the target Y is invariant to a different subset of $\{\mathcal{G}_{\text{rot}}, \mathcal{G}_{\text{flip}}, \mathcal{G}_{\text{color}}\}$, i.e., invariant to all three groups, to two, to one, invariant to none (and sensitive to the remaining groups). We consider the following subsets of the 3 groups: **i)** $\{\mathcal{G}_{\text{rot}}, \mathcal{G}_{\text{color}}, \mathcal{G}_{\text{vertical-flip}}\}$, **ii)** $\{\mathcal{G}_{\text{rot}}, \mathcal{G}_{\text{vertical-flip}}\}$, **iii)** $\{\mathcal{G}_{\text{color}}\}$, **iv)** $\emptyset$, and generate $\mathcal{G}_{\mathcal{I}}$ from these subsets. We generate $\mathcal{G}_{\mathcal{D}}$ from the subset $\{\mathcal{G}_{\text{rot}}, \mathcal{G}_{\text{flip}}, \mathcal{G}_{\text{color}}\} \setminus \mathcal{G}_{\mathcal{I}}$ (our choices ensure that $\mathcal{G}_{\mathcal{I}} \trianglelefteq \mathcal{G}_{\mathcal{D} \cup \mathcal{I}}$, thus satisfying the conditions of Theorem 2).

Training data: $X^{(\text{hid})}$ is the canonically ordered image in the MNIST datasets. The training data is sampled via Equation (4) using an economical data generation process, which means obtaining the observed input $X^{(\text{tr, obs})}$ through the decomposition: $X^{(\text{tr,obs})} = T_{U_{\mathcal{I}}, U_{\mathcal{D}}} \circ X^{(\text{hid})} = T_{U'_{\mathcal{I}}|U_{\mathcal{D}}} \circ T_{U_{\mathcal{D}}} \circ X^{(\text{hid})}$, where $U_{\mathcal{I}}$ and $U'_{\mathcal{I}}|U_{\mathcal{D}}$ are appropriately defined such that $P(T_{U'_{\mathcal{I}}|U_{\mathcal{D}}} = T_{\mathcal{I}}) = 1$, for some transformation $T_{\mathcal{I}} \in \mathcal{G}_{\mathcal{I}}$, and the random transformations $T_{U_{\mathcal{D}}}$ have full support $\mathcal{G}_{\mathcal{D}}$. In other words, $\mathcal{G}_{\mathcal{I}}$ transforms the images in the training data with a single transformation $T_{\mathcal{I}} \in \mathcal{G}_{\mathcal{I}}$. For instance, if $\mathcal{G}_{\mathcal{I}} = \mathcal{G}_{\text{rot, vertical-flip}}$ and $\mathcal{G}_{\mathcal{D}} = \mathcal{G}_{\text{color}}$, then the training data consists of upright and unflipped images ($T_{\mathcal{I}}$ chosen to be identity transformation) with different permutations of the channels. The task is to

Table 2: **(MNIST-34.)** Validation and Extrapolation test accuracies (%) with 95% confidence intervals for different CG-regularization strength λ in Equation (12). λ is chosen only based on the validation accuracy: maximum λ that achieves the within 5% of the best validation accuracy (shown in **bold**).

		$\mathcal{I} \subseteq \{\text{rot}, \text{color}, \text{vflip}\}$							
		rot,color,vflip		rot,vflip		color		$\emptyset$	
Model	λ	Val. acc (%)	Test acc (%)	Val. acc (%)	Test acc (%)	Val. acc (%)	Test acc (%)	Val. acc (%)	Test acc (%)
VGG + CG-reg	0.0	99.94 (0.17)	49.51 (2.36)	99.83 (0.09)	43.57 (3.69)	97.15 (0.27)	15.71 (5.46)	95.65 (0.39)	96.30 (0.68)
	0.1	99.92 (0.09)	78.72 (25.75)	99.86 (0.21)	73.98 (16.33)	96.48 (0.77)	96.27 (1.01)	94.95 (0.54)	95.56 (0.61)
	1.0	99.71 (0.22)	85.42 (29.66)	99.77 (0.25)	75.64 (20.52)	96.12 (1.26)	96.20 (1.11)	94.01 (1.51)	94.42 (1.38)
	2.0	99.55 (0.33)	94.88 (0.84)	99.56 (0.66)	82.59 (28.92)	95.23 (0.99)	95.61 (1.75)	**94.05 (1.50)**	**94.49 (1.49)**
	10.0	**99.00 (1.18)**	**94.89 (7.49)**	**98.43 (2.00)**	**95.78 (7.11)**	**93.34 (8.42)**	**94.16 (6.43)**	88.42 (19.36)	88.68 (20.13)

Table 3: **(MNIST.)** Validation and Extrapolation test accuracies (%) with 95% confidence intervals for different CG-regularization strength λ in Equation (12). λ is chosen only based on the validation accuracy: maximum λ that achieves the within 5% of the best validation accuracy (shown in **bold**).

		$\mathcal{I} \subseteq \{\text{rot}, \text{color}, \text{vflip}\}$							
		rot,color,vflip		rot,vflip		color		$\emptyset$	
Model	λ	Val. acc (%)	Test acc (%)	Val. acc (%)	Test acc (%)	Val. acc (%)	Test acc (%)	Val. acc (%)	Test acc (%)
VGG + CG-reg	0.0	99.17 (0.17)	11.93 (1.87)	98.80 (0.14)	25.81 (0.92)	91.50 (0.35)	4.19 (2.12)	91.80 (0.60)	91.60 (0.32)
	0.1	98.62 (0.05)	29.48 (0.98)	98.34 (0.17)	30.12 (4.05)	90.11 (0.58)	87.23 (3.68)	88.30 (1.21)	88.48 (1.17)
	1.0	98.49 (0.24)	44.23 (15.45)	98.29 (0.21)	40.13 (4.83)	90.24 (0.46)	90.23 (0.99)	88.76 (1.28)	88.65 (1.30)
	2.0	98.45 (0.13)	55.24 (2.29)	98.34 (0.34)	47.14 (15.17)	89.98 (0.24)	89.71 (0.89)	89.50 (1.35)	89.45 (1.43)
	10.0	**97.76 (0.74)**	**64.99 (2.76)**	**95.21 (6.55)**	**62.68 (6.02)**	**88.80 (2.11)**	**88.69 (2.11)**	**90.54 (1.04)**	**90.89 (0.43)**

predict the original label of the image (i.e., the digit) and the transformation $T_{\mathcal{D}}$ that was applied. In the above example, the task is to predict the digit and its color.

Extrapolation task: The extrapolation test data consists of samples from the coupled random variable $X^{(\text{te, cf})}$ (Definition 1) obtained by defining $\tilde{U}_{\mathcal{I}}$ such that the support of the random transformation $T_{\tilde{U}_{\mathcal{I}}, U_{\mathcal{D}}}$ is the entire group $\mathcal{G}_{\mathcal{D} \cup \mathcal{I}}$, hence $X^{(\text{te, cf})} = T_{\tilde{U}_{\mathcal{I}}, U_{\mathcal{D}}} \circ X^{(\text{hid})}$, and Y is as before. Once again, if $\mathcal{G}_{\mathcal{I}} = \mathcal{G}_{\text{rot, vertical-flip}}$ and $\mathcal{G}_{\mathcal{D}} = \mathcal{G}_{\text{color}}$, then the extrapolation test data consists of images randomly rotated, flipped and channel permuted, while the task is the same: predict the digit and its color.

In order to evaluate the models, we use 5-fold cross-validation procedure as follows. We divide the training and test datasets that are pre-split in MNIST and MNIST-34 datasets into 5 folds each. We use the above procedure to transform the training data and the test data. Then in each iteration i of the cross-validation procedure, we leave out i-th fold of the transformed training data and i-th fold of the extrapolated test data. Further, we use 20% of the training data as validation data for hyperparameter tuning and early stopping.

Baselines and Architecture. For all methods, we use a VGG architecture (Simonyan and Zisserman, 2014) with 8 convolutional layers each having 128 channels except the first layer which has 64 channels. All convolutional layers have a receptive field of size 3×3, stride 1 and padding 1. A max-pooling layer is added after every two convolutional layers. Two feedforward layers at the end give the final output. We compare our approach with the standard CNNs and Group-equivariant CNNs (G-CNNs) (Cohen et al., 2016) with the $p4m$ group. We modified G-CNN such that it has invariances to all the 3 groups strictly enforced via a) coset-pooling (Cohen et al., 2016) after each layer and b) adding together the 3 input RGB channels. For our approach, we replace the standard convolutional layer in the VGG architecture by CG-invariant layers with bases constructed from $\mathcal{G}_{\text{rot}}, \mathcal{G}_{\text{color}}$ and $\mathcal{G}_{\text{vertical-flip}}$. An example architecture with only 2 convolutional layers is shown in Figure 3.

We optimize all models using SGD with momentum with learning rate in $\{10^{-2}, 10^{-3}, 10^{-4}\}$ and a batch size of 64. We use early stopping on validation loss to select the best model. Further, we use validation loss to select the best set of hyperparameters for each model. Tables 2 and 3 show the effect of regularization strength on the performance of the model. We observe that a constant value of $\lambda = 10$ performs considerably well across all tasks. Note however that we choose the maximum value of λ that is within a 5% threshold of the maximum validation accuracy obtained from any value of λ.

D.2 SEQUENCES

Dataset & Tasks. For Sequence tasks, we generate $X^{(\text{hid})} = (X_i)_{i=1}^{10}$ as a sequence of $n = 10$ canonically ordered integers uniformly sampled with replacement from a fixed vocabulary set $\{1, \ldots, 99\}$. The canonical ordering is fixed for a given set of integers sampled: the corresponding sequence $X^{(\text{hid})}$ is always either in an increasing order or a decreasing order.

Groups. We consider $m = \binom{n}{2}$ pairwise permutation groups: $\{\mathcal{G}_{i,j}\}_{1 \leq i < j \leq n}$. We choose 4 different subsets of the given m groups shown in the first column of the Table 4. $\mathcal{G}_{\mathcal{D}}$ is always the identity group to ensure that $\mathcal{G}_{\mathcal{I}} \trianglelefteq \mathcal{G}_{\mathcal{D} \cup \mathcal{I}}$. The label for the sequence $X^{(\text{hid})}$ is obtained by applying an arithmetic function to $X^{(\text{hid})}$ that is invariant to the chosen group $\mathcal{G}_{\mathcal{I}}$. The arithmetic functions are given in the second column of Table 4.

Table 4: Sequence tasks

$\mathcal{G}_{\mathcal{I}}$	Target Y
$\langle \{\mathcal{G}_{i,j}\}_{1 \leq i < j \leq n} \rangle$	$Y_{\{1 \ldots n\}} = \sum_{i=1}^{10} X_i$
$\langle \{\mathcal{G}_{i,j}\}_{2 \leq i < j \leq n} \rangle$	$Y_{\{2 \ldots n\}} = \sum_{i=2}^{10} X_i$
$\langle \{\mathcal{G}_{i,i+2k}\}_{1 \leq i < i+2k \leq n} \rangle$	$Y_{\{\text{even}\},\{\text{odd}\}} = \sum_{i=1}^{5} (X_{2i} - X_{2i-1})$
$\{\text{Id}\}$	$Y_{\emptyset} = \sum_{i=1}^{10} \prod_{j=1}^{i} \mathbf{1}(X_j \geq 20)$

Since $\mathcal{G}_{\mathcal{D}}$ is the identity group and the training data is economically sampled, $X^{(\text{tr, obs})} = T_{U_{\mathcal{D}}, U_{\mathcal{I}}} \circ X^{(\text{hid})} = T_{U_{\mathcal{I}}} \circ X^{(\text{hid})}$ in training for a single $T_{U_{\mathcal{I}}} \in \mathcal{G}_{\mathcal{I}}$. In the extrapolated test data, $X^{(\text{te, cf})} = T_{U_{\mathcal{D}}, \widetilde{U}_{\mathcal{I}}} \circ X^{(\text{hid})} = T_{\widetilde{U}_{\mathcal{I}}} \circ X^{(\text{hid})}$ for any $T_{\widetilde{U}_{\mathcal{I}}} \in \mathcal{G}_{\mathcal{I}}$. Sizes of the training data and the extrapolated test data are fixed at 8000 and 2000 respectively. We repeat all the experiments for 5 different random seeds.

Baselines and Architecture. We compare our approach with a) standard sequence models, specifically Transformers (Vaswani et al., 2017) and GRUs (Cho et al., 2014), and b) forced permutation-invariant set models, specifically DeepSets (Zaheer et al., 2017), SetTransformer (Lee et al., 2019) and Janossy Pooling (Murphy et al., 2018). An example of the proposed CG-invariant feedforward architecture is depicted in Figure 4.

We optimize all models using Adam (Kingma and Ba, 2014) with an initial learning rate in $\{10^{-2}, 10^{-3}, 10^{-4}\}$ and a batch size of 128. We use validation loss for early-stopping and to select the best hyperparameters for all models. Once again, we choose the best value for the CG-regularization strength λ by choosing the maximum value of λ that is within a 5% threshold of the maximum validation accuracy obtained from any λ.

Table 5 shows the complete set of results for all the models. The table clearly shows the issue with standard sequence models (cannot extrapolate when $\mathcal{I} \neq \emptyset$) and the issue with forced G-invariant models (fail when $\mathcal{I} \subsetneq \{1, \ldots, m\}$). In Table 4 of the main text, we show the results for the best model out of all the permutation-invariant models in the column Best FF+G-inv. Table 6 shows the

Table 5: (**Sequence tasks**) Extrapolation test accuracies (%) with 95% confidence intervals for all the models.

	$\mathcal{G}_{\mathcal{I}}$			
Model	$\langle \{\mathcal{G}_{i,j}\}_{1 \leq i < j \leq n} \rangle$	$\langle \{\mathcal{G}_{i,j}\}_{2 \leq i < j \leq n} \rangle$	$\langle \{\mathcal{G}_{i,i+2k}\}_{1 \leq i < i+2k \leq n} \rangle$	$\{\text{Id}\}$
DeepSets (Zaheer et al., 2017)	**100.00 (0.00)**	2.36 (2.37)	0.97 (0.60)	16.12 (8.21)
Janossy pooling (Murphy et al., 2018)	96.64 (3.13)	9.55 (1.61)	0.78 (0.52)	21.22 (2.94)
Set Transformer (Lee et al., 2019)	**99.57 (0.33)**	10.68 (1.49)	0.75 (0.28)	23.38 (1.88)
Transformer (Vaswani et al., 2017)	20.26 (32.08)	12.15 (16.05)	0.85 (0.37)	**100.00 (0.00)**
GRU (Cho et al., 2014)	0.48 (0.48)	0.47 (0.38)	0.90 (0.77)	**99.41 (1.58)**
FF + CG-reg. (ours)	**100.00 (0.00)**	**42.08 (18.99)**	**71.85 (26.61)**	95.70 (3.05)

Table 6: **(Sequence Tasks)** Validation and Extrapolation test accuracies (%) with 95% confidence intervals for different CG-regularization strength λ in Equation (12). λ is chosen only based on the validation accuracy: maximum λ that achieves the within 5% of the best validation accuracy (shown in **bold**).

		$\mathcal{G}_{\mathcal{I}}$							
		$\langle\{\mathcal{G}_{i,j}\}_{1\leq i<j\leq n}\rangle$		$\langle\{\mathcal{G}_{i,j}\}_{2\leq i<j\leq n}\rangle$		$\langle\{\mathcal{G}_{i,i+2k}\}_{1\leq i<i+2k\leq n}\rangle$		$\{\text{Id}\}$	
Model	λ	Val. acc (%)	Test acc (%)	Val. acc (%)	Test acc (%)	Val. acc (%)	Test acc (%)	Val. acc (%)	Test acc (%)
FF + CG-reg.	0.0	80.80 (84.15)	54.34 (87.19)	100.00 (0.00)	80.36 (74.04)	99.95 (0.10)	22.78 (14.52)	99.92 (0.27)	99.86 (0.15)
	0.1	80.83 (84.04)	59.18 (91.12)	100.00 (0.00)	65.13 (80.43)	99.99 (0.05)	60.66 (49.83)	99.95 (0.10)	99.98 (0.05)
	1.0	80.72 (84.48)	80.03 (87.52)	99.04 (4.22)	61.81 (66.24)	100.00 (0.00)	68.34 (36.98)	99.81 (0.55)	99.76 (0.65)
	2.0	82.56 (72.85)	63.16 (99.44)	100.00 (0.00)	77.97 (48.87)	99.99 (0.05)	69.20 (31.40)	99.46 (0.53)	99.37 (0.53)
	10.0	80.97 (74.10)	62.83 (100.17)	**98.14 (2.71)**	**42.08 (18.99)**	**100.00 (0.00)**	**71.85 (26.61)**	**95.56 (3.34)**	**95.70 (3.05)**
	100.0	**100.00 (0.00)**	**100.00 (0.00)**	15.65 (3.63)	2.29 (0.96)	93.42 (14.90)	27.64 (24.85)	65.92 (10.38)	65.42 (10.30)

effect of regularization strength on the performance of the model. We choose the maximum value of λ that is within a 5% threshold of the maximum validation accuracy obtained from any value of λ. We observe that although $\lambda = 10$ performs comparably to the rest in validation accuracy and is chosen consistently, it does not achieve the best possible extrapolation accuracy.