GroupifyVAE: from Group-based Definition to VAE-based Unsupervised Representation Disentanglement

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Abstract
The key idea of the state-of-the-art VAE-based unsupervised representation disentanglement methods is to minimize the total correlation of the latent variable distributions. However, it has been proved that VAE-based unsupervised disentanglement can not be achieved without introducing other inductive bias. In this paper, we address VAE-based unsupervised disentanglement by leveraging the constraints derived from the Group Theory based definition as the non-probabilistic inductive bias. More specifically, inspired by the \textit{nth dihedral group} (the \textit{permutation group} for regular polygons), we propose a specific form of the definition and prove its two equivalent conditions: isomorphism and “the constancy of permutations”. We further provide an implementation of isomorphism based on two Group constraints: the Abel constraint for the exchangeability and Order constraint for the cyclicity. We then convert them into a self-supervised training loss that can be incorporated into VAE-based models to bridge their gaps from the Group Theory based definition. We train 1800 models covering the most prominent VAE-based models on five datasets to verify the effectiveness of our method. Compared to the original models, the \textit{Groupified} VAEs consistently achieve better mean performance with smaller variances, and make meaningful dimensions controllable. Project page at https://github.com/ThomasMrY/Groupified-VAE.

1. Introduction
Learning independent and semantic representations of which individual dimension has interpretable meaning, usually referred to as disentangled representations learning, is important for artificial intelligence research. Such disentangled representations are useful for many tasks (Bengio et al., 2013): domain adaptation (Li et al., 2019; Zou et al., 2020), zero-shot learning (Lake et al., 2017), and adversarial attacks (Alemi et al., 2016), etc. Intuitively, for a disentangled representation, each latent unit is only sensitive to changes in an individual generative factor. Higgins et al. (2018) propose a formal mathematical definition of disentangled representations from a perspective of Group Theory and Group Representation Theory, which is widely accepted (Greff et al., 2019; Mathieu et al., 2019; Khemakhem et al., 2020).

Recently, Caselles-Dupré et al. (2019); Quessard et al. (2020) propose to learn disentangled representation based on the \textit{group} \textsuperscript{1}-based definition of Higgins et al. (2018). However, these methods can only work on toy datasets and require the ground truth (the \textit{World States} in Higgins et al. (2018)) of the generative factors, as they rely on interaction with the environment. Subsequently, Painter et al. (2020) propose to estimate the actions (e.g., interactions with the environment) by policy gradient to get rid of World States. However, interaction with the environment is still required.

Most of the state-of-the-art methods (Higgins et al., 2016; Burgess et al., 2018; Kim & Mnih, 2018; Chen et al., 2018; Kumar et al., 2017) are based on Variational Autoencoders (VAEs) (Kingma & Welling, 2013), which learn disentangled representations from the perspective of probabilistic inference, i.e., by enforcing a factorized aggregated posterior. These methods are \textit{fully unsupervised} and can be applied to a variety of complex datasets. However, based on Measure Theory, Locatello et al. (2019b) prove that \textit{VAE-based unsupervised disentanglement is fundamentally impossible}.

1The terms in Group Theory are marked in bold italics in this paper and explained in Appendix A.
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without introducing inductive bias on both models and data. Therefore, it is necessary to find some non-probabilistic inductive bias and introduce it to VAE-based disentangled representation learning. Furthermore, these models do not consider the definition of Higgins et al. (2018). Motivated by the above observations, we derive constraints from the group-based definition and introduce them into these VAE-based models as a non-probabilistic inductive bias to facilitate unsupervised disentangled representation disentanglement.

In Group Theory, the nth dihedral group (Judson, 2020) is a set of all permutations of polygons vertices, forming a group under the operation of composition (Miller, 1973). There are several basic generators in an nth dihedral group, e.g., flip and rotation, which can be regarded as the disentangled factors. Inspired by the nth dihedral group, which is a subgroup generated by some basic generators and also a permutation group, we assume the group G in the definition of Higgins et al. (2018) (see Section 3.1) is a subgroup generated by disentangled factors; We further define a permutation group Φ based on the existing VAE-based models using group actions (see Section 3.2 and Figure 2), which has the same form as the nth dihedral group. In this setting, as shown in Figure 1, first, we can find two conditions equivalent to the definition (Higgins et al., 2018), as Theorem 1 in Section 3.2 shows: isomorphism (between G and Φ) and the constancy of permutations (which requires World State). We then prove (in Section 3.4) that the isomorphism condition is equivalent to two Group constraints (which are self-supervision signals): Abel constraint (for the exchangeability) and Order constraint (for the cyclicity). We map the latent representation of VAE into an nth roots of unity group by applying the sine and cosine functions (see Figure 2 (a) and Section 3.3), which makes the existing VAE-based models groupifiable (i.e., based on which Φ can be defined) so that these two constraints can be applied (see Figure 2 (b)) to meet one of the necessary conditions (i.e., isomorphism) of disentangled representation. With these two Group constraints as the non-probabilistic inductive bias, our method consistently achieves statistically better performance in prominent metrics (higher means and lower variances for different VAE-based models on five datasets). Besides, we can even make the meaningful dimensions controllable for AnnealVAE (Burgess et al., 2018).

Our main contributions are summarized as:

- For unsupervised representation disentanglement learning, to our best knowledge, we are the first to unify the formal group-based mathematical definition with the existing VAE-based probability inference models by groupifying existing models.
- We map the formal group-based mathematical definition into two specific conditions (isomorphism and constancy of permutations), where isomorphism acts as a non-probabilistic inductive bias, to facilitate unsupervised disentangled representation learning.
- We propose to use the sine and cosine functions to make the existing VAE-based models groupifiable so that the Group constraints can be applied. We then convert the proposed isomorphism condition into a loss function specifically applicable to the VAE-based models.

2. Related Works

Different definitions have been proposed for disentangled representation (Bengio et al., 2013; Higgins et al., 2018; Suter et al., 2019). However, only the group-based definition proposed by Higgins et al. (2018) focuses on the disentangled representation itself and is mathematically rigorous, which is well accepted (Caselles-Dupré et al., 2019; Quessard et al., 2020; Painter et al., 2020; Diane Bouchacourt, 2021). Nevertheless, Higgins et al. (2018) do not propose a specific method based on their definition. Before this rigorous definition was proposed, there have been some success in identifying generative factors in static datasets (without environment), such as β-VAE (Higgins et al., 2016), Anneal-VAE (Burgess et al., 2018), β-TCVAE (Chen et al., 2018), and FactorVAE (Kim & Mnih, 2018). These VAE-based unsupervised methods are based on probabilistic inference. Locatello et al. (2019b) proved by Measure Theory (which is the basis of Probability Theory) that these methods theoretically have infinitely many solutions. Therefore, introducing non-probabilistic inductive bias into them would help to reduce the solution space.

It is not straightforward to reconcile the probabilistic inference methods with the group-based definition framework (Quessard et al., 2020). Caselles-Dupré et al. (2019); Quessard et al. (2020); Painter et al. (2020) leverage the interaction with the environment (assuming it is available) as supervision instead of minimizing the total correlation as the VAE-based methods do. Consequently, the effectiveness of these methods is limited to the datasets with the environment available. Pfau et al. (2020) propose a non-parametric method to unsupervisedly learn linear disentangled planes in data manifold under a metric by leveraging the lie group. However, as pointed out by the authors, the method does not generalize to held-out data and performs poorly when trying to disentangle directly from pixels.

To summarize, the probabilistic inference methods lack theoretical support and non-probabilistic inductive bias, while the application scope of existing methods based on the group-based mathematical definition (Higgins et al., 2018) is limited. Therefore, unifying the probabilistic inference methods and the group-based definition framework is essential for learning disentangled representations. To the best of
Figure 2. Overview of GroupifyVAE. (a) Illustration of permutation group \( \Phi = \{ \varphi_g | g \in G \} \) defined on a VAE-based model, where \( G \) is a sub group generated by disentangled factors. Here we take a dataset \( X \) of four images as an example. (i) Notations. \( z \in Z \) marked with dashline box denotes the representation of an image \( x \in X \). The groupifiable function \( h \) denotes the mapping from \( z \) to congruence class \( \pi \), i.e., \( \pi = h(z) = \exp((2\pi i z)/N) \) (implemented by the sine and cosine functions, \( N \) denotes the Group Order). The VAE-based models with \( \pi \) become groupifiable. \( e_i \) and \( e_j \) are identical elements of dimension \( i \) and \( j \) respectively, \( \alpha_i(\pi) = z + e_i \) and \( \alpha_i(\pi) = z + e_j \) denote group actions of \( e_i, e_j \in G \) on \( Z \). (ii) Permutation. The generators \( \varphi_i \) and \( \varphi_j \) are group actions of \( e_i, e_j \in G \) on \( Z \). For example, \( \varphi_i \) is defined on the VAE-based model as the orange solid arrows illustrate, and also is a permutation on \( X \) (orange dash arrow). Specifically, when GroupifyVAE is optimized, \( \varphi_i \) and \( \varphi_j \) are horizontal and vertical movement of the white square in images respectively (i.e., disentangled). (iii) Groupifying a model is to: make all of the permutations form a permutation group \( \Phi \) that is isomorphic to \( G \), including making models groupifiable and introducing the Isomorphism Loss to the models. (b) The Isomorphism Loss, which is converted from the isomorphism condition, includes Abel Loss \( \mathcal{L}_a \) which constrains the exchangeability of \( \varphi_i \) and \( \varphi_j \), and Order Loss \( \mathcal{L}_o \) which constrains the cyclicity of \( \varphi_i \).

our knowledge, our work is the first to reconcile the probabilistic generative methods with the inherently deterministic group-based definition framework of Higgins et al. (2018).

3. Groupifying VAE-based Models

We first review the group-based mathematical definition of disentangled representation (Higgins et al., 2018) in Section 3.1. We then map the definition into two equivalent conditions: one related to the World States, the other not (isomorphism). The isomorphism is used as a non-probabilistic inductive bias for the VAE-based models (Section 3.2), after making the VAE-based models groupifiable (Section 3.3). Section 3.4 describes how to convert the isomorphism condition into a specific loss to be incorporated into existing VAE-based models.

3.1. Disentangled Representations

We assume some basic familiarity with the fundamentals of Group Theory and Group Representation Theory. Please refer to Appendix A for some basic concepts. In this section, we briefly introduce the group-based definition of disentangled representation (Higgins et al., 2018). Some of the settings and mathematical symbols in this section are used later when introducing our method.

Let \( W \) be a set of World States. We assume that the data \( X \) is obtained through a generation process \( f : W \rightarrow X \), which maps from the World States to observations (we focus on images in this paper). Let \( Z \) be a set of representations, and we have an inference process (done by the encoder) \( b : X \rightarrow Z \), which maps from observations to representations. Then, we consider the function composition \( c = f \circ b \).

Consider a group \( G \) acting on \( W \) and \( Z \) via group action \( \cdot W \) and group action \( \cdot Z \) respectively. We state: the mapping \( c \) is equivariant between the actions on \( W \) and \( Z \) if

\[
g \cdot c(w) = c(g \cdot w), \quad \forall g \in G, \quad \forall w \in W:
\]

Assume \( G \) can be decomposed as \( G = G_1 \times G_2 \times \cdots \times G_m \). The set \( Z \) is disentangled with respect to \( G \) if: (i) the mapping \( c \) is equivariant between the actions on \( W \) and \( Z \). (ii) There is a decomposition \( Z = Z_1 \times Z_2 \times \cdots \times Z_m \) such that each \( Z_i \) is affected only by the corresponding \( G_i \).

3.2. Introducing Non-probabilistic Inductive Bias

It is not straightforward to apply the definition above to existing VAE-based unsupervised disentanglement models. A specific form for the definition is required to introduce the definition into those VAE-based models as a non-probabilistic inductive bias.
As mentioned in Section 1, we assume $G$ is a subgroup generated by disentangled factors, i.e., direct product of $m$ cyclic groups: $G = \mathbb{Z}/n\mathbb{Z} \times \mathbb{Z}/n\mathbb{Z} \times \cdots \times \mathbb{Z}/n\mathbb{Z}$, where $n$ is the factor size. To get a non-probabilistic inductive bias from the definition without requiring the World States, the key is to define a permutation group based on the VAE-based model, inspired by the $n$th dihedral group as discussed in Section 1. Considering an ideal VAE-based model, where the encoder $b$ and the decoder $d$ are inversion of each other, the group action of $g$ on $X$ is defined as:

$$\varphi_g(x) \triangleq d(g \cdot b(x)) \triangleq d(g + b(x)), \forall x \in X, \forall g \in G,$$  

where $\varphi_g$ is a permutation on $X$, and "overlin" indicates congruence class (equivalence class under congruence relation). $g \cdot b(x)$ denotes the group action of $g$ on $Z$, which is defined as the addition on congruence class. Therefore, the set $\{\varphi_g\}$ is the group action of generators $\{\varphi_g\}$ forms a permutation group $\Phi$ under the operation of composition as shown in Figure 2, where $\Phi \subseteq S(X)$, $S(X)$ denotes the symmetry group on $X$. In this setting, the group-based definition is equivalent to two conditions as shown in Theorem 1. The proof is provided in Appendix B.

**Theorem 1** For the group $G = \mathbb{Z}/n\mathbb{Z} \times \mathbb{Z}/n\mathbb{Z} \times \cdots \times \mathbb{Z}/n\mathbb{Z}$ and a decomposition $Z = Z_1 \times Z_2 \times \cdots \times Z_n$, if (i) there exists an isomorphism between $G$ and $\Phi$, i.e., $G \sim \Phi = \langle \varphi_1, \varphi_2, \ldots, \varphi_m \rangle$, and (ii) the constancy of permutations; for $\forall w \in W$ and $\varphi_i, i = 1, \ldots, m$, we have $\varphi_i(f(w)) = f(w + c_i)$, where $c_i$ is an unknown constant, then $Z$ is disentangled with respect to $G$.

$\Phi = \langle \varphi_1, \varphi_2, \ldots, \varphi_m \rangle$ denotes that $G$ is generated by generators $\{\varphi_i, i = 1, \ldots, m\}$ (see the toy examples in Figure 2 (a)). The isomorphism condition requires no World States. Therefore, we can apply it to the existing VAE-based models as a self-supervision signal. The isomorphism condition is the non-probabilistic inductive bias.

In this paper, “groupifying a VAE-based model” means forming a permutation group $\Phi$ (isomorphic to $G$) based on the model as discussed above. In Section 3.3, we discuss how to introduce congruence class into existing VAE-based models to achieve group action of $G$ on $Z$, which is necessary for a permutations group $\Phi$. Then in Section 3.4 we convert the isomorphism condition into a loss function, which can be applied to VAE-based models, as a necessary condition to achieve disentangled representations.

### 3.3. Making Models Groupifiable

The existing VAE-based models can not form the permutation group $\Phi$ for lacking of congruence class. In this section, we map the representation $z$ of the VAE-based models to the $n$-th root unity group for implementing congruence class into the models. Based on this, the permutation group $\Phi$ can be defined and the isomorphism condition can be established.

The congruence classes form a direct product of cyclic groups $G = \mathbb{Z}/N\mathbb{Z} \times \mathbb{Z}/N\mathbb{Z} \times \cdots \times \mathbb{Z}/N\mathbb{Z}$, where $N$ is the order of the groups. To implement congruence classes, we need a group that the representation $z$ can be mapped to with a differentiable function (to allow back-propagation) and that is isomorphic to $G_z$. From Group Theory, we know there is an isomorphism between $G_z$ and the $n$-th root unity group:

$$\left\{ \exp \left( \frac{2\pi iz}{N} \right) \mid z \in \mathbb{Z}^m \right\}. \tag{3}$$

Therefore, the representation $z$ is mapped to $\tau$ by groupifying function $h$ as $\tau = h(z) = \exp((2\pi iz)/N)$ (see Figure 2 (a)). However, $\tau$ can not be mapped to directly for it has complex numbers, but we can use Euler’s formula: $\exp((2\pi iz)/N) = \sin((2\pi z)/N) + i \cos((2\pi z)/N)$ to map $z$ to its real and imaginary part, i.e., vector $\sin((2\pi z)/N)$ and $\cos((2\pi z)/N)$. The two vectors are fed to the decoder after concatenation. Then the congruence class is implemented for the VAE-based models. In practice, the functions should multiply a scaling coefficient for better optimization (Sitzmann et al., 2020). We refer to such updated VAE-based models as groupifiable models.

### 3.4. Isomorphism Loss

The group $\Phi$ is similar to the $n$th dihedral group: (i) it can be generated by several generators, which is guaranteed by the isomorphism condition (i.e., $\Phi$ and $G$ are isomorphic); (ii) the elements of the group are permutations. Inspired by this, we convert the isomorphism condition into two constraints on the generators. Furthermore, we convert these constraints into an Isomorphism Loss on the groupifiable models we build. The group $G = \mathbb{Z}/n\mathbb{Z} \times \mathbb{Z}/n\mathbb{Z} \times \cdots \times \mathbb{Z}/n\mathbb{Z}$ is a direct product of the cyclic groups. Therefore, the group $\Phi$, being isomorphic to $G$, is expected to be commutative and cyclic. The constraints on the generators thus should include two parts: one is exchangeability, the other is cyclicity. Based on this observation, we derive two constraints that together are equivalent to the isomorphism condition, as shown in Theorem 2. Please refer to Appendix C for the proof.

**Theorem 2** The permutation group we defined $\Phi = \langle \varphi_1, \varphi_2, \ldots, \varphi_m \rangle$ is isomorphic to $G = \mathbb{Z}/n\mathbb{Z} \times \mathbb{Z}/n\mathbb{Z} \times \cdots \times \mathbb{Z}/n\mathbb{Z}$ if and only if: (i) for $\forall$ generators $\varphi_i, \varphi_j \in \Phi, 0 \leq i, j \leq m$, we have $\varphi_i \varphi_j = \varphi_j \varphi_i$, and (ii) $\forall \varphi_i \in \Phi, 0 \leq i \leq m$, we have $\varphi_i^n = e$, where $e$ is the identity element of group $\Phi$.

The first condition in Theorem 2 suggests that: first performing permutation $\varphi_1$ and then permutation $\varphi_j$ on images should be equal to first performing permutation $\varphi_j$ then permutation $\varphi_i$. Intuitively, a good disentanglement model should meet the constraint. The second suggests
Abel Loss. For a given VAE-based model, the generator \( \varphi_i \) of group \( \Phi \) is defined as \( d(a_i(b(x))), \forall x \in X \), where \( e_i \) is identical element of dimension \( i \) in \( G \) and \( a_i(b(x)) = b(x) + e_i \), denotes group actions of \( e_i \) on \( Z \), as shown in Figure 2 (a). We implement \( a_i \) by adding the action scale \( \tau \) on the \( i \)-th dimension of \( z \), then mapping it to \( \tau \) by the sine and cosine functions. Here we focus on the Abel constraint: \( \forall \varphi_i, \varphi_j \in \Phi, 0 \leq i, j \leq m, \) we have \( \varphi_i \varphi_j = \varphi_j \varphi_i \). We minimize \( \| \varphi_i(\varphi_j(x)) - \varphi_j(\varphi_i(x)) \|, \forall x \in X \) to make the first condition satisfied.

Denote the set of factors learned by a VAE-based model as \( I \). The Abel Loss function needs to constrain any two factors learned for the exchangeability. Therefore, the Abel Loss is the sum of the losses on the combination of factors. Denote the set containing factors combinations as \( C = \{(i, j) | i, j \in I\} \). Finally, the Abel Loss of the groupifiable VAE-based model is as follows:

\[
\mathcal{L}_a = \sum_{x \in X} \sum_{(i,j) \in C} \| \varphi_i(\varphi_j(x)) - \varphi_j(\varphi_i(x)) \|.
\]

Order Loss. For the Order constraint: \( \forall \varphi_i \in \Phi, 0 \leq i \leq m, \) we have \( \varphi_i^n = \varphi_i \varphi_i^{n-1} = \varphi_i \), where \( e \) is the identity element in group \( \Phi \) (identity mapping). \( \varphi_i(x)^n = e \) is rewritten as \( \{d(a_i(b(x)))\}^n = x, \forall x \in X \), where the exponent operation does not mean multiplication but composition instead. Note that with \( n \) times composition of \( \varphi_i \), it is difficult for the gradient to back-propagate. Recall that the decoder \( d \) is approximately equal to the inverse of the encoder \( b^{-1} \), so \( \varphi_i^{-1}(x) = \{d(a_i(b(x)))\}^{-1} \) can be approximated as \( d(a_i^{-1}(b(x))) \), where \( a_i^{-1}(b(x)) = b(x) + (n-1)e_i \). With this approximation, there are only two times of composition, which is easy to be optimized. Besides, because

\[
b(x) + e_i + b(x) + (n-1)e_i = b(x) + ne_i = b(x),
\]

where \( a_i^{-1} \) is the inverse of \( a_i \). Therefore, we implement \( a_i^{-1} \) by adding \( (N-1)\tau \) on the \( i \)-th dimension of \( z \) (let \( n = N \), and mapping it to \( \tau \) by the sine and cosine functions. Similar to Abel Loss, we minimize \( \| \varphi_i(\varphi_i^{-1}(x)) - x \|, \forall x \in X \) to make the second condition satisfied. The whole process is illustrated in Figure 2 (b). However, this conversion is not symmetrical, which leads to bias in the optimization process. Therefore, we convert the Order constraint into a symmetrical form: \( \varphi_i \varphi_i^{-1} = \varphi_i^{-1} \varphi_i = e \). There is an Order Loss for each element of \( I \). Therefore, the Order Loss is as follows:

\[
\mathcal{L}_o = \sum_{x \in X} \sum_{i \in I} (\| \varphi_i(\varphi_i^{-1}(x)) - x \| + \| \varphi_i^{-1}(\varphi_i(x)) - x \|),
\]

see Appendix E for the details of implementation. With the above two loss functions optimized, the isomorphism condition is satisfied. This can be illustrated by Theorem 3. Please refer to Appendix D for the proof.

Theorem 3 If the decoder \( d = b^{-1} \), where \( b \) is the encoder, the following two conditions are equivalent: (i) \( \forall \varphi_i, \varphi_j \in \Phi, 0 \leq i, j \leq m, \) we have \( \varphi_i \varphi_j = \varphi_j \varphi_i \) and \( \forall \varphi_i \in \Phi, 0 \leq i \leq m, \) we have \( \varphi_i^n = e \) (ii) the Abel Loss function (Equation 4) and the Order Loss function (Equation 6) are optimized.

Since the Abel Loss and Order Loss are equally important for meeting the isomorphism condition, we assign equal weight for them. Thus, the Isomorphism Loss is \( \mathcal{L}_i = \mathcal{L}_a + \mathcal{L}_o \). We name the groupifiable VAE optimized with this loss as groupified VAE.

4. Experiments

We first verify the effectiveness of groupified models quantitatively in enhancing the ability to learn disentangled representations on several datasets and several models. Then, we show their effectiveness qualitatively on two typical datasets. After that, we perform a case study on the dSprites dataset to analyze the effectiveness and ablation studies on the losses and hyperparameters. Furthermore, we evaluate the performance of two downstream tasks trained on the representations learned by the groupified models: abstract reasoning (Van Steenkiste et al., 2019) and fairness evaluation (Locatello et al., 2019a). For more comprehensive results, please see Appendix G.

4.1. Datasets and Baseline Methods

To evaluate our method, we consider several datasets: dSprites (Higgins et al., 2016), Shapes3D (Kim & Mnih, 2018), Cars3D (Reed et al., 2015), and the variants of dSprites introduced by Locatello et al. (2019b): Color-dSprites and Noisy-dSprites. Please refer to Appendix F for the details of the datasets.

We choose the following four baseline methods as repre-
4.2. Quantitative Evaluations

This section performs quantitative evaluations on the datasets and models introduced with different random seeds and different hyperparameters. Then, we evaluate the performance of the original and groupified models in terms of several popular metrics: BetaVAE score (Higgins et al., 2016), DCI disentanglement (Eastwood & Williams, 2018) (DCI in short), MIG (Chen et al., 2018), and FactorVAE score (Kim & Mnih, 2018). We assign three or four hyperparameter settings for each model on each dataset. We run it with 10 random seeds for each hyperparameter setting to minimize the influence of random seeds. Therefore, we totally run \((3 \times 10 \times 3 + 10 \times 3 \times 3) \times 2 \times 5 = 1800\) models. We evaluate each metric’s mean and variance for each model on each dataset to demonstrate the effectiveness of our method. As shown in Table 1, these groupified models have better performance (numbers marked bold in Table 1) than the original models on almost all the cases. Please refer to Appendix G for more results.

On Shapes3d, the groupified models outperform the original ones on all the metrics except for BetaVAE scores, suggesting that there is some disagreement between BetaVAE scores and other metrics. Similar disagreement is also observed between the variances of MIG and other metrics on Cars3d. Note that the qualitative evaluation in Appendix H shows that the disentanglement ability of groupified VAEs is better on Shapes3d and Cars3d.

4.3. Qualitative Evaluations

By groupifying the VAEs, we qualitatively show they achieve better disentanglement than the originals. As shown in Figure 6, the traversal results of groupified \(\beta\)-TCVAE on Shape3d and Car3d are less entangled. For more qualitative evaluation, please refer to Appendix H.

4.4. Visualization of the Learned Latent Space

To demystify how the groupifying helps the VAE-based models to improve the disentanglement ability, we take dSprites as an example, visualize the learned latent space, and show the typical score distributions of the metrics. First, we visualize the space spanned by the three most dominant factors (x position, y position, and scale). Figure 4 is plot as follows: (i) We traverse all the related World States to get the images; (ii) feed them into the encoder get the representations; (iii) take the three corresponding dimensions as the location of the points in the 3D space and use different colors to indicate different images. As shown in Figure 4 (for more results, please refers to Appendix J), the spaces learned by the original models collapses, while the spaces of the groupified models only bend a little bit. The main reason is that the Isomorphism Loss, serving as a self-supervision signal, suppresses the representation space distortion and encourages the disentanglement of the learned factors. As Figure 3 shows, the groupified models consistently achieve better mean performance with smaller variances. The Group constraints reduce the search space of the network so that the groupified model converges to the ideal disentanglement solution with higher probability.

An interesting observation is that meaningful dimensions can be controlled in groupified AnnealVAE. As shown in Figure 5, the KL divergence increases continuously on these assigned dimensions after the Isomorphism Loss is applied to them. Note that the KL divergence loss in AnnealVAE indicates the amount of information encoded. As Figure 5 (b) shows, the KL divergence of assigned dimensions increases
Table 1. Performance (mean ± variance) on different datasets and different models with different metrics. We evaluate β-VAE, AnnealVAE, FactorVAE, and β-TCVAE on dSprites, Cars3d, Shapes3d, Noisy-dSprites, and Color-dSprites for 1800 settings. These settings include different random seeds and hyperparameters, refer to Appendix F for the details. We only show the first three datasets here. For more results, please refer to Appendix G.

| dSprites | DCI | BetaVAE | MIG | FactorVAE |
|----------|-----|---------|-----|-----------|
| β-VAE    | 0.23 ± 0.10 | 0.46 ± 0.085 | 0.86 ± 0.051 | 0.37 ± 0.089 |
| AnnealVAE| 0.28 ± 0.10 | 0.39 ± 0.056 | 0.87 ± 0.0067 | 0.34 ± 0.061 |
| FactorVAE| 0.38 ± 0.10 | 0.41 ± 0.074 | 0.89 ± 0.020 | 0.31 ± 0.061 |
| β-TCVAE  | 0.30 ± 0.15 | 0.36 ± 0.11 | 0.861 ± 0.038 | 0.06 ± 0.024 |

| Cars3d   | DCI | BetaVAE | MIG | FactorVAE |
|----------|-----|---------|-----|-----------|
| β-VAE    | 0.18 ± 0.059 | 0.24 ± 0.041 | 0.99 ± 1.6e−3 | 0.11 ± 0.032 |
| AnnealVAE| 0.22 ± 0.046 | 0.25 ± 0.046 | 0.99 ± 1.5e−4 | 0.10 ± 0.014 |
| FactorVAE| 0.21 ± 0.054 | 0.25 ± 0.040 | 1.0 ± 0.0 | 0.11 ± 0.033 |
| β-TCVAE  | 0.24 ± 0.049 | 0.26 ± 0.046 | 1.0 ± 0.0 | 0.11 ± 0.033 |

| Shapes3d | DCI | BetaVAE | MIG | FactorVAE |
|----------|-----|---------|-----|-----------|
| β-VAE    | 0.44 ± 0.176 | 0.56 ± 0.10 | 0.91 ± 0.072 | 0.28 ± 0.18 |
| AnnealVAE| 0.52 ± 0.051 | 0.60 ± 0.078 | 0.82 ± 0.076 | 0.48 ± 0.047 |
| FactorVAE| 0.47 ± 0.10 | 0.49 ± 0.065 | 0.86 ± 0.055 | 0.43 ± 0.11 |
| β-TCVAE  | 0.66 ± 0.10 | 0.72 ± 0.061 | 0.97 ± 0.039 | 0.47 ± 0.090 |

Table 2. Ablation study on the action scale τ, group order N, and Isomorphism Loss. DCI disentanglement are listed (mean ± variance).

| Original | Group Order N = 10 | Action Scale τ = N/2 | Group Order N = 10, Action Scale τ = 5 |
|----------|-------------------|---------------------|----------------------------------------|
| DCI      | 0.27 ± 0.10       | 0.38 ± 0.055        | 0.38 ± 0.055                           |
| τ = 1    | 0.31 ± 0.093      | 0.33 ± 0.084        | 0.33 ± 0.062                           |
| τ = 3    | 0.34 ± 0.062      | 0.38 ± 0.055        | 0.38 ± 0.064                           |
| τ = 5    | 0.34 ± 0.062      | 0.38 ± 0.055        | 0.38 ± 0.064                           |
| N = 5    | 0.38 ± 0.055      | 0.38 ± 0.055        | 0.38 ± 0.055                           |
| N = 10   | 0.38 ± 0.055      | 0.38 ± 0.055        | 0.38 ± 0.055                           |
| N = 15   | 0.38 ± 0.055      | 0.38 ± 0.055        | 0.38 ± 0.055                           |

Figure 4. The latent space spanned by the learned factors original (bottom row) and groupified models (top row). The localization of each point is the disentangled representation of the corresponding image. And an ideal result is all the points form a cube and color variation is continuous. The increase of hyperparameter \( C_{max} \) results in a collapse of latent space of the original VAE. The collapse is suppressed by the Isomorphism Loss, which leads to better disentanglement.
We perform ablation study on the action scale $\tau$, Group order $N$, Abel Loss $L_a$, and Order Loss $L_o$. We take the Anneal-VAE trained on dSprites as an example. We only consider the DCI disentanglement metric here. To illustrate the influence of the action scale, we vary $\tau$ from 1 to 5 with $N$ set to 10, and the full Isomorphism Loss is applied. Similarly, we set the action scale to $N/2$, and investigate the influence of Group size $N$. Besides, to evaluate the effectiveness of the two constraints, the models with the Abel Loss alone or Order Loss alone are also evaluated. In this setting, we fix $\tau$ to 5 and $N$ to 10. We compute the mean and variance of the performance for 30 settings of hyperparameters and random seeds. Table 2 shows that a larger action scale leads to better performance, as a larger action scale makes the isomorphism condition harder to be satisfied, which requires better disentanglement. The isomorphism condition plays a role of cycle consistency in the latent space, leading to better disentanglement. The performance is robust to the Group order $N$, as the models learn to adapt to different $N$ in the training process. The models with only the Abel Loss or Order Loss applied have improved performance compared to the originals. The former performs better than the latter, suggesting that exchangeability plays a more important role.

In this paper, we unify the group-based mathematical definition of disentangled representation with the existing VAE-based probability inference models by groupifying them. Inspired by the $n$th dihedral group, we map the group-based mathematical definition of unsupervised representation disentanglement into two equivalent conditions: isomorphism and the constancy of permutations. We use the former as a self-supervision signal, which is converted into Group constraints. These constraints are converted to the Abel Loss for the exchangeability and Order Loss for the cyclicity, summation as Isomorphism Loss. After making the VAE-based models groupifiable by mapping the representation into the $n$-throot unity group, we form a VAE-based permutation group, and apply Isomorphism Loss to meet the isomorphism condition. We observe through our extensive experiments that the Group constraints narrows down the optimization space, and by incorporating this non-probabilistic inductive bias, the groupified VAEs achieve better average performance with smaller variances and controllable meaningful dimensions. For future work, extending Groupify-VAE by leveraging the lie group (Hall, 2015) (which is also a manifold) is an interesting direction.

### 4.6. Abstract Reasoning and Fairness Evaluation

As pointed out by Locatello et al. (2019b), the disentangled representation’s downstream tasks should also be verified. Therefore, we verify the effectiveness of the representations learned by the groupified VAE-based models on Shapes3d in two downstream tasks: abstract reasoning (Van Steenkiste et al., 2019) and fairness evaluation (Locatello et al., 2019a). As Table 3 shows, the performance of the abstract reasoning models fine-tuned on the representation learned by the groupified FactorVAEs is better than the original ones. In terms of fairness evaluation, we can observe that the unfairness scores of the representation learned by the groupified FactorVAEs are lower than the original ones.

### 5. Conclusion

In this paper, we unify the group-based mathematical definition of disentangled representation with the existing VAE-based probability inference models by groupifying them. Inspired by the $n$th dihedral group, we map the group-based mathematical definition of unsupervised representation disentanglement into two equivalent conditions: isomorphism and the constancy of permutations. We use the former as a self-supervision signal, which is converted into Group constraints. These constraints are converted to the Abel Loss for the exchangeability and Order Loss for the cyclicity, summation as Isomorphism Loss. After making the VAE-based models groupifiable by mapping the representation into the $n$-throot unity group, we form a VAE-based permutation group, and apply Isomorphism Loss to meet the isomorphism condition. We observe through our extensive experiments that the Group constraints narrows down the optimization space, and by incorporating this non-probabilistic inductive bias, the groupified VAEs achieve better average performance with smaller variances and controllable meaningful dimensions. For future work, extending Groupify-VAE by leveraging the lie group (Hall, 2015) (which is also a manifold) is an interesting direction.

### Table 3. Downstream task performance on the models trained on the representation learned by original and groupified FactorVAE.

|                      | Abstract reasoning↑ | Unfairness scores↓ |
|----------------------|---------------------|---------------------|
| Original             | $0.948 \pm 0.031$   | $0.023 \pm 0.007$   |
| Groupified           | $0.954 \pm 0.028$   | $0.018 \pm 0.008$   |

Figure 5. Visualization of meaningful dimensions of groupified Anneal-VAE. From the image traversal results (b), position x (row 1), y (row 2), scale (row 5), orientation (row 3,4) are learned in the targeted dimensions (0 to 4) (a). There is no semantics in the remaining dimensions.

Figure 6. Visual traversal comparison between original and groupified β-TCVAE. The traversal results of Groupified model are less entangled.

(a) Original

(b) Groupified
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