

MUTIPLE INVERTIBLE AND EQUIVARIANT TRANSFORMATION FOR DISENTANGLEMENT IN VAES

Anonymous authors

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ABSTRACT

Disentanglement learning is a core issue for understanding and re-using trained information in Variational AutoEncoder (VAE), and effective inductive bias has been reported as a key factor. However, the actual implementation of such bias is still vague. In this paper, we propose a novel method, called *Multiple Invertible and Equivariant transformation (MIE-transformation)*, to inject inductive bias by 1) guaranteeing the invertibility of latent-to-latent vector transformation while preserving a certain portion of equivariance of input-to-latent vector transformation, called *Invertible and Equivariant transformation (IE-transformation)*, 2) extending the form of prior and posterior in VAE frameworks to an unrestricted form through a learnable conversion to an approximated exponential family, called *Exponential Family conversion (EF-conversion)*, and 3) integrating multiple units of IE-transformation and EF-conversion, and their training. In experiments on 3D Cars, 3D Shapes, and dSprites datasets, MIE-transformation improves the disentanglement performance of state-of-the-art VAEs.

1 INTRODUCTION

Disentanglement learning to learn more interpretable representations is broadly useful in artificial intelligence fields such as classification (Singla et al., 2021), zero-shot learning (Tenenbaum, 2018), and domain adaptation (Li et al., 2019; Zou et al., 2020). The disentangled representation is defined as a change in a single dimension, which corresponds to unique semantic information. Several works have been conducted based on this framework.

A major model for enhancing the disentanglement learning is Variational AutoEncoder (VAE) (Kingma & Welling, 2013). Based on VAE, unsupervised disentangled representation learning has been elaborated (Higgins et al., 2017; Chen et al., 2018; Kim & Mnih, 2018; Jeong & Song, 2019; Li et al., 2020) through the factorizable variations and control of uncorrelatedness of each dimension of representations. Moreover, VAE models to handle the shape of prior as a Gaussian mixture (Dilokthanakul et al., 2016) or von Mises-Fisher (Davidson et al., 2018) were also developed, but the disentanglement is still incomplete. As a critical point, there is a report that unsupervised disentanglement learning is impossible without inductive bias (Locatello et al., 2019).

Recently, such inductive bias has been introduced in various perspectives on transformation of latent vector space. Intel-VAE (Miao et al., 2021) proposed the benefit of *invertible* transformation of the space to another latent space to provide better data representation, which includes hierarchical representations. Group theory based bias also shows significant improvement of disentanglement (Zhu et al., 2021; Yang et al., 2021), whose definition follows Higgins et al. (2018a), which is based on the group theory. The works show that *equivariant* transformation between input and latent vector space has a key role of disentanglement.

Inspired by the above works, we propose a *Multiple Invertible and Equivariant transformation (MIE-transformation)* method¹, which is simply insertable to VAEs. The method adopts the matrix exponential to hold the invertible property of *latent-to-latent (L2L)* vector transformation. Then, to preserve at least some potential equivariance between *input-to-latent (I2L)* vector transformation, we constrain the L2L transformation to a symmetric matrix exponential, called *invertible and*

¹available on Github, which will be released after publication.

equivariant transformation (IE-transformation). The IE-transformation generates an uncertain form of latent vector distributions, so we provide a training procedure to force them to be close to an exponential family, called *exponential family conversion (EF-conversion)*. This conversion enables the uncertain distribution to work in the typical training framework of VAEs. Then, we mathematically show that the multiple uses of IE-transformation work as β parameters (Higgins et al., 2017) controlled for enhancing disentanglement learning. Also, we propose the *sparse log-normalizer to induce an implicit semantic mask in the latent vector space, different to* Yang et al. (2020). In experiments with quantitative and qualitative analysis, MIE-transformation shows significant improvement in disentangled representation learning in 3D Cars, 3D Shapes, and dSprites tasks. Our main contributions are summarized as follows.

1. We propose to use a symmetric matrix exponential as a latent-to-latent vector transformation function for inducing inductive bias based on invertible and equivariant properties with mathematical analysis.
2. We provide a training procedure and losses for VAEs to learn unknown latent vector distribution as an approximated exponential family.
3. We propose the novel MIE-transformation architecture to integrate multiple IE-transformation and EF-conversion, which is widely applicable to state-of-the-art VAEs.
4. We empirically analyze the properties of MIE-transformation and validate its effectiveness in disentanglement learning on benchmarks.

2 RELATED WORK

Recently, various works have focused on the unsupervised disentanglement learning. One of the branches is InfoGAN (Chen et al., 2016) based works such as IB-GAN (Jeon et al., 2021) and OOGAN (Liu et al., 2020) showed the improvements, but these works regularize informativeness introduced in Lin et al. (2020) to elaborate regularizing MI. The other branch is based on the Variational AutoEncoder (VAE). β -VAE (Higgins et al., 2017) penalizes Kullback-Leibler divergence (KL divergence) with weighted hyper-parameters. Factor VAE (Kim & Mnih, 2018) and β -TCVAE (Chen et al., 2018) are trained with total correlation (TC) to make independent dimensions on a latent vector with discriminator and divided KL divergence term. Differently, we consider the impact based on group theory based on Higgins et al. (2018a).

Following the definitions of disentangled representation learning by group theory, several works have emphasized equivariant and improved disentangled representation learning. Commutative Lie Group VAE (CLG-VAE) (Zhu et al., 2021) proposed direct mapping of the latent vector into Lie algebra to obtain group structure (inductive bias) with constraints: commutative and hessian loss. Furthermore, Groupified VAE (Yang et al., 2021) extends Spatial Broadcast Decoder (Watters et al., 2019) with the group theory, and it also proves the necessity of the proposed abel loss and order loss with cyclic groups and n-th root unity group to improve disentangled representation. Topographic VAE (Keller & Welling, 2021) combines Student’s-t distributions and variational inference. It enforces rotated latent vectors to be equivariant. On the other hand, we apply unrestricted prior and posterior for disentanglement learning.

Other works elaborate uncertainty of exponential family distribution with Bayesian update (Charpentier et al., 2020; 2022b). Other approaches in VAEs, some works have implemented extension prior such as a transformed Gaussian distribution, Gaussian mixture distribution (Kalatzis et al., 2018) or von Mises-Fisher distribution (Davidson et al., 2018). InteL-VAE (Miao et al., 2021) shows that transformed Gaussian distribution by the invertible function trains hierarchical representation with manual function. We show more clear relation of invertibility to disentanglement and improve VAEs to use its unrestricted form of prior.

Invertible and equivariant Deep Neural Networks have been investigated with normalizing flows. As proven by Xiao & Liu (2020), utilized matrix exponential on Neural networks is invertible, but it only provides mathematical foundations of the transformation. Matrix exponential flows are proposed in Hooeboom et al. (2020) for equivariant simultaneously. In our work, we show how to use it for disentanglement learning.

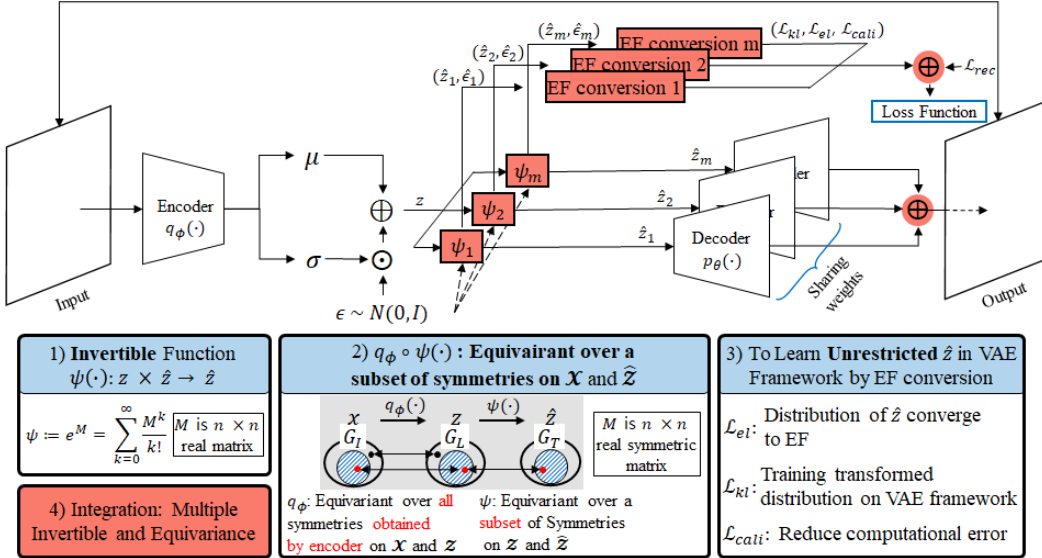


Figure 1: The overall architecture of our proposed *MIET*-VAE. The invertible and equivariant function $\psi(\cdot)$ consists of a symmetric matrix exponential to be 1) invertible and 2) partially equivariant. Then 3) EF conversion module converges the distribution of unrestricted \hat{z} to the power density function of EF with \mathcal{L}_{el} loss. Also, it applies KL divergence loss (\mathcal{L}_{kl}) between the transformed posterior and prior, which are expressed by the power density function of EF. In the last, EF conversion reduces the computational error (\mathcal{L}_{cali}) between approximated and true KL divergence. 4) The reddish color represents the integration parts. The details of the gray box are in Fig. 2a.

3 METHOD

The overview of a VAE equipped with MIE-transformation is shown in Fig. 1. The MIE-transformation has three main components: 1) *IE-Transformation Unit* to transform latent vectors with invertible and equivariant properties, 2) *EF-conversion Unit* to extend VAEs to learn the exponential family distribution of latent vectors, and 3) integrated training and generation process for multiple uses of IE-transformation and EF-conversion.

3.1 INVERTIBLE AND EQUIVARIANT TRANSFORMATION

Invertible Property by Using Matrix Exponential To guarantee the invertible property of IE-transformation, we use a function $\psi(\cdot) = e^M * \cdot$ for the transformation, where M is in $n \times n$ real number matrix set $M_n(\mathbb{R})$ (Xiao & Liu, 2020). The operator $*$ is matrix multiplication, and $e^M = \sum_k \frac{M^k}{k!}$. Intel-VAE effectively extracts hierarchical representation which includes low-level features (affect to a specific factor) and high-level features (affect to complex factors) with invertible transformation function (Miao et al., 2021). Our motivation is to use the benefits of injecting explicit inductive bias for disentanglement Locatello et al. (2019); Miao et al. (2021).

Why Should L2L Transformation Be Equivariant? Let’s consider equivariance between the input space and the final latent vector space directly used for a decoder in the VAE frameworks. We assume that previous works are equivariant over a subset of symmetries on the input and the latent vector space because these methods have improved disentanglement learning. However, if we apply the unrestricted L2L transformation to the VAE, then there is no guarantee to be equivariant between the input and final space. This problem is more precisely shown in Fig. 2a, which illustrates equivariance over the input space \mathcal{X} , latent vector space \mathcal{Z} , and its transformed latent vector space $\hat{\mathcal{Z}}$ with a corresponding group of symmetries G_I , G_L , and G_T , respectively. In the VAEs literature, it has not been reported to restrict L2L transformation to guarantee equivariant function between two spaces, so we propose a solution to guarantee at least a part of symmetries to be equivariant.

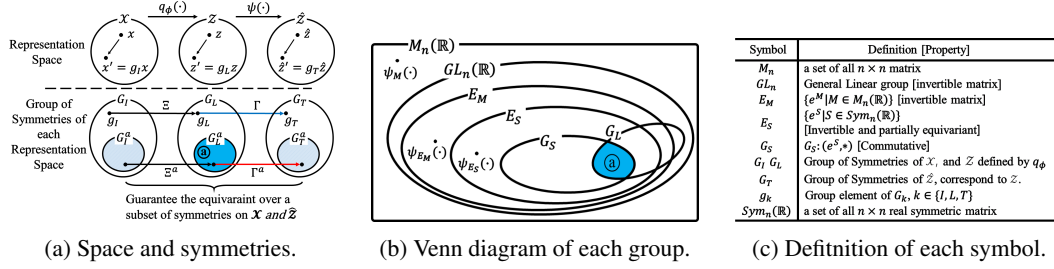


Figure 2: G_I and G_L are obtained through q_ϕ . Fig. 2a shows the relation between each space and symmetries. If q_ϕ and $\psi(\cdot)$ is equivariant function over all G_I , G_L , and G_T , then there exist Ξ , and Γ , respectively, where $\Xi : G_I \rightarrow G_L$, and $\Gamma : G_L \rightarrow G_T$, and $\Xi \circ \Gamma : G_I \rightarrow G_T$. However, unrestricted $\psi(\cdot)$ has no guarantee to be equivariant. The red arrows represent our method.

Equivariance Property with Symmetric Matrix Exponential To enhance the equivariance of L2L transformation, we set M of $\psi(\cdot)$ to a symmetric matrix. We show that 1) a group with the constraint guarantees equivariance of $\psi(\cdot)$ in the group, 2) $\psi(\cdot)$ being equivariant over subset of symmetries between the input transformed latent vector space, and 3) the constraint increases the probability of $\psi(\cdot)$ to be in the group.

We distinguish $M_n(\mathbb{R})$, E_M , E_S , and G_S as shown in Fig 2b, and 2c. The intersection $@ : G_S \cap G_L$ is shown in Fig. 2a, and 2b. We particularly call the transformations as *symmetries* (Higgins et al., 2022) to distinguish them from IE- and I2L-transformations. For the generality of our method, we consider an arbitrary VAE model that has no restriction on creating intersections to any set as Fig. 2b.

Proposition 1. Any $\psi(\cdot) \in G_S$, notated as $\psi_{G_S}(\cdot)$, is equivariant to group G_S .

Proof. The group G_S is closed to matrix multiplication, and its element is always a symmetric matrix by definition. Then, any two elements in G_S are commutative because if matrix multiplication of two symmetric matrices is symmetric then both are commutative. As a result, $\psi_{G_S}(\cdot)$ and group elements of G_S are commutative (G_S is an abelian group). Because of the commutativity, $\psi_{G_S}(g_s \circ z) = e^{\mathbf{S}} g_s z = g_s e^{\mathbf{S}} z = g_s \circ \psi_{G_S}(z)$ for $g_s \in G_S$ if the group action \circ is set to matrix multiplication, where $\psi_{G_S} \in G_S$. This equation satisfies the general definition of an equivariant function that a function $f(\cdot)$ is equivariant if $f(g \circ z) = g \circ f(z)$ for all g in a group G by matching f , g , and G to ψ_{G_S} , g_s , and G_S , respectively. ■

Proposition 2. If q_ϕ is equivariant over defined on group of symmetries G_I^a and G_L^a , then $\psi_{G_S}(q_\phi(\cdot))$ is equivariant to symmetries in G_I corresponding to $@$ and G_T corresponding to $@$ by the equivariance of q_ϕ .

Proof. The function $\psi_{G_S}(\cdot)$ is an equivariant function over group elements in $@$ by Proposition 1. Then, the composite function, $\psi_{G_S}(\cdot)$ and q_ϕ , is an equivariant function of G_I corresponding to $@$ and G_T corresponding to $@$ (see Appendix C.2). ■

In other words, $\psi_{G_S}(\cdot)$ guarantees to preserve the equivariance of I2L-transformation to certain symmetries in $@$ after IE-transformation.

Let $P(B)$ be the probability of $\psi(\cdot) \in B$ for a subset $B \subset M_n(\mathbb{R})$ after VAE training. Then,

Proposition 3. $Pr(\psi_{E_S}(\cdot) \in G_S) > Pr(\psi_{E_M}(\cdot) \in G_S) > Pr(\psi_M(\cdot) \in G_S)$.

Proof. All $e^{\mathbf{S}} \in E_S$ are in E_M since $Sym_n(\mathbb{R}) \subset M_n(\mathbb{R})$. However, $E_M \not\subset E_S$ because $e^{\mathbf{S}}$ is always symmetric, but $e^{\mathbf{M}}$ can be an asymmetric matrix (see Appendix C.1). Therefore, the probability $Pr(\psi_{E_M}(\cdot) \in G_S) = \frac{P(G_S)}{P(E_M)}$ is greater than $Pr(\psi_{E_S}(\cdot) \in G_S) = \frac{P(G_S)}{P(E_S)}$. In the same way, $Pr(\psi_{E_M}(\cdot) \in G_S) > Pr(\psi_M(\cdot) \in G_S) = \frac{P(G_S)}{P(M_n(\mathbb{R}))}$ because $E_M \subset M_n(\mathbb{R})$ and non-invertible functions are only in $M_n(\mathbb{R})$. ■

Therefore, ψ_{E_S} clearly increases the probability of preserving a certain type of equivariance compared to unrestricted ψ functions.

dSprites	Disentanglement Metric							
	FVM \uparrow		MIG \uparrow		SAP \uparrow		DCI \uparrow	
	original	MIET	original	MIET	original	MIET	original	MIET
β -VAE	69.15(\pm 5.88)	74.19 (\pm 5.62)	9.49(\pm 8.30)	19.72 (\pm 11.37)	2.43(\pm 2.07)	5.08 (\pm 2.90)	18.57(\pm 12.41)	28.81 (\pm 10.19)
β -TCVAE	78.50(\pm 7.93)	79.87 (\pm 5.80)	26.00(\pm 9.06)	35.04 (\pm 4.07)	7.31(\pm 0.61)	7.70 (\pm 1.63)	41.80(\pm 8.55)	47.83 (\pm 5.01)
CLG-VAE	79.06(\pm 6.83)	81.80 (\pm 3.17)	23.40(\pm 7.89)	36.34 (\pm 5.55)	7.37(\pm 0.96)	8.03 (\pm 0.83)	37.68(\pm 7.83)	44.73 (\pm 5.11)

3D Shapes	Disentanglement Metric							
	FVM \uparrow		MIG \uparrow		SAP \uparrow		DCI \uparrow	
	original	MIET	original	MIET	original	MIET	original	MIET
β -VAE	71.76(\pm 12.26)	75.19 (\pm 8.16)	37.33(\pm 22.34)	47.37 (\pm 10.13)	7.48(\pm 4.12)	9.20 (\pm 2.44)	52.07(\pm 17.92)	54.95 (\pm 8.99)
β -TCVAE	76.62(\pm 10.23)	80.59 (\pm 8.57)	52.93(\pm 20.5)	54.49 (\pm 9.44)	10.64(\pm 5.93)	11.58 (\pm 3.32)	65.32(\pm 11.37)	66.22 (\pm 7.32)
CLG-VAE	77.04(\pm 8.22)	80.17 (\pm 8.43)	49.74(\pm 8.18)	53.87 (\pm 7.41)	9.20(\pm 2.44)	12.83 (\pm 3.01)	57.70(\pm 8.60)	60.74 (\pm 7.77)

3D Cars	Disentanglement Metric							
	FVM \uparrow		MIG \uparrow		SAP \uparrow		DCI \uparrow	
	original	MIET	original	MIET	original	MIET	original	MIET
β -VAE	89.48(\pm 5.22)	88.95(\pm 5.94)	6.90(\pm 2.70)	7.27 (\pm 1.99)	1.30(\pm 0.48)	1.88 (\pm 1.12)	19.85 (\pm 4.87)	18.90(\pm 4.49)
β -TCVAE	95.84(\pm 3.40)	96.43 (\pm 2.42)	11.87 (\pm 2.90)	10.80(\pm 1.22)	1.55(\pm 0.38)	1.88 (\pm 1.12)	27.91 (\pm 4.31)	26.08(\pm 2.47)
CLG-VAE	86.11(\pm 7.12)	91.06 (\pm 5.09)	6.19(\pm 2.42)	8.51 (\pm 2.11)	2.06 (\pm 0.60)	1.99(\pm 0.93)	16.91(\pm 4.01)	18.31 (\pm 2.83)

Table 1: Performance (mean \pm std) of four metrics on dSprites, 3D Shapes, and 3D Cars. The $\alpha = 1$ and $\gamma = 1$ of β -TCVAE as Chen et al. (2018).

p -value	VAEs				CLG-VAE				β -TCVAEs			
	FVM	MIG	SAP	DCI	FVM	MIG	SAP	DCI	FVM	MIG	SAP	DCI
dSprites	0.000	0.000	0.000	0.000	0.030	0.000	0.005	0.000	<i>0.281</i>	0.000	<i>0.170</i>	0.009
3D Shapes	0.080	0.007	0.016	<i>0.191</i>	<i>0.085</i>	0.029	0.000	<i>0.088</i>	<i>0.111</i>	<i>0.383</i>	<i>0.277</i>	<i>0.390</i>
3D Cars	0.659	<i>0.250</i>	0.003	0.583	0.003	0.000	0.630	<i>0.071</i>	<i>0.278</i>	0.923	<i>0.119</i>	0.933

Table 2: p -value of t-test for original vs MIET results of Table 1, which are averaged over models (bold: positive and significant, italic: positive but insignificant, normal: lower performance).

In practice, however, there are uncertain and undefinable conditions to derive the total probability of preserving all existing equivariance. For example, probability distribution $P(\cdot)$ varies by training settings, so Proposition 3 holds with only uniform or equal distributions determined by training settings for $\psi_{E_M}(\cdot)$ and $\psi_{E_S}(\cdot)$. Additionally, the area of $G_L \setminus G_S$ and its probability are uncertain and depend on I2L transformation functions such as encoders of VAEs. We empirically validate the impact of equivariance with the uncertain $P(\cdot)$ to disentanglement in Section 5.1.

Independence of Latent Variables In addition to invertible and equivariant properties, our IE-transformation also guarantees zero Hessian matrix, which enhances disentanglement without any additional loss of Peebles et al. (2020). Hessian matrix of the transformation $\nabla_z^2 \psi(\mathbf{z}) = \nabla_z (\nabla_z e^{\mathbf{M}z}) = 0$ because of the irrelevance of \mathbf{M} to \mathbf{z} . By this property, $\psi(\cdot)$ leads that independently factorizes each dimension (Peebles et al., 2020), and it injects group theory based inductive bias simultaneously. This is because the group decomposition of \mathbf{z} space $G = G_1 \times G_2 \times \dots \times G_k$ corresponds to group decomposition of the transformed latent vector $\hat{\mathbf{z}}$ space $G' = G'_1 \times G'_2 \times \dots \times G'_k$ such that each G'_i is fixed by the action of all the G_j for $j \neq i$ (Yang et al., 2021; Higgins et al., 2018b). This correspondence of decomposition is expected to transfer the independence between dimensions of \mathbf{z} to the space of $\hat{\mathbf{z}}$ (Higgins et al., 2018a).

3.2 EXPONENTIAL FAMILY CONVERSION

The generated latent variables by IE-transformation may not follow a Gaussian distribution generally used for the training of VAEs in a non-parametric perspective. As a solution, we present a training procedure for VAEs to build an exponential family distribution from a latent variable of an arbitrary distribution. Then, we introduce training losses obtained from the unit IE-transformation function and EF-conversion, and more details of each procedure are in Appendix B.

Posterior Approximation As an Exponential Family The procedure represents a posterior distribution in the exponential family by adopting the following form:

$$p(\boldsymbol{\theta}|\mathbf{X}, \xi, \nu) \propto \exp(\boldsymbol{\theta}^\top (\sum_{n=1}^N T(\mathbf{x}_n) + \nu\xi) - A(\boldsymbol{\theta})), \quad (1)$$

where *sufficient statistics* $T(\cdot)$ and *log-normalizer*, $A(\cdot)$ are known functions, samples $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$ from distribution, and *natural parameter* of posterior $\boldsymbol{\theta}$ and of prior ξ (Bishop,

dataset	Metrics			
	FVM	IMG	SAP	DCI
dSprites				

Table 3: Impact of the number of MIE-transformation function on the β -TCVAE and β -VAE with dSprites, 3D Shapes, and 3D Cars datasets in terms of the four metrics. The blue and red box plots represent each model’s single and multiple IE-transformation cases, respectively. (A- n : MIET- β -TCVAE (4), B- n : MIET- β -TCVAE (6), C- n : MIET- β -VAE, n : the number of MIE-transformation)

2006). The functions $T(\cdot)$, and $A(\cdot)$ are deterministic functions to maximize posterior distribution. The *evidence* is implemented as learnable parameters $\nu \in \mathbb{R}^{n \times n}$. The natural parameter is generated by a multi-layer perceptron as Charpentier et al. (2022a). This general form approximating an exponential family distribution with learnable parameters can extend VAEs to use a wider distribution for latent variables by simply matching \mathbf{X} to generated latent variables. After IE-transformation, we can apply the form by using the \hat{z}_m , $\theta_{\hat{z}_m}$, and $\theta_{\hat{\epsilon}_m}$ for \mathbf{X} , θ , and ξ , respectively. More details of the background, conjugate prior, posterior, and assumptions are in Appendix B.3.

EF similarity Loss We added a loss to converge the unrestricted distributions of \hat{z} to the power density function of the exponential family by constraining the posterior maximization as:

$$\text{maximize } \log p(\theta_{\hat{z}_m} | \hat{z}_m, \theta_{\hat{\epsilon}_m}, \nu_m) \quad \text{s.t. } D_{\text{KL}}(f_{\mathbf{x}}(\mathbf{x} | \theta_{\hat{z}_m}) || f_{\mathbf{x}}(\mathbf{x} | \theta_{\hat{\epsilon}_m})) \geq 0 \quad (2)$$

$$\Rightarrow \mathcal{L}_s(\hat{z}_m, \hat{\epsilon}_m) = \log p(\theta_{\hat{z}_m} | \hat{z}_m, \theta_{\hat{\epsilon}_m}, \nu_m) + \lambda_m D_{\text{KL}}(f_{\mathbf{x}}(\mathbf{x} | \theta_{\hat{z}_m}) || f_{\mathbf{x}}(\mathbf{x} | \theta_{\hat{\epsilon}_m})) \quad (3)$$

$$\Rightarrow \mathcal{L}_{el} := \|\nabla_{\hat{z}_m, \hat{\epsilon}_m, \lambda_m} \mathcal{L}_s\|_2^2 = 0. \quad (4)$$

This provides EF similarity loss in Eq. 9. The notation θ_k is a generated natural parameter by a given $k \in \{\hat{z}, \hat{\theta}\}$, and $f_{\mathbf{x}}(\mathbf{x} | \theta)$ is a power density function of the exponential family. Moreover, λ_m is a trainable parameter for optimizing the Lagrange multiplier, and $D_{\text{KL}}(f_{\mathbf{x}}(\mathbf{x} | \theta_{\hat{z}_m}) || f_{\mathbf{x}}(\mathbf{x} | \theta_{\hat{\epsilon}_m}))$ is a KL divergence of the exponential family to guarantee KL divergence of the transformed distribution always being positive. More details of Eq. 4 are in Appendix B.3.

KL Divergence for Evidence of Lower Bound The KL divergence of Gaussian distribution (Kingma & Welling, 2013) is computed using mean and variance, which are the parameters of a Gaussian distribution. To introduce a loss as the KL divergence of Gaussian distribution, we compute KL divergence of the exponential family in Eq. 1 using the learnable parameter $T(\cdot)$ and $A(\cdot)$ with given natural parameter $\theta_{\hat{z}}$ and $\theta_{\hat{\epsilon}}$, expressed as:

$$\mathcal{L}_{kl} := D_{\text{KL}}(f_{\mathbf{x}}(\mathbf{x} | \theta_{\hat{z}_m}) || f_{\mathbf{x}}(\mathbf{x} | \theta_{\hat{\epsilon}_m})) = A(\theta_{\hat{\epsilon}}) - A(\theta_{\hat{z}}) + \theta_{\hat{z}}^T \nabla_{\theta_{\hat{z}}} A(\theta_{\hat{z}}) - \theta_{\hat{\epsilon}}^T \nabla_{\theta_{\hat{\epsilon}}} A(\theta_{\hat{\epsilon}}). \quad (5)$$

More details of Eq. 5 are in Appendix B.2.

KL divergence calibration loss To reduce the error between the approximation and true matrix for the matrix exponential² (Bader et al., 2019), we add a loss to minimize the difference of their KL divergence measured by mean squared error (MSE) as:

$$\mathcal{L}_{cali} = \text{MSE}(D_{\text{KL}}(q_{\phi}(\mathbf{z} | \mathbf{x}) || p_{\theta}(\mathbf{z})), D_{\text{KL}}(f_{\mathbf{x}}(\mathbf{x} | \theta_{\hat{z}_m}) || f_{\mathbf{x}}(\mathbf{x} | \theta_{\hat{\epsilon}_m}))), \quad (6)$$

which is the KL divergence calibration loss (\mathcal{L}_{cali}).

Sparse log-normalizer We propose sparse log-normalizer to improve disentanglement learning. We apply mask matrix \mathcal{M} which consists of 0 or 1 element to log-normalizer to prevent less effective weight flow as:

$$\mathcal{M}_{ij} = \begin{cases} 1 & \text{if } |\mathcal{W}_{ij}| \geq \mu_{|\mathcal{W}_{ij}|} - \lambda \sigma_{|\mathcal{W}_{ij}|} \\ 0 & \text{otherwise} \end{cases}, \quad (7)$$

²https://pytorch.org/docs/1.10/generated/torch.matrix_exp.html#torch.matrix_exp

where \mathcal{W} is the weight of log-normalizer, λ is a hyper-parameter, $\mu_{|\mathcal{W}_{i,j}|}$, and $\sigma_{|\mathcal{W}_{i,j}|}$ are the mean, and standard deviation of weight respectively. Previous work (Yang et al., 2020) utilizes a semantic mask in input space directly, but we inject the semantic mask implicitly on the latent space.

3.3 INTEGRATION FOR MULTIPLE IE-TRANSFORMATION AND EF-CONVERSION

We mathematically extend IE-transformation to MIE-transformation, which is the equivalent process of β -VAE to enhance disentanglement. The equivalence is proven in Appendix B.1. Each IE-transformation function operates independently, then $p_\theta(\mathbf{x}|\hat{z}_1, \hat{z}_2, \dots, \hat{z}_k) = \prod_{i=1}^k p_\theta(\mathbf{x}|\hat{z}_i)$. Therefore, the reconstruction error term (\mathcal{L}_{rec}) for given all \hat{z}_i in Eq. 9 is

$$\mathcal{L}_{rec} := \sum_{i=1}^k \left[\int q_i(\hat{z}_i|\mathbf{x}) \log p_\theta(\mathbf{x}|\hat{z}_i) d\hat{z}_i \prod_{j=1, j \neq i}^k \int q_j(\hat{z}_j|\mathbf{x}) d\hat{z}_j \right] = \sum_{i=1}^k E_{q_{\phi, \psi_i}(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\psi_i(\mathbf{z})), \quad (8)$$

where $\hat{z}_i = \psi_i(\mathbf{z})$. However, according to the following Eq. 8, k samples are generated, and each sample is disentangled for different factors. We implement the output as the average of the sum of the k samples to obtain a single sample with a superposition effect of disentanglement from k samples, as shown in Fig. 1. More derivation details of Eq. 8 are in Appendix B.1.

The VAEs equipped with MIE-transformation (MIET-VAEs) can be trained with the following loss:

$$\mathcal{L}(\phi, \theta, \psi_{i \in [1, k]}; \mathbf{x}) = \frac{1}{k} \mathcal{L}_{rec} - \mathcal{L}_{kl} - \mathcal{L}_{el} - \mathcal{L}_{cali}. \quad (9)$$

More derivation details of our proposed evidence of lower bound (ELBO) in Appendix B.

4 EXPERIMENT SETTINGS

Models As baseline models, we select VAE, β -VAE, β -TCVAE, and CLG-VAE. These models are compared to their extension to adopt MIET, abbreviated by adding the MIET prefix. We apply the proposed method to β -TCVAE only with the EF similarity loss term because β -TCVAE penalizes the divided KL divergence terms. We set the same encoder and decoder architecture in each model to exclude the overlapped effects. More details of model architecture are in Table 8-9, and Appendix D.

Datasets We use following datasets: dSprites (Matthey et al., 2017), 3D Shapes (Burgess & Kim, 2018), and 3D cars (Reed et al., 2015). More information of datasets are in Appendix E.

Training We set 256 mini-batch size in the datasets (dSprites, 3D Shapes, and 3D Cars), Adam optimizer with learning rate 4×10^{-4} , $\beta_1 = 0.9$, and $\beta_2 = 0.999$ as a common setting for all the comparative methods. For the comparison, we follow training and inference on the whole dataset. We train each model for 30, 67, and 200 epochs on the dSprites, 3D Shapes, and 3D Cars, respectively, as introduced in Kim & Mnih (2018); Ren et al. (2022). More details of the setting are in Appendix D.

Evaluation We evaluate four disentanglement metrics for a less biased understanding of the actual states of disentanglement. The used metrics include FactorVAE metric (FVM) (Kim & Mnih, 2018), MIG metric (Chen et al., 2018), SAP metric (Kumar et al., 2018), and DCI metric (Eastwood & Williams, 2018). More details of the evaluation metric are in Appendix F.

5 RESULTS AND DISCUSSION

5.1 QUANTITATIVE ANALYSIS

Disentanglement Metrics We set the number of IE-transformation functions to be equal to balancing hyper-parameter β on β -VAE because of Eq. 9. The number of IE-transform functions of β -TCVAE is 3. However, in the case of CLG-VAE, we set it to 1 because its approach is based on the group theory, not directly controlling a KL divergence term such as β -VAE. We average each

3D Cars	β -VAE			β -TCVAE		
	MIET	MIET (w/o E)	MIET (w/o EF)	MIET	MIET (w/o E)	MIET (w/o EF)
FVM \uparrow	88.95 (± 5.94)	82.09(± 11.33)	45.23(± 6.39)	96.43 (± 2.42)	91.34(± 4.75)	91.43(± 4.86)
MIG \uparrow	7.27 (± 1.99)	6.77(± 2.41)	0.04(± 0.02)	10.80 (± 1.22)	9.79(± 1.07)	9.81(± 1.10)
SAP \uparrow	1.88 (± 1.12)	1.76(± 1.06)	0.18(± 0.12)	1.88 (± 1.12)	1.35(± 0.30)	1.35(± 0.30)
DCI \uparrow	18.90 (± 4.49)	17.21(± 5.57)	1.67(± 1.26)	26.08 (± 2.47)	25.12(± 3.72)	25.16(± 3.82)

Table 4: Ablation study for the equivariant property (w/o E), and EF-conversion (w/o EF). Each metric is averaged over 40 and 20 settings of β -VAE and β -TCVAE, respectively.

mask ratio	β -VAE (1)				CLG-VAE (0.5)			
	FVM \uparrow	MIG \uparrow	SAP \uparrow	DCI \uparrow	FVM \uparrow	MIG \uparrow	SAP \uparrow	DIC \uparrow
0.0	90.46(± 6.50)	4.84(± 2.32)	1.29(± 0.81)	16.76(± 4.68)	90.06 (± 4.44)	9.28 (± 2.09)	1.82(± 0.82)	19.12 (± 3.41)
0.5	91.35(± 5.52)	5.37(± 2.74)	1.17(± 0.67)	16.65(± 3.76)	88.69(± 4.78)	6.90(± 1.96)	1.85(± 0.67)	17.52(± 3.16)
1.0	91.78 (± 6.20)	4.99(± 2.27)	1.36(± 0.81)	16.50(± 2.53)	83.60(± 11.48)	8.12(± 3.66)	2.37 (± 1.50)	17.07(± 3.89)
1.5	90.04(± 5.88)	7.22 (± 2.87)	1.36 (± 0.48)	18.23 (± 2.84)	84.76(± 6.86)	7.70(± 2.11)	2.05(± 0.73)	17.06(± 2.77)
2.0	87.79(± 8.88)	4.75(± 2.49)	1.01(± 0.99)	16.64(± 3.75)	85.78(± 4.18)	7.83(± 1.79)	1.91(± 0.96)	17.26(± 2.07)
∞	89.43(± 11.72)	3.74(± 2.32)	0.77(± 0.39)	15.45(± 4.59)	82.96(± 11.84)	8.07(± 2.52)	2.32(± 1.02)	17.46(± 4.07)

Table 5: Impact of the mask (mean \pm std.) and its ratio λ in Eq. 7 on 3D Cars. (∞ : no masking case, gray box: the best setting over all metrics, bold text: the best in each metric.) Each model runs with ten random seeds.

model performance value with 40, 20, and 30 cases in VAEs, β -TCVAEs, and Commutative Lie Group VAE (CLG-VAEs) respectively.

As shown in Table 1, MIET-VAEs disentanglement performance is broadly improved with four metrics on each dataset. In particular, most FVM results significantly affect the model performance and stability on all datasets. Therefore, our proposed method obtains a specific dimension that corresponds to a specific single factor. These results imply that applied to MIE-transformation functions on VAEs elaborate disentangled representation learning.

We additionally estimate the p -value of each metrics over models in Table 2. Previous work shows the average case of each models (Yang et al., 2021).

We divide each case into four categories: 1) Positive & Significant, 2) Positive & Insignificant, 3) Negative & Insignificant, and 4) Negative & Significant, where positive is when the mean value is higher than baseline and significant is statistically significant. We estimate the probability of each category: 1) 50%, 2) 36.11%, and 3) 13.89%. As shown in Table 2 and the results, half of the cases are statistically significant, and 86.11% of cases are improved model performance. Even though our method shows a lower value than the baseline, it is not significantly decreased (13.89%). In addition, averaged results show that our method impacts to model itself without hyper-parameter tuning. β -TCVAEs is partially using our method (paragraph Models in Section 4), so it does not show the whole effect of MIET, but it improves model performance in many cases.

Sensitivity to the Number of IE-transformation and EF-conversion We investigate the impact of the MIE-transformation function. As presented in Table. 3, MIE-transformation is better than IE-transformation for disentanglement learning on each dataset. Indeed, MIET- β -VAEs results more clearly show the impact of the MIE-transformation function. Our derivation in Section 3.3 and Appendix B clearly explains MIE-transformation impact. This result shows the impact of the multiple uses of IE-transformation and EF-conversion. More details are in Appendix H.

Ablation Study We conduct an ablation study to evaluate the separate impact of equivariant property and the EF-conversion. We have already presented the impact of the multiple uses of IE-transform and EF-conversion in the previous paragraph. We evaluate the impact of the other properties by setting MIE-transformation 1) without equivariant (w/o E), which is implemented as an asymmetric matrix, and

dSprites	3D Shapes	3D Cars
0.58	0.56	0.67

Table 6: The ratio of seeds to show better performance with symmetric matrix

2) without EF-conversion (w/o EF). To exclude group theory interference with other methods, we select β -VAE and β -TCVAE. As the results are shown in Table 4, most of the results show that MIET-VAEs performance is better than other cases. In particular, MIET (w/o EF) results are lower than MIET (w/o E) results and are clearly shown in all cases. More details are in Appendix I.

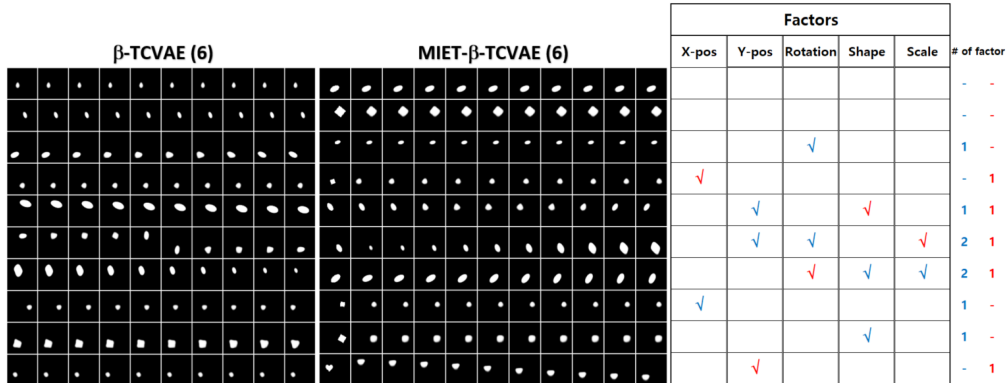


Figure 3: dSprites

Figure 4: Qualitative results on dSprites. The left-side grids are input images and their variants by changing activations of each dimension of latent vectors. The first row shows input images. The right-side table shows matching pre-defined factors of the dataset (red: MIET, blue: no MIET).

Impact of Symmetric Matrix Exponential We empirically show the benefit of using a symmetric matrix for ψ . Table 6 shows the ratio of runs with a symmetric matrix, which shows better performance than unrestricted matrices, to the total 240 (60 models \times 4 metrics) runs for each dataset. All results are higher than 0.5, which implies that the constraint enhances I2L equivariance even with uncertain factors.

Impact of Sparse Log-normalizer We set masking hyper-parameter λ from $\{0.0, 0.5, \dots, 2.0, \infty\}$, and each model has different λ for best case. In Table 5, VAE and CLG-VAE with masked log-normalizer show better and well-balanced results than the models without masking, which implies improvement of disentanglement.

5.2 QUALITATIVE ANALYSIS

We randomly sample an image for each dimension of the latent vector space and creates 10 variants of its generated latent vector by selecting values from $\{-2, 2\}$ with 10 intervals for the dimension, then generate their corresponding output images. For the generation, we select β -TCVAE (6), which shows the best FVM scores in dSprites dataset. Thereafter, we evaluate the semantic roles of each dimension before and after applying MIE-transformation function.

In Fig. 3, β -TCVAE struggles with y-position and rotation, as shown on the 6th row, and with scale and shape represented on the 7th row. On the contrary, MIET- β -TCVAE separates y-position and rotation factor (10th, and 7th rows), also the activated dimensions of MIET- β -TCVAE are not overlapped with each factor. Applied our method on β -TCVAE shows better disentangled representation on dSprites dataset. These results also show that our proposed method improves disentangled representation learning. More results are in Appendix K.

6 CONCLUSION

In this paper, we address the problem of injecting inductive bias for learning unsupervised disentangled representations. To build the bias in VAE frameworks, we propose MIE-transformation composed of 1) IE-transformation for the benefits of invertibility and equivariance in disentanglement, 2) a training loss and module to adapt unrestricted prior and posterior to an approximated exponential family, and 3) integration of multiple units of IE-transformation function and EF-conversion for more expressive bias. The method is easily equipped on state-of-the-art VAEs for disentanglement learning and shows significant improvement on dSprites, 3D Shapes, and 3D Cars datasets. We expect that our method can be applied to more VAEs, and extended to downstream applications. Our work is limited to holding potential equivariance of I2L transformation, so more direct methods to induce it can be integrated in the future.

7 REPRODUCIBILITY STATEMENT

In this section, we summarize detail contents for reproducing our theoretical and empirical results.

- Equations for MIET Method Implementation
 1. Objective function: Equation 9, Appendix B.1.
 2. EF family equation: Equation 1, Appendix B.3.
 3. EF similarity loss: Equation 2-4.
 4. KL Divergence of EF family: Equation 5, Appendix B.2.
 5. Reconstruction loss: Equation 8, Appendix 9.
- Motivation Proofs
 1. Proposition 1-3 : Appendix C.
- Experiment setting details
 1. Hyper-parameters: Appendix D.1.
 2. Training procedure and model configuration: Appendix D.2.
 3. Datasets: Appendix E.
 4. Quantitative analysis setting: Appendix F.
 5. Code description for running experiments: Supplementary material.

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A NOTATION

\mathbf{z}	Latent vector from encoder	$\psi(\cdot)$	Invertible function
$\hat{\mathbf{z}}_m$	Transformed latent vector by $\psi_m(\cdot)$	$\hat{\epsilon}_m$	Transformed prior samples by $\psi_m(\cdot)$
$\theta_{\hat{\mathbf{z}}_m}$	Natural Parameter of posterior	$\theta_{\hat{\epsilon}_m}$	Natural Parameter of prior
T	Sufficient Statistics	A	Log-Normalizer
ν	Evidence	$D_{\text{KL}}(\cdot \cdot)$	Kullback-Leibler divergence
$f_{\mathbf{x}}(\cdot)$	Power Density Function	$M_n(\mathbb{R})$	A set of $n \times n$ real matrix
$Sym_n(\mathbb{R})$	A set of $n \times n$ symmetric real matrix	E_M	$\{\mathbf{e}^M M \in M_n(\mathbb{R})\}$
E_S	$\{\mathbf{e}^S S \in Sym_n(\mathbb{R})\}$	G_S	$G_S : (\mathbf{e}^S, *)$
G_I	Group of input space for symmetries	G_L	Group of latent space for symmetries (equivariant to G_I)
$\psi_M(\cdot)$	$\psi_M(\cdot) \in M_n(\mathbb{R})$	$\psi_{E_M}(\cdot)$	$\psi_{E_M}(\cdot) \in E_M$
$\psi_{E_S}(\cdot)$	$\psi_{E_S}(\cdot) \in E_S$	$\mathbf{0}$	zero vector
$\mathbf{0}_{n,n}$	n by n zero matrix	\mathcal{X}	Input space
\mathcal{Z}	Latent vector space	$\hat{\mathcal{Z}}$	Transformed latent vector space
Ξ	$G_I \times G_L \rightarrow G_L$	Γ	$G_L \times G_T \rightarrow G_T$

B OBJECTIVE FUNCTION

B.1 EVIDENCE OF LOWER BOUND (ELBO)

The log likelihood of $p(\mathbf{x})$ can be derived as follows:

$$\log p_{\theta}(\mathbf{x}) = \int q_1(\hat{\mathbf{z}}_1|\mathbf{x})q_2(\hat{\mathbf{z}}_2|\mathbf{x}) \cdots q_k(\hat{\mathbf{z}}_k|\mathbf{x}) \log p_{\theta}(\mathbf{x}) d\hat{\mathbf{z}}' \quad (10)$$

$$= \int q_1(\hat{\mathbf{z}}_1|\mathbf{x})q_2(\hat{\mathbf{z}}_2|\mathbf{x}) \cdots q_k(\hat{\mathbf{z}}_k|\mathbf{x}) \log \frac{p_{\theta}(\mathbf{x}, \hat{\mathbf{z}}_1, \hat{\mathbf{z}}_2, \cdots, \hat{\mathbf{z}}_k)}{p_{\theta}(\hat{\mathbf{z}}_1, \hat{\mathbf{z}}_2, \cdots, \hat{\mathbf{z}}_k|\mathbf{x})} d\hat{\mathbf{z}}' \quad (11)$$

$$= \int q_1(\hat{\mathbf{z}}_1|\mathbf{x})q_2(\hat{\mathbf{z}}_2|\mathbf{x}) \cdots q_k(\hat{\mathbf{z}}_k|\mathbf{x}) \cdot \quad (12)$$

$$\left[\log \frac{p_{\theta}(\mathbf{x}, \hat{\mathbf{z}}_1, \hat{\mathbf{z}}_2, \cdots, \hat{\mathbf{z}}_k)}{q(\hat{\mathbf{z}}_1, \hat{\mathbf{z}}_2, \cdots, \hat{\mathbf{z}}_k|\mathbf{x})} - \log \frac{p_{\theta}(\hat{\mathbf{z}}_1, \hat{\mathbf{z}}_2, \cdots, \hat{\mathbf{z}}_k|\mathbf{x})}{q(\hat{\mathbf{z}}_1, \hat{\mathbf{z}}_2, \cdots, \hat{\mathbf{z}}_k|\mathbf{x})} \right] d\hat{\mathbf{z}}'$$

$$\geq \int q_1(\hat{\mathbf{z}}_1|\mathbf{x})q_2(\hat{\mathbf{z}}_2|\mathbf{x}) \cdots q_k(\hat{\mathbf{z}}_k|\mathbf{x}) \log \frac{p_{\theta}(\mathbf{x}, \hat{\mathbf{z}}_1, \hat{\mathbf{z}}_2, \cdots, \hat{\mathbf{z}}_k)}{q(\hat{\mathbf{z}}_1, \hat{\mathbf{z}}_2, \cdots, \hat{\mathbf{z}}_k|\mathbf{x})} d\hat{\mathbf{z}}' \quad (13)$$

$$= \int q_1(\hat{\mathbf{z}}_1|\mathbf{x})q_2(\hat{\mathbf{z}}_2|\mathbf{x}) \cdots q_k(\hat{\mathbf{z}}_k|\mathbf{x}) \cdot \quad (14)$$

$$\left[\log p_{\theta}(\mathbf{x}|\hat{\mathbf{z}}_1, \hat{\mathbf{z}}_2, \cdots, \hat{\mathbf{z}}_k) + \log \frac{p(\hat{\mathbf{z}}_1, \hat{\mathbf{z}}_2, \cdots, \hat{\mathbf{z}}_k)}{q(\hat{\mathbf{z}}_1, \hat{\mathbf{z}}_2, \cdots, \hat{\mathbf{z}}_k|\mathbf{x})} \right] d\hat{\mathbf{z}}',$$

where $d\hat{\mathbf{z}}' = d\hat{\mathbf{z}}_1 d\hat{\mathbf{z}}_2 \cdots d\hat{\mathbf{z}}_k$. Each IE-transformation operates independently, then

$$p_{\theta}(\mathbf{x}|\hat{\mathbf{z}}_1, \hat{\mathbf{z}}_2, \cdots, \hat{\mathbf{z}}_k) = \prod_{i=1}^k p_{\theta}(\mathbf{x}|\hat{\mathbf{z}}_i).$$

$$\log p_\theta(\mathbf{x}) \geq \frac{1}{k} \sum_{i=1}^k \left[\int q_i(\hat{\mathbf{z}}_i|\mathbf{x}) \log p_\theta(\mathbf{x}|\hat{\mathbf{z}}_i) d\hat{\mathbf{z}}_i \prod_{j=1, j \neq i}^k \int q_j(\hat{\mathbf{z}}_j|\mathbf{x}) d\hat{\mathbf{z}}_j \right] \quad (15)$$

$$\begin{aligned} & - \int q_1(\hat{\mathbf{z}}_1|\mathbf{x}) q_2(\hat{\mathbf{z}}_2|\mathbf{x}) \cdots q_k(\hat{\mathbf{z}}_k|\mathbf{x}) \log \frac{q_1(\hat{\mathbf{z}}_1|\mathbf{x}) q_2(\hat{\mathbf{z}}_2|\mathbf{x}) \cdots q_k(\hat{\mathbf{z}}_k|\mathbf{x})}{p(\hat{\mathbf{z}}_1) p(\hat{\mathbf{z}}_2) \cdots p(\hat{\mathbf{z}}_k)} d\hat{\mathbf{z}}' \\ & = \frac{1}{k} \sum_{i=1}^k \mathbb{E}_{q(\hat{\mathbf{z}}_i|\mathbf{x})} \log p_\theta(\mathbf{x}|\hat{\mathbf{z}}_i) - \sum_{i=1}^k \left[D_{\text{KL}}(q_\phi(\hat{\mathbf{z}}_i|\mathbf{x})||p(\hat{\mathbf{z}}_i)) \prod_{j=1, j \neq i}^k \int q_j(\hat{\mathbf{z}}_j|\mathbf{x}) d\hat{\mathbf{z}}_j \right] \end{aligned} \quad (16)$$

$$= \frac{1}{k} \sum_{i=1}^k \mathbb{E}_{q_\phi(\hat{\mathbf{z}}_i|\mathbf{x})} \log p_\theta(\mathbf{x}|\hat{\mathbf{z}}_i) - \sum_{i=1}^k D_{\text{KL}}(q_\phi(\hat{\mathbf{z}}_i|\mathbf{x})||p(\hat{\mathbf{z}}_i)) \quad (17)$$

$$= \frac{1}{k} \sum_{i=1}^k \mathbb{E}_{q_{\phi, \psi_i}(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\psi_i(\mathbf{z})) - \sum_{i=1}^k D_{\text{KL}}(q_{\phi, \psi_i}(\mathbf{z}|\mathbf{x})||p_{\psi_i}(\mathbf{z})). \quad (18)$$

Therefore, we define ELBO as:

$$\mathcal{L}'(\phi, \theta, \psi_{i \in [1, k]}; \mathbf{x}) = \underbrace{\frac{1}{k} \sum_{i=1}^k \mathbb{E}_{q_{\phi, \psi_i}(\mathbf{z}_i|\mathbf{x})} \log p_\theta(\mathbf{x}|\psi_i(\mathbf{z}))}_{\text{① reconstruction loss}} - \underbrace{\sum_{i=1}^k D_{\text{KL}}(q_{\phi, \psi_i}(\mathbf{z}|\mathbf{x})||p_{\psi_i}(\mathbf{z}))}_{\text{② KL divergence}}. \quad (19)$$

However, following Eq. 19, k samples are generated, and each sample is disentangled for different factors. We implement the output as the average of the sum of the k samples to obtain a single sample with a superposition effect from k samples. Moreover, the KL divergence term in Eq. 19 represents that increasing number of MIE-transformation is equal to increasing β hyper-parameter in β -VAE (Higgins et al., 2017).

B.2 EXPONENTIAL FAMILY KULLBACK-LEIBLER DIVERGENCE

The second term of Eq. 19 is equal to $D_{\text{KL}}(f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}})||f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{e}}}))$ because power density function of posterior and prior are $f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}})$ and $f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{e}}})$, respectively.

$$D_{\text{KL}}(f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}})||f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{e}}})) = \int_{-\infty}^{\infty} f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}}) \log f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}}) d\mathbf{x} - \int_{-\infty}^{\infty} f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}}) \log f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{e}}}) d\mathbf{x}. \quad (20)$$

We designed sufficient statistics as matrix multiplication (multi-layer perceptron).

$$\int_{-\infty}^{\infty} f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}}) \log f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}}) d\mathbf{x} = \int_{-\infty}^{\infty} f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}}) [\theta_{\hat{\mathbf{z}}}^T \mathbf{T}(\mathbf{x}) - A(\theta_{\hat{\mathbf{z}}}) + B(\mathbf{x})] d\mathbf{x} \quad (21)$$

$$= -A(\theta_{\hat{\mathbf{z}}}) \int_{-\infty}^{\infty} f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}}) d\mathbf{x} + \int_{-\infty}^{\infty} f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}}) [\theta_{\hat{\mathbf{z}}}^T \mathbf{T}(\mathbf{x}) + B(\mathbf{x})] d\mathbf{x} \quad (22)$$

$$= -A(\theta_{\hat{\mathbf{z}}}) + \theta_{\hat{\mathbf{z}}}^T \int_{-\infty}^{\infty} T(\mathbf{x}) f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}}) d\mathbf{x} + \int_{-\infty}^{\infty} B(\mathbf{x}) f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}}) d\mathbf{x}, \quad (23)$$

and

$$\int_{-\infty}^{\infty} f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}}) \log f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{e}}}) d\mathbf{x} = -A(\theta_{\hat{\mathbf{e}}}) + \theta_{\hat{\mathbf{e}}}^T \int_{-\infty}^{\infty} T(\mathbf{x}) f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{e}}}) d\mathbf{x} + \int_{-\infty}^{\infty} B(\mathbf{x}) f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{e}}}) d\mathbf{x}. \quad (24)$$

$$\begin{aligned} \therefore D_{\text{KL}}(f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}})||f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{e}}})) & = A(\theta_{\hat{\mathbf{e}}}) - A(\theta_{\hat{\mathbf{z}}}) + \theta_{\hat{\mathbf{z}}}^T \int_{-\infty}^{\infty} T(\mathbf{x}) f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{z}}}) d\mathbf{x} \\ & \quad - \theta_{\hat{\mathbf{e}}}^T \int_{-\infty}^{\infty} T(\mathbf{x}) f_{\mathbf{x}}(\mathbf{x}|\theta_{\hat{\mathbf{e}}}) d\mathbf{x}. \end{aligned} \quad (25)$$

The mean of the sufficient statistic is followed as:

$$\int_{-\infty}^{\infty} T(\mathbf{x})f_{\mathbf{x}}(\mathbf{x}|\boldsymbol{\theta})d\mathbf{x} = \frac{\partial A^*(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \approx \frac{\partial A(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} \quad \because A^*(\boldsymbol{\theta}) = \boldsymbol{\theta}^\top A^*, \quad (26)$$

where $A^*(\cdot)$ is a true log-partition function of the exponential family (ideal case of $A(\cdot)$). However, estimating A^* is difficult, and there is no direct method without random samplings, such as mini-batch weighted sampling or mini-batch stratified sampling (Chen et al., 2018). Then, we approximate A^* to A , and train A to be close to A^* . Consequently, we obtain KL divergence of the exponential family as:

$$\int_{-\infty}^{\infty} f_{\mathbf{x}}(\mathbf{x}|\boldsymbol{\theta}_{\hat{\mathbf{z}}}) \log f_{\mathbf{x}}(\mathbf{x}|\boldsymbol{\theta}_{\hat{\mathbf{z}}}) = -A(\boldsymbol{\theta}_{\hat{\mathbf{z}}}) + \boldsymbol{\theta}_{\hat{\mathbf{z}}}^\top \frac{\partial A(\boldsymbol{\theta}_{\hat{\mathbf{z}}})}{\partial \boldsymbol{\theta}_{\hat{\mathbf{z}}}} + \int_{-\infty}^{\infty} f_{\mathbf{x}}(\mathbf{x}|\boldsymbol{\theta}_{\hat{\mathbf{z}}})B(\mathbf{x})d\mathbf{x}, \quad (27)$$

$$\int_{-\infty}^{\infty} f_{\mathbf{x}}(\mathbf{x}|\boldsymbol{\theta}_{\hat{\mathbf{z}}}) \log f_{\mathbf{x}}(\mathbf{x}|\boldsymbol{\theta}_{\hat{\boldsymbol{\epsilon}}}) = -Z(\boldsymbol{\theta}_{\hat{\boldsymbol{\epsilon}}}) + \boldsymbol{\theta}_{\hat{\boldsymbol{\epsilon}}}^\top \frac{\partial A(\boldsymbol{\theta}_{\hat{\boldsymbol{\epsilon}}})}{\partial \boldsymbol{\theta}_{\hat{\boldsymbol{\epsilon}}}} + \int_{-\infty}^{\infty} f_{\mathbf{x}}(\mathbf{x}|\boldsymbol{\theta}_{\hat{\mathbf{z}}})B(\mathbf{x})d\mathbf{x}. \quad (28)$$

Therefore, the final Kullback-Leibler divergence of exponential family is followed as:

$$D_{\text{KL}}(f_{\mathbf{x}}(\mathbf{x}|\boldsymbol{\theta}_{\hat{\mathbf{z}}})||f_{\mathbf{x}}(\mathbf{x}|\boldsymbol{\theta}_{\hat{\boldsymbol{\epsilon}}})) = A(\boldsymbol{\theta}_{\hat{\boldsymbol{\epsilon}}}) - A(\boldsymbol{\theta}_{\hat{\mathbf{z}}}) + \boldsymbol{\theta}_{\hat{\mathbf{z}}}^\top \frac{\partial A(\boldsymbol{\theta}_{\hat{\mathbf{z}}})}{\partial \boldsymbol{\theta}_{\hat{\mathbf{z}}}} - \boldsymbol{\theta}_{\hat{\boldsymbol{\epsilon}}}^\top \frac{\partial A(\boldsymbol{\theta}_{\hat{\boldsymbol{\epsilon}}})}{\partial \boldsymbol{\theta}_{\hat{\boldsymbol{\epsilon}}}}. \quad (29)$$

B.3 BACKGROUND OF EXPONENTIAL FAMILY

Power density function of the exponential family (PDF) generalized formulation:

$$\begin{aligned} f_{\mathbf{x}}(\mathbf{x}|\boldsymbol{\theta}) &= h(\mathbf{x})\exp(\boldsymbol{\theta}^\top T(\mathbf{x}) - A(\boldsymbol{\theta})) \\ &= \exp(\boldsymbol{\theta}^\top T(\mathbf{x}) - A(\boldsymbol{\theta}) + B(\mathbf{x})), \end{aligned} \quad (30)$$

where *sufficient statistics* $T(\cdot)$, *log-normalizer* $A(\cdot)$, and *carrier or base measure* $B(\cdot)$ are known functions, samples \mathbf{x} from distribution, and *natural parameter* $\boldsymbol{\theta}$. However, we set $T(\cdot)$, $A(\cdot)$, and $B(\cdot)$ are deterministic functions by maximizing conjugate prior for parameter ξ . To determine the *natural parameter* of posterior and prior $\boldsymbol{\theta}_{\hat{\mathbf{z}}_m}$, and $\hat{\boldsymbol{\epsilon}}_m$, we use a natural parameter generator (NPG) designed by multi-layer perceptron (Charpentier et al., 2022a). As introduced in Bishop (2006); Charpentier et al. (2022a), we assume exponential family always admits a conjugate prior:

$$q(\boldsymbol{\theta}|\xi, \boldsymbol{\nu}) = \exp(\boldsymbol{\nu}\boldsymbol{\theta}^\top \xi - \boldsymbol{\nu}A(\boldsymbol{\theta}) + B'(\xi, \boldsymbol{\nu})), \quad (31)$$

where $B'(\cdot)$ is a *normalize coefficient* and $\boldsymbol{\nu}$ is evidence, and it is expressed by prior natural parameter ξ . However, generated natural parameter $\boldsymbol{\theta}_{\hat{\mathbf{z}}_m}$ is not guaranteed as the appropriate parameter of the exponential family corresponds to conjugate prior. To satisfy this condition, we assume observation is a set of independent identically distributed, then Eq. 30 is modified: $p(\mathbf{X}|\boldsymbol{\theta}) = \prod_{n=1}^N h(\mathbf{x}_n)\exp(\boldsymbol{\theta}^\top \sum_{n=1}^N T(\mathbf{x}_n) - A(\boldsymbol{\theta}))$ (Bishop, 2006), where observation $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$. In the next, we multiply the modified formation by the prior Eq. 31 to obtain the posterior distribution (Bishop, 2006) as Eq. 1.

C PROOF

C.1 $E_M \not\subset E_S$

All elements of E_S are symmetric because of the matrix exponential property that $\mathbf{e}^{M^\top} = (\mathbf{e}^M)^\top$. If M is a symmetric matrix then $\mathbf{e}^{M^\top} = \mathbf{e}^M = (\mathbf{e}^M)^\top$. Therefore, if M is symmetric then the exponential of M is also symmetric. We show a counter example to $E_M \subset E_S$. When $M =$

$$\begin{aligned}
& \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \\
e^M &= \sum_{k=0}^{\infty} \frac{1}{k!} M^k \\
&= I + \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} + \frac{1}{2!} \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}^2 + \cdots + \frac{1}{(n-1)!} \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}^{(n-1)} + \cdots \\
&= I + \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} + \frac{1}{2!} \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} + \cdots + \frac{1}{(n-1)!} \begin{bmatrix} 1 & n-1 \\ 0 & 1 \end{bmatrix} + \cdots \\
&= I + \begin{bmatrix} \sum_{n=0}^{\infty} \frac{1}{n!} & 1 + \sum_{n=0}^{\infty} \frac{1}{(n-1)!} \\ 0 & \sum_{n=0}^{\infty} \frac{1}{n!} \end{bmatrix} \\
&= \begin{bmatrix} 1 + \sum_{n=0}^{\infty} \frac{1}{n!} & 1 + \sum_{n=0}^{\infty} \frac{1}{(n-1)!} \\ 0 & 1 + \sum_{n=0}^{\infty} \frac{1}{n!} \end{bmatrix} \\
&= \begin{bmatrix} 1+e & 1+e \\ 0 & 1+e \end{bmatrix}.
\end{aligned} \tag{32}$$

The matrix e^M is asymmetric and not in E_S . Therefore $E_M \not\subset E_S$.

C.2 TRANSITIVITY OF EQUIVARIANCE

We show that ψ_{G_S} preserves equivariance between group elements of latent space in $\textcircled{\text{a}}$ and input space. If there exists equivariance between input and latent vector space, there should be a group G_L for a latent space and its corresponding group G_I in an input space by definition of equivariance ($q_\phi(g_I x) = g_L q_\phi(x)$).

Let g_L^a be a group element in $\textcircled{\text{a}}$, and g_I^a is a group element in G_I corresponding to $\textcircled{\text{a}}$, and g_T^a is a group element where corresponding to $\textcircled{\text{a}}$ on the latent vector space transformed from the original latent vector space. Then, group element g_T^a is equal to g_L^a :

$$\hat{z}_1 = \psi_{G_S}(z_1), \text{ and} \tag{33}$$

$$\hat{z}_2 = \psi_{G_S}(z_2) = \psi_{G_S}(g_L^a z_1) = g_L^a \psi_{G_S}(z_1) (\because \text{Proposition 1}), \tag{34}$$

$$\text{then } g_L^a \psi_{G_S}(z_1) = g_T^a \psi_{G_S}(z_1) (\because \hat{z}_2 = g_T^a \hat{z}_1) \tag{35}$$

$$\Rightarrow (g_L^a - g_T^a) \psi_{G_S}(z_1) = \mathbf{0}, \tag{36}$$

where $\mathbf{0}$ is a zero vector. Eq. 35 is defined when $\forall z \in \mathcal{Z}$ by the equivariance definition. In other words, Eq. 35 is satisfied only if the kernel (linear algebra) of $g_L^a - g_T^a$, notated as $\ker(g_L^a - g_T^a)$, includes the basis of \mathbb{R}^n vector space. If the standard basis of \mathbb{R}^n vector space is in $\ker(g_L^a - g_T^a)$, then $(g_L^a - g_T^a) = \mathbf{0}_{n,n}$, where $\mathbf{0}_{n,n}$ is an n by n zero matrix. Other bases of \mathbb{R}^n vector space are expressed by the standard basis. Therefore $g_L^a - g_T^a = \mathbf{0}_{n,n}$.

Then, $\psi_{G_S}(g_L^a z_1) = g_L^a \psi_{G_S}(z_1) = g_T^a \psi_{G_S}(z_1)$. The encoder is an equivariant function over input space \mathcal{X} as $q_\phi(g_I^a \mathbf{x}_1) = g_L^a q_\phi(\mathbf{x}_1)$. Mixing two equivariance property, we can derive another equivariance relation $g_T^a \psi_{G_S}(q_\phi(\mathbf{x}_1)) = \psi_{G_S}(q_\phi(g_I^a \mathbf{x}_1))$. This result implies that the equivariance between input space and a latent space is preserved for $\textcircled{\text{a}}$ if the latent vector z is transformed by ψ_{G_S} .

D MODEL AND TRAINING PROCEDURE DETAILS

D.1 HYPER-PARAMETERS

We set 256 mini-batch size in the datasets (dSprites, 3D Shapes, and 3D Cars), Adam optimizer with learning rate 4×10^{-4} , $\beta_1 = 0.9$, $\beta_2 = 0.999$, and epochs from $\{30, 67, 200\}$ as a common setting

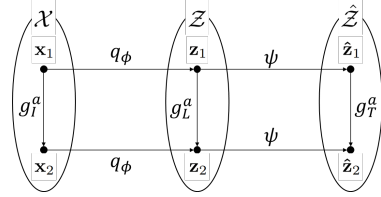


Figure 5: Equivariant map: \mathcal{X} , \mathcal{Z} , and $\hat{\mathcal{Z}}$ are input space, latent vector space, and transformed latent vector space by L2L transformation function $\psi(\cdot) : \mathbb{R}^n \rightarrow \mathbb{R}^n$, respectively. $\mathbf{x} \in \mathcal{X}$, $\mathbf{z} \in \mathcal{Z}$, and $\hat{\mathbf{z}} \in \hat{\mathcal{Z}}$.

models	hyper-parameters	values
common	batch size	256
	epoch	{30, 200}
	optim	Adam
	lr	4e-4
	lr for MIET	4e-4
	weight decay	1e-4
β -VAE	latent dim	10
	# of IE and EF	{1, 2, 4, 10}
β -TCVAE	β	{4, 6}
	# of IE and EF	{1, 3}
commut-VAE	α, γ	1.0
	λ_{decomp}	40
	λ_{hessian}	40
	forward group	0.2
commut-VAE	group reconst	{0.2, 0.5, 0.7}

(a) dSprites and 3D Cars: epochs for dSprites and 3D cars are 30 and 200, respectively.

models	hyper-parameters	values
common	batch size	256
	epoch	67
	optim	Adam
	lr	4e-4
	lr for MIET	4e-4
β -VAE	# of IE and EF	{1, 2, 4, 10}
	weight decay	0.0
	latent dim	6
β -TCVAE	β	{4, 6}
	# of IE and EF	{1, 3}
	α, γ	1.0
	weight decay	1e-4
	latent dim	6
commut-VAE	λ_{decomp}	40
	λ_{hessian}	40
	forward group	0.2
	group reconst	{0.2, 0.5, 0.7}
	weight decay	0.0
	latent dim	10

(b) 3D Shapes

Table 7: Notation commut-VAE is CLG-VAEs, lr is learning rate, latent dim is dimension size of latent vector, group reconst is group reconstruction, and forward group is forward group pass.

for all the comparative methods. For the comparison, we follow training and inference on the whole dataset. We train each model for 30, 67, and 200 epochs on the dSprites, 3D Shapes, and 3D Cars, respectively, as introduced in Kim & Mnih (2018); Ren et al. (2022). We tune β from {1, 2, 4, 10} and {4, 6} for β -VAE and β -TCVAE, respectively. We set the dimension size of the latent vectors from {6, 10} for 10 on dSprites and 3D Cars datasets and 6 for 3D Shapes, but we set 10 for CLG-VAE because it sets 10 dimensions size on 3D Shapes in Zhu et al. (2021). Regarding the CLG-VAE, we fix λ_{decomp} , λ_{hessian} , and forward group features as 40, 20, and 0.2, respectively. Because the hyper-parameters showed the best result in Zhu et al. (2021). We set group reconstruction from {0.2, 0.5, 0.7}. In addition, we set masking ratio λ from {0.0, 0.5, . . . 2.0, ∞ }. **To check the impact of MIE-transformation, we do not consider the Groupified VAE because the latter is implemented with an extended decoder (different capacity).**

D.2 TRAINING PROCEDURE AND MODEL

We present the model architecture for each dataset in Table 8 and 9. For MIET architecture reproduction, Algorithm 2 to Algorithm 4. To estimate EF similarity loss, we directly implement $\nabla_{\hat{z}, \hat{\epsilon}} \lambda_m p(\theta | \mathbf{X}, \mathcal{X}, \nu) + \lambda_m D_{\text{KL}}(f_{\hat{z}}(\hat{z} | \theta_{\hat{z}}) || f_{\hat{\epsilon}}(\hat{\epsilon} | \theta_{\hat{\epsilon}}))$, instead of implementing posterior, in our supplement materials. More details of this algorithm are in `ie_transformation.py` file.

Encoder	Decoder
Input 64×64 binary image	input $\in \mathbb{R}^{10}$
4×4 conv. 32 ReLU. stride 2	FC. 128 ReLU.
4×4 conv. 32 ReLU. stride 2	FC. $4 \times 4 \times 64$ ReLU.
4×4 conv. 64 ReLU. stride 2	4×4 upconv. 64 ReLU. stride 2.
4×4 conv. 64 ReLU. stride 2	4×4 upconv. 32 ReLU. stride 2.
FC. 128. FC. 2×10	4×4 upconv. 32 ReLU. stride 2.
	4×4 upconv. 1. stride 2

Table 8: VAE architecture for dSprites dataset.

Algorithm 1 Unit Invertible and Equivariant Transformation Function (UIET-function)

Input: matrices M_1 , and M_2

Output: Invertible and Equivariant Transformation Function $\psi(\cdot)$

$$M_1, M_2 \leftarrow \frac{1}{2}(M_1 + M_1^T), \frac{1}{2}(M_2 + M_2^T)$$

$$\psi(\cdot) \leftarrow M_1^T M_2$$

Encoder	Decoder
Input $64 \times 64 \times 3$ RGB image	input $\in \mathbb{R}^6$ (3D Shapes), \mathbb{R}^{10} (3D Cars)
4×4 conv. 32 ReLU. stride 2	FC. 256 ReLU.
4×4 conv. 32 ReLU. stride 2	FC. $4 \times 4 \times 64$ ReLU.
4×4 conv. 64 ReLU. stride 2	4×4 upconv. 64 ReLU. stride 2.
4×4 conv. 64 ReLU. stride 2	4×4 upconv. 32 ReLU. stride 2.
FC. 256. FC. 2×10	4×4 upconv. 32 ReLU. stride 2.
	4×4 upconv. 3. stride 2

Table 9: VAE architecture for 3D Shapes, and 3D Cars datasets. For exceptional case, CLG-VAE, we use ten dimension size on 3D Shapes dataset (Zhu et al., 2021).

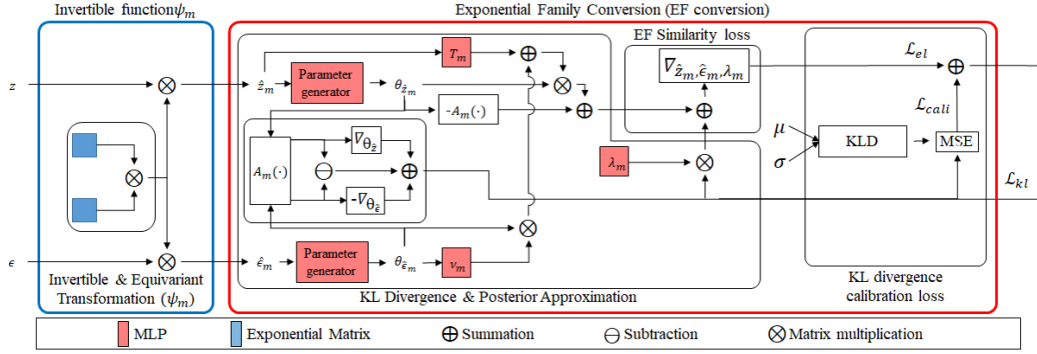


Figure 6: The overall architecture of our proposed *MIET-VAE*. KLD is the KL divergence of Gaussian Distribution in Kingma & Welling (2013). $\nabla_{\hat{z}_m, \hat{\epsilon}_m, \lambda_m}$ is in Eq. 4, and MSE is a mean squared error. More details of our proposed method are introduced in Section 3.

Algorithm 2 IE-Transformation

Input: latent vector z , and samples from prior ϵ

Output: transformed latent vector \hat{z} , and transformed normal Gaussian distribution samples $\hat{\epsilon}$

$$\begin{aligned} \psi(\cdot) &\leftarrow \text{UIET-function } (M_1, M_2) \\ \hat{z}, \hat{\epsilon} &\leftarrow \psi(z), \psi(\epsilon) \end{aligned}$$

Algorithm 3 KL Divergence & Posterior Estimator

Input: latent vector \hat{z}_m , prior samples $\hat{\epsilon}_m$,

Natural Parameter Generator $\Omega_1(\cdot), \Omega_2(\cdot)$

log-normalizer A , *sufficient statistics* T , and *evidence* ν .

Output: KL divergence $D_{\text{KL}}(f_{\hat{z}}(\hat{z}|\theta_{\hat{z}})||f_{\hat{\epsilon}}(\hat{\epsilon}|\theta_{\hat{\epsilon}}))$, and posterior $p(\theta|\mathbf{X}, \mathcal{X}, \nu)$

$$\theta_{\hat{z}}, \theta_{\hat{\epsilon}} \leftarrow \Omega_1(\hat{z}), \Omega_2(\hat{\epsilon})$$

$$A \leftarrow \text{sparse log-normalizer}(A)$$

▷ Equation 7

$$p(\theta|\mathbf{X}, \mathcal{X}, \nu) \leftarrow \exp\left[\theta_{\hat{z}}\left(\sum_{i=1}^B T(\hat{z}_i) + \nu\theta_{\hat{\epsilon}}\right) - A(\theta_{\hat{z}})\right]$$

▷ Equation 1

$$D_{\text{KL}}(f_{\hat{z}}(\hat{z}|\theta_{\hat{z}})||f_{\hat{\epsilon}}(\hat{\epsilon}|\theta_{\hat{\epsilon}})) \leftarrow A(\theta_{\hat{\epsilon}}) - A(\theta_{\hat{z}}) + \theta_{\hat{z}}^\top \frac{\partial A(\theta_{\hat{z}})}{\partial \theta_{\hat{z}}} - \theta_{\hat{\epsilon}}^\top \frac{\partial A(\theta_{\hat{\epsilon}})}{\partial \theta_{\hat{\epsilon}}}$$

▷ Equation 5

Algorithm 4 EF-Conversion Loss

Input: KL divergence $D_{\text{KL}}(f_{\hat{z}}(\hat{z}|\theta_{\hat{z}})||f_{\hat{\epsilon}}(\hat{\epsilon}|\theta_{\hat{\epsilon}}))$, posterior $p(\theta|\mathbf{X}, \mathcal{X}, \nu)$, μ, σ

Output: Regularization \mathcal{L}_{reg}

$$\mathcal{L}_{\text{el}} \leftarrow p(\theta|\mathbf{X}, \mathcal{X}, \nu) + \lambda_m D_{\text{KL}}(f_{\hat{z}}(\hat{z}|\theta_{\hat{z}})||f_{\hat{\epsilon}}(\hat{\epsilon}|\theta_{\hat{\epsilon}}))$$

$$\mathcal{L}_{\text{el}} \leftarrow \|\nabla_{\hat{z}_m, \hat{\epsilon}_m, \lambda_m} \mathcal{L}_{\text{el}}\|_2^2$$

$$D_{\text{KL}}(q_\phi(z|\mathbf{x})||p(z)) \leftarrow 0.5 \sum_{d=1}^D (1 + 2 \log \sigma_j - \mu_j^2 - \sigma_j^2) \quad \triangleright \text{Reference (Kingma \& Welling, 2013)}$$

$$\mathcal{L}_{\text{cali}} \leftarrow \text{MSE}(D_{\text{KL}}(f_{\hat{z}}(\hat{z}|\theta_{\hat{z}})||f_{\hat{\epsilon}}(\hat{\epsilon}|\theta_{\hat{\epsilon}})), D_{\text{KL}}(q_\phi(z|\mathbf{x})||p(z)))$$

▷ Equation 6

$$\mathcal{L} \leftarrow \mathcal{L}_{\text{el}} + \mathcal{L}_{\text{cali}}$$

▷ Equation 9

E DATASET DETAILS

We compare well-known VAEs to CHIC-VAEs: VAE, β -VAE, β -TCVAE, and CLG-VAE on the following data sets with 1) dSprites (Matthey et al., 2017) which consists of 737,280 binary 64×64 images of dSprites with five independent ground truth factors(number of values), *i.e.* shape(3), orientation(40), scale(6), x-position(32), and y-position(32). 2) 3D Shapes (Burgess & Kim, 2018) which consists of 480,000 RGB $64 \times 64 \times 3$ images of 3D Shapes with six independent ground truth factors: shape(4) orientation(15), scale(8), wall color(10), floor color(10), and object color(10). 3) 3D Cars (Reed et al., 2015) which consists of 17,568 RGB $64 \times 64 \times 3$ images of 3D Shapes with three independent ground truth factors: car models(183), azimuth directions(24), and elevations(4).

F QUANTITATIVE ANALYSIS SETTING

We conduct experiments on NVIDIA A100, RTX 2080 Ti, and RTX 3090. We set 100 samples to evaluate global empirical variance in each dimension and run it a total of 800 times to estimate the FVM score introduced in Kim & Mnih (2018). For the other metrics, we follow default values introduced in Michlo (2021), training and evaluation 100 and 50 times with 100 mini-batches, respectively.

G QUANTITATIVE ANALYSIS WITH MORE BASELINES AND DATASETS

We investigate more baseline and dataset. We add Factor-VAE (Kim & Mnih, 2018) and Control-VAE (Shao et al., 2020) model, and smallNORB (LeCun et al., 2004) dataset. We represent additional results in Table 10. The proposed method improves the disentanglement performance on Control-VAE, and Factor-VAE. Also, in the large-scale task, smallNORB (96×96), our method shows better results than the original cases.

dSprites	Disentanglement Metric							
	FVM \uparrow		MIG \uparrow		SAP \uparrow		DCI \uparrow	
	original	MIET	original	MIET	original	MIET	original	MIET
Factor-VAE	59.28(± 6.93)	59.55 (± 5.62)	3.30(± 1.97)	3.64 (± 1.42)	1.09 (± 0.84)	0.92(± 0.56)	10.46(± 2.76)	11.49 (± 3.15)
Control-VAE	62.36(± 8.62)	67.71 (± 6.41)	4.36(± 2.86)	7.34 (± 4.10)	2.11 (± 1.88)	1.93(± 1.63)	10.40(± 3.42)	15.18 (± 4.61)
3D Shapes	Disentanglement Metric							
	FVM \uparrow		MIG \uparrow		SAP \uparrow		DCI \uparrow	
	original	MIET	original	MIET	original	MIET	original	MIET
Factor-VAE	41.86(± 6.90)	49.22 (± 10.58)	2.47(± 1.88)	7.47 (± 9.48)	1.18(± 0.97)	2.04 (± 1.96)	10.40(± 4.20)	13.08 (± 10.24)
Control-VAE	71.05(± 14.35)	71.89 (± 8.33)	24.88(± 13.68)	32.28 (± 10.74)	6.60(± 3.59)	7.14 (± 2.09)	40.08(± 13.45)	43.06 (± 8.68)
3D Cars	Disentanglement Metric							
	FVM \uparrow		MIG \uparrow		SAP \uparrow		DCI \uparrow	
	original	MIET	original	MIET	original	MIET	original	MIET
Factor-VAE	82.81(± 8.32)	84.84 (± 9.30)	1.22(± 0.68)	2.00 (± 1.40)	0.68(± 0.52)	0.85 (± 0.68)	11.67 (± 4.74)	9.63(± 2.72)
Control-VAE	88.76(± 7.66)	89.10 (± 6.90)	4.68(± 2.67)	5.08 (± 2.68)	1.16(± 0.74)	1.45 (± 0.86)	14.70(± 3.84)	15.22 (± 4.15)
smallNORB 96 \times 96	Disentanglement Metric							
	FVM \uparrow		MIG \uparrow		SAP \uparrow		DCI \uparrow	
	original	MIET	original	MIET	original	MIET	original	MIET
CLG-VAE	32.01(± 4.72)	32.71 (± 5.59)	17.30 (± 0.75)	16.75(± 2.57)	8.82(± 0.60)	9.26 (± 1.39)	11.92(± 1.75)	13.26 (± 2.03)
Control-VAE	34.41(± 7.17)	34.46 (± 8.64)	17.37(± 1.74)	17.42 (± 1.92)	9.28(± 1.02)	9.74 (± 1.20)	16.73(± 2.70)	17.76 (± 2.84)

Table 10: The smallNORB 64×64 represents the centered cropped version of smallNORB. We set the hyper-parameter γ of Factor-VAE from $\{5, 10, 15\}$, and run total 30 seeds. And we set the maximum KL divergence value of Control-VAE from $\{10, 12, 14, 16, 18, 20\}$, and run total 60 seeds.

G.1 ADDITIONAL DATASET

The smallNORB (LeCun et al., 2004) dataset consists of total 96×96 24,300 grayscale images with five factors, which are category(5), elevation(9), azimuth(18), light(6), right-left(2).

H SENSITIVITY TO THE NUMBER OF IE-TRANSFORMATION

We present the sensitivity of the number of IE-transformation results of 3D Shapes and 3D Cars in Table 11. These results also show that the disentanglement performance of multiple units of IE-transformation is higher than a single unit.

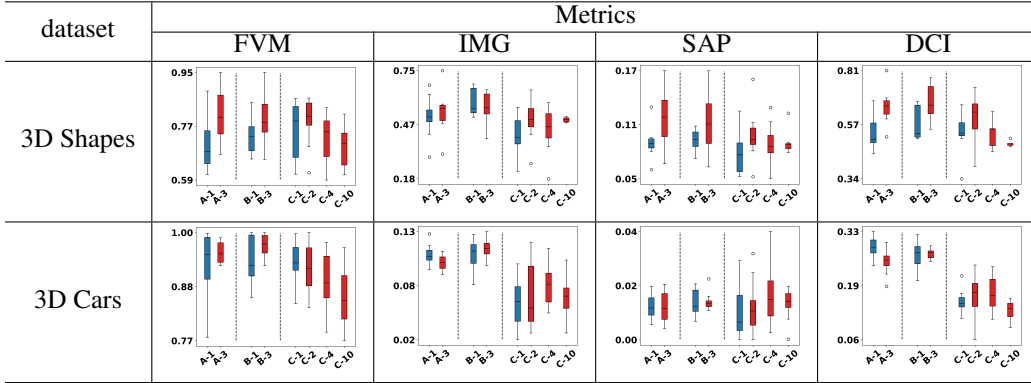


Table 11: Impact of the number of MIE-transformation function on the β -TCVAE and β -VAE with dSprites, 3D Shapes, and 3D Cars datasets in terms of the four metrics. The blue and red box plots represent each model’s single and multiple IE-transformation cases, respectively. (A- n : MIET- β -TCVAE (4), B- n : MIET- β -TCVAE (6), C- n : MIET- β -VAE, n : the number of MIE-transformation)

I ABLATION STUDY

Ablation studies with dSprites and 3D Shapes datasets are presented in Table 12.

dSprites	β -VAE			β -TCVAE		
	MIET	MIET (w/o E)	MIET (w/o EF)	MIET	MIET (w/o E)	MIET (w/o EF)
FVM	74.19 (± 5.62)	71.54(± 8.66)	25.83(± 1.16)	79.87 (± 5.80)	76.39(± 7.44)	77.44(± 7.15)
MIG	19.72 (± 11.37)	19.29(± 11.79)	0.02(± 0.01)	35.04 (± 4.07)	33.83(± 8.06)	21.88(± 8.42)
SAP	5.08 (± 2.90)	4.91(± 3.25)	0.21(± 0.10)	7.70 (± 1.63)	7.64(± 2.03)	6.84(± 1.87)
DCI	28.81 (± 10.19)	27.51(± 11.49)	1.81(± 0.08)	47.83 (± 5.01)	45.10(± 6.92)	37.84(± 8.85)

3D Shapes	β -VAE			β -TCVAE		
	MIET	MIET (w/o E)	MIET (w/o EF)	MIET	MIET (w/o E)	MIET (w/o EF)
FVM	75.19 (± 8.16)	74.91(± 10.46)	22.27(± 1.29)	80.59 (± 8.57)	77.90(± 8.66)	66.38(± 7.57)
MIG	47.37(± 10.13)	47.45 (± 8.98)	0.28(± 0.09)	54.49 (± 9.44)	51.37(± 11.54)	36.08(± 17.42)
SAP	9.20(± 2.44)	9.43 (± 2.59)	0.26(± 0.07)	11.58 (± 3.32)	10.23(± 3.13)	7.13(± 3.09)
DCI	54.95 (± 8.99)	54.23(± 9.05)	0.10(± 0.02)	66.22 (± 7.32)	61.18(± 8.87)	56.85(± 11.72)

Table 12: Ablation study of the impact of the equivariant property (w/o E), and EF-conversion (w/o EF). We conduct 40 β -VAE models and 20 β -TCVAE with different hyper-parameters on the four disentanglement metrics.

J ADDITIONAL EXPERIMENT OF COMPUTING COMPLEXITY

We additionally estimate the computing complexity depending on the number of IE-transformation. The results are in Table 13 and represent the training time complexity compare to baselines (when the number of IE is equal to 0).

# of IE	Complexity
0	$\times 1.00$
1	$\times 0.75$
3	$\times 0.50$
4	$\times 0.33$

K QUALITATIVE ANALYSIS

We represent more qualitative analysis with all datasets in Fig 7-11.

Table 13: Training computing complexity.

L ADDITIONAL INDUCTIVE BIAS

There are several inductive biases to learning unsupervised disentanglement, such as group theory based and sequential order. In this section, we briefly discuss sequential order inductive bias even though its method is considered in different domains such as text and video frames. To individualize the static (time-invariant) and dynamic (time-variant), Li & Mandt (2018); Bai et al. (2021) proposed the latent variables one (f) is only dependent on the given times series datasets $x_{1:T}$, and the other ($z_{1:T}$) is dependent on the $x_{1:T}$ and

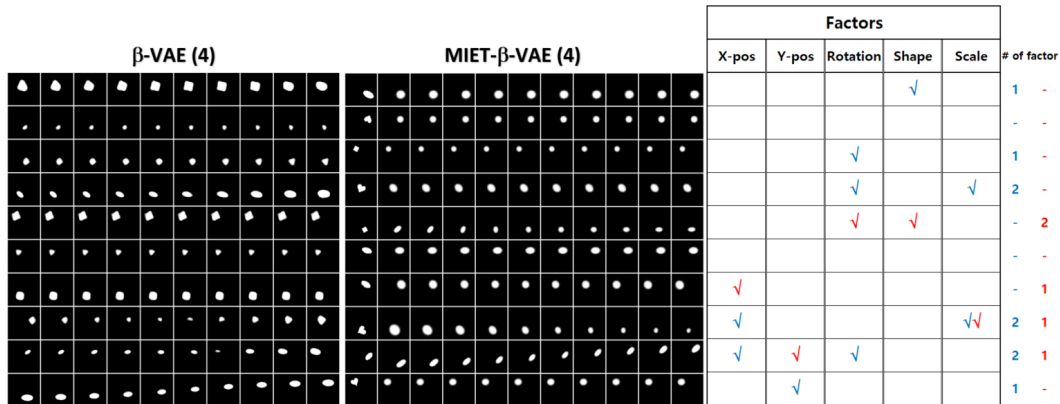


Figure 7: Qualitative analysis result of β -VAE and MIET- β -VAE. As shown in the figure, β -VAE struggles with rotation and scale factors in 4th dimension. Also, it struggles with x-position and scale factors in 8th dimension, and x-position and rotation factors in 9th dimension. However, MIET- β -VAE only struggles with rotation and shape factors in 5th dimension.

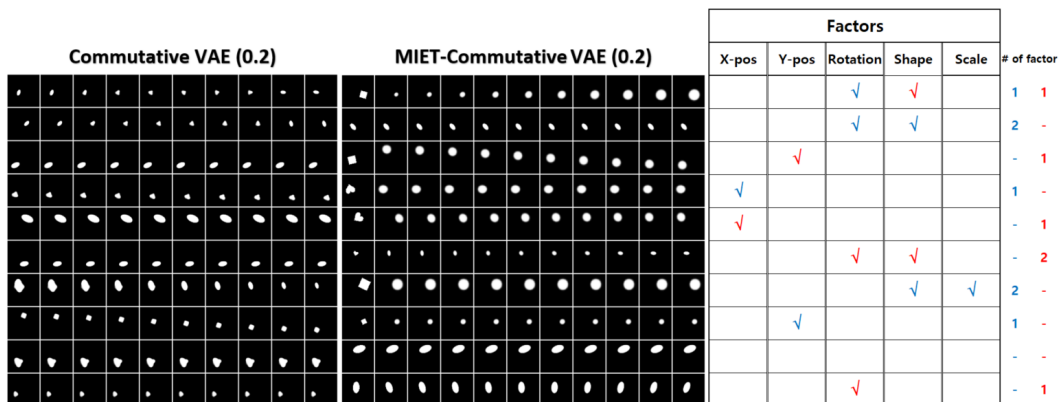


Figure 8: Qualitative analysis result of CLG-VAE (0.2) and MIET-CLG-VAE (0.2) with dSprites. As shown in the results, CLG-VAE struggles with rotation and shape factors in 2nd dimension, and shape and scale factors in 7th dimension. However, MIET-CLG-VAE separates rotation and shape factors in 10th, and 1st dimensions respectively.

f. Moreover Bai et al. (2021) propose the novel ELBO with maximizing mutual information between the input and the latent vectors. These works empirically show that sequential order which includes separated latent vectors improves unsupervised disentanglement learning with diverse qualitative analysis. Differently in group theory based approaches, the proposed methods consider the equivariant function between the input and latent vector space.

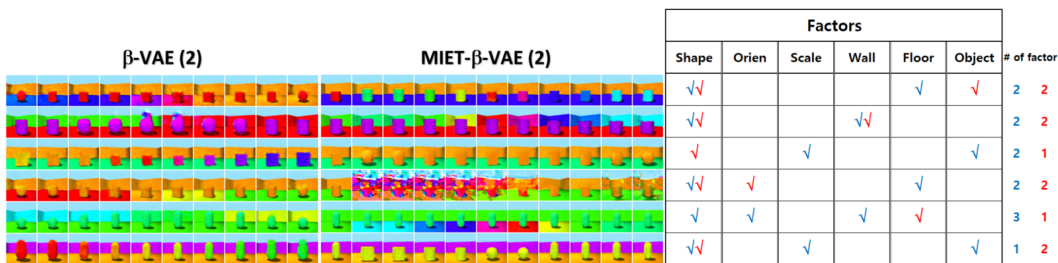


Figure 9: The Shape is object shape, Orien is an orientation of object, Scale is a scale factor of object, Wall is wall color factor, Floor is floor color, and Object is object color factors. As shown in the results, β -VAE struggles with all factors, and only the object color factor is divided in 6th dimension. However, this factor is still activated with scale factor in 3rd dimension. Although MIET- β -VAE struggles with reconstruction, it is less struggle with than β -VAE.

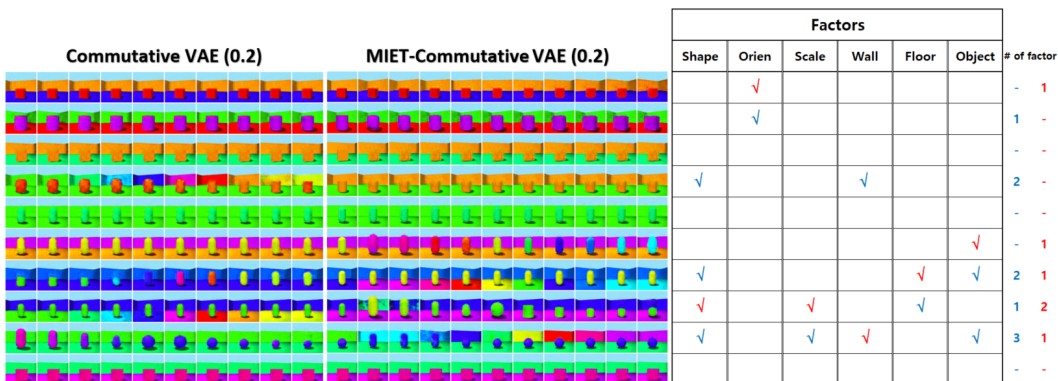


Figure 10: Shape is object shape, Orien is an orientation of object, Scale is scale factor of object, Wall is wall color factor, Floor is floor color, and Object is object color factor. As shown in the result, CLG-VAE struggles with shape and wall color factors in 4th dimension, and shape and object color factors in 7th dimension. In particular, it struggles with tree factors in 9th dimension. On the other hand, MIET-CLG-VAE separates shape, wall, and object color factors.

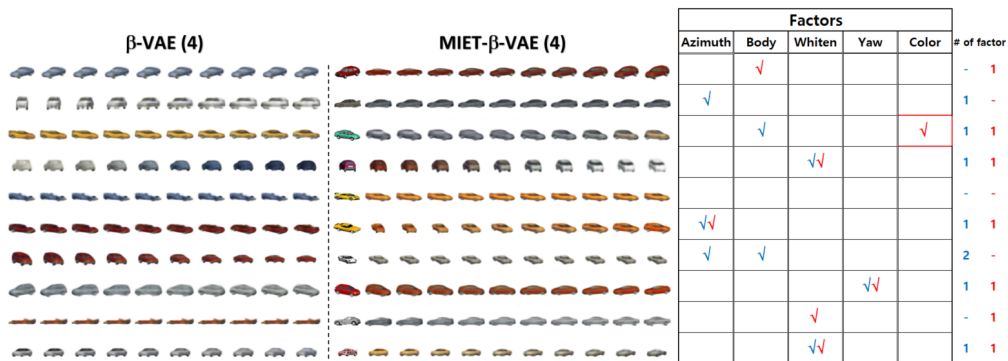


Figure 11: 3D Cars: On the left side is the β -TCVAE result, and it struggles with body, and azimuth factors shown in the 7th row. However, MIET- β -TCVAE separates azimuth (6th row) and body (1st row). In particular, MIET- β -TCVAE learns color factor (3rd row) which does not exist on β -TCVAE.