ABSTRACT

After the success of deep generative models in image generation tasks, learning disentangled latent variable of data has become a major part of deep learning research. Many models have been proposed to learn an interpretable and factorized representation of latent variable by modifying their objective function or model architecture. While disentangling the latent variable, some models show lower quality of reconstructed images and others increase the model complexity which is hard to train. In this paper, we propose a simple disentangling method with traditional principal component analysis (PCA) which is applied to the latent variables of variational auto-encoder (VAE). Our method can be applied to any generative models. In experiment, we apply our proposed method to simple VAE models and experimental results confirm that our method finds more interpretable factors from the latent space while keeping the reconstruction error the same.

Index Terms— Disentanglement, Deep Generative Model, Latent Variable, Representation, Whitening

1. INTRODUCTION

Since variational auto-encoder (VAE) [1] and generative adversarial network (GAN) [2] are proposed, many different deep generative models have been introduced and they have showed remarkable results in image generation tasks. After the success of image generation, disentangling the latent variable of generative models has been a major research point. Disentangled latent variables are important to make models understand our world more conceptually [3, 4, 5].

Many papers have proposed models that learn a disentangled latent variable [4, 5, 6]. \( \beta \)-VAE [5] and Factor-VAE [6] are based on VAE structure and change the original objective function to push the model to factorize their latent variable. Info-GAN [4] is one of the GAN networks and add a feature latent code to the original input latent variable.

Although these models show remarkable results in learning a explainable factorized latent variable, they have drawbacks. For example, \( \beta \)-VAE achieves a better disentangling result [6] at the cost of lower reconstruction quality compared to the original VAE. Factor-VAE overcomes the drawback of \( \beta \)-VAE by introducing a new disentangling method to VAE, but it needs an additional network structure (discriminator). Info-GAN provides good reconstruction quality and disentangling result. However, because it is based on the GAN structure, it has the unstable training issue. Since W-GAN [7] was proposed, GAN models have better training stability, but they still have some issues in hyper-parameter tuning.

In this paper, we introduce a new disentangling method which is simple and easy to apply to any generative models. We apply principal component analysis (PCA) as whitening transformation to latent variable and make a disentangled latent variable space. The original generative models are good to capture important factors behind the input data and the only problem is that each dimension of the latent variable is correlated to others. Therefore, if we can make the latent variable to be uncorrelated to each other, we could get a disentangled latent variable. Whitening with PCA (or PCA whitening) is one of the most frequently used method that converts a set of correlated variables into a set of linearly uncorrelated variables. In this point of view, we propose to apply PCA whitening to the latent variable of the original VAE as a new disentangle method.

To verify the disentangling quality of our proposed method, we analyze and compare several methods on image datasets qualitatively and quantitatively. The qualitative analysis of disentangling methods is just encoding the input image and generating images while traversing each dimension’s value of the latent variable. If the generated images are changed only one factor of image when we change one dimension of the latent variable, it means the latent variable is well disentangled [3]. Despite of the growing interests in research of disentanglement, there is a lack of standard quantitative analysis method for disentanglement. Recently, a few papers suggested various quantitative analysis methods [5, 8, 6], in this paper, we use the method proposed in [6]. We apply our proposed method to the original VAE model and compare to other models (VAE, \( \beta \)-VAE, and Factor-VAE) with three datasets (MNIST, CelebA, 2D Shapes) [9, 10, 11].

The paper is organized as follows. We introduce back-
ground knowledge including deep generative models, and PCA whitening in section 2. In section 3, we review related works like β-VAE, Factor-VAE, Info-GAN. Then, we describe our method to disentangle the latent variable of the models in section 4. The datasets and models that we used in our experiments, and the experiment results are presented in section 5. Finally, we conclude this paper with summary of our work and some future works in section 6.

2. RELATED WORK

2.1. Deep Generative Model

Deep generative models are based on deep neural networks and aim to learn a true data distribution from training data in the unsupervised learning manner. If the model can learn a true data distribution, it is possible to generate new data samples from the learned distribution with some variations. However, sometimes it is not possible to learn a true data distribution. Therefore, deep generative models use deep neural networks to approximate the distribution of model to the true data distribution.

In deep learning, most deep generative models are variations of VAE or GAN. VAE is an auto-encoder with a constraint on the latent space which is forced to be Gaussian. Since the latent space generates samples for the decoder, the reparameterization trick is used to make the gradient information flow through the latent space. After training the model, the latent space keeps most information to reconstruct input data, and it becomes Gaussian as much as possible. In the conventional GAN models, there is no constraint on the latent space. That is, in both VAE and GAN, the dimensions of the latent space might be entangled with each others.

2.2. Whitening with PCA

Whitening with PCA is a preprocessing step to make data linearly uncorrelated. PCA whitening is composed of two steps. First, it applies PCA to the data samples to transform the correlated data distribution to an uncorrelated data distribution. Second, it normalizes each dimension with the square root of the corresponding eigenvalue to make each dimension has the same variance.

2.3. Disentangling Models

Since disentangling latent variable has been drawing much attention, several disentangling models have been proposed [5, 6]. β-VAE changes the original objective function of VAE with a new parameter β as in Eq 1, where z is the latent variable of the model and x is the input data.

$$L_{β-VAE} = E_{q(z|x)}[\log p(x|z)] - \beta(KL(q(z|x)||p(z))),$$  (1)

where $KL(q||p)$ means the KL divergence between q and p.

When β = 1, it is exactly the same as original objective function of VAE. However, with β > 1, it constrains the capacity of model’s latent variable z to make the distribution of z to be more similar to the prior distribution which is an isotropic Gaussian distribution. Also, if β becomes larger, the latent variable can be more disentangled by resembling the isotropic Gaussian. That is, the KL divergence term in the objective function of β-VAE encourages conditional independence (or uncorrelatedness) in q(z|x) [5]. However, there is trade-off between reconstruction error and disentanglement [6]. In other words, the quality of reconstruction is damaged with larger β, with which the latent variable is more disentangled.

To overcome the side effect of β-VAE, Factor-VAE proposes another disentangling method with the VAE structure. To avoid the trade-off in Eq 1, they do not change the objective function of original VAE, and add another KL divergence term to regularize the latent variable to be factorized as in Eq 2.

$$L_{F-VAE} = [E_{q(z|x)}[\log p(x|z)] - (KL(q(z|x)||p(z))) - γKL(q(z)||\bar{q}(z),$$  (2)

where $q(z) = E_{p(x)}[q(z|x)] = \frac{1}{N} \sum_{i=1}^{N} q(z|x(i)), \bar{q} = \prod_{j=1}^{d} q(z_{i})$, and d is the dimension of latent variable.

2.4. Metrics for disentanglement

Despite of the growing interests about disentangling models, there is no standard evaluation metric and lack of labeled data for evaluation. Therefore, the previously proposed disentangling models verify their disentangling quality based on qualitative analysis. Most commonly used analysis is latent variable traversal. If only one factor of generated images is changed while changing the value of one dimension in the latent variable, then the latent variable that the model learned is considered to be well disentangled. This qualitative analysis is easy to understand and intuitive method, but we still need quantitative analysis methods to compare the disentangling ability of various models. Recently several evaluation metrics have been proposed for disentanglement with labeled data for that metrics [5, 8, 6].

3. WHITENING THE LATENT VARIABLE

Our proposed disentangling method, whitening the latent variable with PCA, is simple and easy to apply to various generative models, and its disentangling ability is as good as, if not better than, other disentangling models. Also, while β-VAE has trade-off between disentangling and reconstruction quality as we described above, our proposed method does not sacrifice the reconstruction quality while disentangling the latent variable. Note that our method dose not change the original objective function. To disentangle the latent variable with our
method, we apply PCA to the original latent variable of the trained model, then we rescale the dimensions of projected variable with square root of corresponding eigenvalues. Given input data $X$, the generative model encodes $X$ to $Z$ in the latent space. Then the whitening process is summarized in Table 1. Because our proposed method does not need to change the objective function of the original VAE, the objective function of our model is the same as described in Eq 3.

$$L_{W-VAE} = \mathbb{E}_{q(z|x)}[\log p(x|z)] - KL(q(z|x)||p(z)).$$  

(3)

Since we use the same objective function, the reconstruction quality is not effected by the whitening process, while $\beta$-VAE has trade-off between disentangling and reconstruction. Also, $\beta$-VAE needs sampling and approximating, because $\gamma KL(q(z)||\bar{q}(z))$ term is intractable in practice [6]. Additionally, extra discriminator for density-ratio trick is necessary to minimize the KL divergence term as in Eq 4 [12, 13].

$$TC(z) = KL(q(z)||\bar{q}(z)) = \mathbb{E}_{q(z)}[\log \frac{q(z)}{\bar{q}(z)}]$$

$$\approx \mathbb{E}_{q(z)}[\log \frac{D(z)}{1 - D(z)}],$$

(4)

where $TC(z)$ is total correlation [14] and $D$ is the discriminator. However, our proposed method does not need any extra network, sampling or approximation process.

### Table 1. Algorithm: Whitening the latent variable.

1. Apply the encoder to $X$ to obtain $Z$.
2. Apply PCA to $Z$ to find the eigenvalue $\Lambda$ and eigenvector $U$ of the covariance matrix.
3. Project $Z$ to the eigenspace by $Z_{PCA} = U^T Z$.
4. Rescale the eigenspace by $Z_{PCA,W} = \Lambda^{1/2} Z_{PCA}$.

Fig. 1 shows the model structure of our proposed method applied to VAE, which leads to W-VAE, and how latent variable traversal can be applied. To generate new samples, we control $Z_{PCA,W}$ in the rescaled eigenspace.

### 4. EXPERIMENTS

#### 4.1. Data

We use three different image datasets for our experiments (MNIST, CelebA, and 2D Shapes). These datasets are most frequently used in many papers of deep generative models and disentanglement of latent variable. The first two datasets (MNIST and CelebA) have no label for generative factors while the 2D shapes dataset has labels for generative factors. MNIST consists of 60K and 10K hand written images ($28 \times 28$) for training and testing, respectively. CelebA (aligned and cropped version) has 202,599 RGB face images ($64 \times 64 \times 3$) of celebrities. 2D Shape has 737,280 images ($64 \times 64$) that are generated with 6 generative factors [number of values] (color[1], shape[3], scale[6], orientation[40], position X[32], and position Y[32]). Fig. 2 shows a few sample images of the datasets. We analyze qualitatively the methods on the three datasets, and analyze quantitatively on the 2D Shapes dataset. We compare our proposed method to three different method: VAE, $\beta$-VAE, and Factor-VAE.

![Fig. 1.](image1.png)

(a) Model structure of W-VAE

(b) Process of latent variable traversals

![Fig. 2.](image2.png)

4.2. Models

To compare our proposed method to other models, we use the same VAE architecture for $\beta$-VAE, and Factor-VAE. Encoder consists of convolutional neural networks, and decoder consists of deconvolutional neural networks. For Factor-VAE, we use fully connected layers for the discriminator as in [6].

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apply whitening process to the latent variable, we calculate eigenvalue and eigenvector with the entire training data of each dataset.

4.3. Results

Fig. 3 shows the results of latent variable traversals with our proposed method. It shows that our whitened latent variable has linearly independent factors of face data. Table 2 shows the quantitative analysis results on the 2D Shapes dataset from the three different deep generative models (W-VAE, VAE, and Factor-VAE) with the disentanglement metric proposed in [6]. Our proposed model’s disentanglement score is between Factor-VAE and original VAE. Fig. 4 shows the results of latent variable traversals with other models. Disentangling quality of our model is as good as, if not better than, β-VAE and Factor-VAE, while the latent variable of original VAE model is highly entangled. Also, Fig. 5 shows that the latent variable of our model is disentangled better than original VAE with MNIST.

Fig. 3. Qualitative analysis of our proposed method on the CelebA dataset. The top row of each image is the ground truth image. (a-e) show hair length, background darkness, azimuth, smile, and hair color changing, respectively.

Fig. 4. Qualitative analysis of VAE, β-VAE, and Factor-VAE models on CelebA.

Table 2. The average disentangling score of each models with the disentangling metric proposed in [6]

|                  | W-VAE | VAE  | Factor-VAE |
|------------------|-------|------|------------|
| Disentangling score | 63.4  | 60.1 | 73.0       |

5. CONCLUSION

Learning a disentangled representation of given data set is important for not only deep generative models but also making an artificial intelligence (AI) model to understand our real world more conceptually, which is more similar to human being [3]. Therefore, many disentangling models have been proposed but those models have draw backs: trade-off between disentangling ability and reconstruction quality, complex model structure. However, in this paper, we show that the latent variable can be disentangled by a simple method (PCA whitening) without any change in the objective function or model architecture. The results of qualitative and quantitative analysis shows that our proposed method can disentangle the latent variable as good as other disentangling models while no reduction of reconstruction quality. For the future work, we will apply PCA whitening to the GAN model’s latent variable and try other transformation methods like non-negative matrix factorization (NMF) or independent component analysis (ICA).

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