Shanghai Jiao Tong University
AI3611

VAE

Yan Han (519030910404)

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1 Introduction

Variational AutoEncoders (VAE) is a method for generative modeling, whose goal is to build the bridge between normal distribution and data distribution. Section 2 formularizes the principle of VAE. Section 3 describes some experiments on MNIST. Section 4 introduces our interesting observations. Section 5 draws a conclusion. The source code is available at `https://github.com/wolfball/Intellisense-Cognitive-Practice`.

2 Principle

The problem of "generative modeling" is to deal with models of distributions $P(X)$, where X is the datapoints in some potentially high-dimensional space $\mathcal{X}$. Take handwritten digits for example, the datapoint is the image which has a large number of pixels, and the generative model is aimed at capturing dependences between pixels and judging whether $P(X)$ is high or low. the X's which look like real images should get high probability while that look like random noise should get low probability. Suppose that X is sampled from $P_{gt}(X)$, our goal is to find P such that $P = P_{gt}$.

In the case of handwritten characters, it helps if the model first decide which character to generate before it assigns a value to any specific pixel. Thus we introduce the *latent variable* z sampled from a high-dimensional space Z with $P(Z)$. That is to say, we have a function $f : \mathcal{Z} \times \Theta \to \mathcal{X}$ to generate the images $f(z;\theta)$. With the popularity of neural networks, we use them to model this function with parameters θ. Now our goal is to optimize θ to make $f(z;\theta)$ become more similar to the data in $\mathcal{X}$.

To make the notion precise mathematically, we are aimed at maximizing the probability of each X in the training set:

$$P(X) = \int P(X|z;\theta)P(z)dz \tag{1}$$

where we replace $f(z;\theta)$ by $P(X|z;\theta)$ to build relation between X and z.

For one thing, we need to define z. In [1], we know that any d-dimention distribution can be generated by taking a set of d variables that are normally distributed and mapping them through a sufficiently complicated

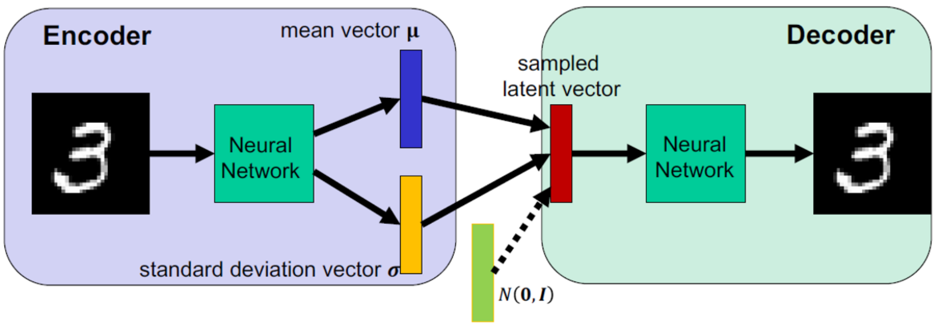


Figure 1: Pipeline

funtion. We can write

$$P(X|z;\theta) = \mathcal{N}(X|f(z;\theta), \sigma^2 I) \tag{2}$$

For another, we need to find out how to integrate over z. Since it is expensive to consider the whole space of Z, we introduce an new function $Q(z|X)$ to narrow the "interesting space". Besides, we will use KL divergence $D[Q||P]$. Then, for arbitrary distribution $Q(z)$,

$$D[Q(z)||P(z|X)] = \mathbb{E}_{z\sim Q}[\log Q(z) - \log P(z|X)] \tag{3}$$

$$= \mathbb{E}_{z\sim Q}[\log Q(z) - \log P(X|z) - \log P(z)] + \log P(X) \tag{4}$$

$$\log P(X) - D[Q(z)||P(z|X)] = \mathbb{E}_{z\sim Q}[\log P(X|z)] - D[Q(z)||P(z)] \tag{5}$$

As we are interested in $P(X)$, it is better to employ those Q that depend on X, thus:

$$\log P(X) - D[Q(z|X)||P(z|X)] = \mathbb{E}_{z\sim Q}[\log P(X|z)] - D[Q(z|X)||P(z)] \tag{6}$$

where $Q(z|X) = \mathcal{N}(z|\mu(X,\theta), \Sigma(X;\theta))$.

The full training equation is:

$$\mathbb{E}_{X\sim D}[\log P(X) - D(Q(z|X)||P(z|X))] \tag{7}$$

$$= \mathbb{E}_{X\sim D}[\mathbb{E}_{z\sim Q}[\log P(X|z)] - D(Q(z|X)||P(z|X))] \tag{8}$$

$$= \mathbb{E}_{X\sim D}[\mathbb{E}_{\epsilon\sim\mathcal{N}(0,I)}[\log P(X|z = \mu(X) + \Sigma^{1/2}(X)\epsilon)] - D(Q(z|X)||P(z|X))] \tag{9}$$

the equation (8) $\rightarrow$ (9) uses a trick called *reparameterization*, which makes sure that given X, ϵ, the function is deterministic and continuous over P, Q.

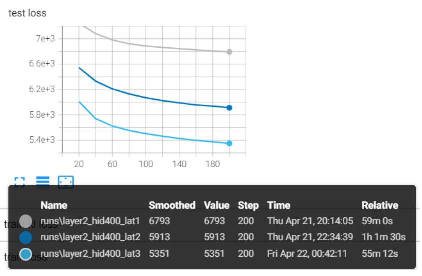
3 Experiment

Experiment setting The pipeline of VAE is in Figure 1. The dataset is MNIST. In our baseline model, the encoder is implemented by an one-layer fully connected layer with ReLU activation, which can map 784d image to 400d hidden vector. And we use two Linear layers to produce μ and Σ respectively, whose dimensions are also hyper parameter called *lat_dim*. The decoder is a two-layer-MLP followed by a Sigmoid activation that can recover a 784d image from a latent point. For optimizer, we use Adam with learning rate as 1e-5. The loss consists of reconstruction loss which is BCELoss, and regularization loss which is the KL-distance between $\mathcal{N}(\mu, \sigma)$ and $\mathcal{N}(0, I)$. We train all the models for 200 epochs. And we use Tensorboard for visualizations.

Visualization Here we mainly introduce four types of visualizations.

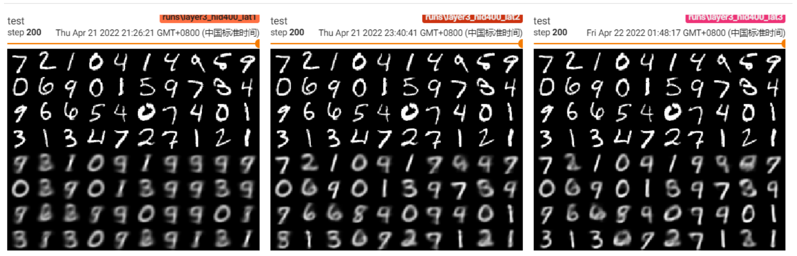
1. Loss curve. Take Figure 5 for example, we will plot the test loss and train KL-loss during training where the x-axis denotes epoch iteration and the y-axis represents the loss value;
2. Reconstructive visualization. Take Figure 2(b) for example, in order to visualize the quality of generated images, we feed the images in first four lines into the network, and the last four lines are the outputs;
3. Sampled visualization. Take Figure 3(a) for example, we evenly sample z from the latent space within a bounded region ([-5, 5] for each dimension), and feed z into decoder. The outputs form this graph. Note that only the latent dimension less than three can be visualized.
4. Latent space visualization. Take Figure 3(b) for example, we input all data into the encoder, which produce responding z. And we visualize these z to form these graphs. Note that only the latent dimension less four can be visualized.

Latent dimension As the dimension of latent variable represents the capability of model, we set different latent dimension to see the performance. In particular, we visualize the result when dimension is less than 3 to better our understanding. We use 3 layers in encoder. From Figure 2.(a), we find that the higher the latent dimension is, the less the test loss will be. And Figure 2.(b) is the reconstruction result on the test data set. When latent dimension is equal to 1, most images can not reconstructed; when latent dimension is equal to 3, we can clearly see that most of them are recognized. From Figure 3.(a), we evenly sample z and feed these z's into the network, the visualization shows that the spatial information of the latent variable is learned, which is more vivid in Figure 3.(b).



	Name	Smoothed	Value	Step	Time	Relative
●	runs\layer2_hid400_lat1	6793	6793	200	Thu Apr 21, 20:14:05	59m 0s
●	runs\layer2_hid400_lat2	5913	5913	200	Thu Apr 21, 22:34:39	1h 1m 30s
●	runs\layer2_hid400_lat3	5351	5351	200	Fri Apr 22, 00:42:11	55m 12s

(a) Loss curve

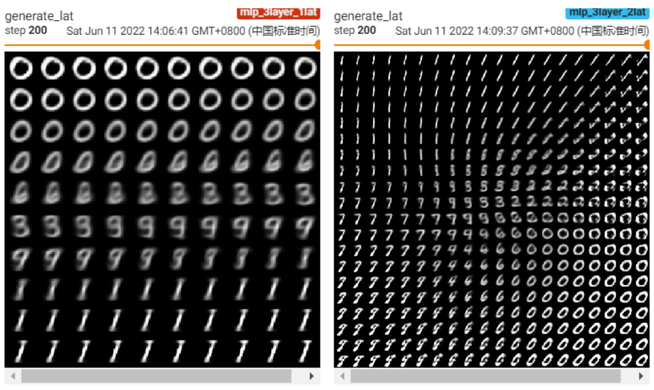

test
runs\layer3_hid400_lat1
step 200
Thu Apr 21 2022 21:26:21 GMT+0800 (中国标准时间)
test
runs\layer3_hid400_lat2
step 200
Thu Apr 21 2022 23:40:41 GMT+0800 (中国标准时间)
test
runs\layer3_hid400_lat3
step 200
Fri Apr 22 2022 01:48:17 GMT+0800 (中国标准时间)

(b) Reconstructive visualization

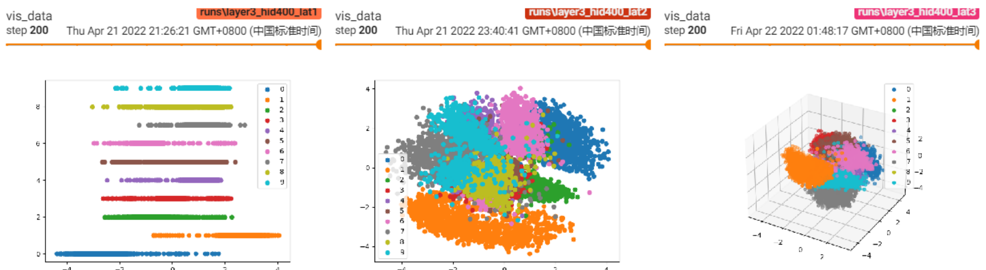
Figure 2: Loss curve and reconstructive visualization with different latent dimensions. In (a), the curves represent latent dimension with 1, 2, and 3 from top to bottom. In (b) the images represent latent dimension with 1, 2 and 3 from left to right.

Number of encoder layers As the number of encoder layers reflects the capability of extracting feature, we set different encoder layers to see the difference. We set latent dimension as 2. From Figure 4, we find that the deeper network in encoder can improve the performance of VAE. The reason may be that the better encoder can capture more robust features and dependences of the images.

Hidden size Hidden size determines the intermediate vector in Encoder and Decoder, which shows the potential ability of modeling. With one layer encoder and 20d latent vector, we have tried 100, 400, 1000 and 2000 hidden size. Figure 5 shows the results. Lager hidden size results in lower test loss, but higher training KL-loss.


generate_lat
mlp_3layer_1lat
step 200
Sat Jun 11 2022 14:06:41 GMT+0800 (中国标准时间)
generate_lat
mlp_3layer_2lat
step 200
Sat Jun 11 2022 14:09:37 GMT+0800 (中国标准时间)

(a) Sampled visualization

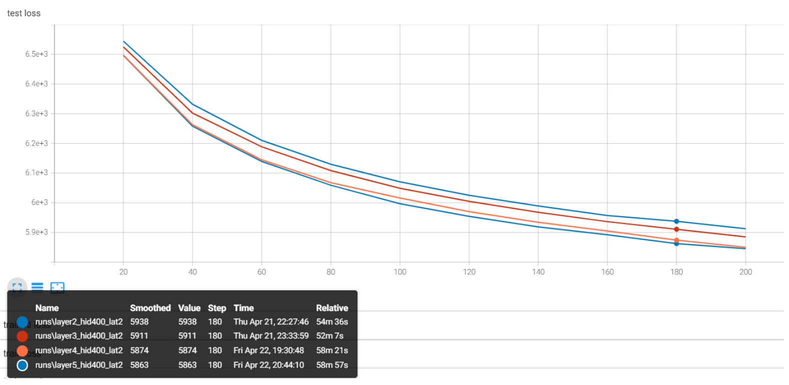


(b) Latent space visualization

Figure 3: Sampled and latent space visualization with different latent dimensions.

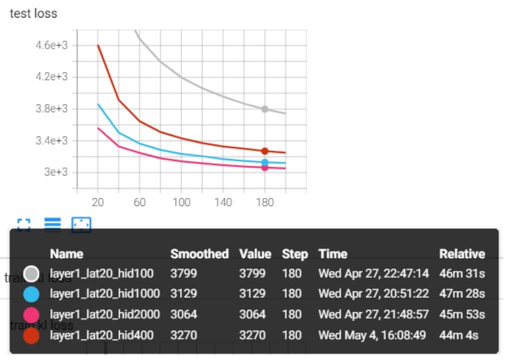
The drop in test loss can be regarded as the improvement of the capacity of the model, and the increase in KL-loss may be to blame for the complexity of data distribution (not normal distribution).

Noise augmentation Since adding noise to the training data can improve the robustness of the model, we randomly add white noise (mean=0, std=1e-6) to input images. And clip the noised pixel values to [0,1]. Figure 6 shows the results. Whether adding noise or not will not influence too much, but model with noise augmentation slightly better than the model without it from the values of test loss.



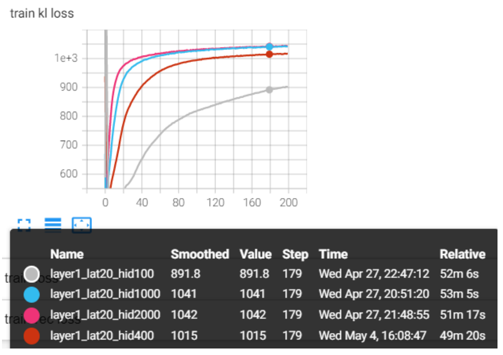
	Name	Smoothed	Value	Step	Time	Relative
●	runs\layer2_hid400_lat2	5938	5938	180	Thu Apr 21, 22:27:46	54m 36s
●	runs\layer3_hid400_lat2	5911	5911	180	Thu Apr 21, 23:33:59	52m 7s
●	runs\layer4_hid400_lat2	5874	5874	180	Fri Apr 22, 19:30:48	58m 21s
●	runs\layer5_hid400_lat2	5863	5863	180	Fri Apr 22, 20:44:10	58m 57s

Figure 4: Test loss curve with different layers.



	Name	Smoothed	Value	Step	Time	Relative
⚪	layer1_lat20_hid100	3799	3799	180	Wed Apr 27, 22:47:14	46m 31s
🔵	layer1_lat20_hid1000	3129	3129	180	Wed Apr 27, 20:51:22	47m 28s
●	layer1_lat20_hid2000	3064	3064	180	Wed Apr 27, 21:48:57	45m 53s
🔴	layer1_lat20_hid400	3270	3270	180	Wed May 4, 16:08:49	44m 4s

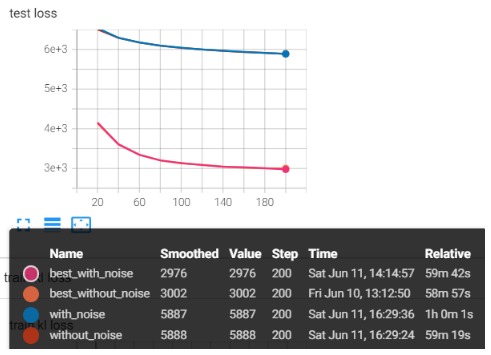
(a) Test loss



	Name	Smoothed	Value	Step	Time	Relative
⚪	layer1_lat20_hid100	891.8	891.8	179	Wed Apr 27, 22:47:12	52m 6s
🔵	layer1_lat20_hid1000	1041	1041	179	Wed Apr 27, 20:51:20	53m 5s
●	layer1_lat20_hid2000	1042	1042	179	Wed Apr 27, 21:48:55	51m 17s
🔴	layer1_lat20_hid400	1015	1015	179	Wed May 4, 16:08:47	49m 20s

(b) Train KL-loss

Figure 5: Test loss and train KL-loss of experiments with different hidden dimensions.



	Name	Smoothed	Value	Step	Time	Relative
●	best_with_noise	2976	2976	200	Sat Jun 11, 14:14:57	59m 42s
🟠	best_without_noise	3002	3002	200	Fri Jun 10, 13:12:50	58m 57s
🔵	with_noise	5887	5887	200	Sat Jun 11, 16:29:36	1h 0m 1s
🔴	without_noise	5888	5888	200	Sat Jun 11, 16:29:24	59m 19s

Figure 6: Experiments on models with or without noise augmentation. ”with_noise” and ”without_noise” are under hidden size 400 and latent dimension 2, while ”best_with_noise” and ”best_without_noise” are under hidden size 2000 and latent dimension 100.

4 Interesting Observations and Thoughts

4.1 Trends in Curve

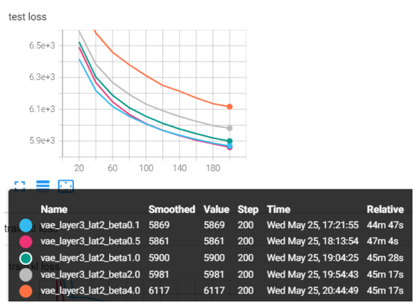
We find that when VAE works well in our experiments, the reconstruction loss always decreases while the KL-loss descends first and rises later (See Figure 8). The possible causes may be that at first, the KL-divergence helps the sampled points representing different numbers to cluster, and later, since the data distributions are actually not standard gaussian distribution, the improvement in reconstruction will result in the drop in similarities between data distribution and gaussian distribution. Finally, these two losses will convergence to comparative orders of magnitude (Here is 3000 and 1000).

4.2 β-VAE

Inspired by [2], while the total loss of VAE consists of two parts: reconstruction loss and regularization loss (KL loss), we will naturally consider adding one parameter β to balance these two items. That is to say, redesign the loss function:

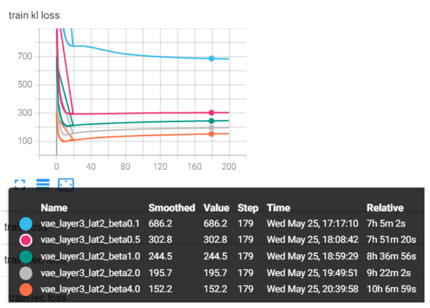
$$\mathcal{L} = \mathcal{L}_{BCE} + \beta \cdot \mathcal{L}_{KL} \tag{10}$$

For $\beta \in \{0.1, 0.5, 1.0, 2.0, 4.0\}$, we do some experiments with 3-layer-encoder and 2d latent vector. Higher β will push the network to focus more on KL-loss, thus resulting in less KL-loss but higher reconstruction loss.



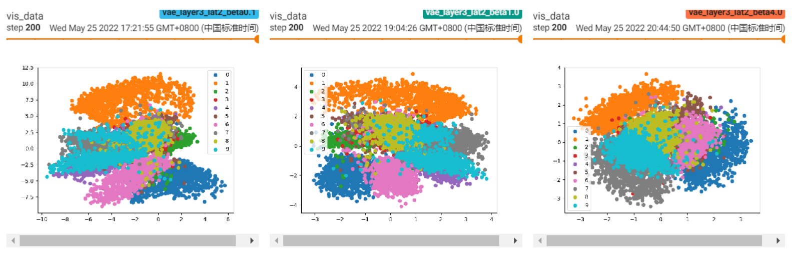
	Name	Smoothed	Value	Step	Time	Relative
●	vae_layer3_lat2_beta0.1	5869	5869	200	Wed May 25, 17:21:55	44m 47s
●	vae_layer3_lat2_beta0.5	5861	5861	200	Wed May 25, 18:13:54	47m 4s
●	vae_layer3_lat2_beta1.0	5900	5900	200	Wed May 25, 19:04:25	45m 28s
●	vae_layer3_lat2_beta2.0	5981	5981	200	Wed May 25, 19:54:43	45m 17s
●	vae_layer3_lat2_beta4.0	6117	6117	200	Wed May 25, 20:44:49	45m 17s

(a) Test loss

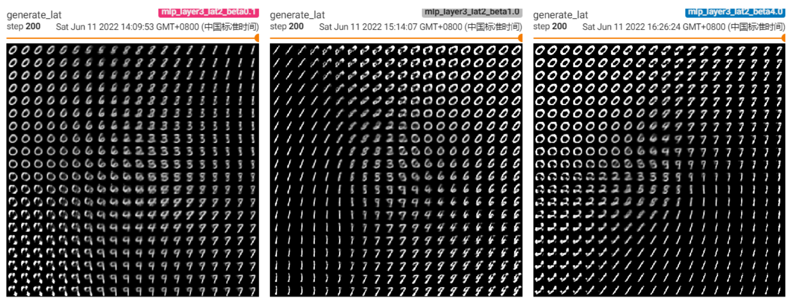


	Name	Smoothed	Value	Step	Time	Relative
●	vae_layer3_lat2_beta0.1	686.2	686.2	179	Wed May 25, 17:17:10	7h 5m 2s
●	vae_layer3_lat2_beta0.5	302.8	302.8	179	Wed May 25, 18:08:42	7h 51m 20s
●	vae_layer3_lat2_beta1.0	244.5	244.5	179	Wed May 25, 18:59:29	8h 36m 56s
●	vae_layer3_lat2_beta2.0	195.7	195.7	179	Wed May 25, 19:49:51	9h 22m 2s
●	vae_layer3_lat2_beta4.0	152.2	152.2	179	Wed May 25, 20:39:58	10h 6m 59s

(b) Train Kl-loss



(c) Visualization


generate_lat
mlp_layer3_lat2_beta0.1
step 200 Sat Jun 11 2022 14:09:53 GMT+0800 (中国标准时间)
generate_lat
mlp_layer3_lat2_beta1.0
step 200 Sat Jun 11 2022 15:14:07 GMT+0800 (中国标准时间)
generate_lat
mlp_layer3_lat2_beta4.0
step 200 Sat Jun 11 2022 16:26:24 GMT+0800 (中国标准时间)

(d) Sampled visualization

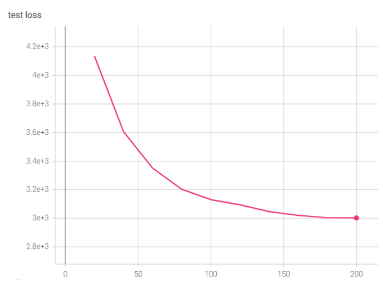
Figure 7: Experiments on different β.

As reconstruction loss is larger than Kl loss, the total loss increases with increasing β (See Figure 7). And the distribution is more like normal distribution under $\beta = 4.0$.

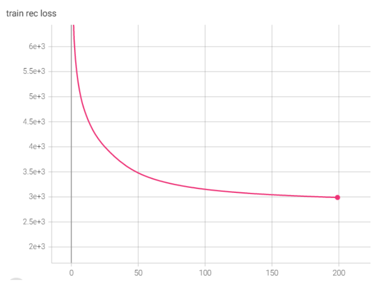
Besides, we find that different β will help different numbers to be "outstanding". For instance, we can hardly see "2" (green points) when $\beta = 4.0$ while it is vivid in low values of β. And "5" (brown points) is on the opposite. Plus, the numbers on the boundary are also different.

5 Conclusion

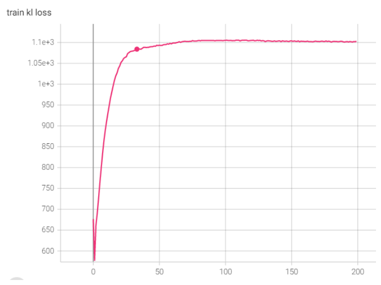
In summary, we introduce the principle of VAE and realize it using Encoder-Decoder architecture. The visualization when latent dimension is one and two is available in this report. Besides, we have designed various experiments to research on the impact of the parameters. Moreover, we find it interesting to use one parameter β to balance between the reconstruction loss and the regularization loss. The lowest test loss is reached under three-layer-encoder, 100d-latent-vector and 2000d-hidden-size with noise augmentation, which is 2976. And the quality of reconstructed images is shown in Figure 9.



(a) Test loss curve



(b) Train reconstruction loss



(c) Train KL loss curve

Figure 8: The loss curve of the best model, who has three-layer-MLP-encoder, 100d-latent-vector and 2000d-hidden-size.

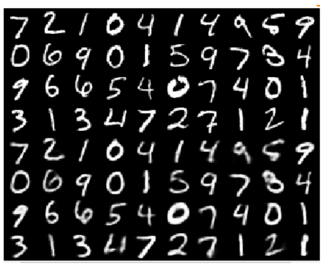


Figure 9: The reconstructive visualization of the best model, who has three-layer-MLP-encoder, 100d-latent-vector and 2000d-hidden-size with noise augmentation.

References

[1] Carl Doersch. Tutorial on variational autoencoders, 2016.

[2] Irina Higgins, Loïc Matthey, Arka Pal, Christopher P. Burgess, Xavier Glorot, Matthew M. Botvinick, Shakir Mohamed, and Alexander Lerchner. beta-vae: Learning basic visual concepts with a constrained variational framework. In *ICLR*, 2017.