Supplementary Information

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ABSTRACT

Variational Autoencoder (VAE) is a generative model from the computer vision community; it learns a latent representation of the images and generates new images in an unsupervised way. Recently, Vanilla VAE has been applied to analyse single-cell datasets, in the hope of harnessing the representation power of latent space to evade the "curse of dimensionality" of the original dataset. However, some research points out that Vanilla VAE is suffering from the issue of the less informative latent space, which raises a question concerning the reliability of Vanilla VAE latent space in representing the high-dimensional single-cell datasets. Therefore a study is set up to examine this issue from the perspective of bioinformatics.
This paper confirms the issue of Vanilla VAE by comparing it to MMD-VAE, a variant of VAE which has overcome this issue, across a series of mass cytometry and single-cell RNAseq datasets. The result shows MMD-VAE is superior to Vanilla VAE in retaining the information not only in the latent space but also the reconstruction space, which suggests that MMD-VAE be a better option for single-cell data analysis.

Supplementary Table

Supplementary table S1

Dataset	F2-Score	MCC
AML	0.970	0.972
PAN	0.990	0.991
SN	0.794	0.793
RBN	0.982	0.983

Table 1. The accuracy of the classifier applied to the original datasets, two metrics are used: F2-Score and MCC.

Supplementary Table S2

vanilla VAE/MMD-VAE						
Dataset	dimension of latent space	training steps	en/decoder structure	learning rate	Activation Function	batch size
AML	3	10,000	[24, 16, 8], [8, 16, 24]	1e-3	Relu	256
PAN	3	12,000	[36, 18, 9], [9, 18, 36]			
SN	10	10,000	[40, 24, 8], [8, 24, 40]			
RBN	3	10,000	[24, 12, 6], [6, 12, 24]			

Table 2. The parameters of variational autoencoder; parameters are training over Vanilla VAE per dataset.

Supplementary Table S3

Supplement figure

Supplementary Figure S1

Neural Network Classifier								
Dataset	VAE Space	structure	dropout	epoch	learning rate	l2 regularization	Activation Function	batch size
AML	Recons/Latent	[12,6]	0	20	0.001	0	Relu	128
PAN	Reconstruction	[36,18,9]	0	20	0.001	0.01		
	Latent	[36,24,12,6]			0.1	0		
SN	Reconstruction	[40,15]	0.1	500	0.02	0.01		
	Latent	[12,6,3]	0	1000		0		
RBN	Reconstruction	[20,10,5]	0	100	0.001	0		
	Latent	[12,6,3]		200	0.02			

Table 3. The parameters of neural network classifier for the original space, latent space and reconstruction space per dataset, parameters are trained over the output of Vanilla VAE per space per dataset.

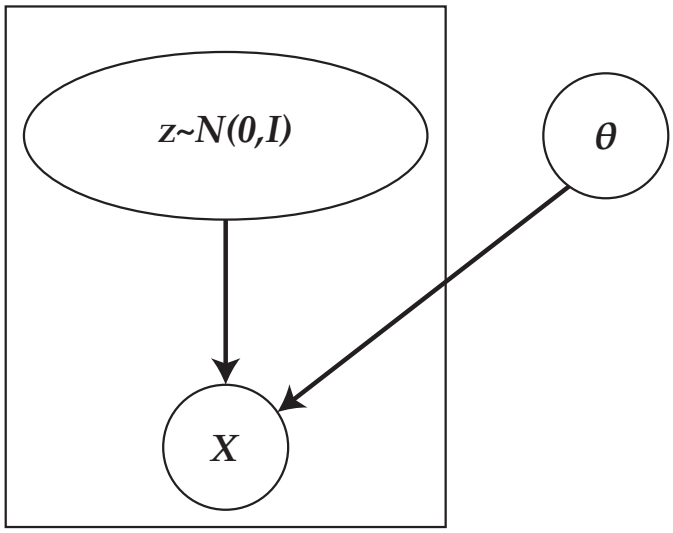

Figure 1. A graphical model representing Variational Autoencoder (VAE)

Data availability

Data and code that contributes to the reproducibility of the results in this manuscript, as well as other technical details, are available at: https://research-project.gitlab.io/mmd-vae/