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1 INTRODUTION

Variational auto-encoder (VAE) model is a stochastic inference and learning algorithm based on variational Bayes (VB) inference proposed by Kingma and Welling (2014). This is a generative that enforces a *prior* on the low-dimensional latent space that can be mapped back into a realistic-looking image. Therefore, the most important characteristic of VAEs, in the context of Monte Carlo methods with Markov chains, is their ability to represent high-dimensional parametric spaces in a low-dimensional latent space.

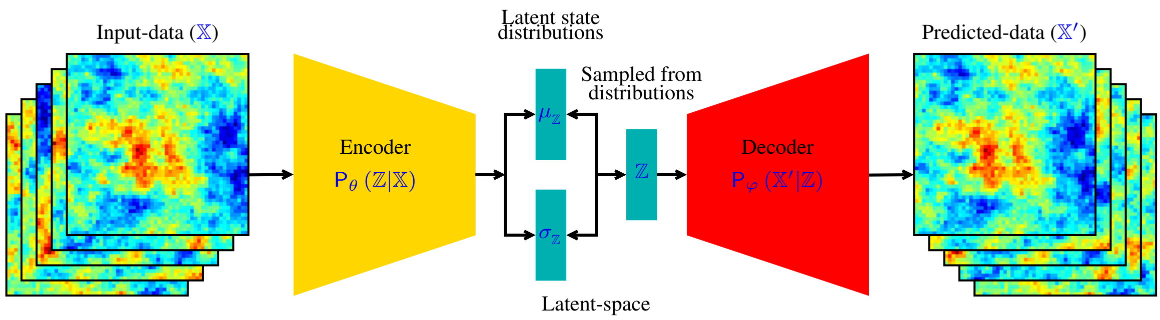
Higgins et al. (2016) introduced the β-VAE, a modification of the original VAE, that introduces an adjustable hyperparameter β to balance latent channel capacity and independence constraints with reconstruction accuracy. They demonstrate that with tuned values of β ($\beta > 1$) the β-VAE outperforms VAE ($\beta = 1$).

Makhzani et al. (2016); Louizos et al. (2017); Burda et al. (2016); Zheng et al. (2019); Vahdat and Kautz (2020)

2 ZHANG ET AL. (2022)

Zhang et al. (2022) proposed a method to reconstruct porous media based on VAE and Fisher information with good quality and efficiency.

Consider the input data set $\mathbb{X} = \left\{\boldsymbol{x}^{(i)}\right\}_{i=1}^{\mathsf{N}}$ ($\boldsymbol{x}^{(i)} \in \mathbb{R}^{\mathsf{N}_x}$) consisting of N *i*ndependent and *i*dentically *d*istributed (*i.i.d.*) samples of the continuous (or discrete) variable drawn from the *prior* distribution $p(\boldsymbol{x})$.



$$\mathbb{Z} = \mu_{\mathbb{Z}} + \sigma_{\mathbb{Z}} \cdot \varepsilon, \quad \text{where} \quad \varepsilon \sim \mathbb{N}\left(0, 1\right) \tag{1}$$

The reconstruction loss is used to ensures that input image is reconstructes at the output one and, here, is given by the mean squared error (MSE):

$$\mathcal{L}_{\mathsf{MSE}}(\theta, \phi, \boldsymbol{x}) = \frac{1}{\mathsf{N}_b} \sum_{i=1}^{\mathsf{N}_b} \left[\boldsymbol{x}^{(i)} - \mathsf{D}_\phi\left(\mathsf{E}_\theta\left(\boldsymbol{x}^{(i)}\right)\right)\right]^2, \tag{2}$$

where E and D represent the encoder and decoder and θ, ϕ are their parameters, respectively.

In VAE, we assume that both *prior* distribution $p(\mathbb{Z}) \simeq \mathbb{N}(0, 1)$ and *posterior* approximation of the latent space follow a standard Gaussian distribution, i.e., $q(\mathbb{Z}|\boldsymbol{x}) \simeq \mathbb{N}(0, 1)$.

To keep the encoder outputs $\mathbb{Z}$ close to a standard normal distribution and sufficiently diverse we use the Kullback–Leibler divergence ($\mathcal{D}_{\mathsf{KL}}$, also called relative entropy and I-divergence). $\mathcal{D}_{\mathsf{KL}}$ is a measure of divergence between two distributions (Kullback and Leibler, 1951; Csiszar, 1975):

$$\mathcal{D}_{\mathsf{KL}}\left(p(\mathbb{Z})||\mathbb{N}(0, 1)\right) = -\frac{1}{2}\sum_{i=1}^{\mathsf{N}_z}\left[1 + \log\left(\sigma_{\mathbb{Z}_i}^2\right) - {\mu_{\mathbb{Z}_i}}^2 - \sigma_{\mathbb{Z}_i}^2\right] \tag{3}$$

Zheng et al. (2019) proposed a Fisher autoencoder Xia and Zabaras (2022); Xu et al. (2023); Xia et al. (2023)

Xia et al. (2023) proposed a multiscale Bayesian inference approach based on a multiscale deep generative model (MDGM)

REFERENCES

Yuri Burda, Roger Grosse, and Ruslan Salakhutdinov. Importance weighted autoencoders, 2016.

I. Csiszar. I-Divergence Geometry of Probability Distributions and Minimization Problems. *The Annals of Probability*, 3(1):146 – 158, 1975. doi: 10.1214/aop/1176996454. URL https://doi.org/10.1214/aop/1176996454.

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 *International Conference on Learning Representations*, 2016.

Diederik P Kingma and Max Welling. Auto-encoding variational bayes. In *International conference on learning representations*, pages 14–27, 2014.

S. Kullback and R. A. Leibler. On Information and Sufficiency. *The Annals of Mathematical Statistics*, 22(1):79 – 86, 1951. doi: 10.1214/aoms/1177729694. URL https://doi.org/10.1214/aoms/1177729694.

Christos Louizos, Kevin Swersky, Yujia Li, Max Welling, and Richard Zemel. The variational fair autoencoder, 2017.

Alireza Makhzani, Jonathon Shlens, Navdeep Jaitly, and Ian Goodfellow. Adversarial autoencoders. In *International Conference on Learning Representations*, 2016. URL http://arxiv.org/abs/1511.05644.

Arash Vahdat and Jan Kautz. Nvae: a deep hierarchical variational autoencoder. In *NIPS'20: Proceedings of the 34th International Conference on Neural Information Processing Systems*, number 1650, page 19667–19679, Red Hook, NY, USA, 2020. Curran Associates Inc. ISBN 9781713829546.

Yingzhi Xia and Nicholas Zabaras. Bayesian multiscale deep generative model for the solution of high-dimensional inverse problems. *Journal of Computational Physics*, 455:111008, 2022. ISSN 0021-9991. doi: https://doi.org/10.1016/j.jcp.2022.111008. URL https://www.sciencedirect.com/science/article/pii/S0021999122000705.

Yingzhi Xia, Qifeng Liao, and Jinglai Li. Vi-dgp: A variational inference method with deep generative prior for solving high-dimensional inverse problems. *Journal of Scientific Computing*, 97(16), 2023.

Zhihang Xu, Yingzhi Xia, and Qifeng Liao. A domain-decomposed VAE method for bayesian inverse problems. *CoRR*, abs/2301.05708, 2023. doi: 10.48550/arXiv.2301.05708. URL https://doi.org/10.48550/arXiv.2301.05708.

REFERENCES

Ting Zhang, Tu Hongyan, Xia Pengfei, and Du Yi. Reconstruction of porous media using an information variational auto-encoder. *Transport in Porous Media*, 143(2):271–295, 2022. doi: 10.1007/s11242-022-01769-5. URL https://doi.org/10.1007/s11242-022-01769-5.

Huangjie Zheng, Jiangchao Yao, Ya Zhang, Ivor Tsang, and Jia Wang. Understanding vaes in fisher-shannon plane. *Proceedings of the AAAI Conference on Artificial Intelligence*, 33: 5917–5924, 07 2019. doi: 10.1609/aaai.v33i01.33015917.

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