ENM 540: Data-driven modeling and probabilistic scientific computing

Conditional variational auto-encoders

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druGAN: An Advanced Generative Adversarial Autoencoder Model for de Novo Generation of New Molecules with Desired Molecular Properties in Silico

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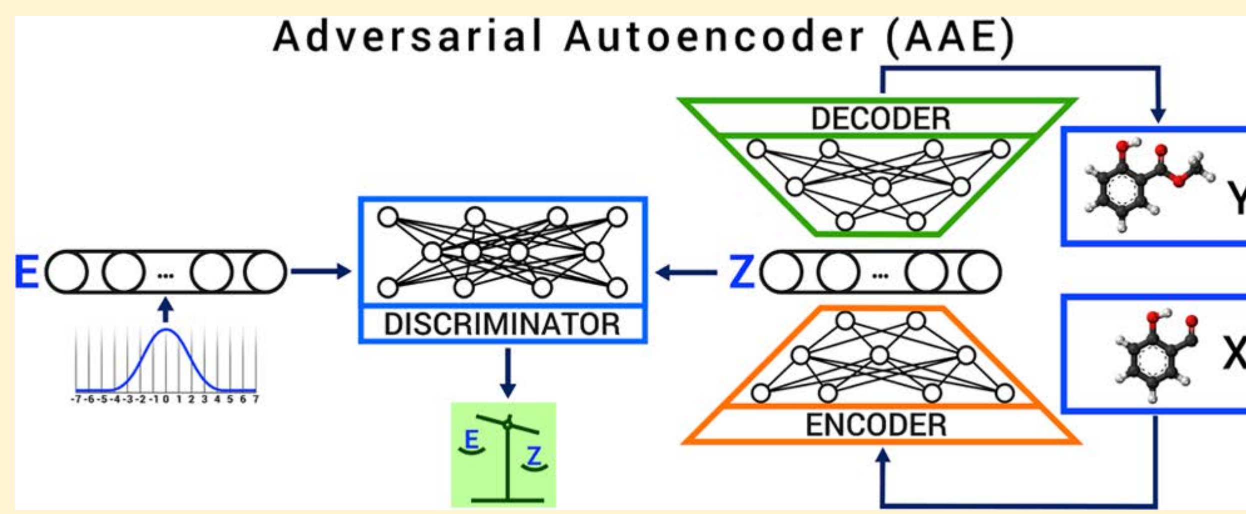
ABSTRACT: Deep generative adversarial networks (GANs) are the emerging technology in drug discovery and biomarker development. In our recent work, we demonstrated a proof-of-concept of implementing deep generative adversarial autoencoder (AAE) to identify new molecular fingerprints with predefined anticancer properties. Another popular generative model is the variational autoencoder (VAE), which is based on deep neural architectures. In this work, we developed an advanced AAE model for molecular feature extraction problems, and demonstrated its advantages compared to VAE in terms of (a) adjustability in generating molecular fingerprints; (b) capacity of processing very large molecular data sets; and (c) efficiency in unsupervised pretraining for regression model. Our results suggest that the proposed AAE model significantly enhances the capacity and efficiency of development of the new molecules with specific anticancer properties using the deep generative models.



KEYWORDS: *adversarial autoencoder, deep learning, drug discovery, variational autoencoder, generative adversarial network*

Extracting a biologically relevant latent space from cancer transcriptomes with variational autoencoders

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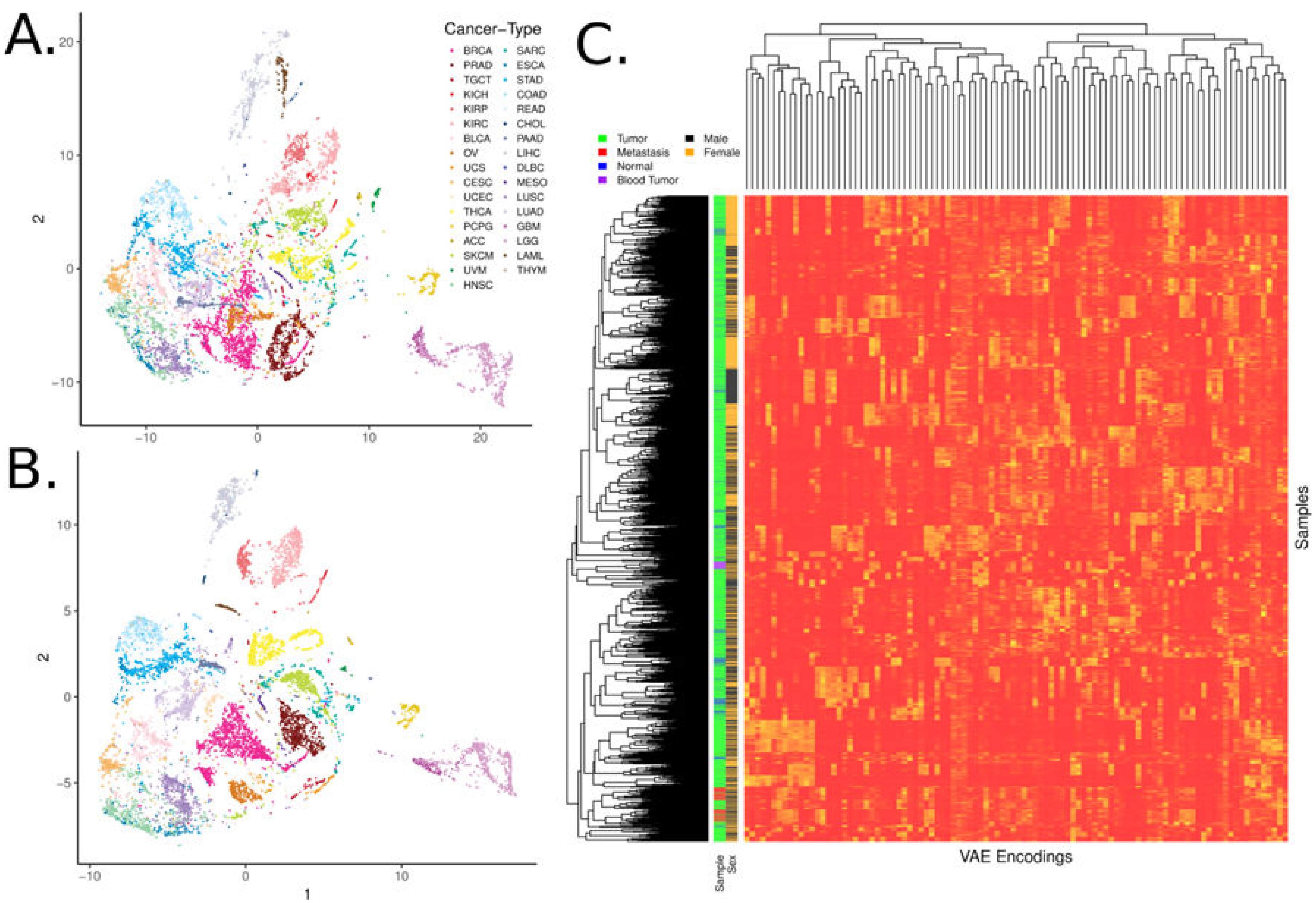

Fig. 2. Samples encoded by a variational auto-encoder retain biological signals
(**A**) t-distributed stochastic neighbor embedding (t-SNE) of TCGA pan-cancer tumors with Tybalt encoded features. (**B**) t-SNE of 0-1 normalized gene expression features. Tybalt retains similar signals as compared to uncompressed gene expression data. (**C**) Full Tybalt encoding features by TCGA pan-cancer sample heatmap. Given on the y axis are the patients sex and type of sample.

Enabling Dark Energy Science with Deep Generative Models of Galaxy Images

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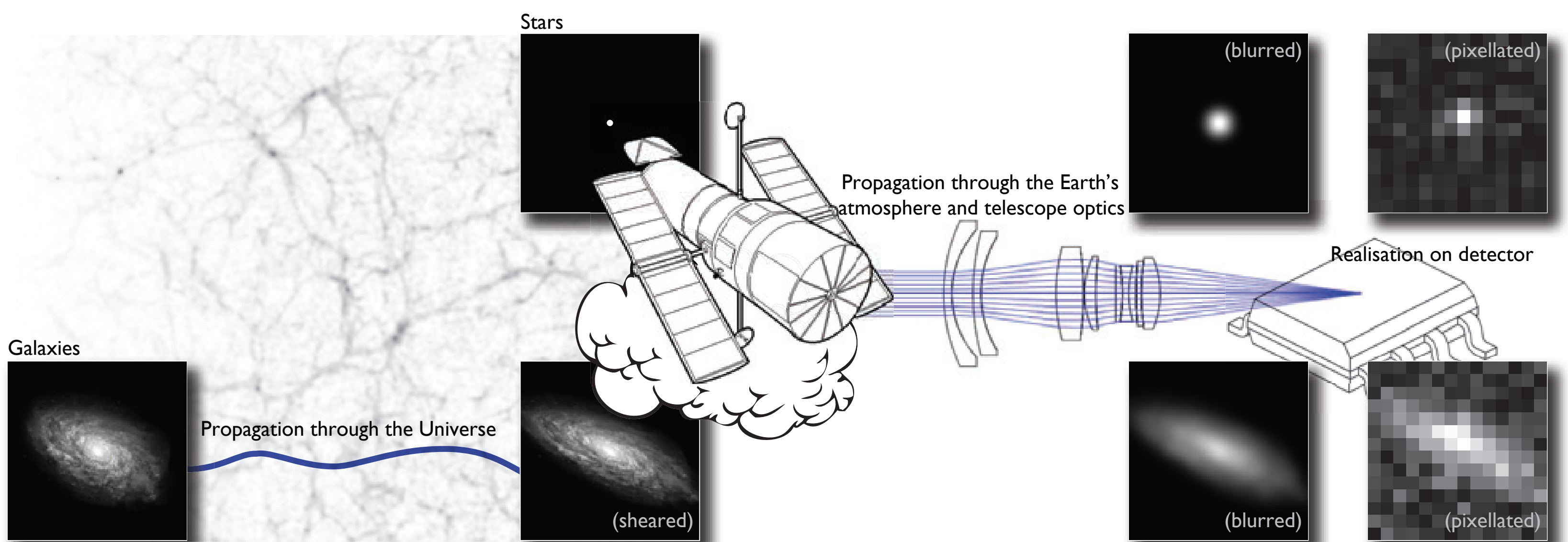


Illustration of the processes involved in the measurement of weak gravitational lensing. The light from distant galaxies is deflected by the matter in the Universe, causing a shearing of the galaxy images, which are then further blurred by the atmosphere and the telescope optics and finally pixelated into a noisy image by the imaging sensor.

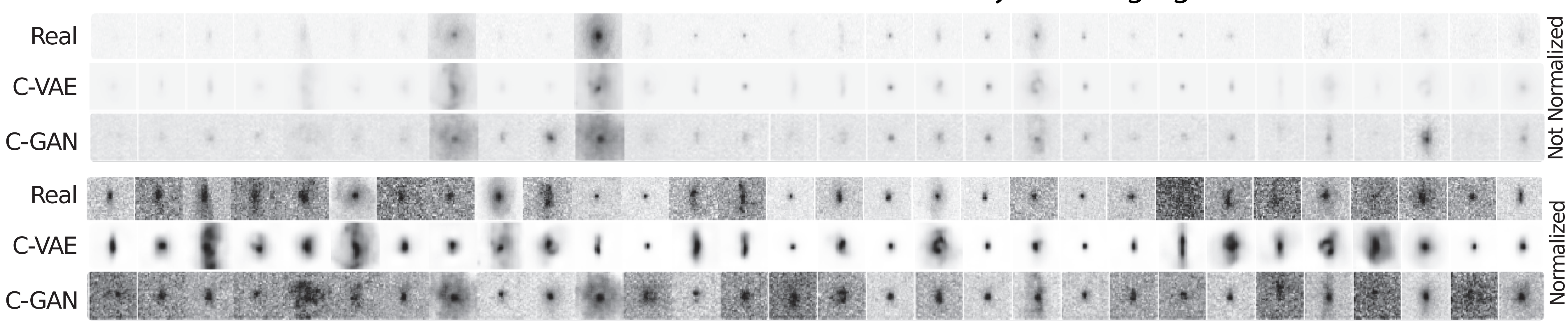
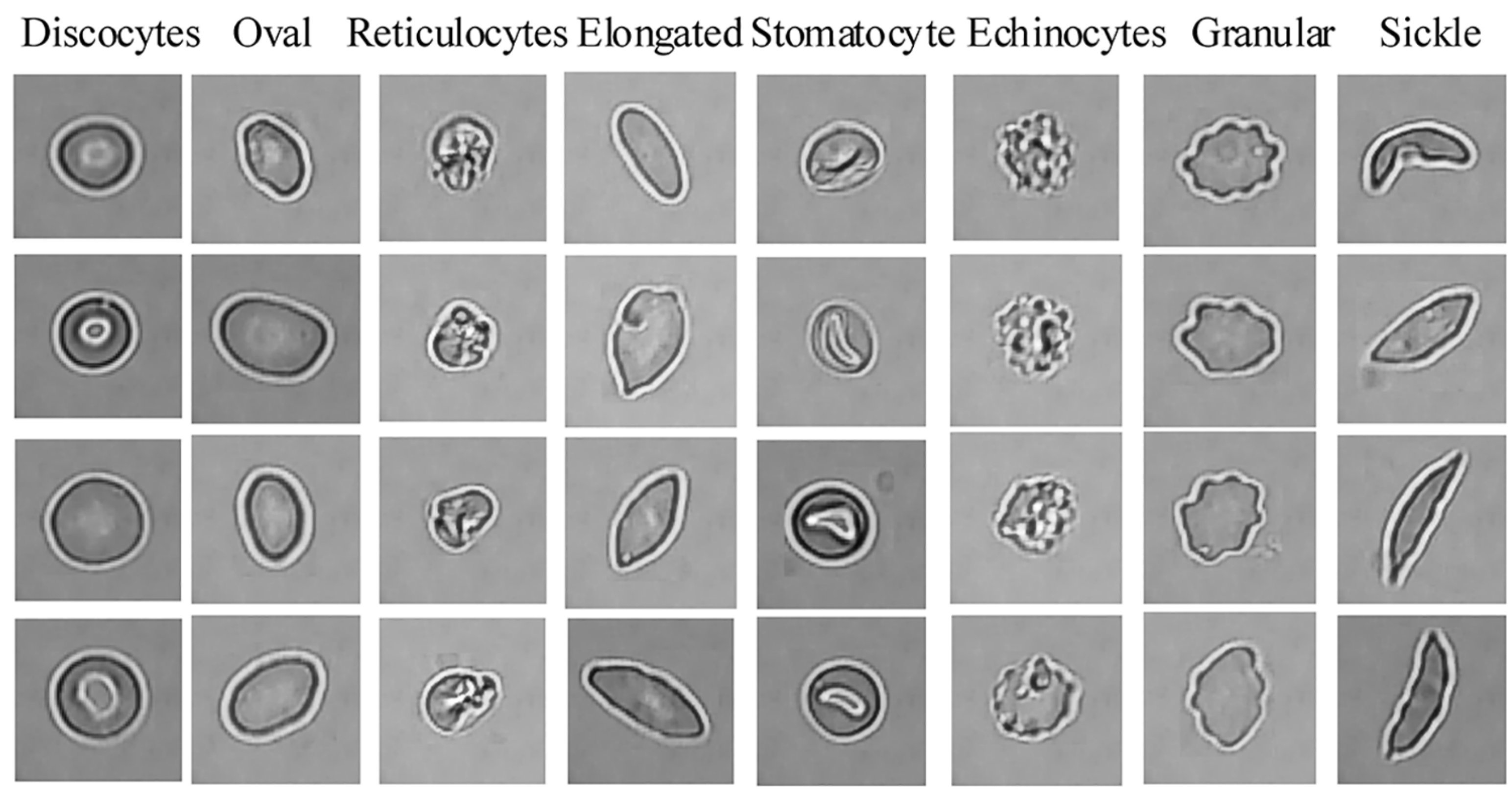


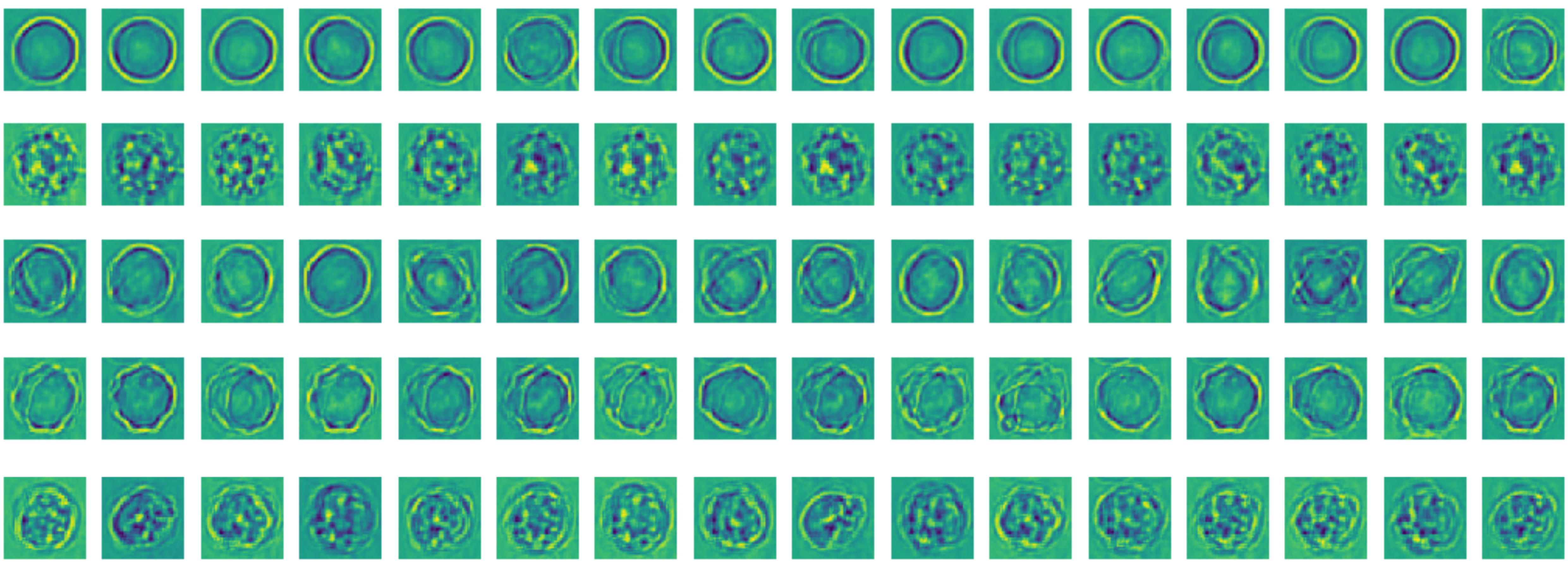
Figure 3: Samples from the COSMOS dataset and generated samples using the conditional variational autoencoder (C-VAE, scheme I) and our variation on conditional generative adversarial network (C-GAN). Each column image shows three 64×64 images (here inverted) produced by conditioning on the same set of features $y \in \Re^3$ in the test-set. Due to its high dynamic range, most figures are very faint. In the bottom three rows, each image is individually normalized.

Semi-supervised learning with VAEs

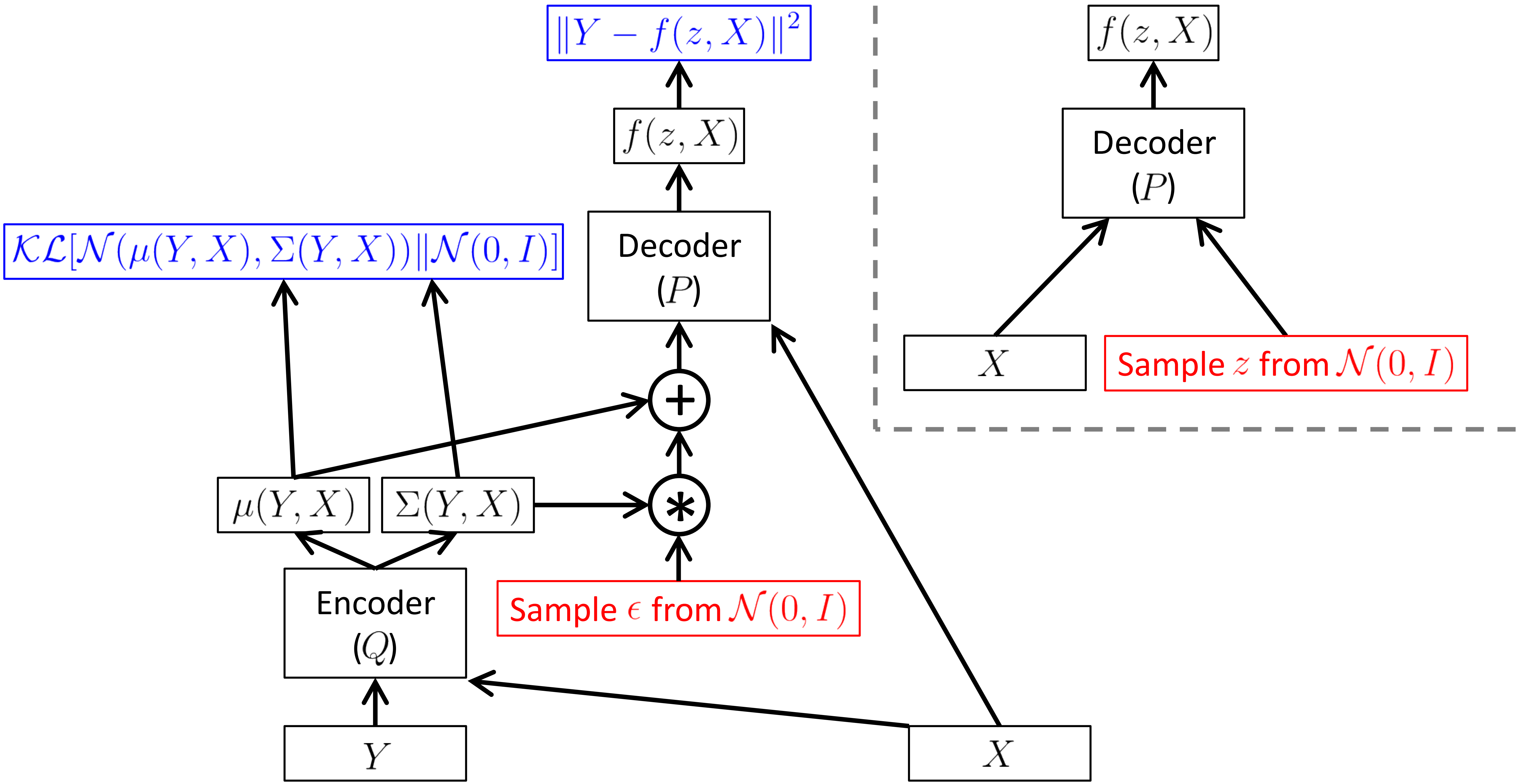
Kingma, D. P., Mohamed, S., Rezende, D. J., & Welling, M. (2014). Semi-supervised learning with deep generative models. In Advances in Neural Information Processing Systems (pp. 3581-3589).

Semi-supervised learning with VAEs





Supervised learning with VAEs



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Doersch, C. (2016). Tutorial on variational autoencoders. arXiv preprint arXiv:1606.05908.