ENM531: Data-driven modeling and probabilistic scientific computing

Lecture #26: Generative adversarial networks

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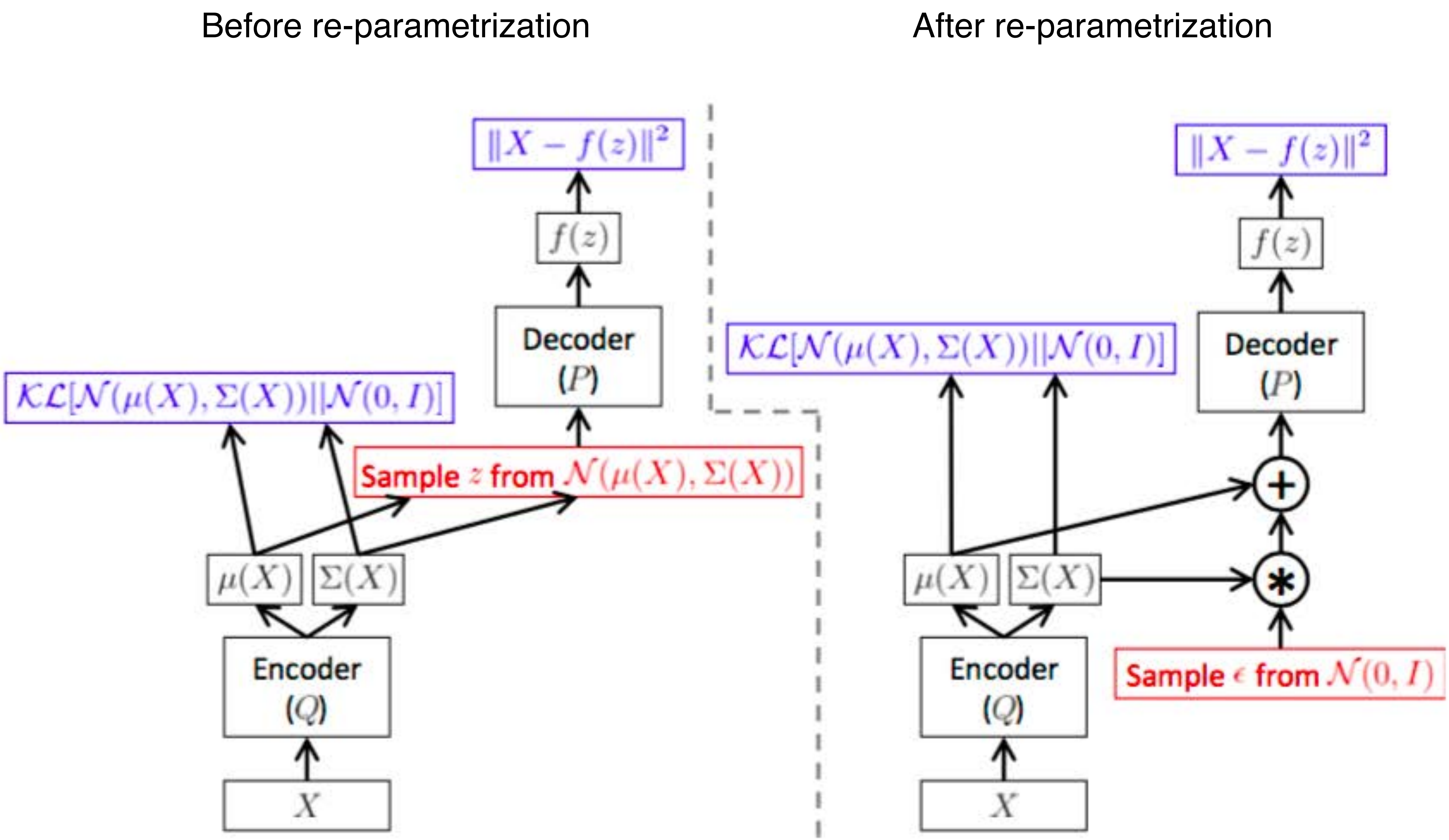
Tricks of the trade

- Variational bounds
- Density re-parametrizations
- Density ratio estimation
- Variational optimization/evolution strategies
- Adversarial games

Variational auto-encoders



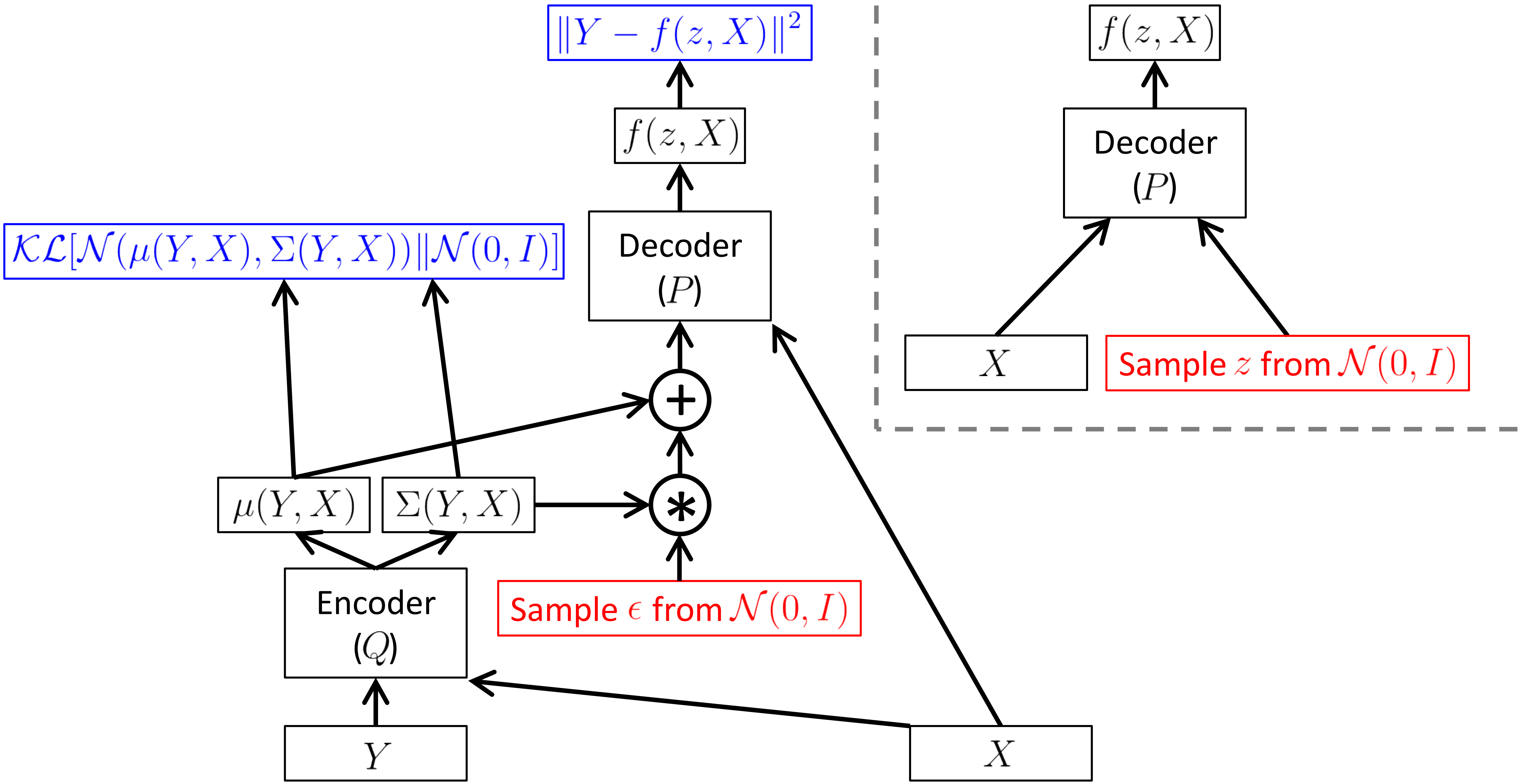
Kingma, D. P., & Welling, M. (2013). Auto-encoding variational bayes. arXiv preprint arXiv:1312.6114.

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

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).

Supervised learning with VAEs



Conditional variational auto-encoder

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

The density ratio trick

The central task in the above five statistical quantities is to efficiently compute the ratio $r(x)$. In simple problems, we can compute the numerator and the denominator separately, and then compute their ratio. Direct estimation like this will not often be possible: each part of the ratio may itself involve intractable integrals; we will often deal with high-dimensional quantities; and we may only have samples drawn from the two distributions, not their analytical forms.

This is where the ***density ratio trick*** *or formally, density ratio estimation*, enters: it tells us to construct a binary classifier $S(x)$ that distinguishes between samples from the two distributions. We can then compute the density ratio using the probability given by this classifier:

$$r(x) = \frac{\rho(x)}{q(x)} = \frac{S(x)}{1 - S(x)}$$

To show this, imagine creating a data set of $2N$ elements consisting of pairs (data x, label y):

- N data points are drawn from the distribution ρ and assigned a label +1.
- The remaining N data points are drawn from distribution q and assigned label −1.

http://blog.shakirm.com/2018/01/machine-learning-trick-of-the-day-7-density-ratio-trick/

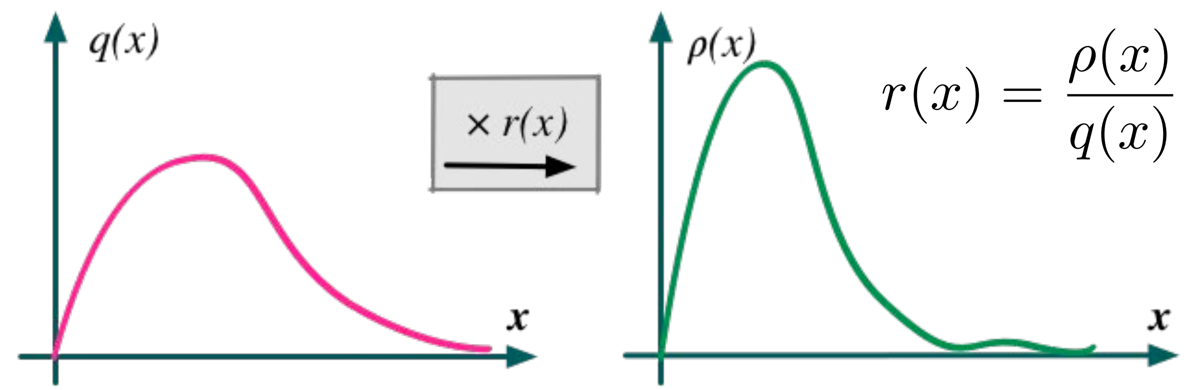
Density ratio estimation by probabilistic classification

$$\mathbb{KL}[p(\boldsymbol{x})||q(\boldsymbol{x})] := \int \log \frac{p(\boldsymbol{x})}{q(\boldsymbol{x})} p(\boldsymbol{x}) d\boldsymbol{x} = \mathbb{E}_{p(\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x})}{q(\boldsymbol{x})} \right]$$

Estimating density ratios is a challenging task:

- Each part of the ratio may itself involve intractable integrals
- We often deal with high-dimensional quantities.
- We may only have samples drawn from the two distributions, not their analytical forms.

This is where the ***density ratio trick*** enters: it allows us to construct a binary classifier that distinguishes between samples from the two distributions.

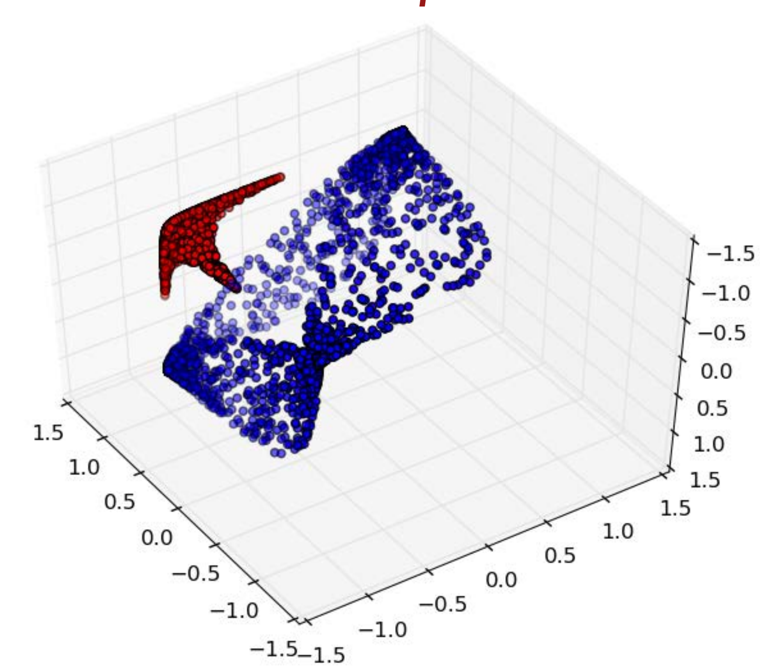


The density ratio gives the correction factor needed to make two distributions equal.

$$r(x) = \frac{\rho(x)}{q(x)} = \frac{p(x|y=+1)}{p(x|y=-1)}$$

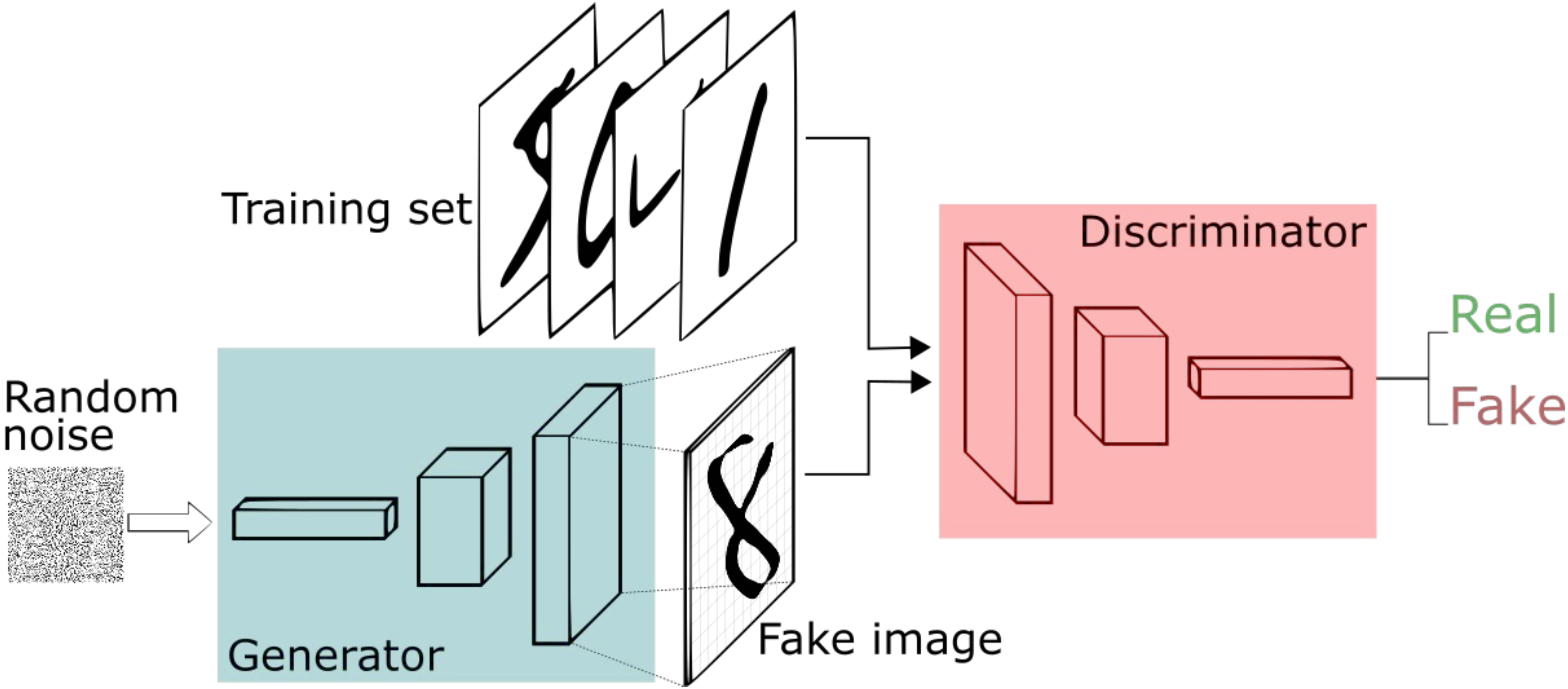
$$= \frac{p(y=+1|x)p(x)}{p(y=+1)} \Big/ \frac{p(y=-1|x)p(x)}{p(y=-1)}$$

$$= \frac{p(y=+1|x)}{p(y=-1|x)} = \frac{p(y=+1|x)}{1-p(y=+1|x)} = \frac{\mathcal{S}(x)}{1-\mathcal{S}(x)}$$



http://blog.shakirm.com/2018/01/machine-learning-trick-of-the-day-7-density-ratio-trick/

Generative adversarial networks



$$\min_G \max_D V(D,G) = \mathbb{E}_{q(\mathbf{x})}[\log(D(\mathbf{x}))] + \mathbb{E}_{p(\mathbf{z})}[\log(1 - D(G(\mathbf{z})))]$$

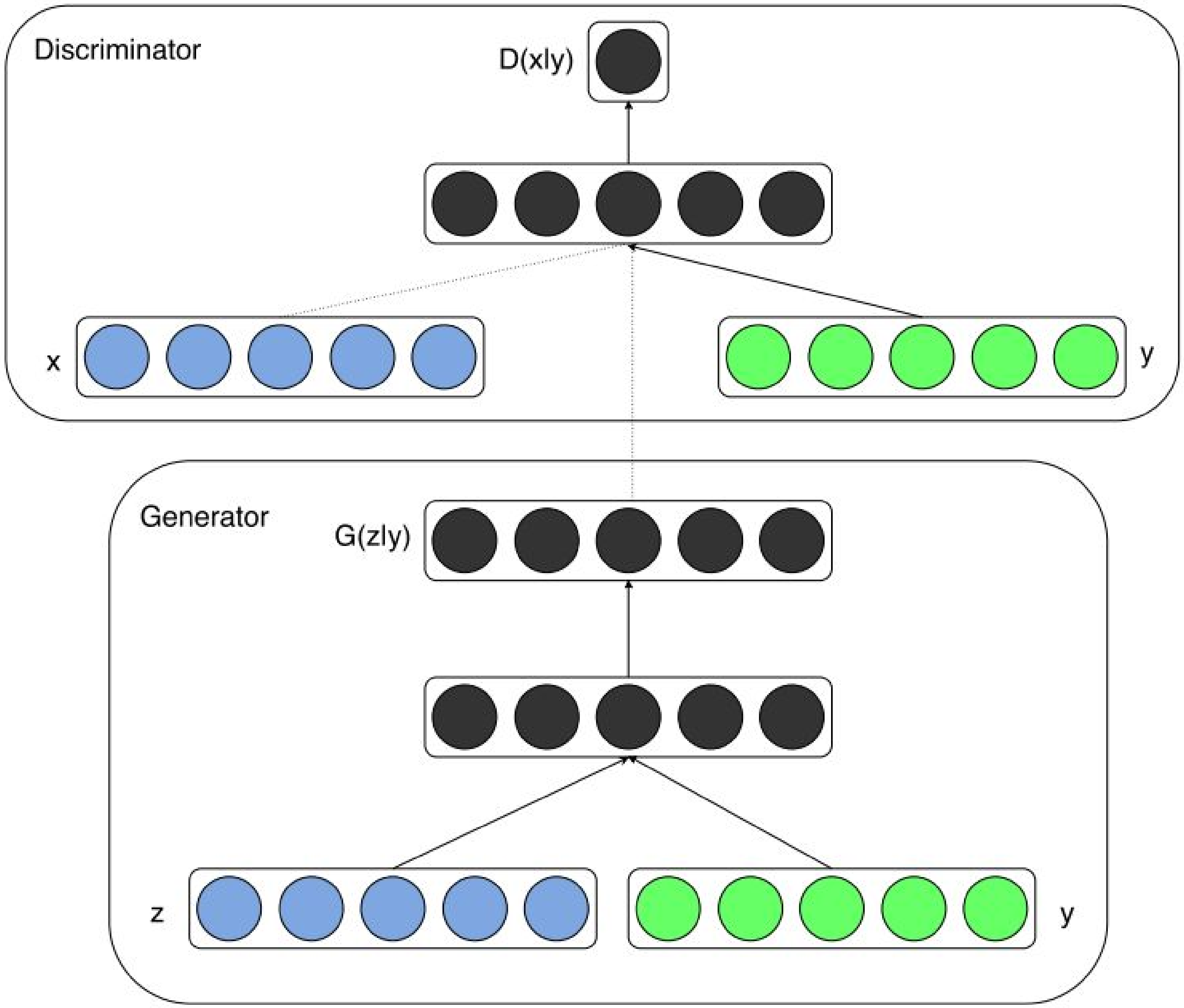
Goodfellow, I., Pouget-Abadie, J., Mirza, M., Xu, B., Warde-Farley, D., Ozair, S., ... & Bengio, Y. (2014). Generative adversarial nets. In Advances in neural information processing systems (pp. 2672-2680).

Generative adversarial networks

Karras, T., Aila, T., Laine, S., & Lehtinen, J. (2017). Progressive growing of gans for improved quality, stability, and variation. arXiv preprint arXiv:1710.10196.

Conditional generative adversarial networks

Mirza and Osindero (2014)



GAN $\min_G \max_D V(D,G) = \mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z}\sim p_z(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z})))]$

CGAN $\min_G \max_D V(D,G) = \mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x}|\boldsymbol{y})] + \mathbb{E}_{\boldsymbol{z}\sim p_z(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z}|\boldsymbol{y})))]$

Conditional generative adversarial networks

High-Resolution Image Synthesis and Semantic Manipulation with Conditional GANs

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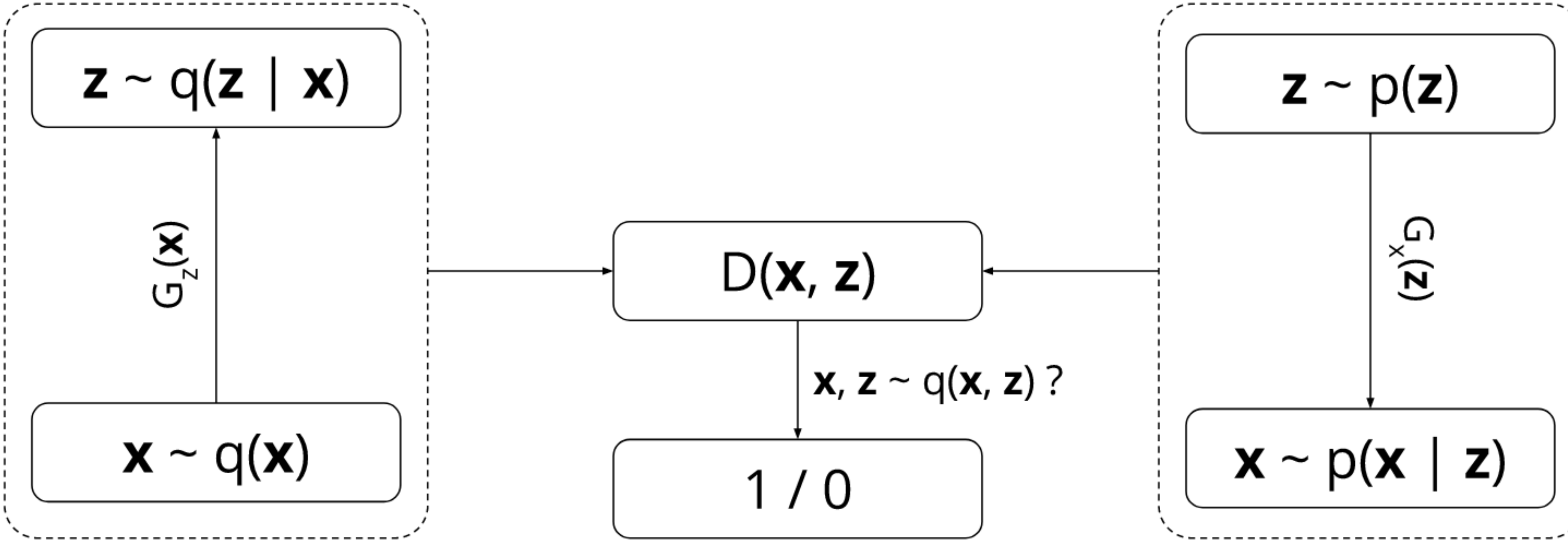
[1]NVIDIA Corporation [2]University of California, Berkeley

Wang, T. C., Liu, M.Y., Zhu, J.Y., Tao, A., Kautz, J., & Catanzaro, B. (2018). High-resolution image synthesis and semantic manipulation with conditional gans. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (pp. 8798-8807).

Adversarially learned inference

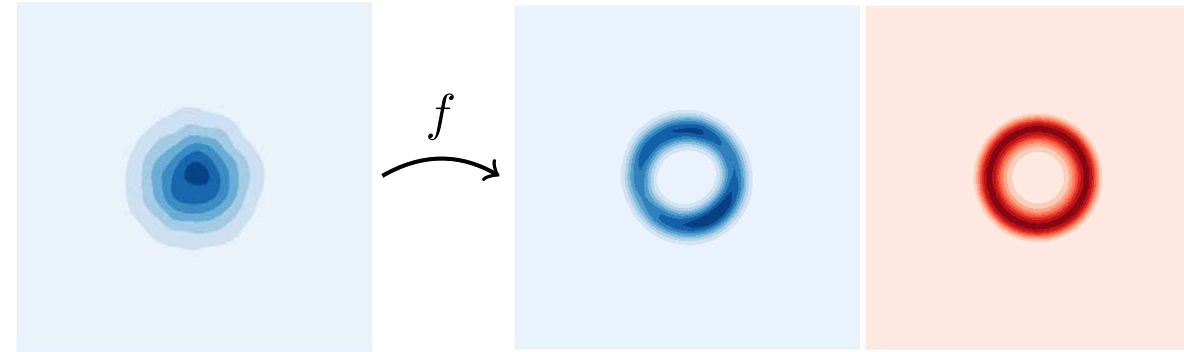


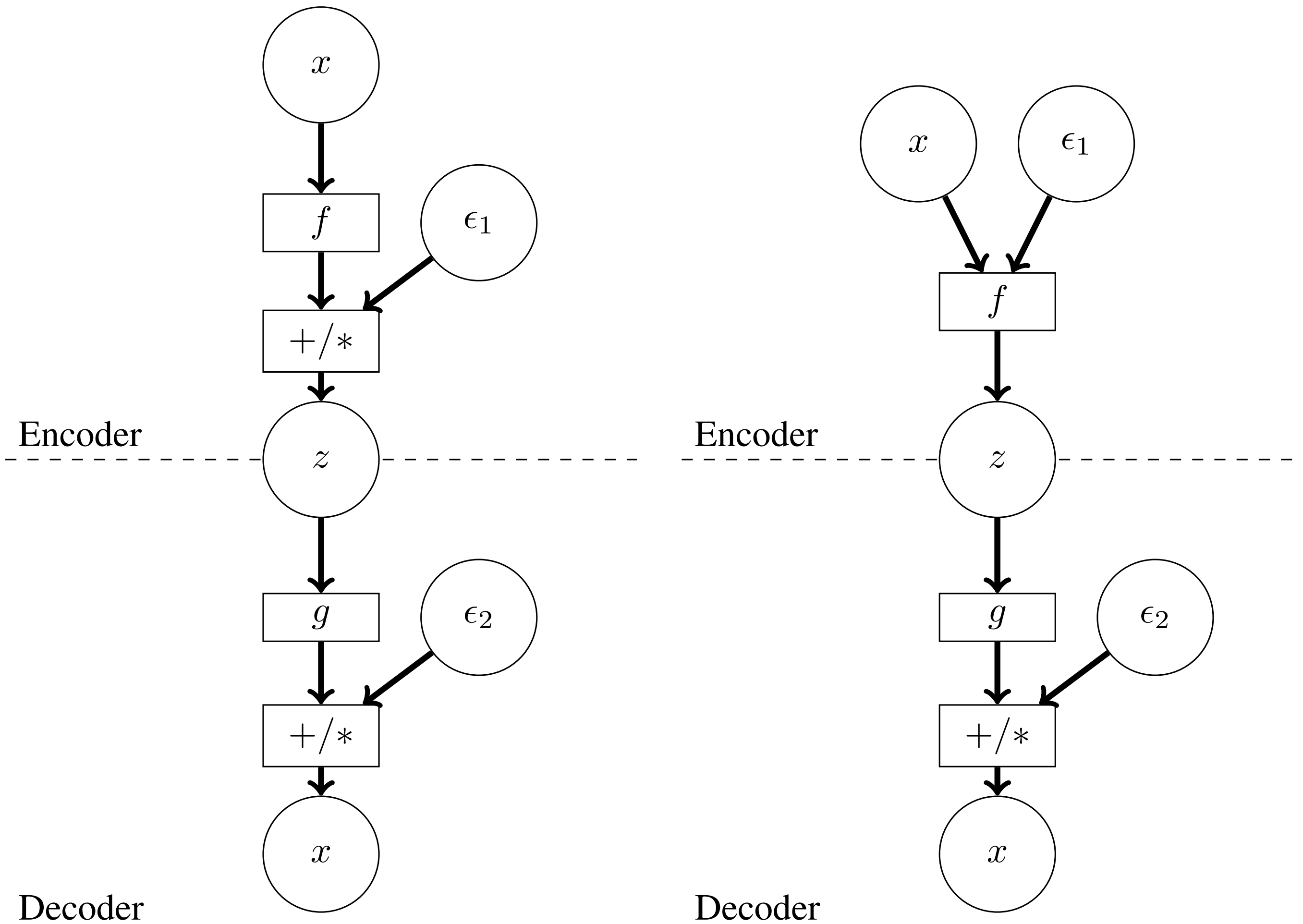
$$\min_G \max_D V(D, G) = \mathbb{E}_{q(\mathbf{x})}[\log(D(\mathbf{x}, G_z(\mathbf{x})))] + \mathbb{E}_{p(\mathbf{z})}[\log(1 - D(G_x(\mathbf{z}), \mathbf{z}))]$$

Dumoulin, V., Belghazi, I., Poole, B., Mastropietro, O., Lamb, A., Arjovsky, M., & Courville, A. (2016). Adversarially learned inference. arXiv preprint arXiv:1606.00704.

Adversarial Variational Bayes

Instead of using approximating distributions of a given pre-defined form (e.g. Gaussian) we can implicitly parametrize them using deep neural networks.





(a) Standard VAE (b) Our model

Algorithm 1 Adversarial Variational Bayes (AVB)

$i \leftarrow 0$
while not converged **do**
  Sample $\{x^{(1)}, \ldots, x^{(m)}\}$ from data distrib. $p_{\mathcal{D}}(x)$
  Sample $\{z^{(1)}, \ldots, z^{(m)}\}$ from prior $p(z)$
  Sample $\{\epsilon^{(1)}, \ldots, \epsilon^{(m)}\}$ from $\mathcal{N}(0, 1)$
  Compute θ-gradient (eq. 3.7):

$$g_\theta \leftarrow \frac{1}{m} \sum_{k=1}^{m} \nabla_\theta \log p_\theta \left(x^{(k)} \mid z_\phi \left(x^{(k)}, \epsilon^{(k)}\right)\right)$$

  Compute ϕ-gradient (eq. 3.7):

$$g_\phi \leftarrow \frac{1}{m} \sum_{k=1}^{m} \nabla_\phi \Big[-T_\psi \left(x^{(k)}, z_\phi(x^{(k)}, \epsilon^{(k)})\right) + \log p_\theta \left(x^{(k)} \mid z_\phi(x^{(k)}, \epsilon^{(k)})\right)\Big]$$

  Compute ψ-gradient (eq. 3.3) :

$$g_\psi \leftarrow \frac{1}{m} \sum_{k=1}^{m} \nabla_\psi \Big[\log \left(\sigma(T_\psi(x^{(k)}, z_\phi(x^{(k)}, \epsilon^{(k)})))\right) + \log \left(1 - \sigma(T_\psi(x^{(k)}, z^{(k)}))\right)\Big]$$

  Perform SGD-updates for θ, ϕ and ψ:
  $\theta \leftarrow \theta + h_i\, g_\theta, \quad \phi \leftarrow \phi + h_i\, g_\phi, \quad \psi \leftarrow \psi + h_i\, g_\psi$
  $i \leftarrow i + 1$
end while

Huszár, F. (2017). Variational inference using implicit distributions. arXiv preprint arXiv:1702.08235.

Mescheder, L., Nowozin, S., & Geiger, A. (2017). Adversarial variational Bayes: Unifying variational autoencoders and generative adversarial networks. arXiv preprint arXiv:1701.04722.

Makhzani, A., Shlens, J., Jaitly, N., Goodfellow, I., & Frey, B. (2015). Adversarial autoencoders. arXiv preprint arXiv:1511.05644.

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

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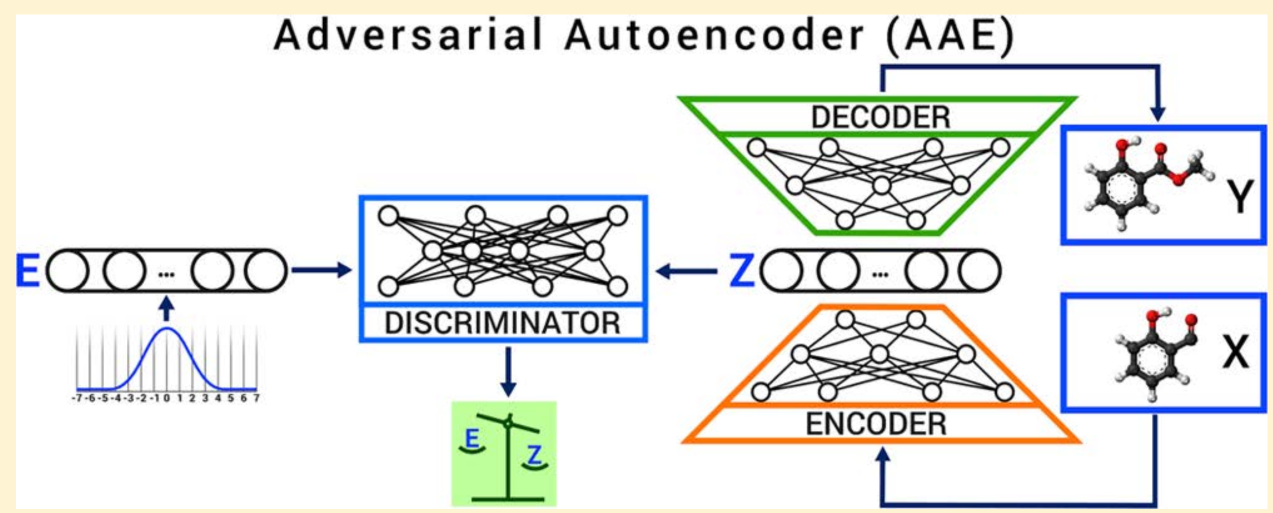
ABSTRACT: Deep generative adversarial networks (GANs) are the emerging technology in drug discovery and biomarker development. In our recent work, we demonstrated a proof-of-concept of implementing deep generative adversarial autoencoder (AAE) to identify new molecular fingerprints with predefined anticancer 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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Casey S. Greene*
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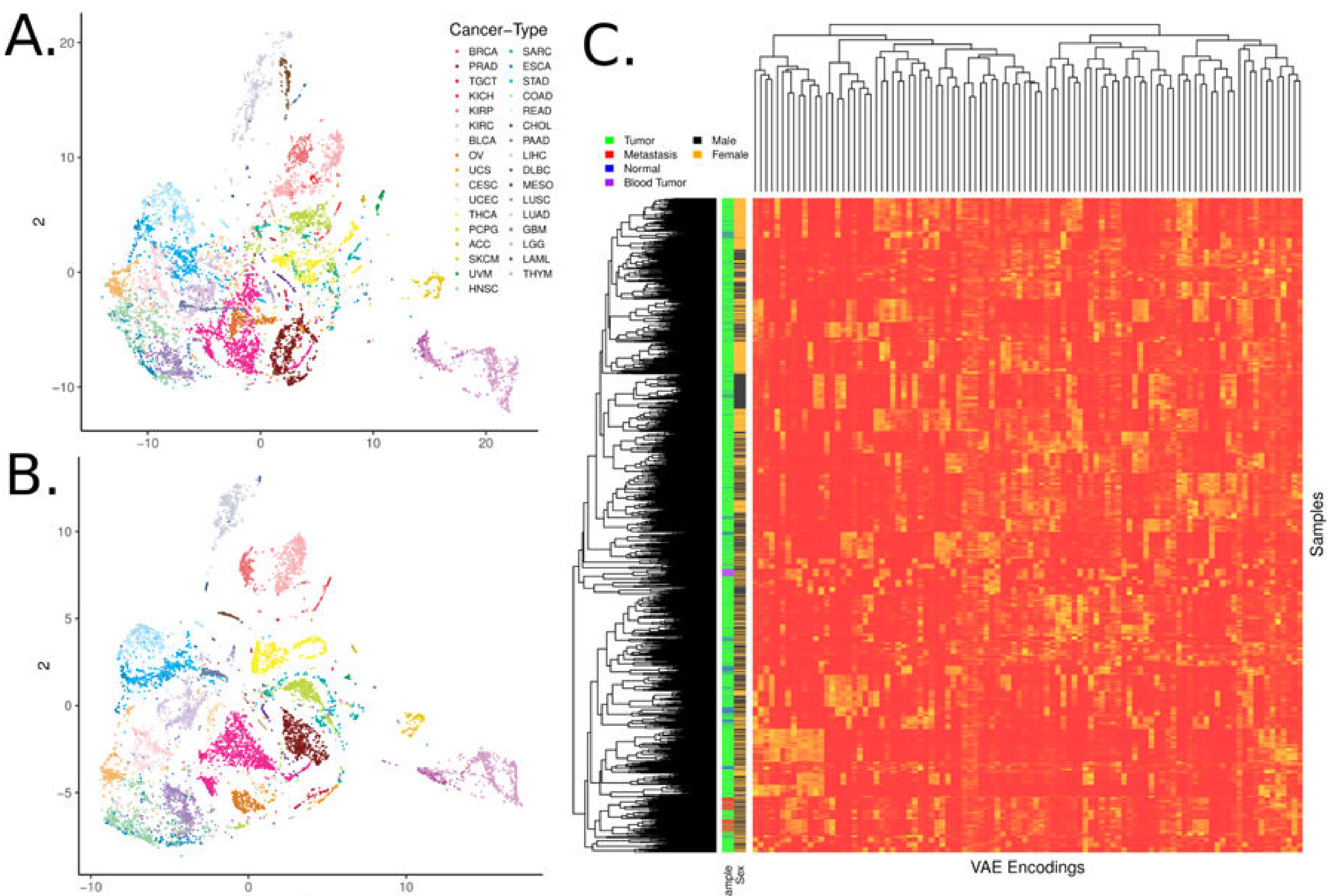

Fig. 2. Samples encoded by a variational auto-encoder retain biological signals
(**A**) t-distributed stochastic neighbor embedding (t-SNE) of TCGA pan-cancer tumors with Tybalt encoded features. (**B**) t-SNE of 0-1 normalized gene expression features. Tybalt retains similar signals as compared to uncompressed 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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Jeff Schneider,[1] **Barnabás Póczos**[1]
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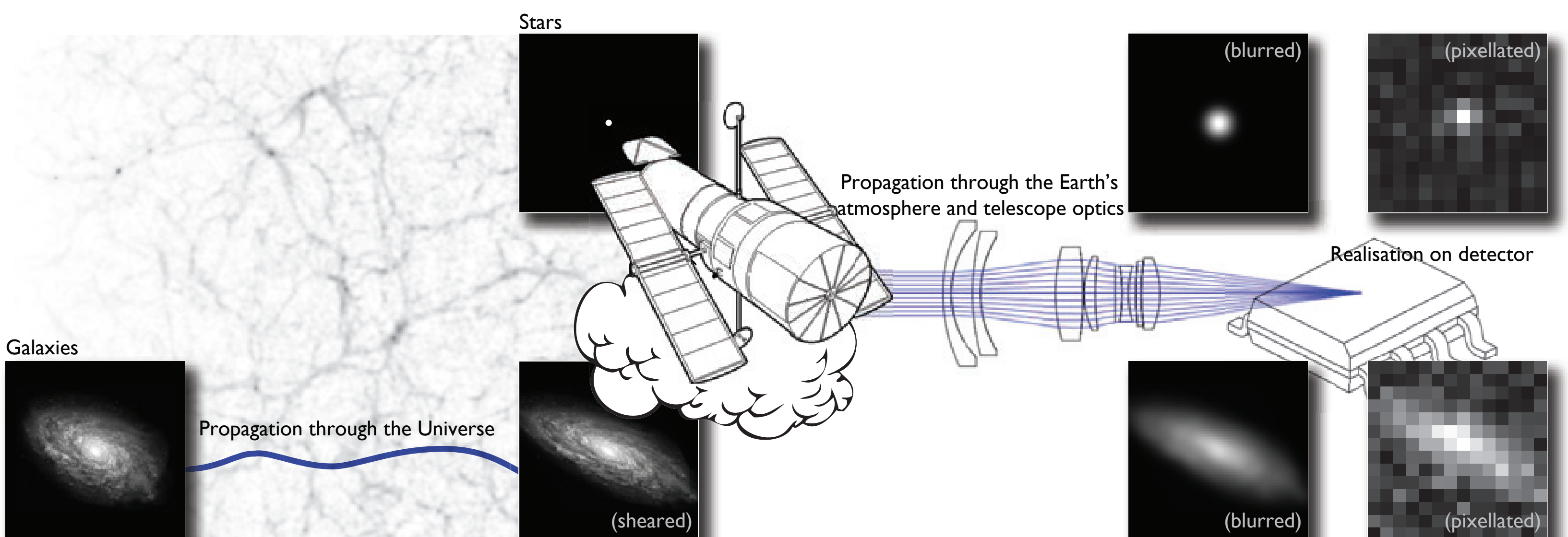

Illustration of the processes involved in the measurement of weak gravitational lensing. The light from distant galaxies is deflected by the matter in the Universe, causing a shearing of the galaxy images, which are then further blurred by the atmosphere and the telescope optics and finally pixelated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

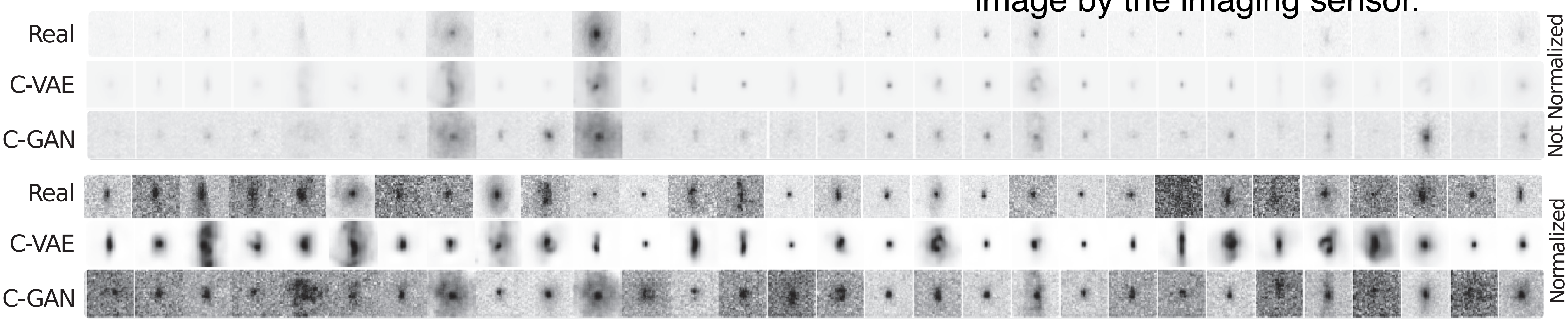

Figure 3: Samples from the COSMOS dataset and generated samples using the conditional variational autoencoder (C-VAE, scheme I) and our variation on conditional generative adversarial network (C-GAN). Each column image shows three 64×64 images (here inverted) produced by conditioning on the same set 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.