Generative models and Variational Autoencoders

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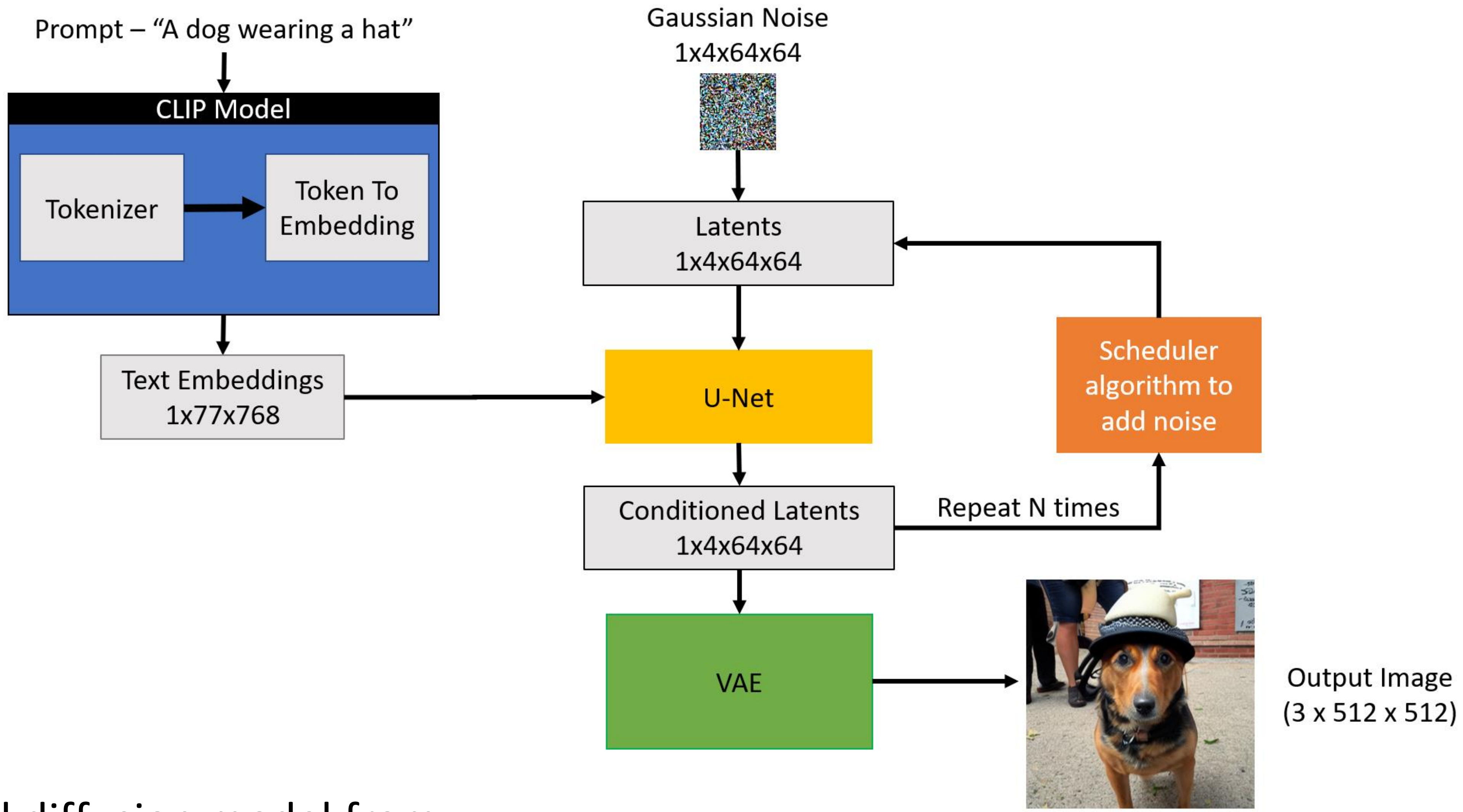
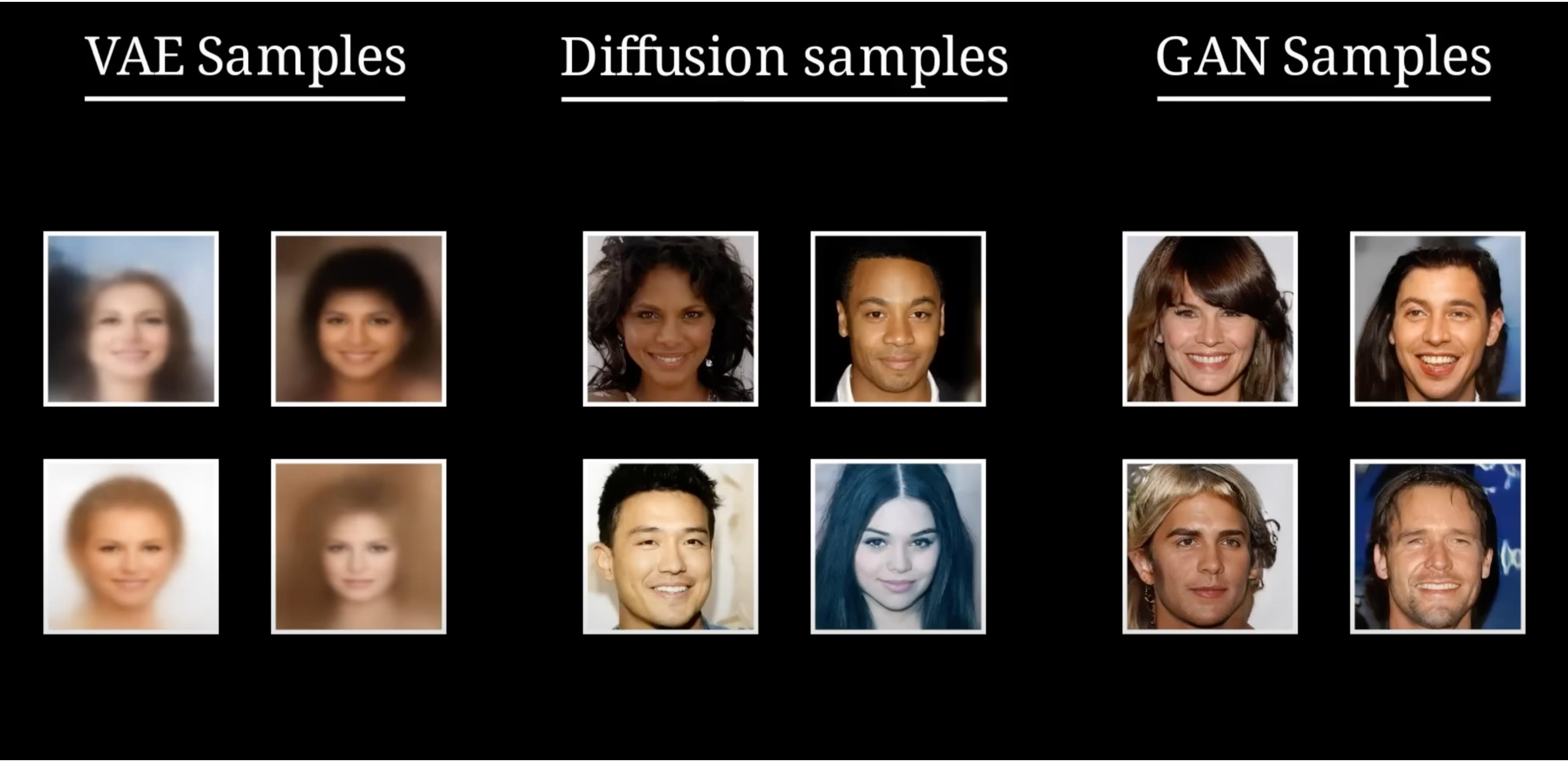
Generative models for general use

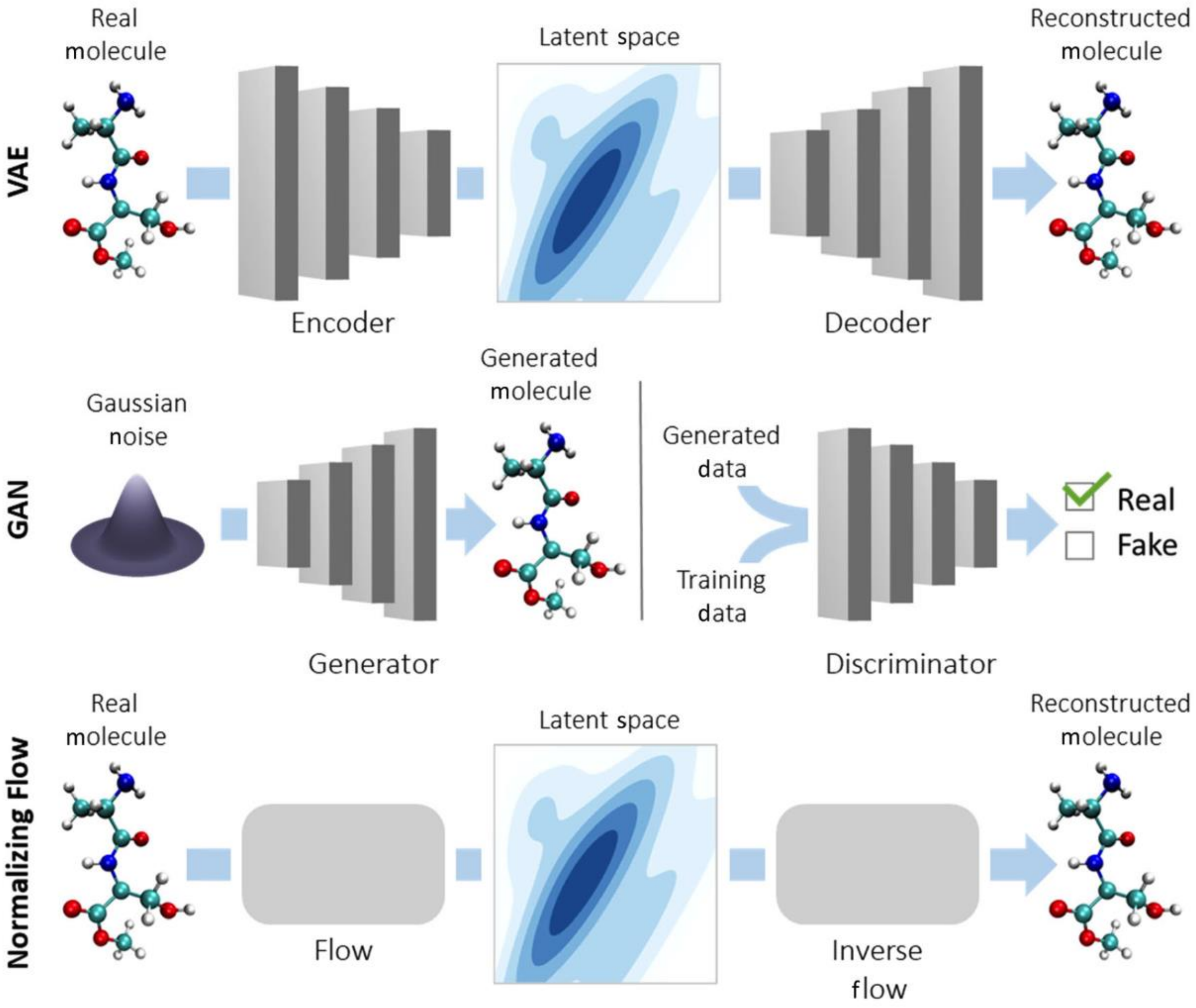


Stabilized diffusion model from Hugging Face



https://www.youtube.com/watch?v=qJeaCHQ1k2w

Types of Generative models for molecules



Generation tries to recover correct molecule reconstruction AND regularization from learned molecular embedding

Generates molecules from Gaussian noise, where a discriminator learns to identify molecules as real or fake. Two networks competing against each other.

Model learns a series of invertible transformations between a prior distribution and molecular data. Can calculate exact data likelihood.

Bilodeau et al. WIREs Computational Molecular Science. (2022)

Latent space optimization for target properties

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Research Article

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Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules

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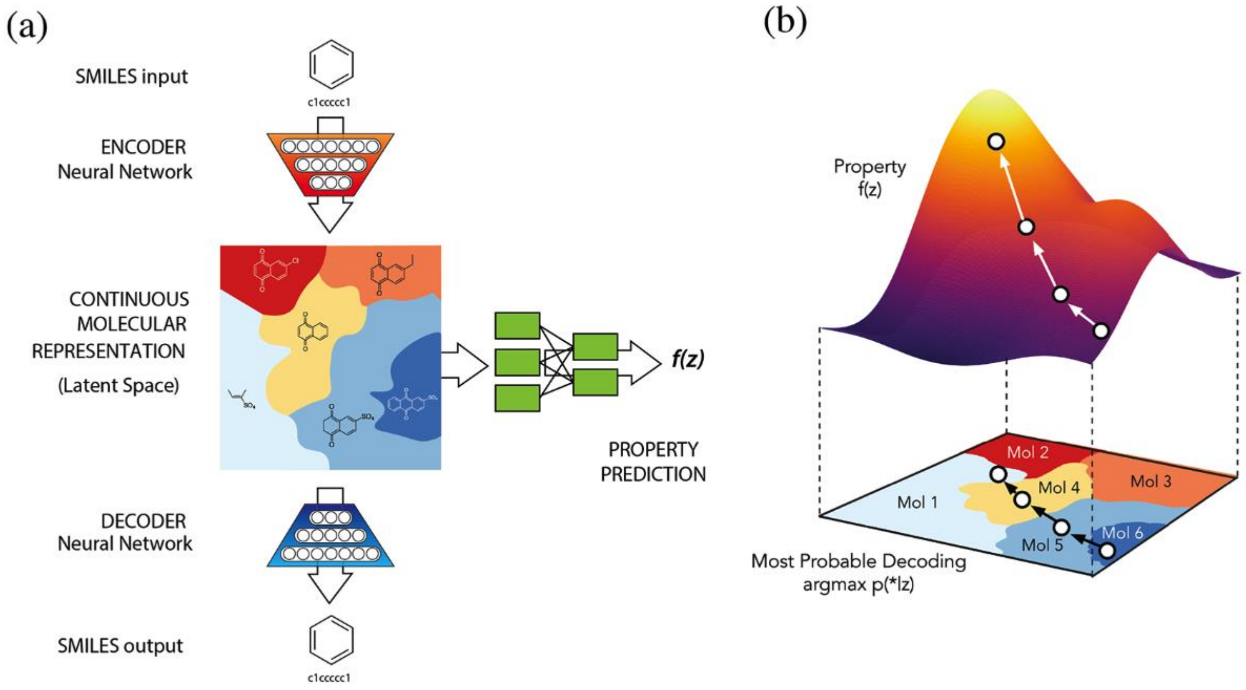
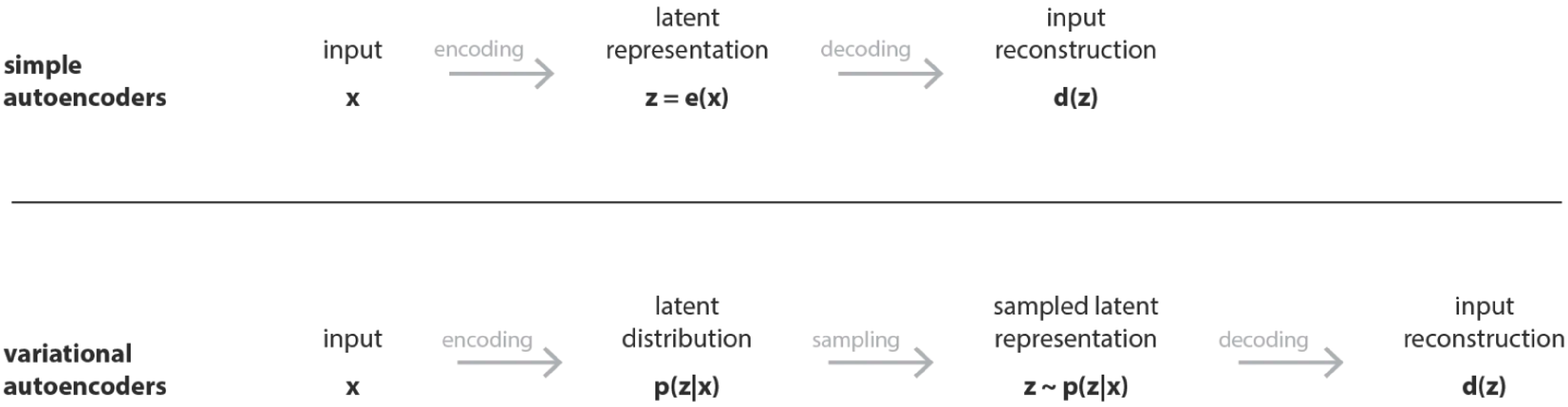


Auto-encoders vs PCA

- PCA is a linear transformation, auto-encoders can describe complicated non-linear processes
- PCA features projects in orthogonal basis. Auto-encoders features optimize for reconstruction, could have correlated features
- PCA is cheaper to compute than autoencoders
- Auto-encoders have a large number of parameters, prone to overfitting

Autoencoder vs variational autoencoder

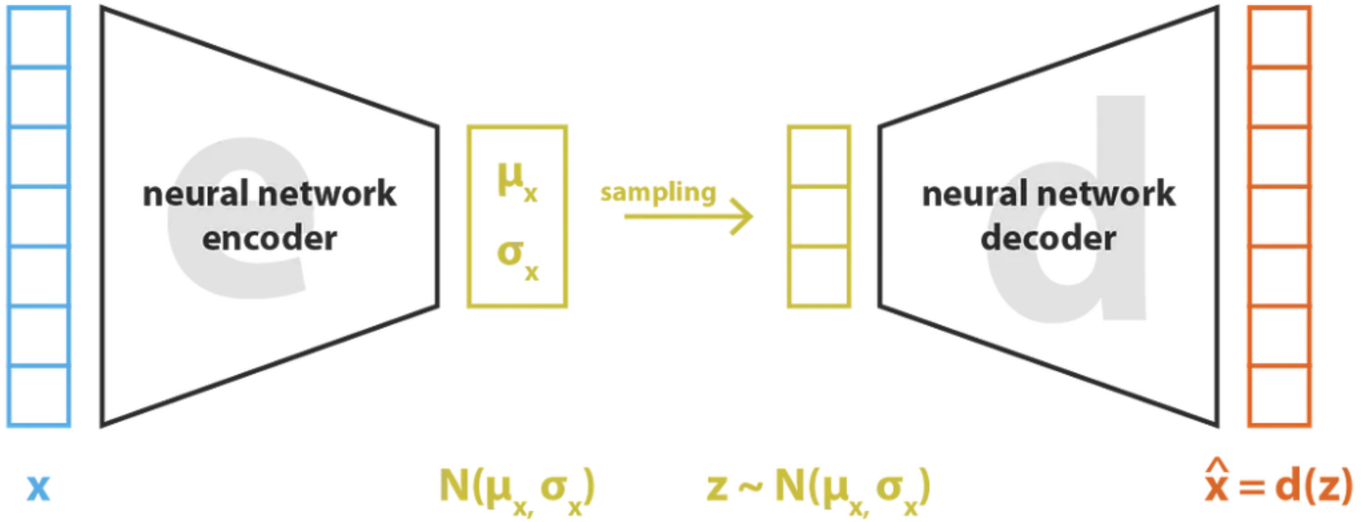
VAE encodes data as probability distribution instead of a single point



https://towardsdatascience.com/understanding-variational-autoencoders-vaes-f70510919f73

Autoencoder vs variational autoencoder

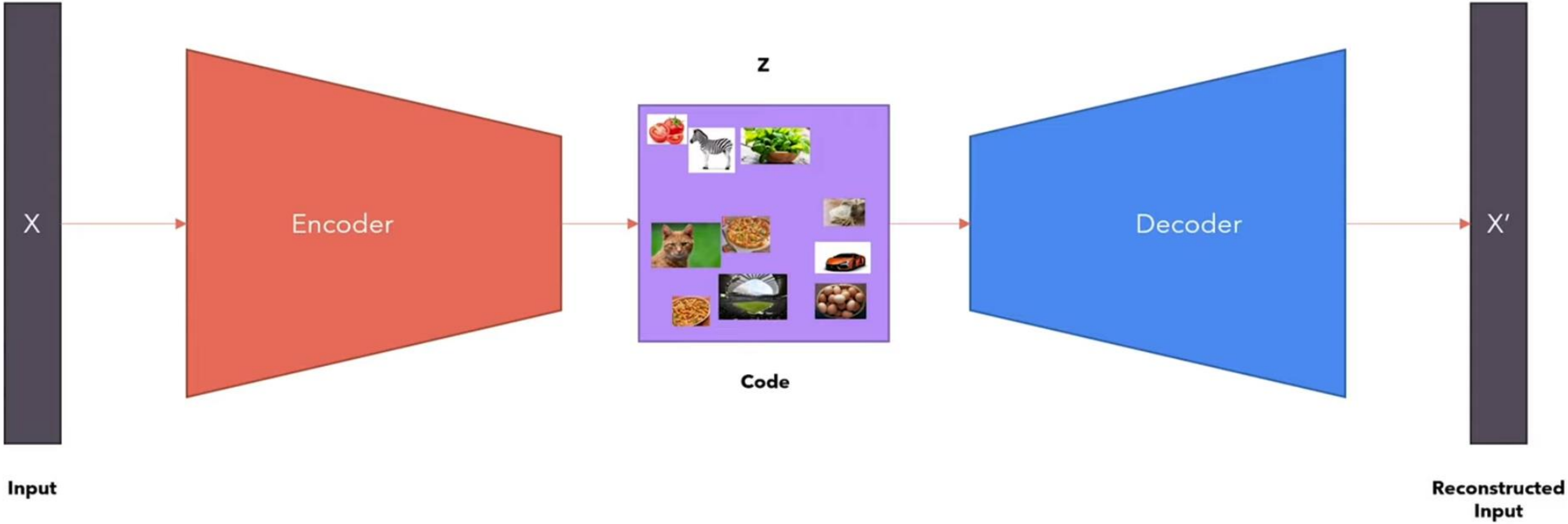
Regularization in the form of the Kullback-Leibler divergence -> this induces better organization in the latent space



$$\text{loss} = \| x - \hat{x} \|^2 + \text{KL}[\, N(\mu_x, \sigma_x), N(0, I) \,] = \| x - d(z) \|^2 + \text{KL}[\, N(\mu_x, \sigma_x), N(0, I) \,]$$

https://towardsdatascience.com/understanding-variational-autoencoders-vaes-f70510919f73

Autoencoder



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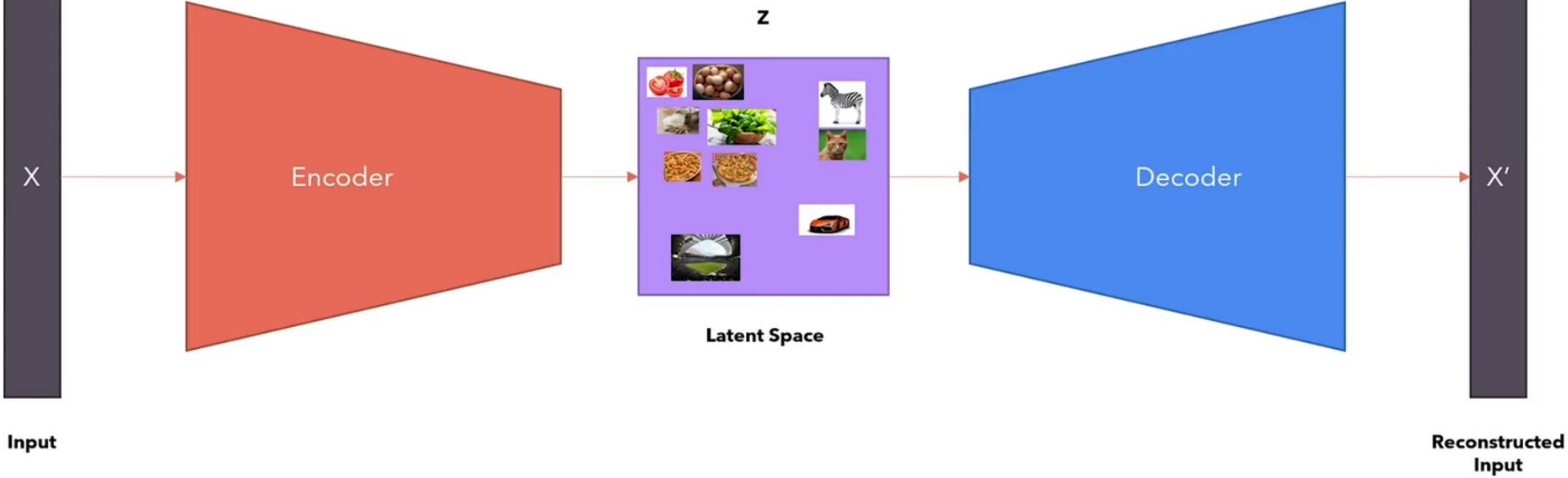
Variational Autoencoder



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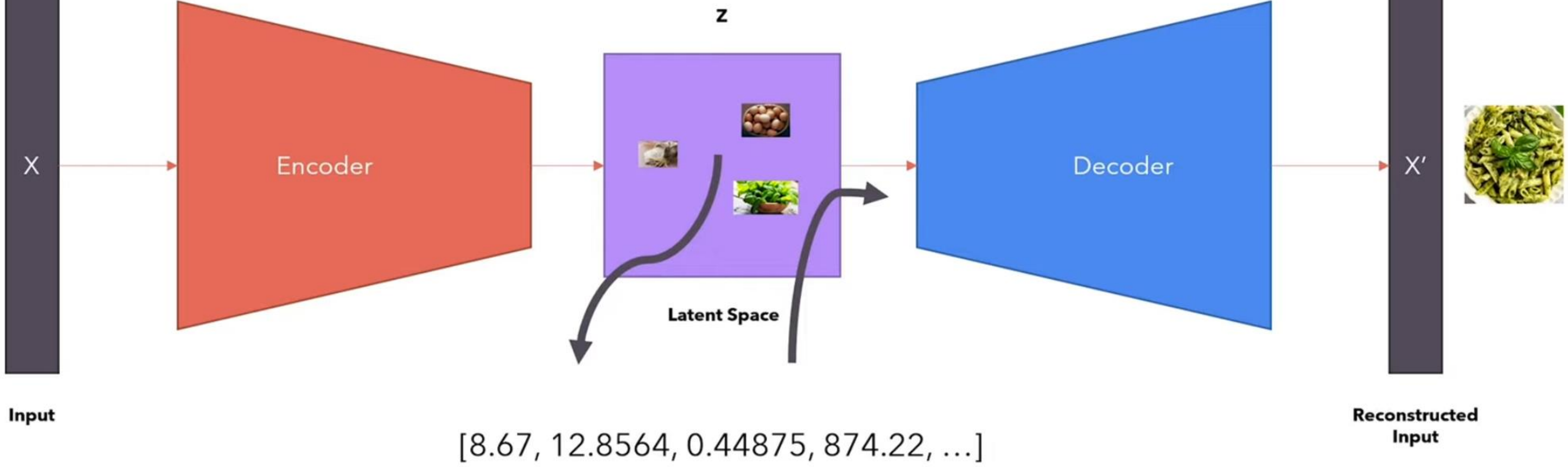
Sampling the latent space



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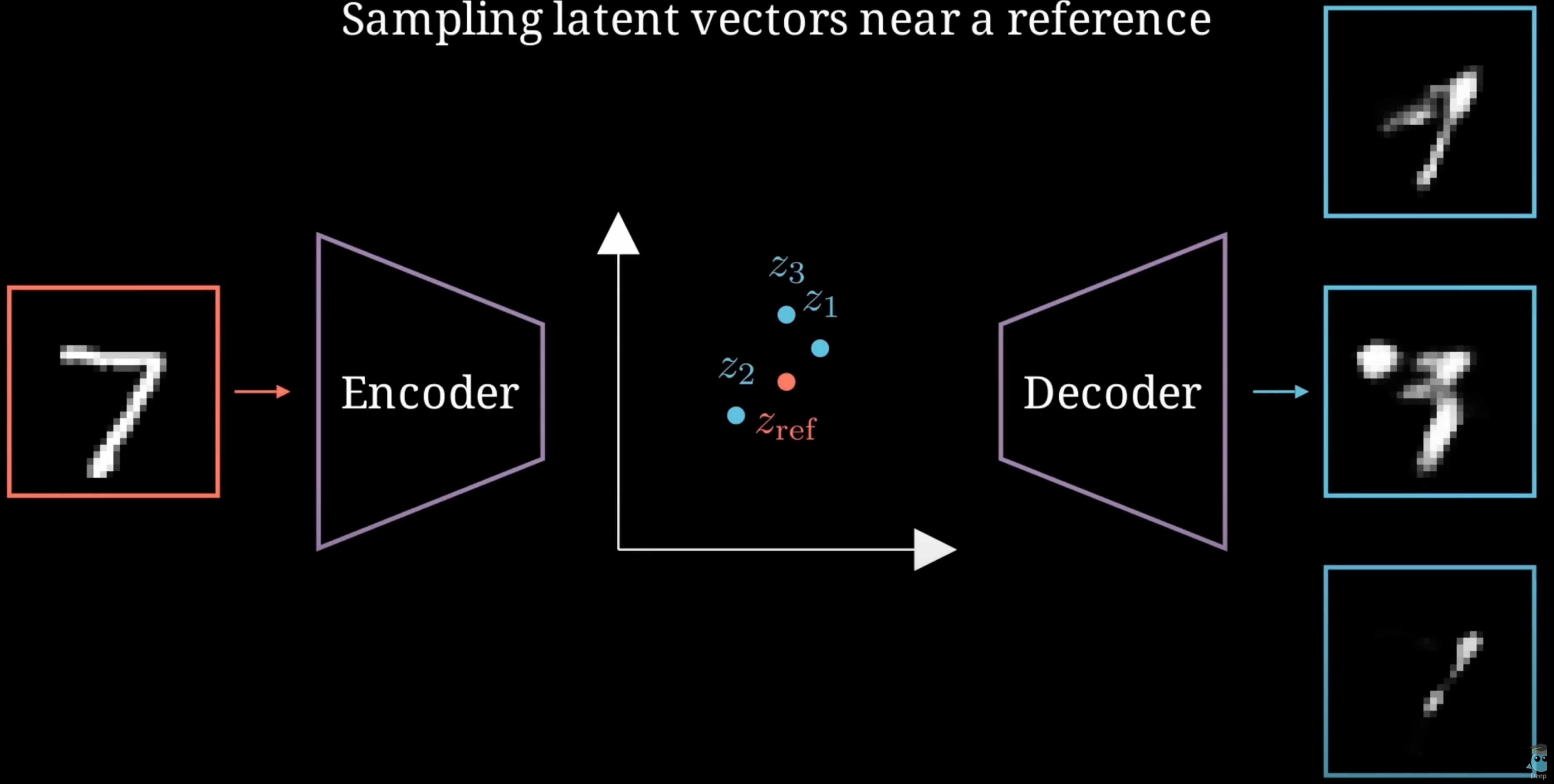
Sampling latent vectors near a reference



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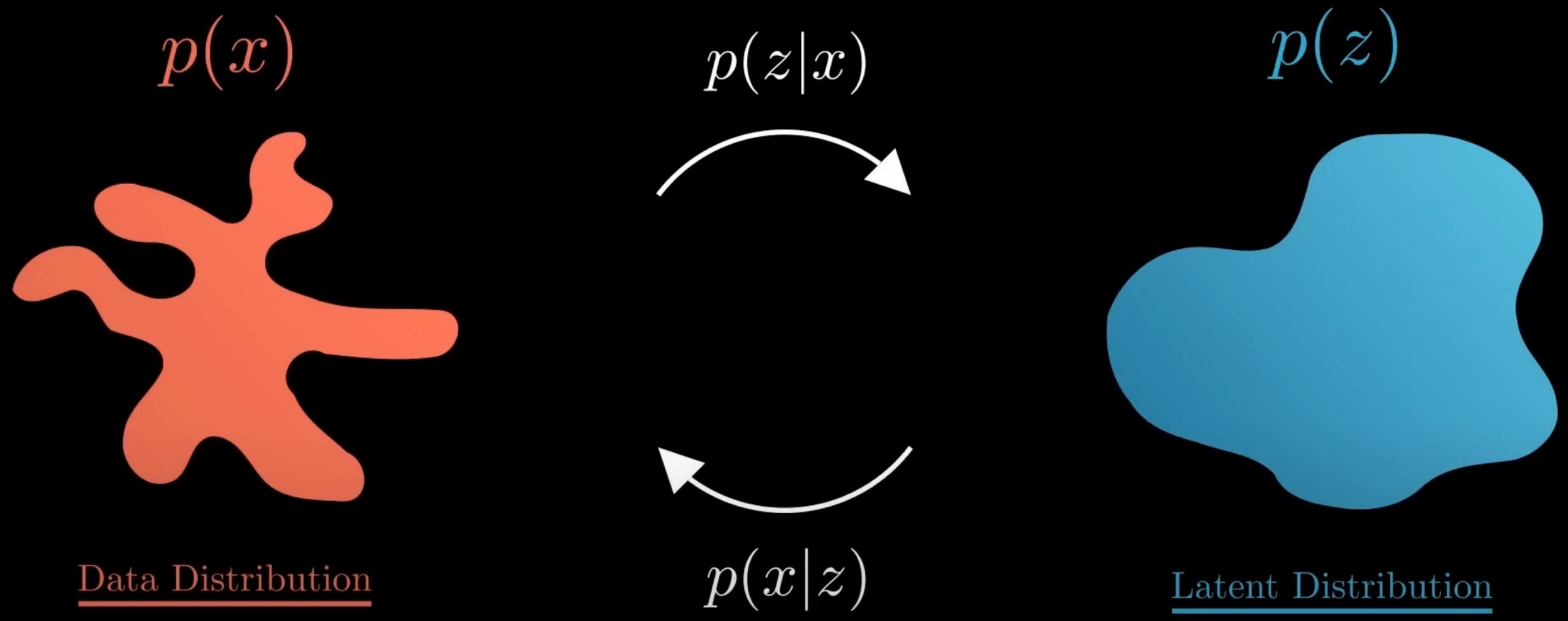

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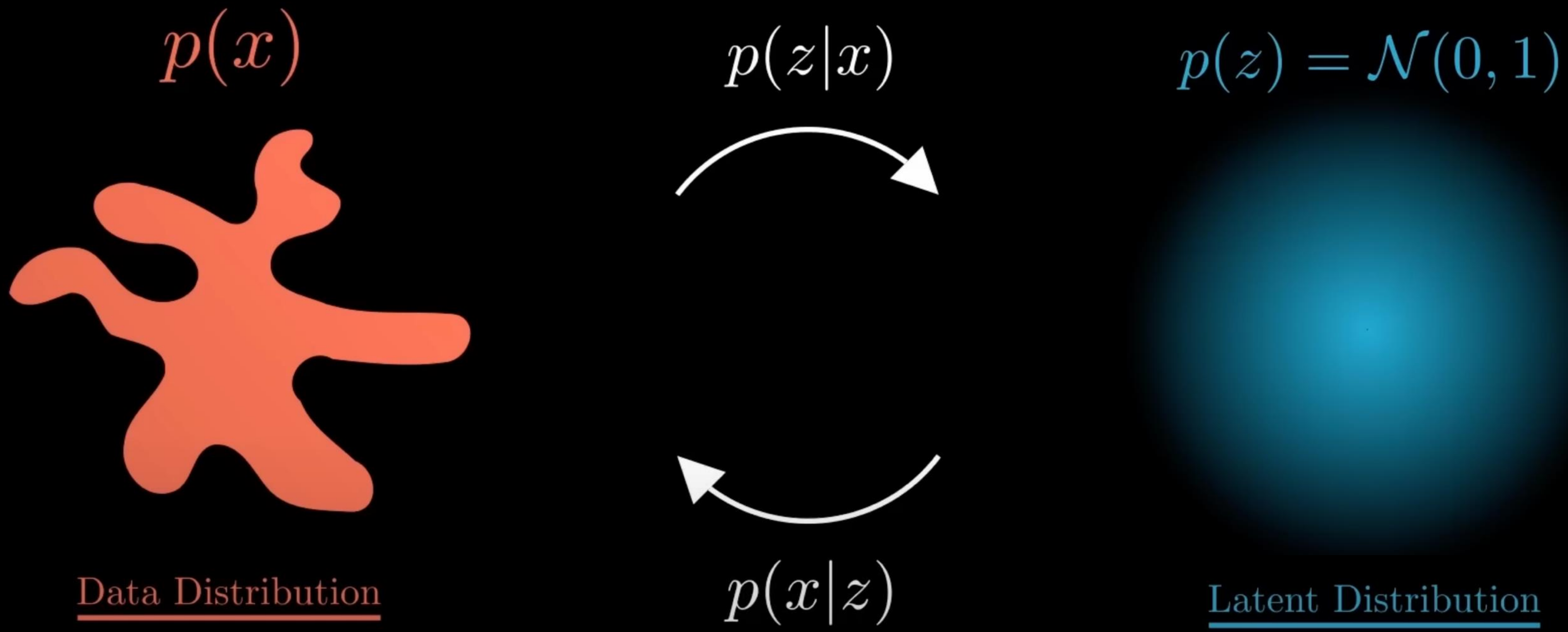

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Loss function

L2/MSE

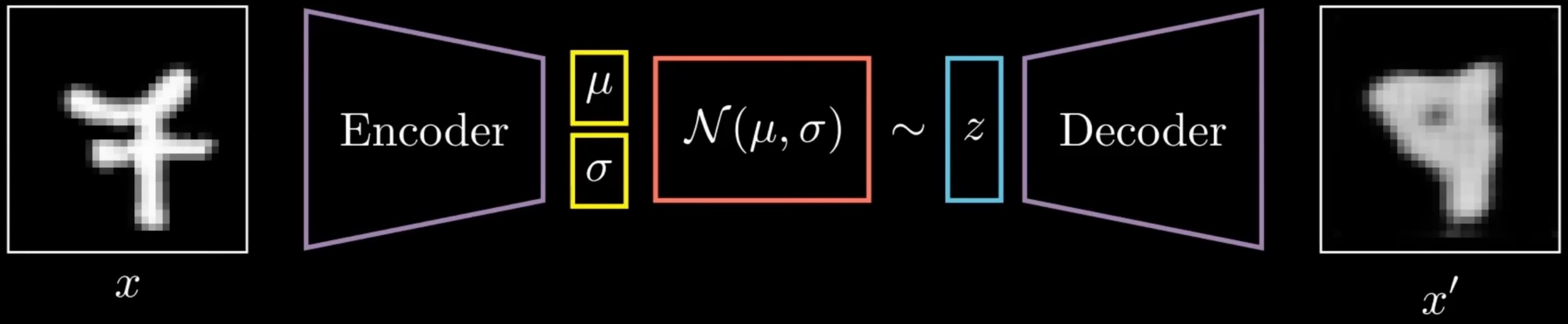
MSE between input molecule and regenerated molecule from latent space

$$\mathcal{L}(x) = \mathbb{E}_{q(z|x)}\left[\log p(x|z)\right] - \mathrm{KL}(q(z|x) \mid p(z))$$

Kullback-Leibler divergence

“regularization”, generalization, how organized the latent space is

https://www.youtube.com/watch?v=qJeaCHQ1k2w



$$\mathcal{L} = \boxed{\mathcal{L}_{KL}(\mathcal{N}(\mu, \sigma) \mid \mathcal{N}(0, 1))} + \mathcal{L}_2(x, x')$$

$$\mathcal{L}_{KL} = -\frac{1}{2}(1 + \log(\sigma^2) - \mu^2 - \sigma^2)$$

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