Advanced Machine Learning

Deep latent variable models

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Outline

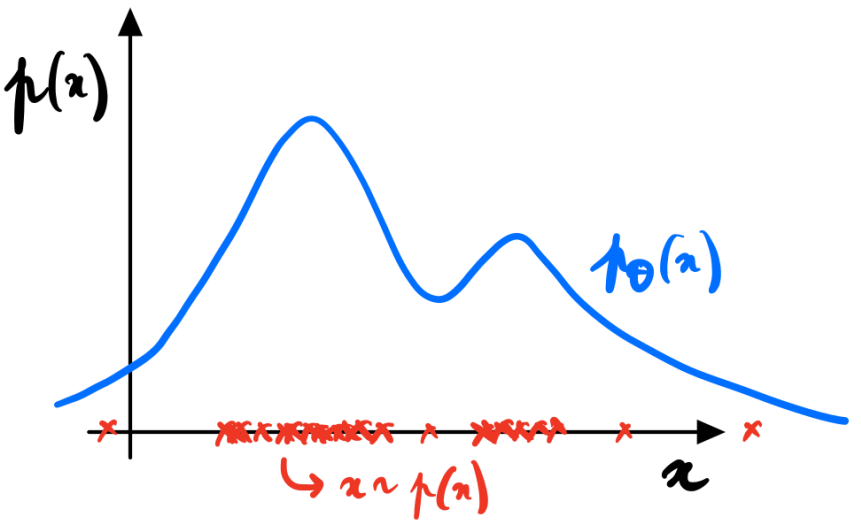
1. Deep generative models
2. Variational auto-encoders
3. Diffusion models

Deep generative models

Generative models

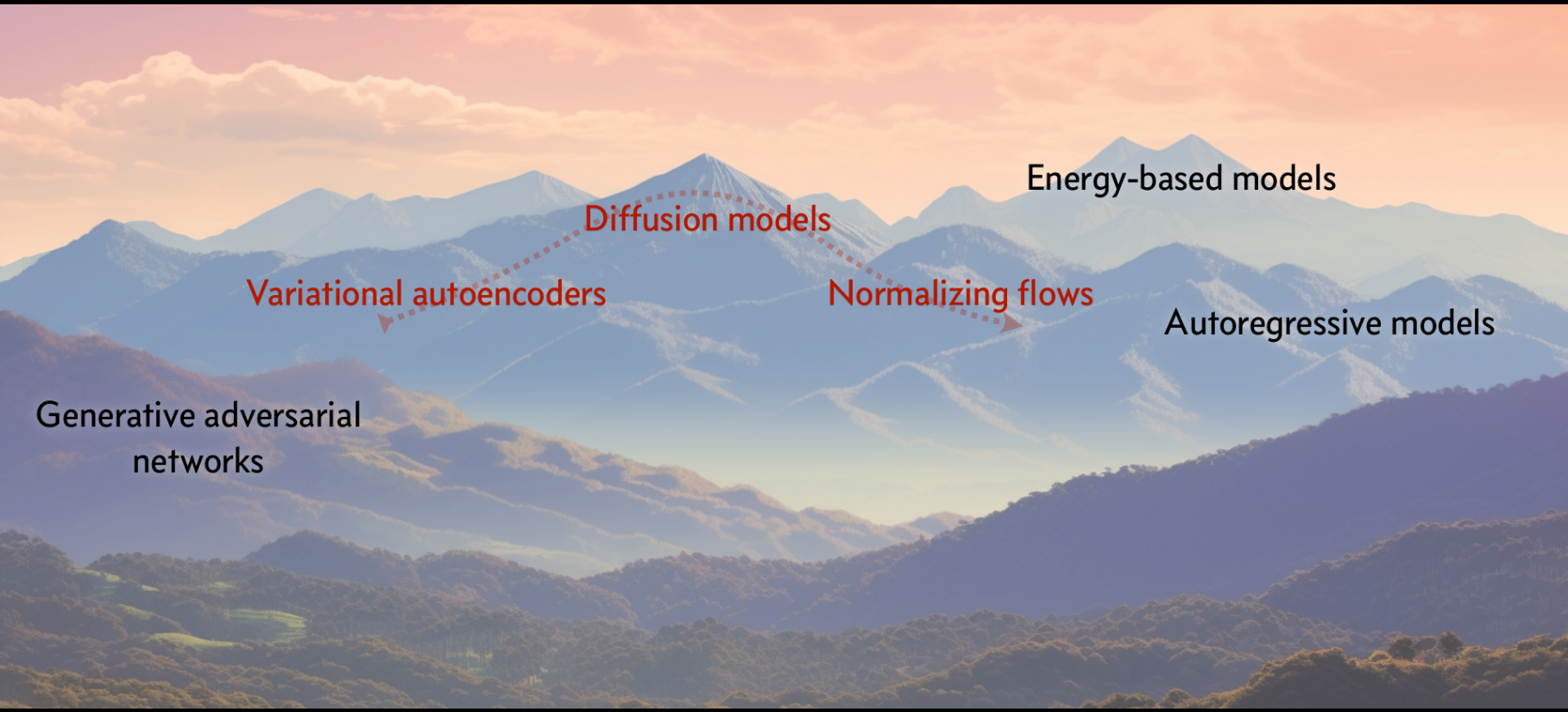
A (deep) generative model is a probabilistic model p_θ that can be used as a simulator of the data.

Formally, a generative model defines a probability distribution $p_\theta(\mathbf{x})$ over the data $\mathbf{x} \in \mathcal{X}$, parameterized by θ.



Variational auto-encoders
(Kingma and Welling, 2013)

Diffusion models
(Midjourney, 2023)



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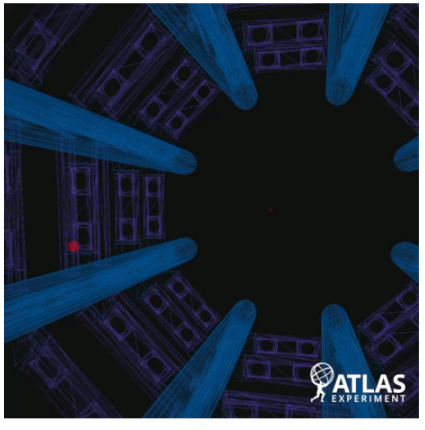
Credits: Karsten et al, 2022; Siddharth Mishra-Sharma, 2023.

Simulators as generative models

A simulator prescribes a generative model that can be used to simulate data $\mathbf{x}$.

Collider data

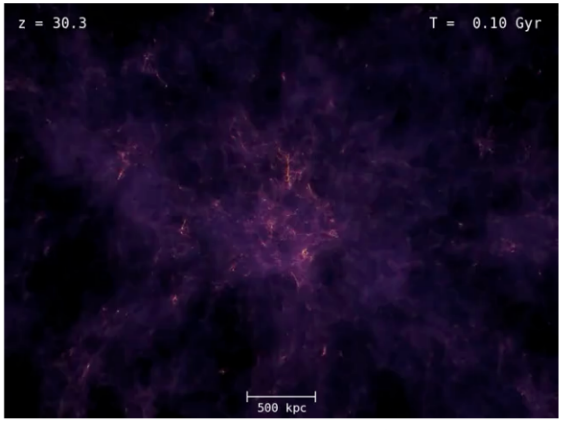
$\text{particles} \sim p(\text{particles})$



[C. Cesarotti with ATLAS]

Cosmology data

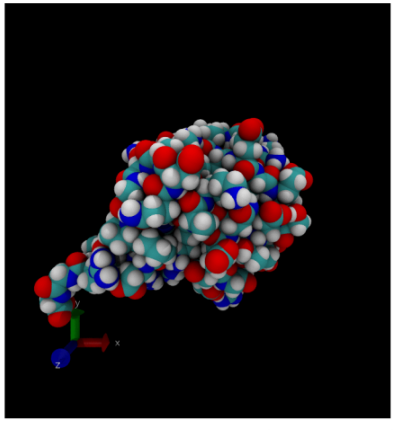
$\text{particles} \sim p(\text{particles})$



[Aquarius simulation]

Molecular dynamics

$\text{configurations} \sim p(\text{configurations})$



[E. Cances et al]

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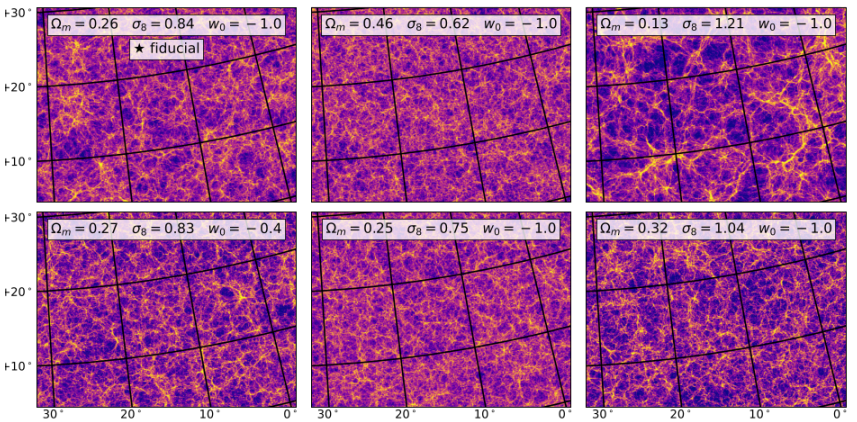
Conditional simulators

A conditional simulator prescribes a way to sample from the likelihood $p(\mathbf{x}|\vartheta)$, where ϑ is a set of conditioning variables or parameters.

Cosmology data

$$\text{map} \sim p(\text{map} \mid \{\Omega_m, \sigma_8, w_0\})$$



[Kacprzak et al 2022]

$$x \sim p(x; \mathscr{M})$$

Model

or

$$x \sim p(x \mid \theta)$$

Model parameters

What can we do with generative models?

Produce samples

$$\mathbf{x} \sim p(\mathbf{x}|\vartheta)$$

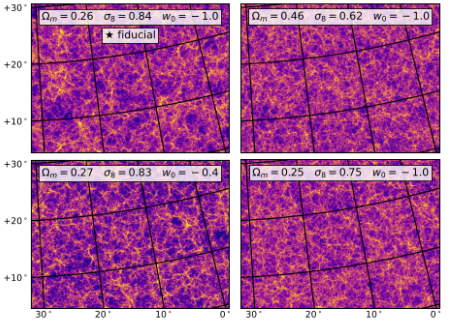
Evaluate densities

$$p(\mathbf{x}|\vartheta)$$

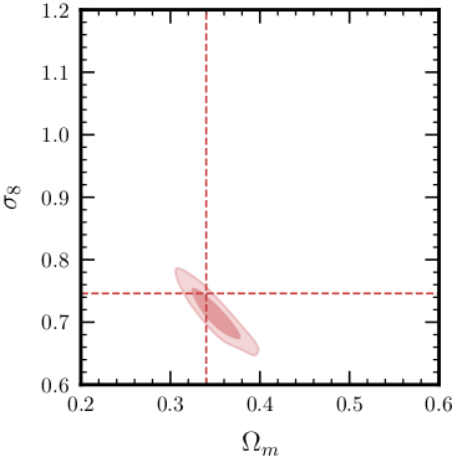
Encode complex priors

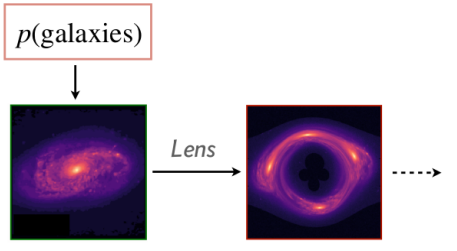
$$p(\mathbf{x})$$

$$p(\vartheta|\mathbf{x}) = \frac{p(\mathbf{x}|\vartheta)p(\vartheta)}{p(\mathbf{x})}$$



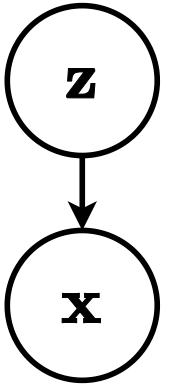
[Kacprzak et al 2022]





Variational auto-encoders

Latent variable model



Consider for now a prescribed latent variable model that relates a set of observable variables $\mathbf{x} \in \mathcal{X}$ to a set of unobserved variables $\mathbf{z} \in \mathcal{Z}$.

The probabilistic model defines a joint probability distribution $p_\theta(\mathbf{x}, \mathbf{z})$, which decomposes as

$$p_\theta(\mathbf{x}, \mathbf{z}) = p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z}).$$

How to fit a latent variable model?

$$
\begin{aligned}
\theta^* &= \arg\max_\theta p_\theta(\mathbf{x}) \\
&= \arg\max_\theta \int p_\theta(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z} \\
&= \arg\max_\theta \mathbb{E}_{p(\mathbf{z})} \left[p_\theta(\mathbf{x}|\mathbf{z}) \right] d\mathbf{z} \\
&\approx \arg\max_\theta \frac{1}{N} \sum_{i=1}^{N} p_\theta(\mathbf{x}|\mathbf{z}_i)
\end{aligned}
$$

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&\approx \arg\max_\theta \frac{1}{N} \sum_{i=1}^{N} p_\theta(\mathbf{x}|\mathbf{z}_i)
\end{aligned}
$$

The curse of dimensionality will lead to poor estimates of the expectation.

Variational inference

Let us instead consider a variational approach to fit the model parameters θ.

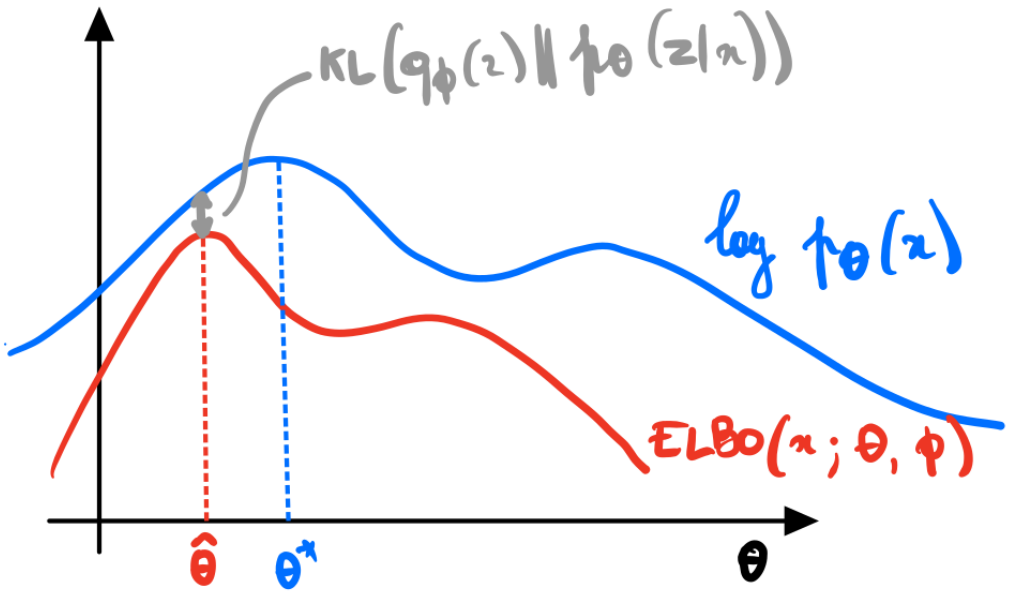
Using a variational distribution $q_\phi(\mathbf{z})$ over the latent variables $\mathbf{z}$, we have

$$\begin{aligned}
\log p_\theta(\mathbf{x}) &= \log \mathbb{E}_{p(\mathbf{z})} \left[p_\theta(\mathbf{x}|\mathbf{z}) \right] \\
&= \log \mathbb{E}_{q_\phi(\mathbf{z})} \left[\frac{p_\theta(\mathbf{x}|\mathbf{z}) p(\mathbf{z})}{q_\phi(\mathbf{z})} \right] \\
&\geq \mathbb{E}_{q_\phi(\mathbf{z})} \left[\log \frac{p_\theta(\mathbf{x}|\mathbf{z}) p(\mathbf{z})}{q_\phi(\mathbf{z})} \right] \quad (\mathrm{ELBO}(\mathbf{x}; \theta, \phi)) \\
&= \mathbb{E}_{q_\phi(\mathbf{z})} \left[\log p_\theta(\mathbf{x}|\mathbf{z}) \right] - \mathrm{KL}(q_\phi(\mathbf{z}) || p(\mathbf{z}))
\end{aligned}$$

Using the Bayes rule, we can also write

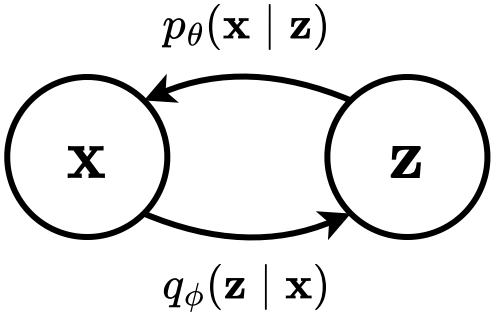
$$\begin{aligned}
\mathrm{ELBO}(\mathbf{x};\theta,\phi) &= \mathbb{E}_{q_\phi(\mathbf{z})}\left[\log \frac{p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{q_\phi(\mathbf{z})}\right] \\
&= \mathbb{E}_{q_\phi(\mathbf{z})}\left[\log \frac{p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{q_\phi(\mathbf{z})}\frac{p_\theta(\mathbf{x})}{p_\theta(\mathbf{x})}\right] \\
&= \mathbb{E}_{q_\phi(\mathbf{z})}\left[\log \frac{p_\theta(\mathbf{z}|\mathbf{x})}{q_\phi(\mathbf{z})}p_\theta(\mathbf{x})\right] \\
&= \log p_\theta(\mathbf{x}) - \mathrm{KL}(q_\phi(\mathbf{z})||p_\theta(\mathbf{z}|\mathbf{x})).
\end{aligned}$$

Therefore, $\log p_\theta(\mathbf{x}) = \mathrm{ELBO}(\mathbf{x};\theta,\phi) + \mathrm{KL}(q_\phi(\mathbf{z})||p_\theta(\mathbf{z}|\mathbf{x}))$.



Provided the KL gap remains small, the model parameters can now be optimized by maximizing the ELBO,

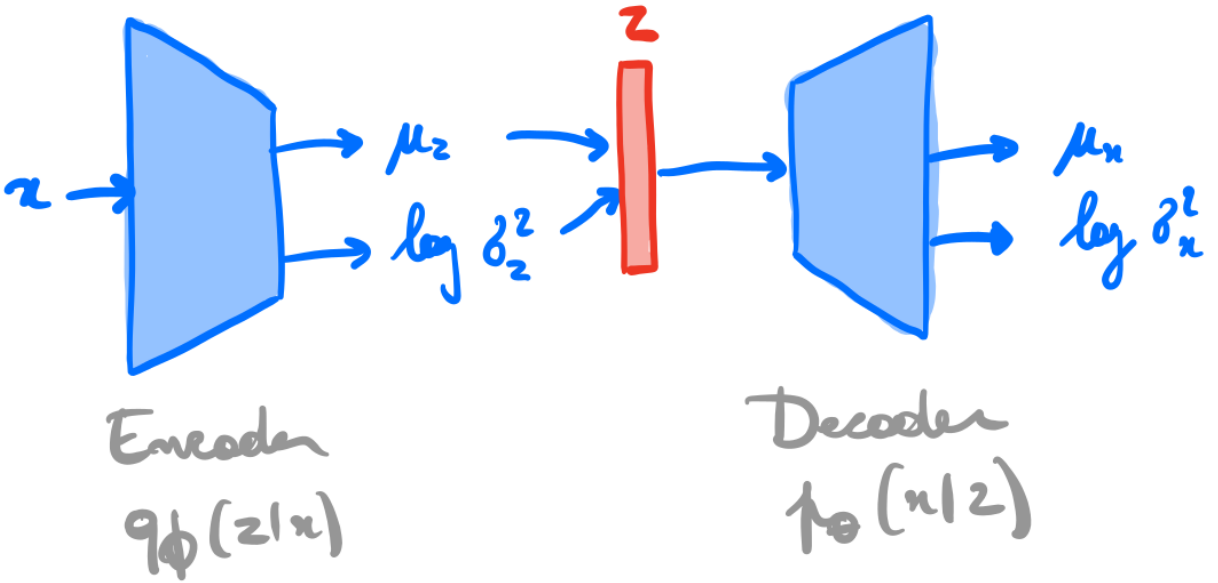
$$\theta^*, \phi^* = \arg\max_{\theta,\phi} \mathrm{ELBO}(\mathbf{x}; \theta, \phi).$$



So far we assumed a prescribed probabilistic model motivated by domain knowledge. We will now directly learn a stochastic generating process $p_\theta(\mathbf{x}|\mathbf{z})$ with a neural network.

We will also amortize the inference process by learning a second neural network $q_\phi(\mathbf{z}|\mathbf{x})$ approximating the posterior, conditionally on the observed data $\mathbf{x}$.

Variational auto-encoders

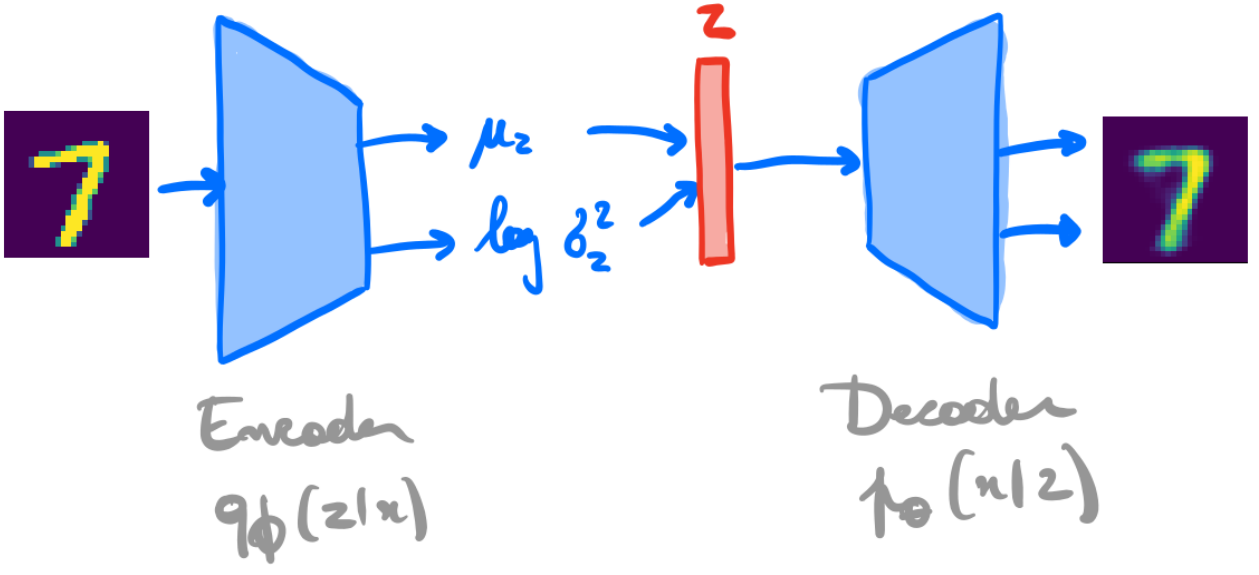


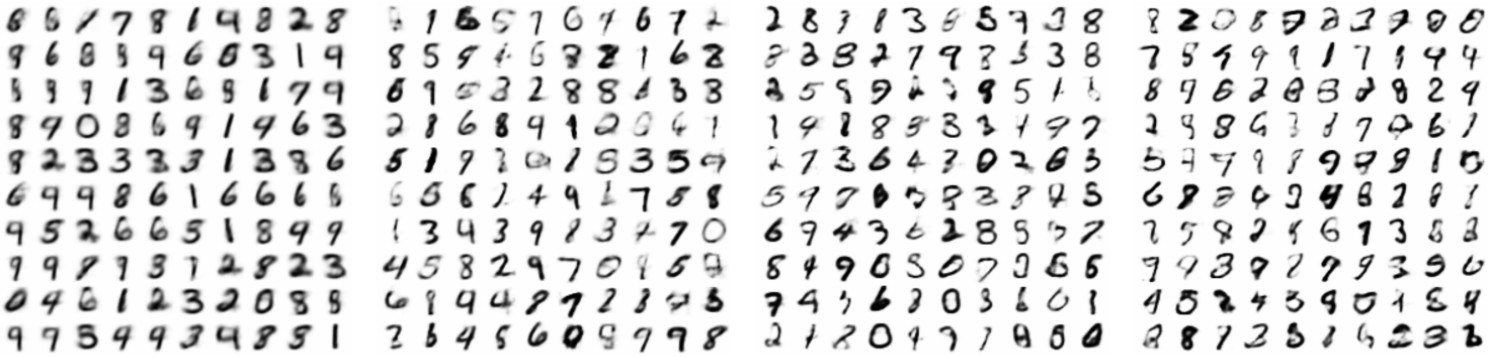
As before, we can use variational inference to jointly optimize the generative and the inference networks parameters θ and ϕ:

$$\begin{aligned}
\theta^*, \phi^* &= \arg\max_{\theta,\phi} \mathbb{E}_{p(\mathbf{x})} \left[\text{ELBO}(\mathbf{x}; \theta, \phi) \right] \\
&= \arg\max_{\theta,\phi} \mathbb{E}_{p(\mathbf{x})} \left[\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} [\log \frac{p_\theta(\mathbf{x}|\mathbf{z}) p(\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}] \right] \\
&= \arg\max_{\theta,\phi} \mathbb{E}_{p(\mathbf{x})} \left[\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \left[\log p_\theta(\mathbf{x}|\mathbf{z}) \right] - \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}) || p(\mathbf{z})) \right].
\end{aligned}$$

Step-by-step example

Consider as data $\mathbf{d}$ the MNIST digit dataset:


z
μ_z
$\log \sigma_z^2$
Encoder
$q_\phi(z|x)$
Decoder
$p_\theta(x|z)$

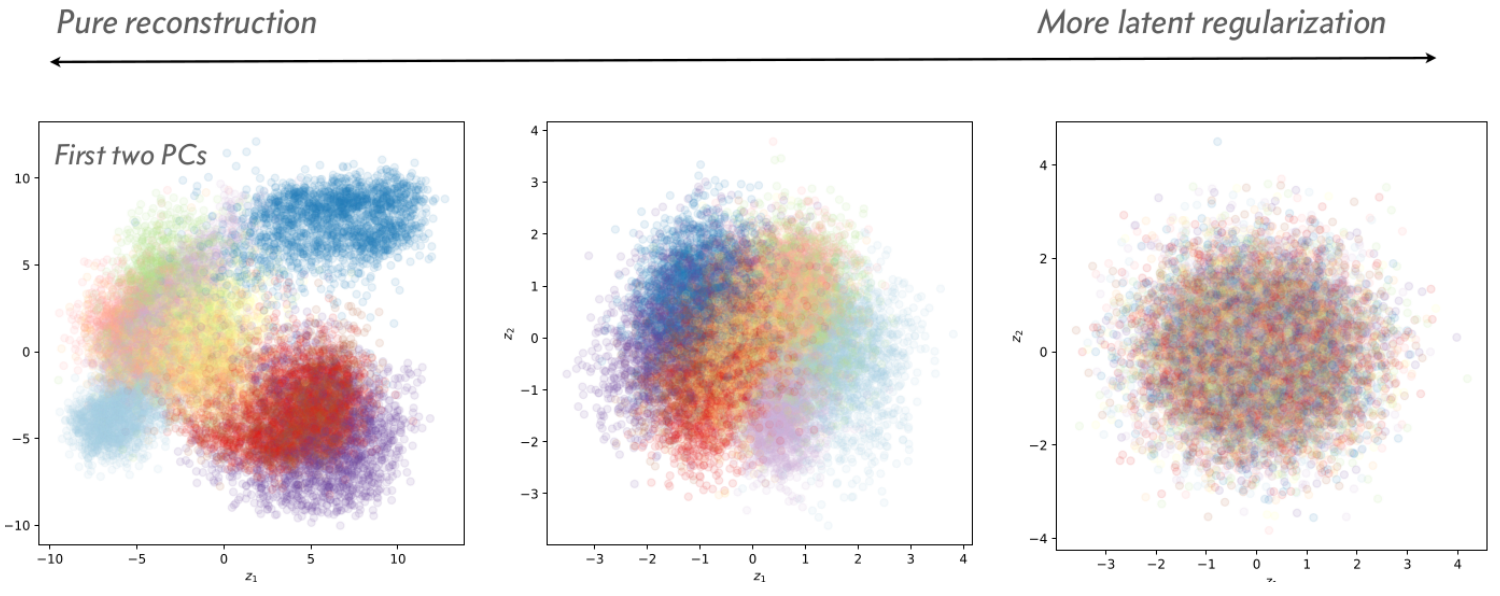


(a) 2-D latent space (b) 5-D latent space (c) 10-D latent space (d) 20-D latent space

(Kingma and Welling, 2013)

A semantically meaningful latent space

The prior-matching term $\mathbf{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))$ enforces simplicity in the latent space, encouraging learned semantic structure and disentanglement.



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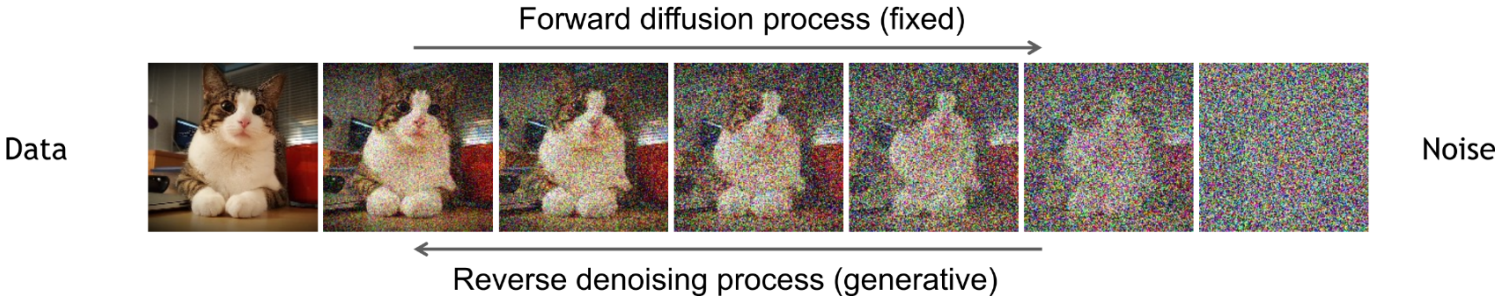
Credits: Siddharth Mishra-Sharma, 2023.

Diffusion models



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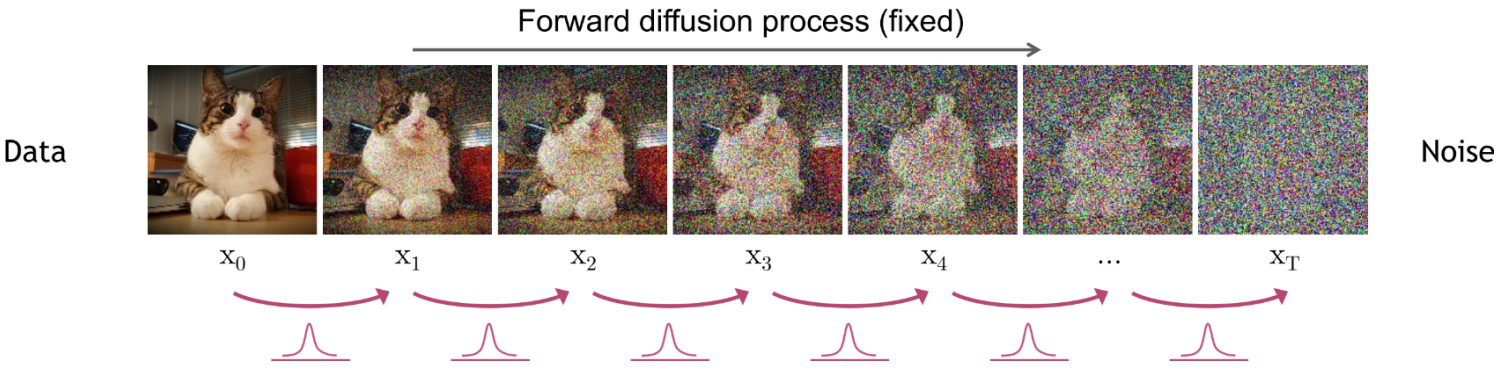
Credits: Kreis et al, 2022.

Forward diffusion process



With $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$, we have

$$\mathbf{x}_t = \sqrt{\alpha_t}\mathbf{x}_{t-1} + \sqrt{1-\alpha_t}\epsilon$$
$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{\alpha_t}\mathbf{x}_{t-1}, (1-\alpha_t)\mathbf{I})$$
$$q(\mathbf{x}_{1:T}|\mathbf{x}_0) = \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1})$$

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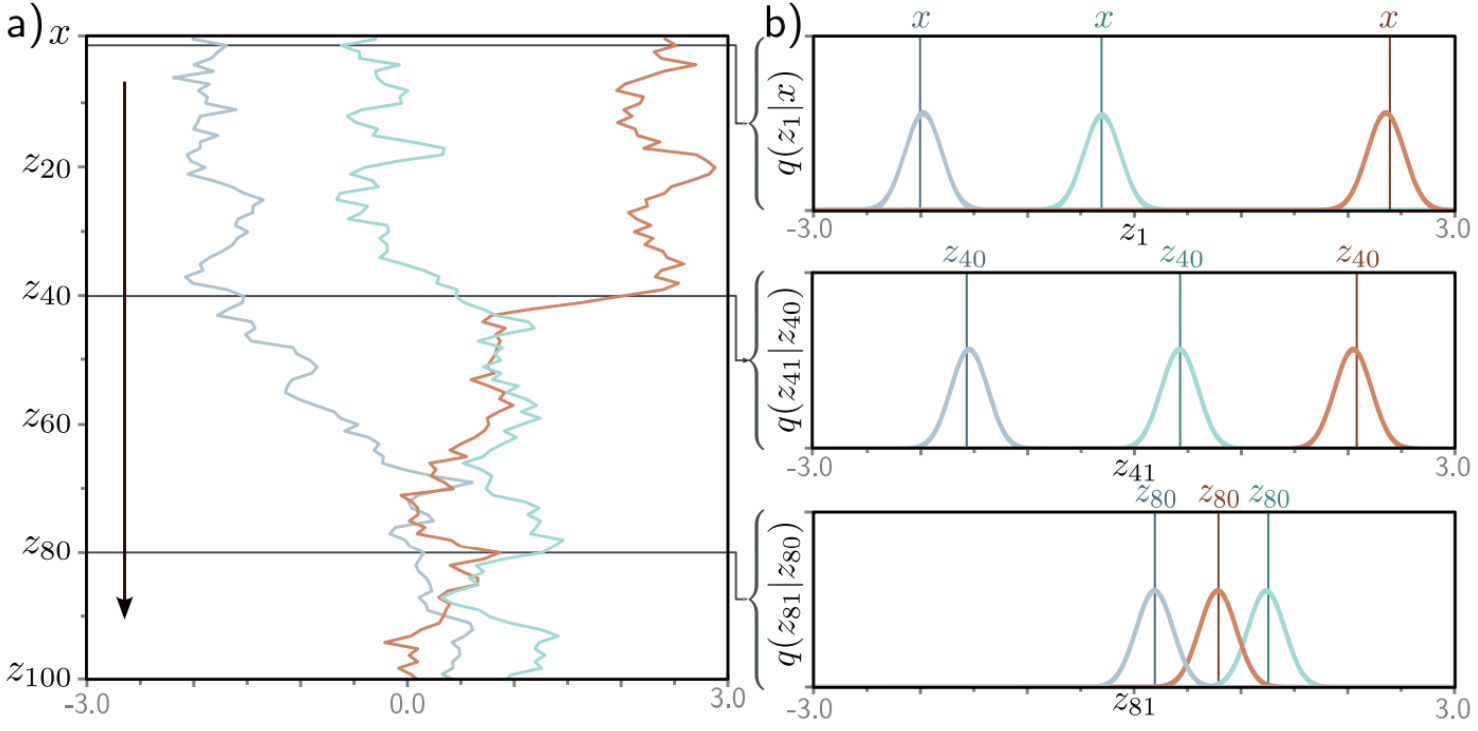
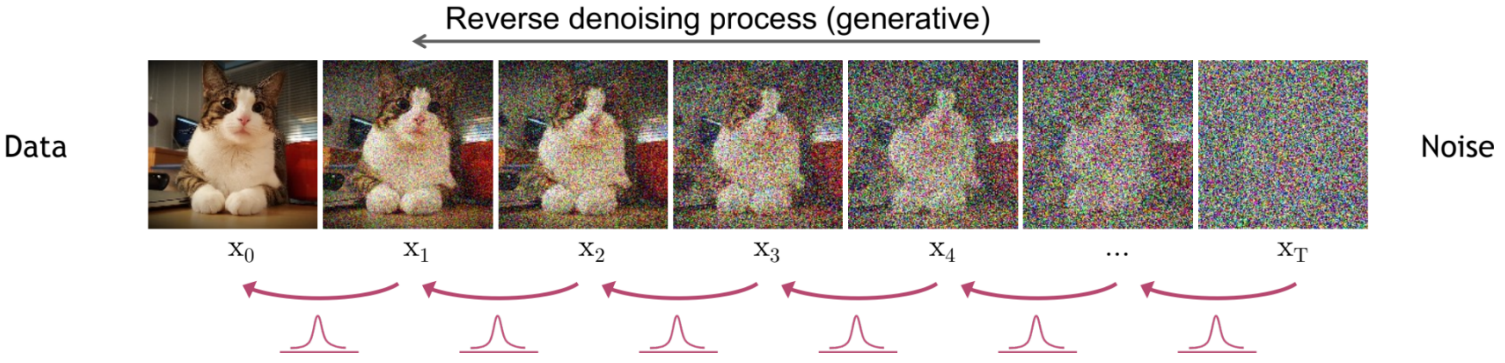
Credits: Kreis et al, 2022.


a)
x
z_{20}
z_{40}
z_{60}
z_{80}
z_{100}
-3.0
0.0
3.0
b)
x
x
x
$q(z_1|x)$
-3.0
z_1
3.0
z_{40}
z_{40}
z_{40}
$q(z_{41}|z_{40})$
-3.0
z_{41}
3.0
z_{80}
z_{80}
z_{80}
$q(z_{81}|z_{80})$
-3.0
z_{81}
3.0

—

Reverse denoising process



$$p(\mathbf{x}_{0:T}) = p(\mathbf{x}_T) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$$

$$p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; \mathbf{0}, I)$$

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \mu_\theta(\mathbf{x}_t, t), \sigma_\theta^2(\mathbf{x}_t, t)\mathbf{I})$$

$$\mathbf{x}_{t-1} = \mu_\theta(\mathbf{x}_t, t) + \sigma_\theta(\mathbf{x}_t, t)\mathbf{z}$$

with $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$.

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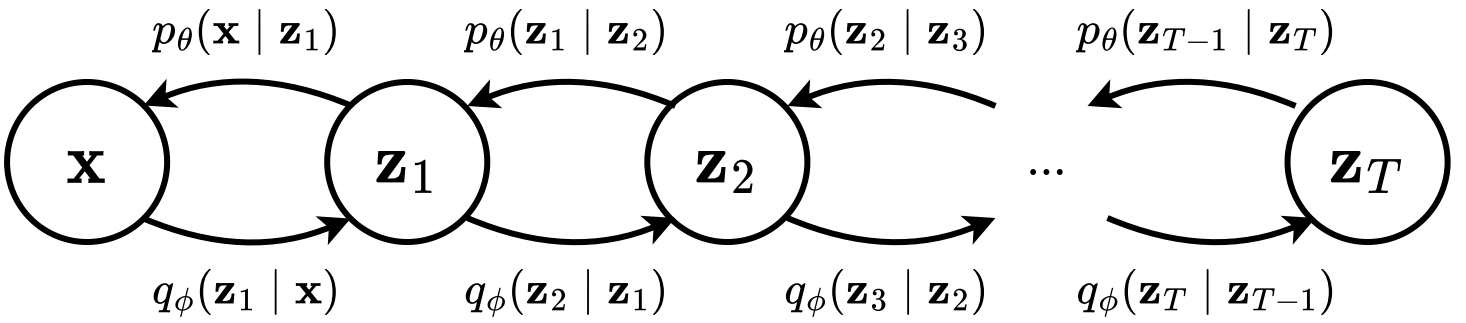
Credits: Kreis et al, 2022.

Markovian Hierarchical VAEs



Similarly to VAEs, training is done by maximizing the ELBO, using a variational distribution $q_\phi(\mathbf{z}_{1:T}|\mathbf{x})$ over all levels of latent variables:

$$\log p_\theta(\mathbf{x}) \geq \mathbb{E}_{q_\phi(\mathbf{z}_{1:T}|\mathbf{x})}\left[\log \frac{p(\mathbf{x}, \mathbf{z}_{1:T})}{q_\phi(\mathbf{z}_{1:T}|\mathbf{x})}\right]$$

Diffusion models are Markovian HVAEs with the following constraints:

- The latent dimension is the same as the data dimension.
- The encoder is fixed to linear Gaussian transitions $q(\mathbf{x}_t|\mathbf{x}_{t-1})$.
- The hyper-parameters are set such that $q(\mathbf{x}_T|\mathbf{x}_0)$ is a standard Gaussian.

Training

For learning the parameters θ of the reverse process, we can form a variational lower bound on the log-likelihood of the data as

$$\mathbb{E}_{q(\mathbf{x}_0)}\left[\log p_\theta(\mathbf{x}_0)\right] \geq \mathbb{E}_{q(\mathbf{x}_0)q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right] := L$$

This objective can be rewritten as

$$
\begin{aligned}
L &= \mathbb{E}_{q(\mathbf{x}_0)q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right] \\
&= \mathbb{E}_{q(\mathbf{x}_0)}\left[L_0 - \sum_{t>1} L_{t-1} - L_T\right]
\end{aligned}
$$

where

- $L_0 = \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)}[\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)]$ can be interpreted as a reconstruction term. It can be approximated and optimized using a Monte Carlo estimate.
- $L_{t-1} = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)}\mathrm{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)||p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))$ is a denoising matching term. The transition $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ provides a learning signal for the reverse process, since it defines how to denoise the noisified input $\mathbf{x}_t$ with access to the original input $\mathbf{x}_0$.
- $L_T = \mathrm{KL}(q(\mathbf{x}_T|\mathbf{x}_0)||p_\theta(\mathbf{x}_T))$ represents how close the distribution of the final noisified input is to the standard Gaussian. It has no trainable parameters.

(Some calculations later...)

$$\arg\min_\theta L_{t-1}$$

$$= \arg\min_\theta \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \frac{1}{2\sigma_t^2} \frac{\bar{\alpha}_{t-1}(1-\alpha_t)^2}{(1-\bar{\alpha}_t)^2} ||\hat{\mathbf{x}}_\theta(\mathbf{x}_t, t) - \mathbf{x}_0||_2^2$$

Interpretation 1: Denoising. Training a diffusion model amounts to learning a neural network that predicts the original ground truth $\mathbf{x}_0$ from a noisy input $\mathbf{x}_t$.

$$
\begin{aligned}
&\arg\min_\theta L_{t-1} \\
&= \arg\min_\theta \mathbb{E}_{\mathcal{N}(\epsilon;\mathbf{0},I)} \frac{1}{2\sigma_t^2} \frac{(1-\alpha_t)^2}{(1-\bar{\alpha}_t)\alpha_t} ||\epsilon_\theta(\underbrace{\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\epsilon}_{\mathbf{x}_t}, t) - \epsilon||_2^2 \\
&\approx \arg\min_\theta \mathbb{E}_{\mathcal{N}(\epsilon;\mathbf{0},I)} ||\epsilon_\theta(\underbrace{\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\epsilon}_{\mathbf{x}_t}, t) - \epsilon||_2^2
\end{aligned}
$$

Interpration 2: Noise prediction. Training a diffusion model amounts to learning a neural network that predicts the noise ϵ that was added to the original ground truth $\mathbf{x}_0$ to obtain the noisy $\mathbf{x}_t$.

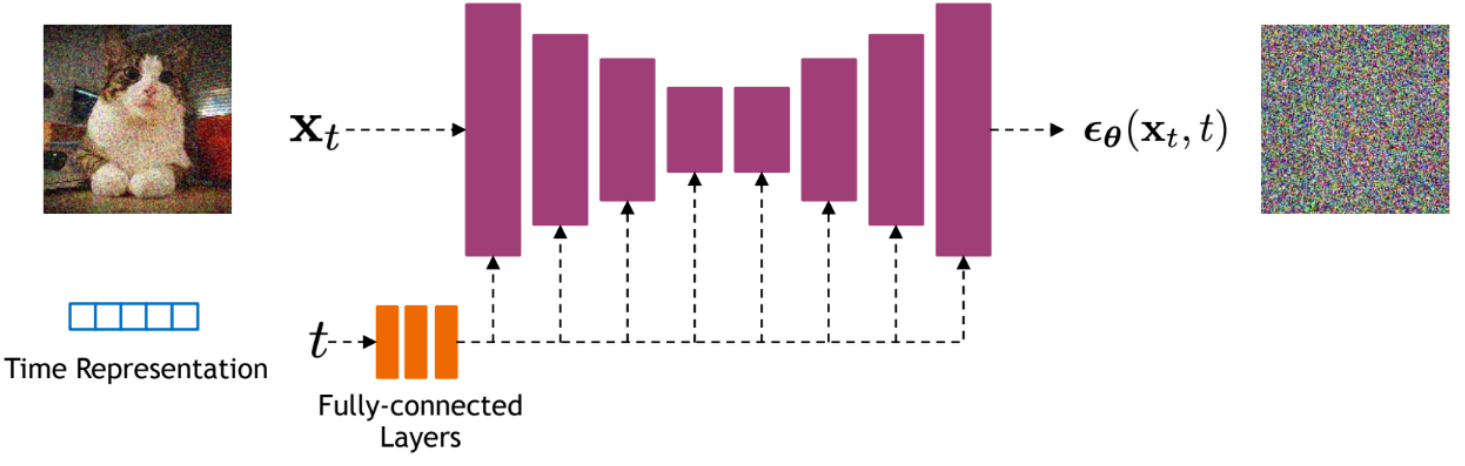
$$\arg\min_\theta L_{t-1}$$

$$= \arg\min_\theta \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \frac{1}{2\sigma_t^2} \frac{(1-\alpha_t)^2}{\alpha_t} ||s_\theta(\mathbf{x}_t, t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x}_0)||_2^2$$

Interpretation 3: Denoising score matching. Training a diffusion model amounts to learning a neural network that predicts the score $\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x}_0)$ of the tractable posterior.

Network architectures

Diffusion models often use U-Net architectures with ResNet blocks and self-attention layers to represent $\hat{\mathbf{x}}_\theta(\mathbf{x}_t, t)$, $\epsilon_\theta(\mathbf{x}_t, t)$ or $s_\theta(\mathbf{x}_t, t)$.



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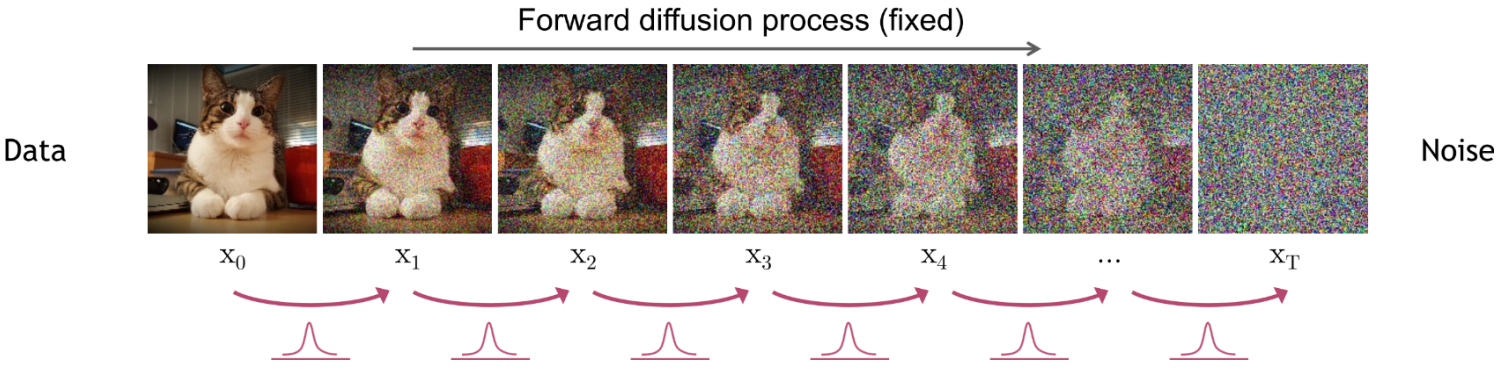
Credits: Kreis et al, 2022.

Continuous-time diffusion models



With $\beta_t = 1 - \alpha_t$, we can rewrite the forward process as

$$\begin{aligned}\mathbf{x}_t &= \sqrt{\alpha_t}\mathbf{x}_{t-1} + \sqrt{1-\alpha_t}\mathcal{N}(\mathbf{0}, \mathbf{I}) \\ &= \sqrt{1-\beta_t}\mathbf{x}_{t-1} + \sqrt{\beta_t}\mathcal{N}(\mathbf{0}, \mathbf{I}) \\ &= \sqrt{1-\beta(t)\Delta_t}\mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta_t}\mathcal{N}(\mathbf{0}, \mathbf{I})\end{aligned}$$

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Credits: Kreis et al, 2022.

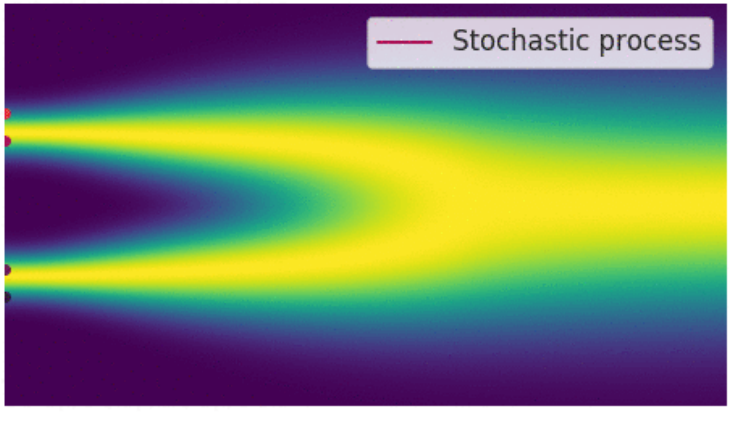
When $\Delta_t \to 0$, we can further rewrite the forward process as

$$\begin{aligned}\mathbf{x}_t &= \sqrt{1-\beta(t)\Delta_t}\mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta_t}\mathcal{N}(\mathbf{0}, \mathbf{I}) \\ &\approx \mathbf{x}_{t-1} - \frac{\beta(t)\Delta_t}{2}\mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta_t}\mathcal{N}(\mathbf{0}, \mathbf{I})\end{aligned}.$$

This last update rule corresponds to the Euler-Maruyama discretization of the stochastic differential equation (SDE)

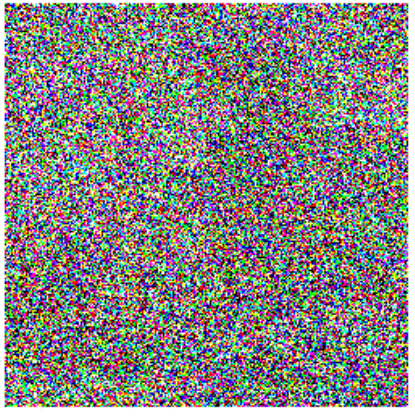
$$\mathrm{d}\mathbf{x}_t = -\frac{1}{2}\beta(t)\mathbf{x}_t\mathrm{d}t + \sqrt{\beta(t)}\mathrm{d}\mathbf{w}_t$$

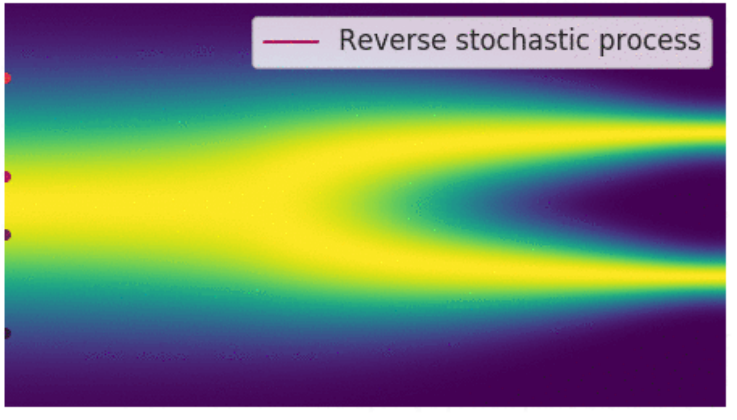
describing the diffusion in the infinitesimal limit.



The reverse process satisfies a reverse-time SDE that can be derived analytically from the forward-time SDE and the score of the marginal distribution $q(\mathbf{x}_t)$, as

$$\mathrm{d}\mathbf{x}_t = \left[-\frac{1}{2}\beta(t)\mathbf{x}_t - \beta(t)\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t) \right] \mathrm{d}t + \sqrt{\beta(t)}\mathrm{d}\mathbf{w}_t.$$





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Credits: Song, 2021.

The end.