Deep generative models

A latent variable model perspective

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Slides, helpful resources, and tutorials can all be found at

https://github.com/glouppe/iaifi-summer-school-2024.

Outline

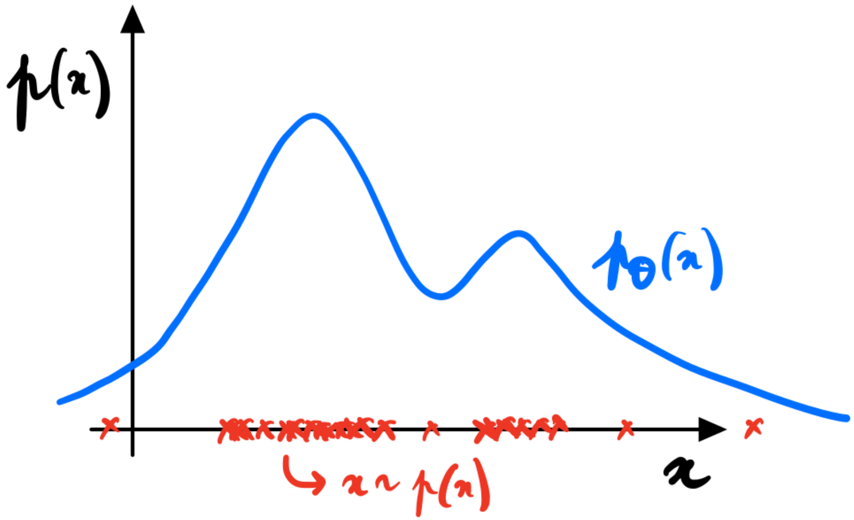
1. Deep generative models
2. Variational auto-encoders
3. Diffusion models
4. Latent diffusion models
5. Normalizing flows

Deep generative models

Generative models

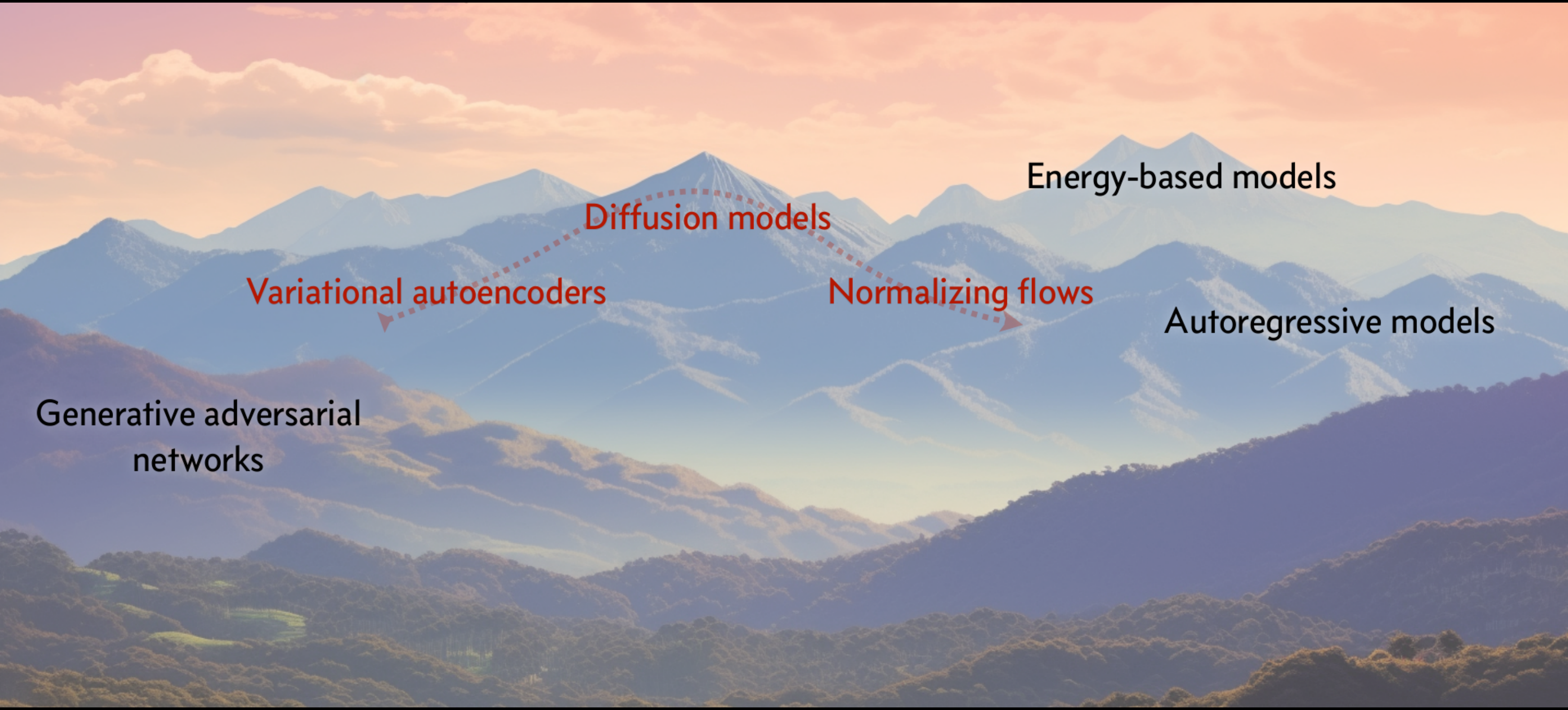
A (deep) generative model is a probabilistic model p_θ that can be used as a simulator of the data.

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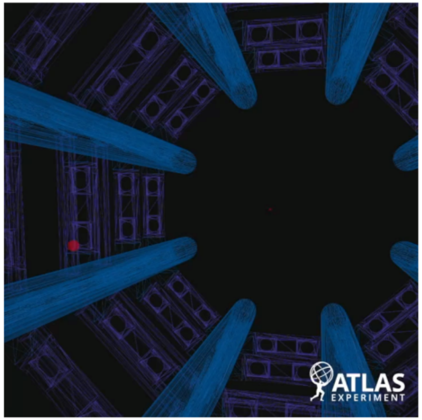
Credits: Karsten et al, 2022; Siddharth Mishra-Sharma, 2023.

Simulators as generative models

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

Collider data

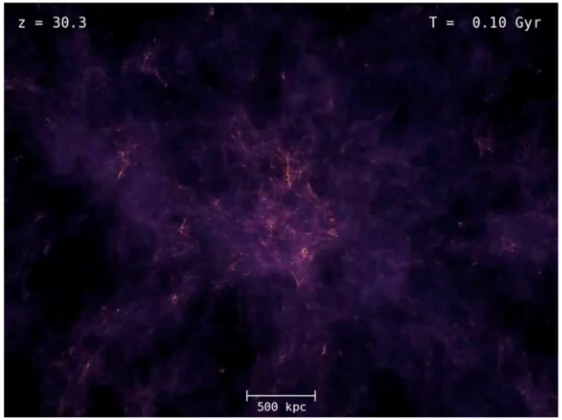
$$\text{particles} \sim p(\text{particles})$$



[C. Cesarotti with ATLAS]

Cosmology data

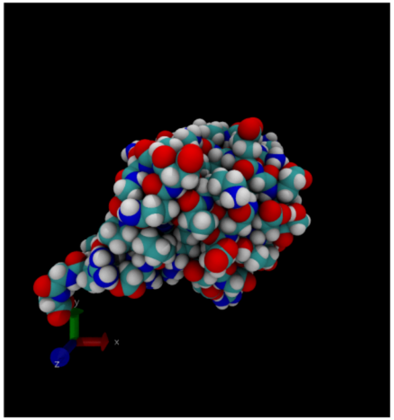
$$\text{particles} \sim p(\text{particles})$$



[Aquarius simulation]

Molecular dynamics

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



[E. Cances et al]

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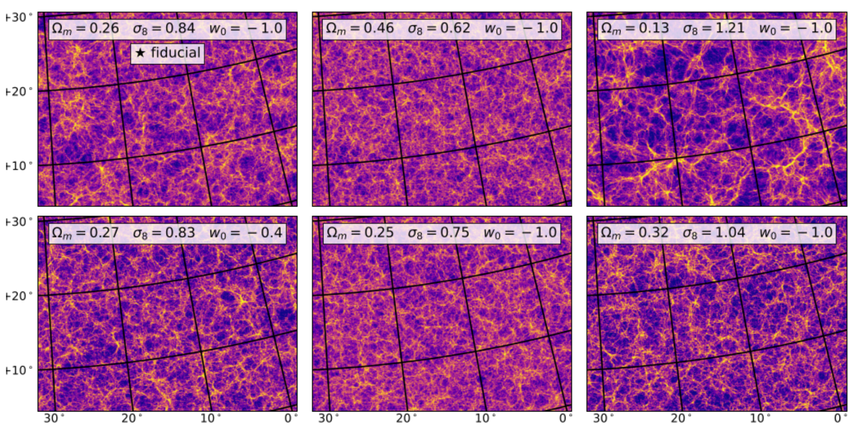
Credits: Siddharth Mishra-Sharma, 2023.

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

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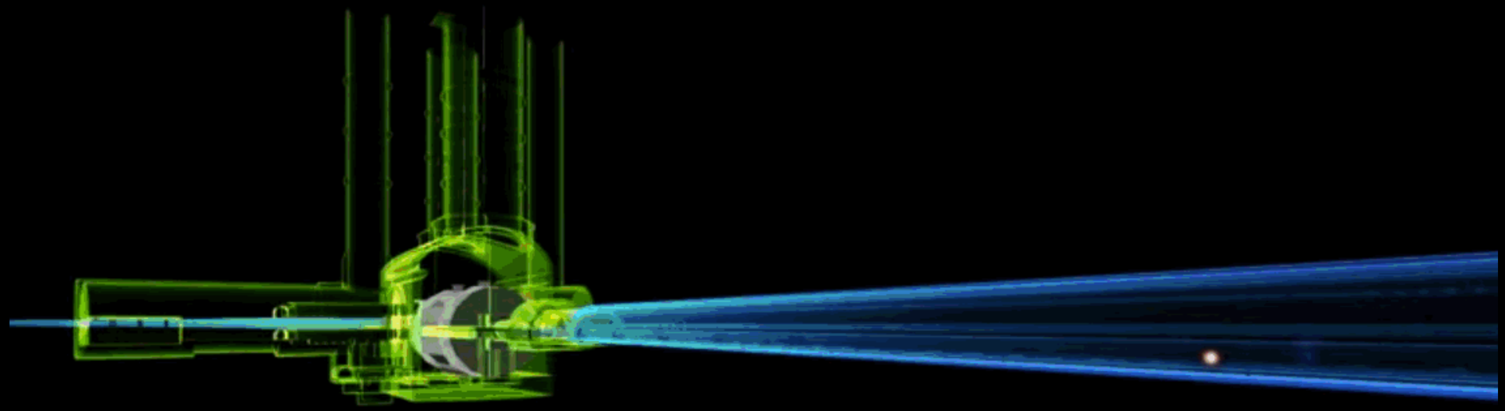
Credits: Siddharth Mishra-Sharma, 2023.



$$p(z_p|\vartheta)$$

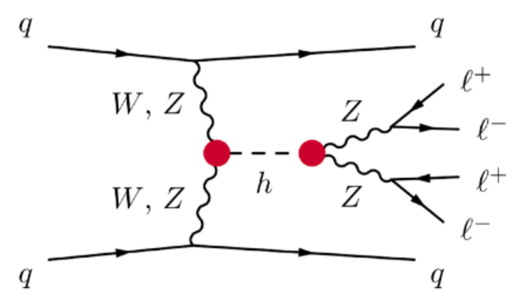
Latent variables

Parameters of interest

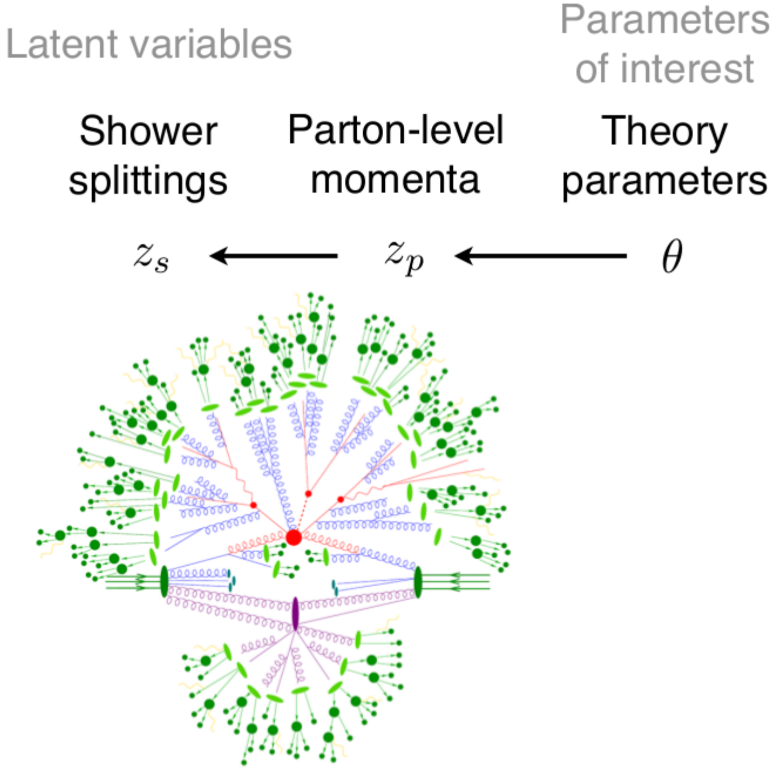
Parton-level momenta

Theory parameters

$$z_p \longleftarrow \theta$$

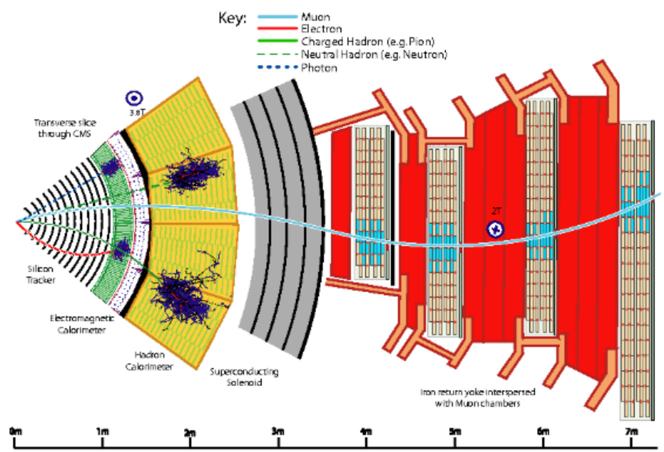


$$p(z_s|\vartheta) = \int p(z_p|\vartheta)p(z_s|z_p)dz_p$$



$$p(z_d|\vartheta) = \iint p(z_p|\vartheta)p(z_s|z_p)p(z_d|z_s)dz_p dz_s$$

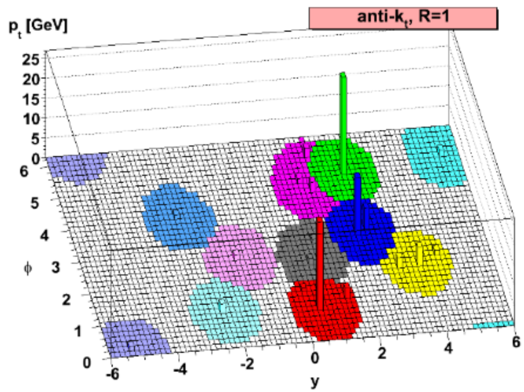
Latent variables			Parameters of interest
Detector interactions	Shower splittings	Parton-level momenta	Theory parameters
z_d ←	z_s ←	z_p ←	θ



$$p(x|\vartheta) = \iiint p(z_p|\vartheta)p(z_s|z_p)p(z_d|z_s)p(x|z_d)dz_p dz_s dx$$

Features	Latent variables			Parameters of interest
Observables	Detector interactions	Shower splittings	Parton-level momenta	Theory parameters
x	z_d	z_s	z_p	θ

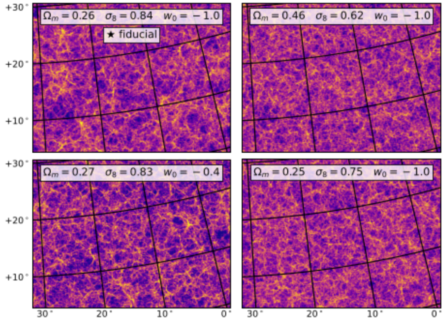
$x \leftarrow z_d \leftarrow z_s \leftarrow z_p \leftarrow \theta$



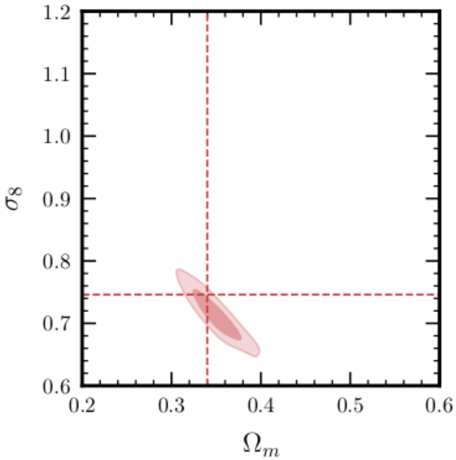
[Image source: M. Cacciari, G. Salam, G. Soyez 0802.1189]

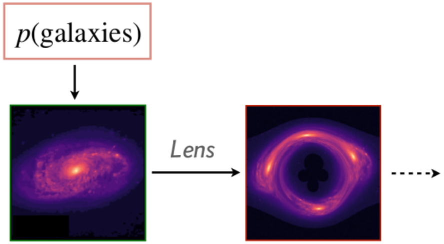
What can we do with generative models?

Produce samples	Inference	Encode complex priors
$\mathbf{x} \sim p(\mathbf{x}\|\vartheta)$	$p(\vartheta\|\mathbf{x}) = \frac{p(\mathbf{x}\|\vartheta)p(\vartheta)}{p(\mathbf{x})}$	$p(\mathbf{x})$



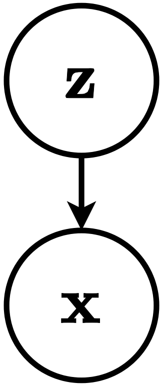
[Kacprzak et al 2022]





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 p_θ?

How to fit a latent variable model p_θ?

$$\theta^* = \arg\max_\theta p_\theta(\mathbf{x})$$

How to fit a latent variable model p_θ?

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

How to fit a latent variable model p_θ?

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

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.

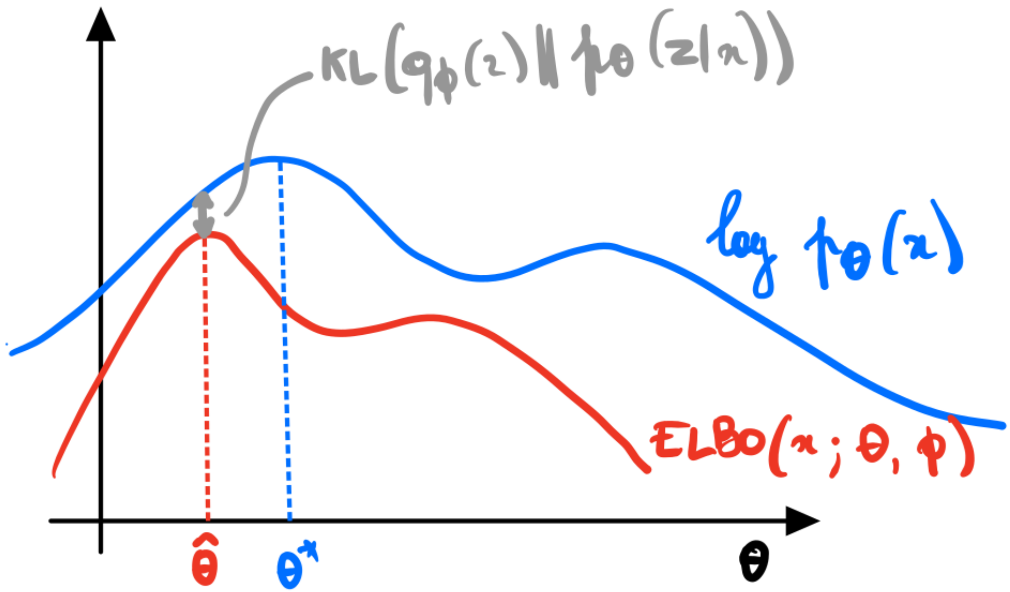
Using a variational distribution $q_\phi(\mathbf{z})$ over the latent variables $\mathbf{z}$, we have

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

Using the Bayes rule, we can also write

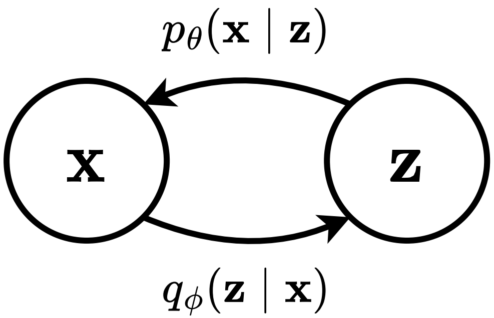
$$\begin{aligned}
\text{ELBO}(\mathbf{x};\theta,\phi) &= \mathbb{E}_{q_\phi(\mathbf{z})}\left[\log \frac{p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{q_\phi(\mathbf{z})}\right] \\
&= \mathbb{E}_{q_\phi(\mathbf{z})}\left[\log \frac{p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{q_\phi(\mathbf{z})}\frac{p_\theta(\mathbf{x})}{p_\theta(\mathbf{x})}\right]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

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



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

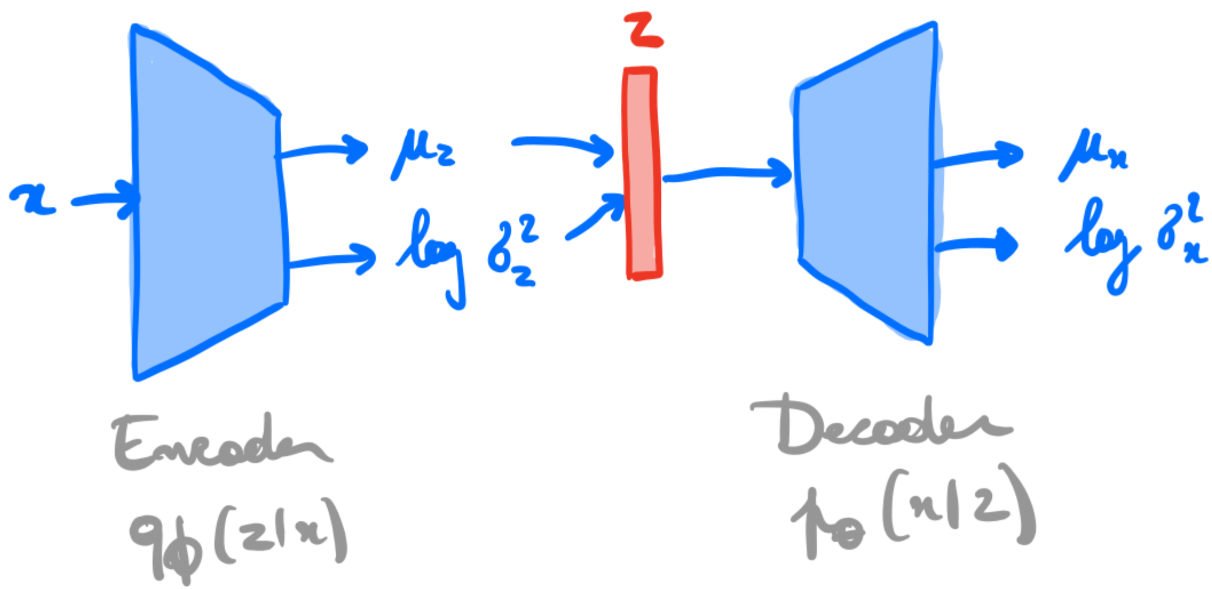
$$\theta^*, \phi^* = \arg\max_{\theta,\phi} \text{ELBO}(\mathbf{x}; \theta, \phi).$$



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

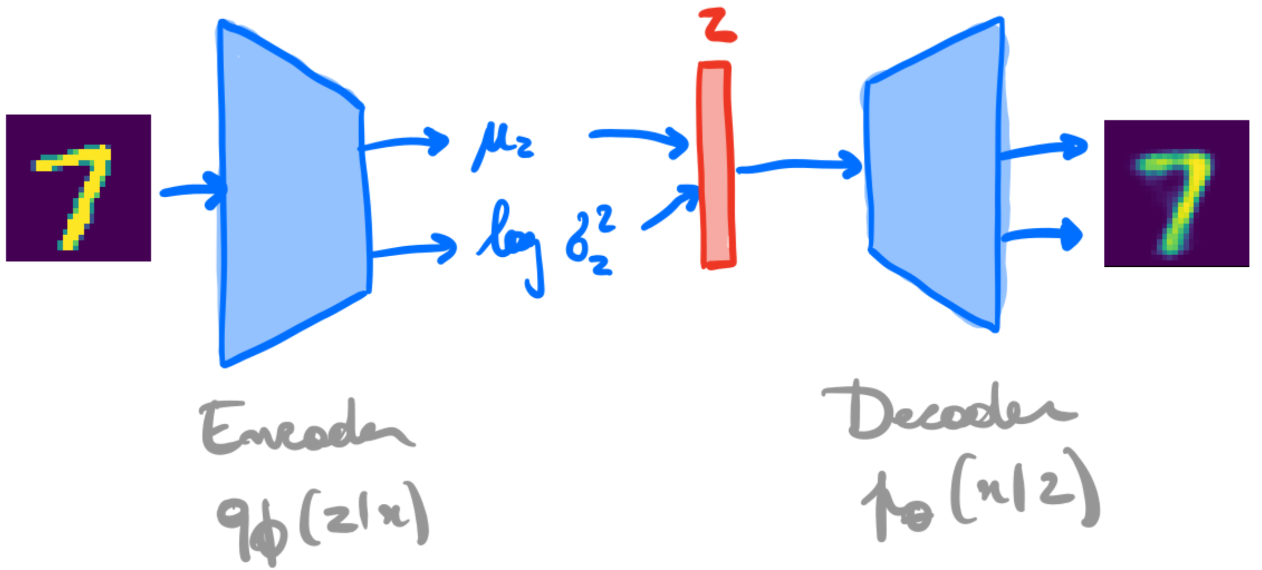


As before, we can use variational inference to jointly optimize the generative and the inference networks parameters θ and ϕ:

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

Step-by-step example

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

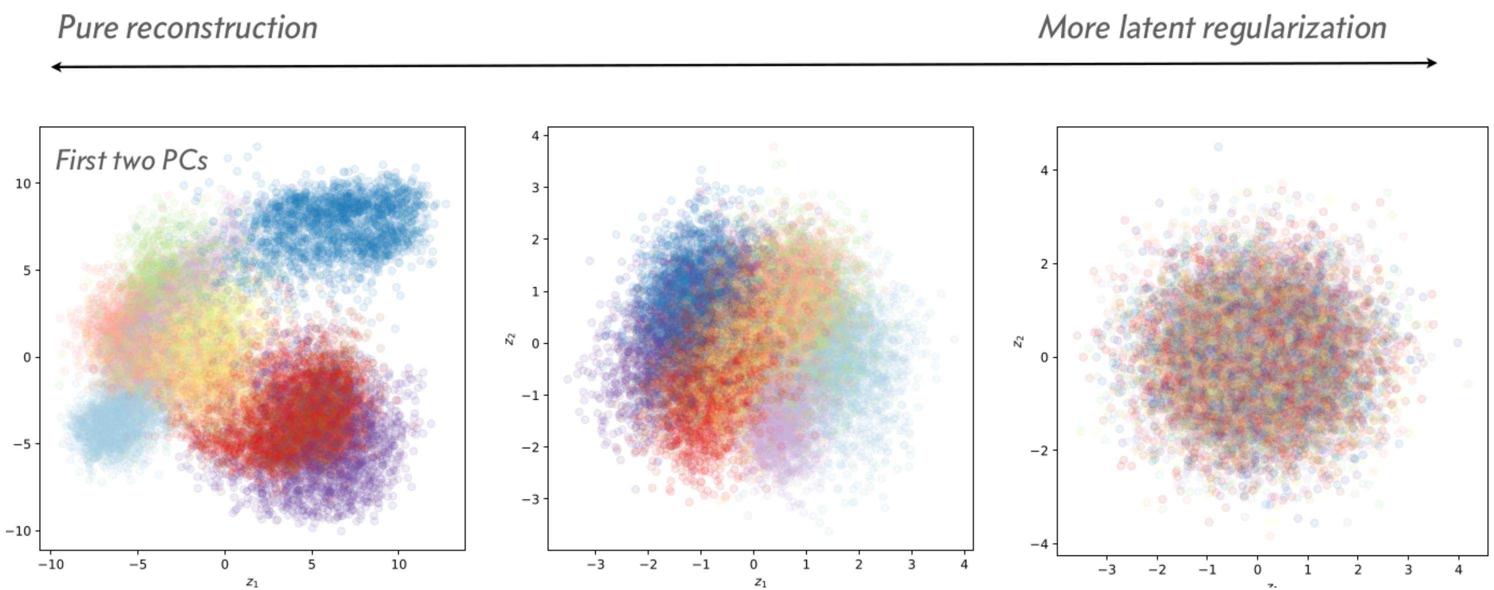

μ_z
$\log \sigma_z^2$
z
Encoder
$q_\phi(z|x)$
Decoder
$p_\theta(x|z)$

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

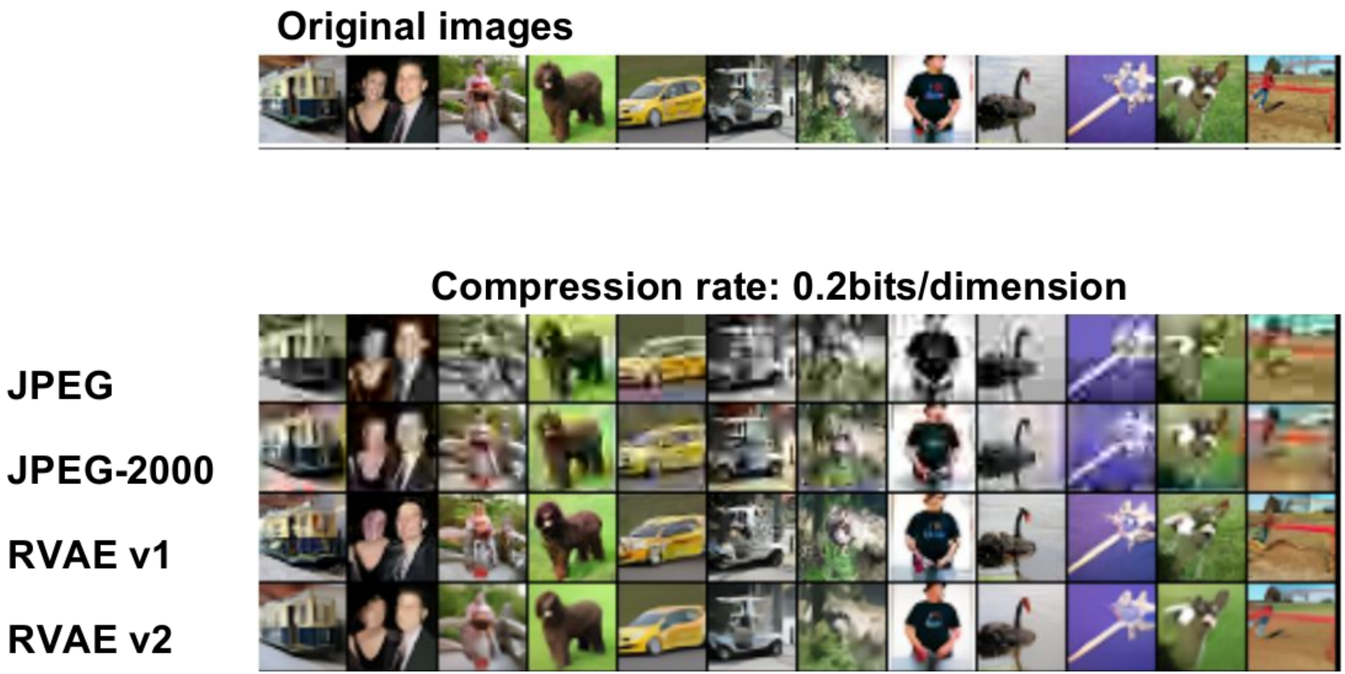
(Kingma and Welling, 2013)

A semantically meaningful latent space

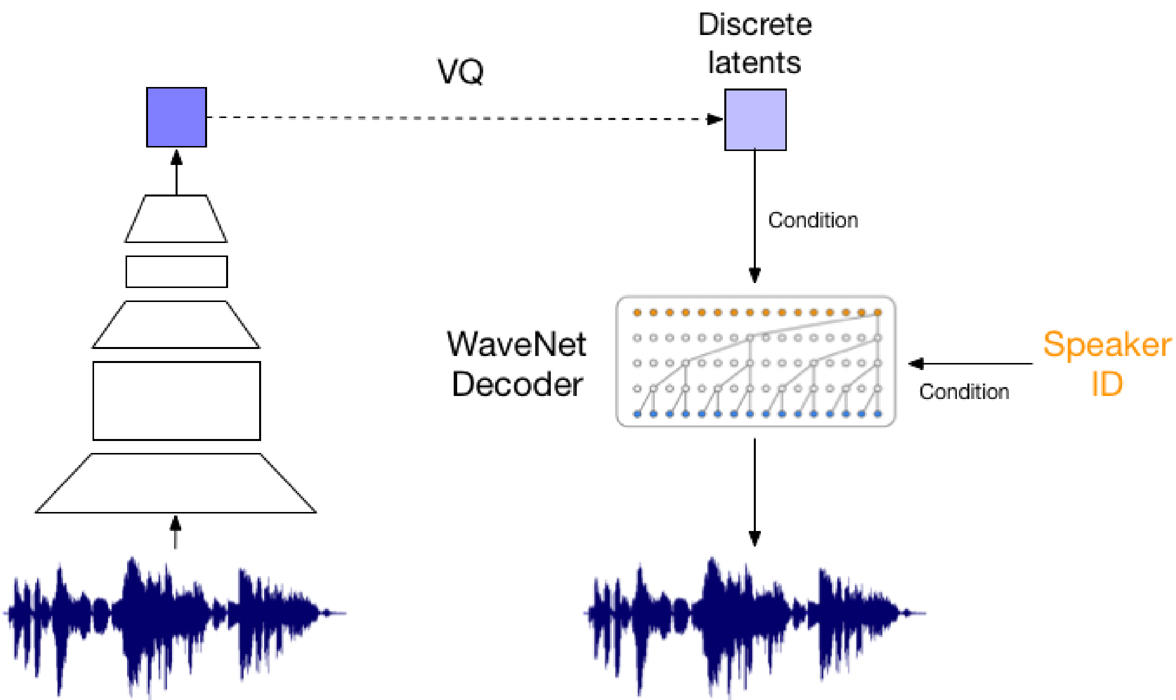
The prior-matching term $\mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))$ enforces simplicity in the latent space, encouraging learned semantic structure and disentanglement.



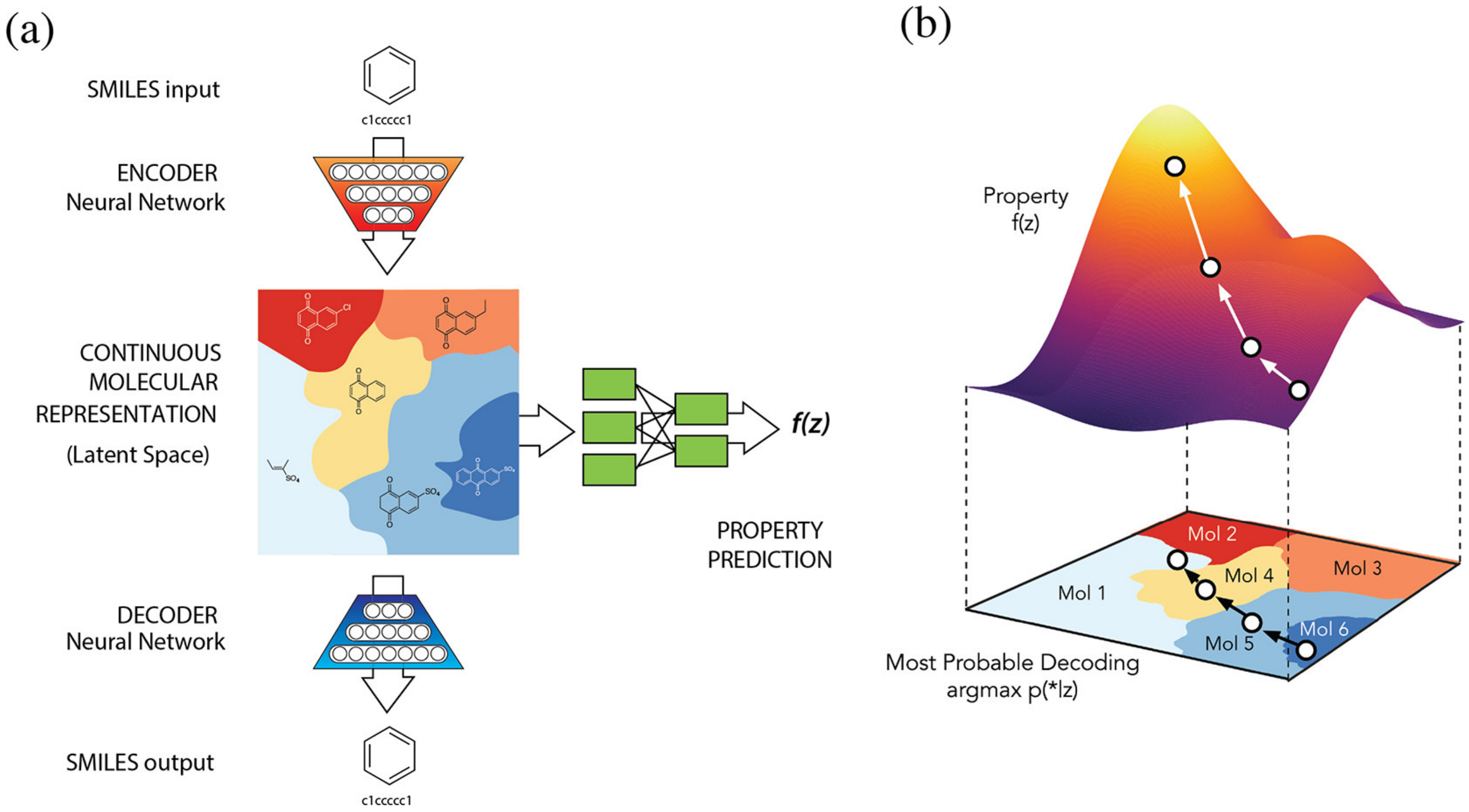
Illustrative applications



Hierarchical **compression of images and other data**,
e.g., in video conferencing systems (Gregor et al, 2016).



Voice style transfer [demo] (van den Oord et al, 2017).

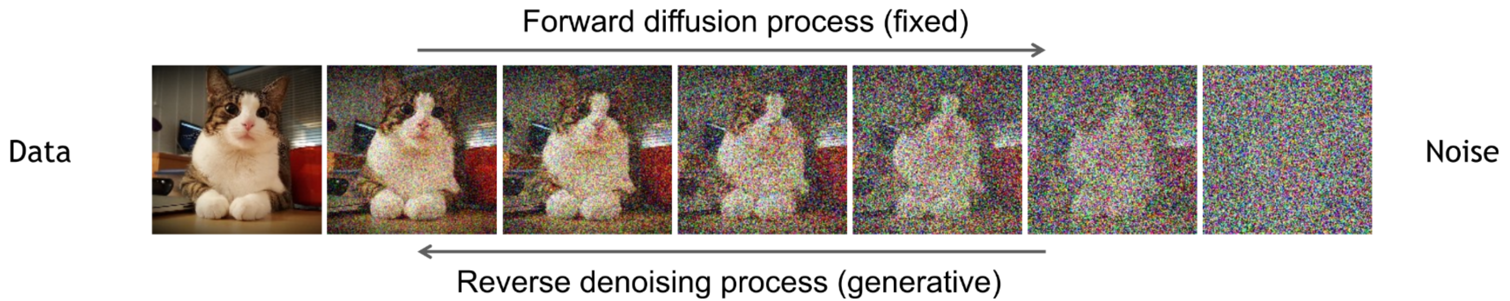


Design of new molecules with desired chemical properties
(Gomez-Bombarelli et al, 2016).

Questions?

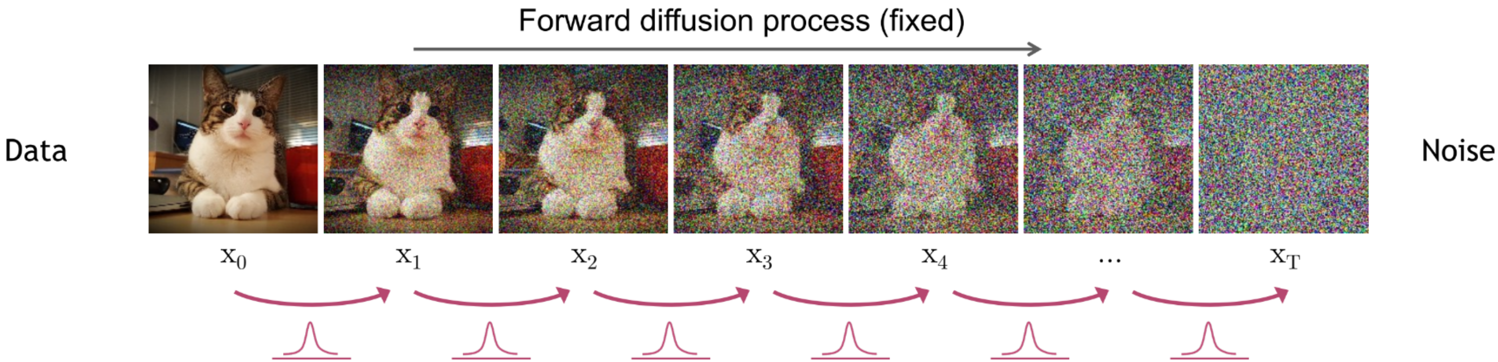
Ask me anything!

Diffusion models



Credits: Kreis et al, 2022.

Forward diffusion process



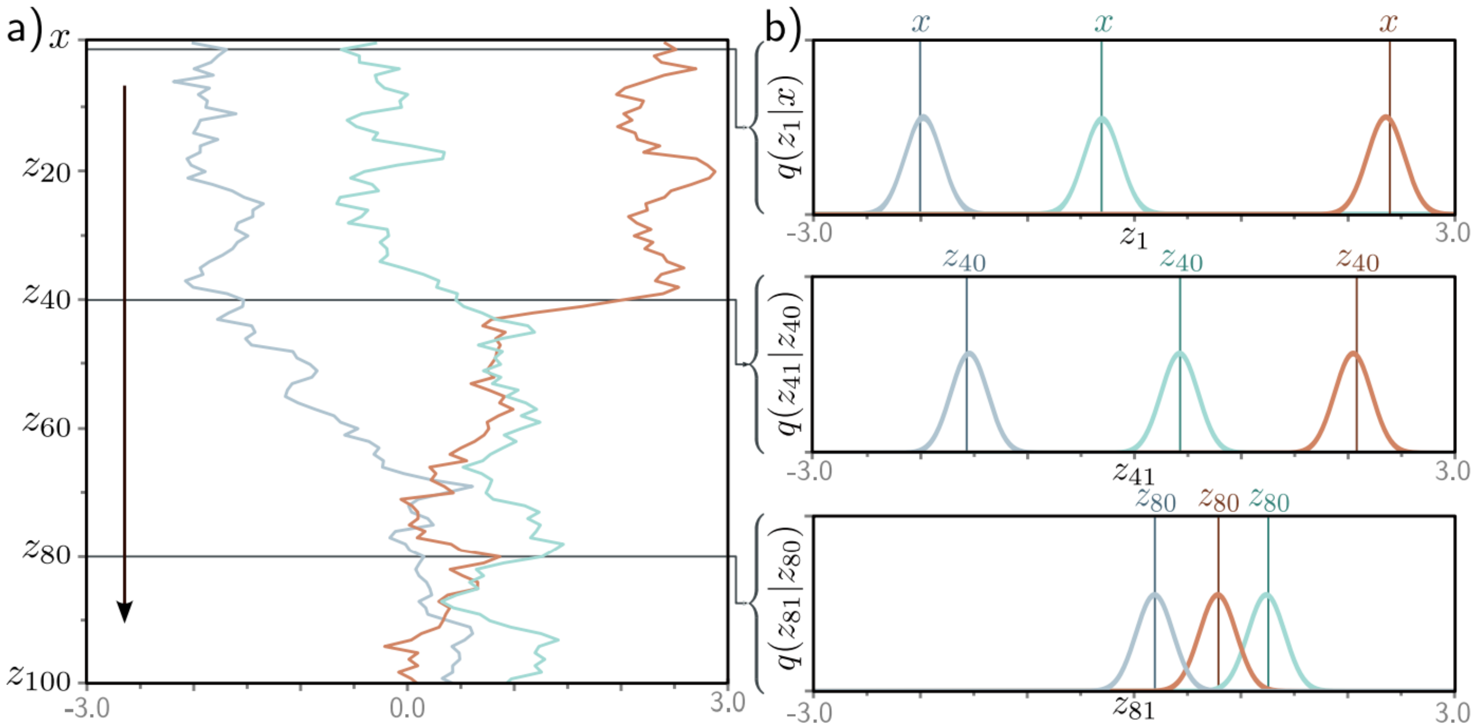
With $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$, we have

$$\mathbf{x}_t = \sqrt{\alpha_t}\mathbf{x}_{t-1} + \sqrt{1-\alpha_t}\epsilon$$

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{\alpha_t}\mathbf{x}_{t-1}, (1-\alpha_t)\mathbf{I})$$

$$q(\mathbf{x}_{1:T}|\mathbf{x}_0) = \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1})$$

Credits: Kreis et al, 2022.



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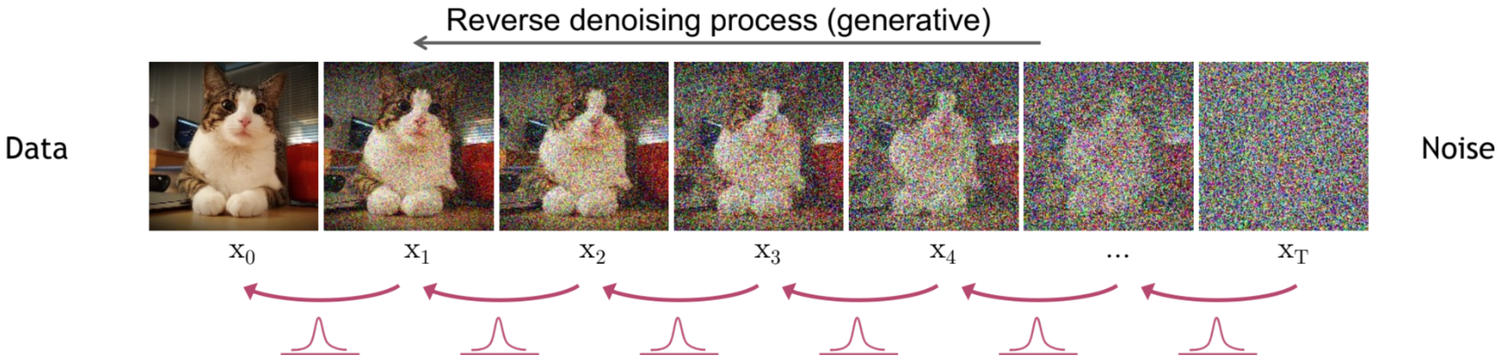
Credits: Simon J.D. Prince, 2023.

Reverse denoising process



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

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

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

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

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

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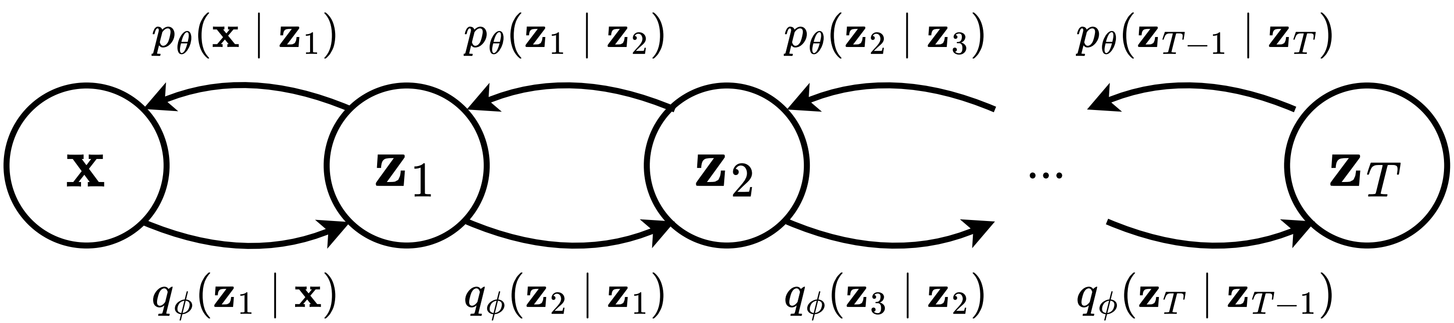
Credits: Kreis et al, 2022.

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.
- $L_{t-1} = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)}\text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)||p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))$ 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 $\mathbf{x}_0$.
- $L_T = \text{KL}(q(\mathbf{x}_T|\mathbf{x}_0)||p_\theta(\mathbf{x}_T))$ represents how close the distribution of the final noisified input is to the standard Gaussian. It has no trainable parameters.

(Some calculations later...)

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

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 $\mathbf{x}_t$.

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

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

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

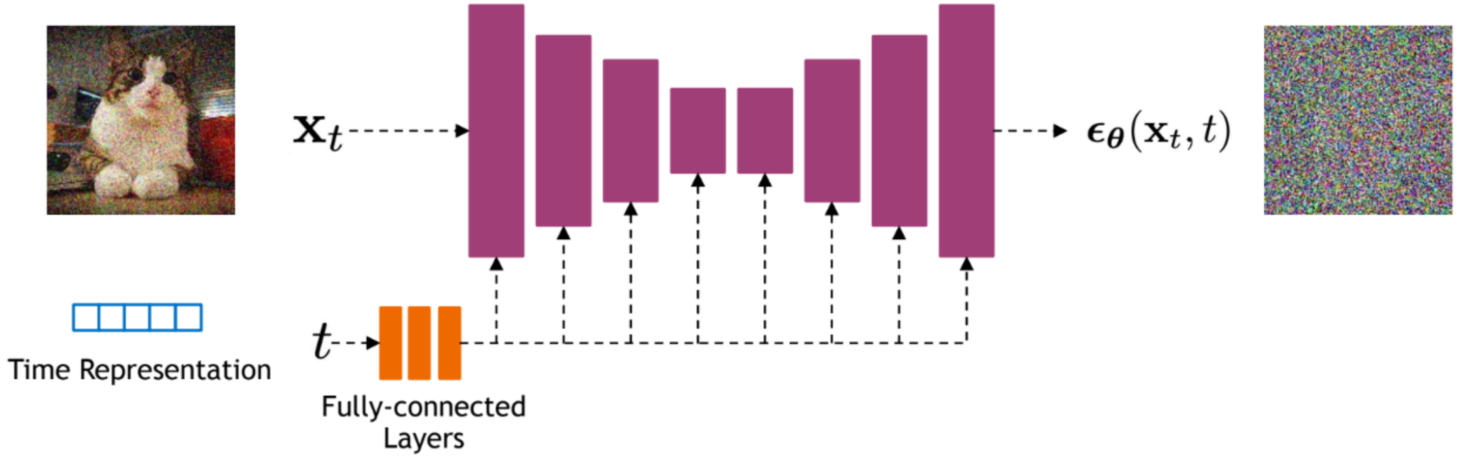
Unfortunately, $\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t)$ is not tractable in general. However, since $s_\theta(\mathbf{x}_t, t)$ is learned in expectation over the data distribution $q(\mathbf{x}_0)$, minimizing instead

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

ensures that $s_\theta(\mathbf{x}_t, t) \approx \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t)$.

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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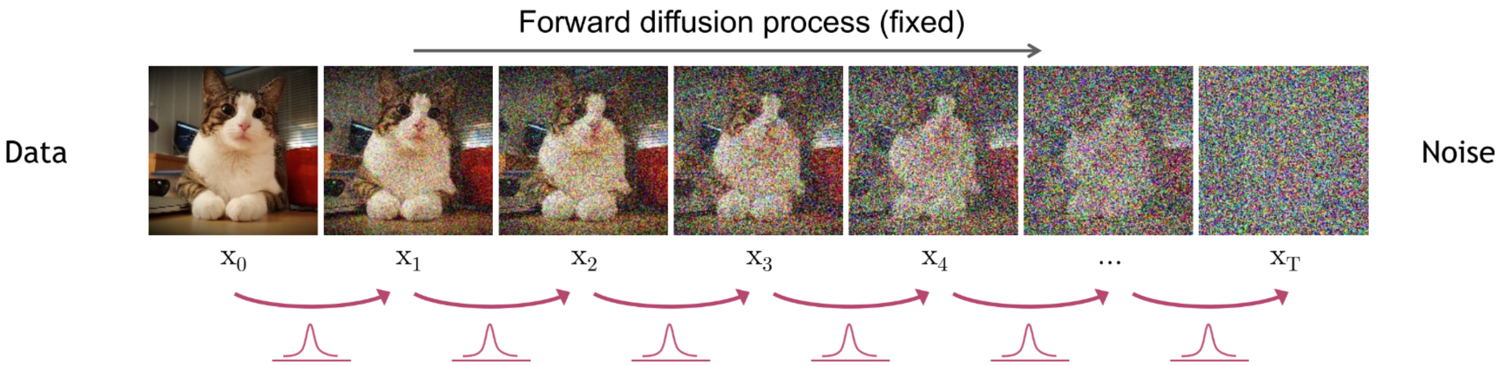
Credits: Kreis et al, 2022.

Continuous-time diffusion models



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

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

—

Credits: Kreis et al, 2022.

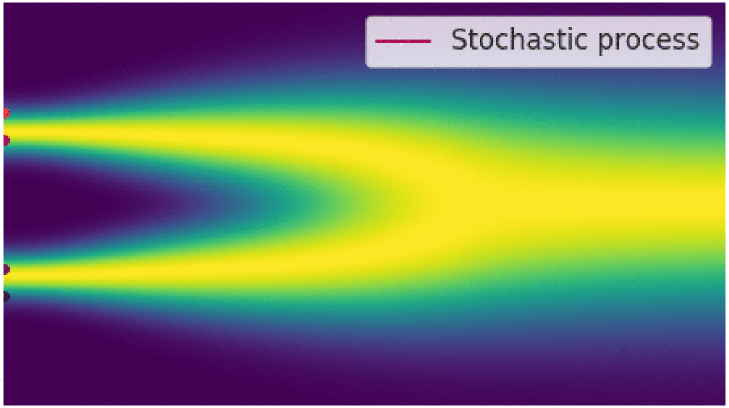
When $\Delta_t \rightarrow 0$, we can further rewrite the forward process as

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

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

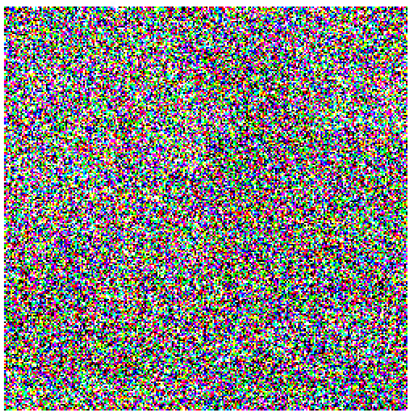
$$\mathrm{d}\mathbf{x}_t = -\frac{1}{2}\beta(t)\mathbf{x}_t \mathrm{d}t + \sqrt{\beta(t)}\mathrm{d}\mathbf{w}_t$$

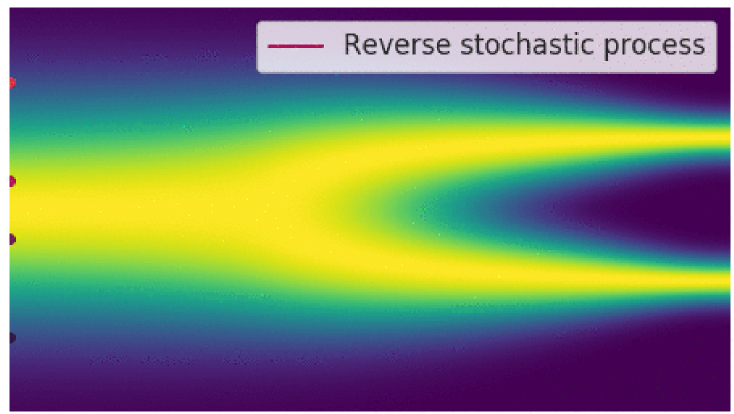
describing the diffusion in the infinitesimal limit.



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

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





Credits: Song, 2021.

Conditional sampling

To turn a diffusion model $p_\theta(\mathbf{x}_{0:T})$ into a conditional model, we can add conditioning information y at each step of the reverse process, as

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

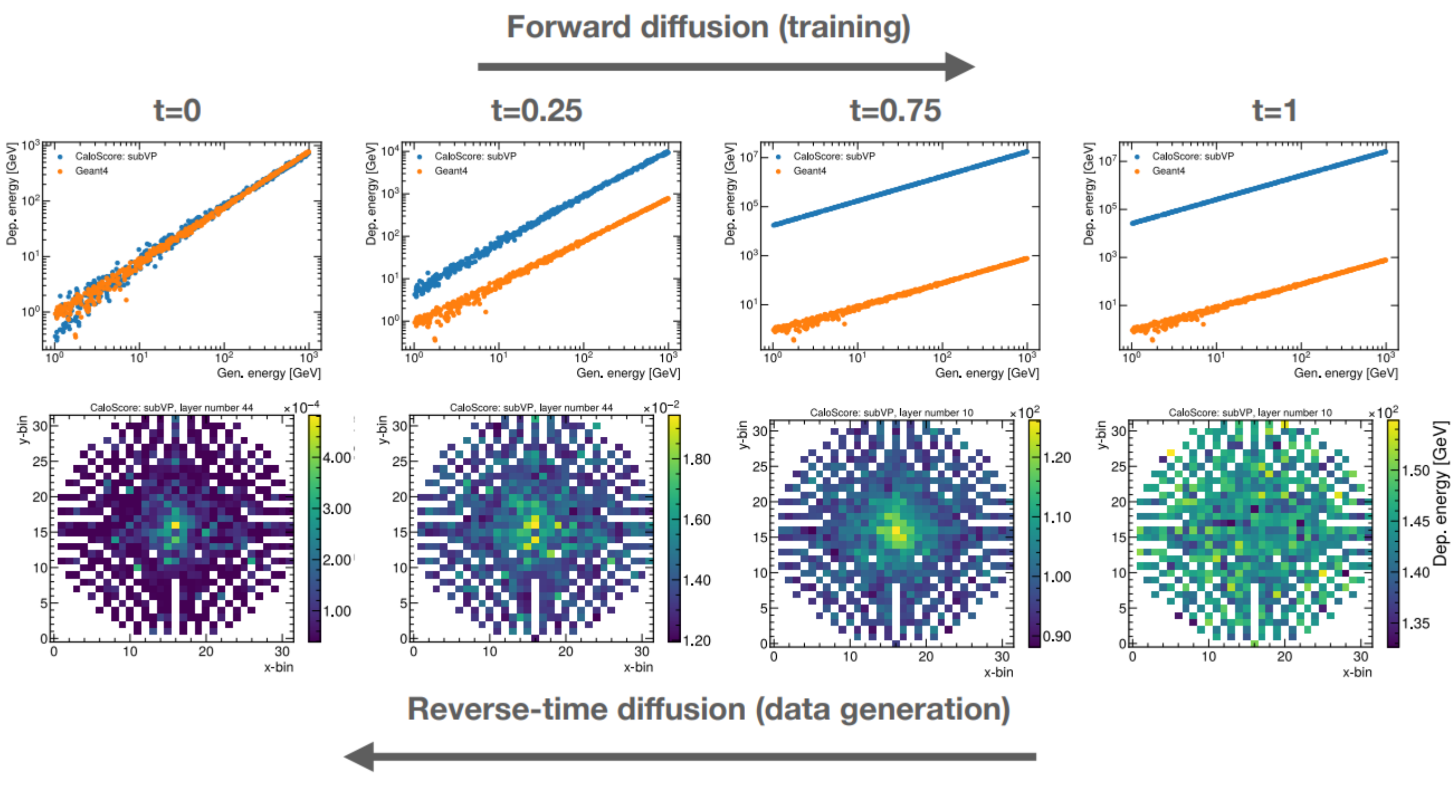
With a score-based model however, we can use the Bayes rule and notice that

$$\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|y) = \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t) + \nabla_{\mathbf{x}_t} \log p(y|\mathbf{x}_t),$$

where we leverage the fact that the gradient of $\log p(y)$ with respect to $\mathbf{x}_t$ is zero.

In other words, controllable generation can be achieved by adding a conditioning signal during sampling, without having to retrain the model. E.g., train an extra classifier $p(y|\mathbf{x}_t)$ and use it to control the sampling process by adding its gradient to the score.

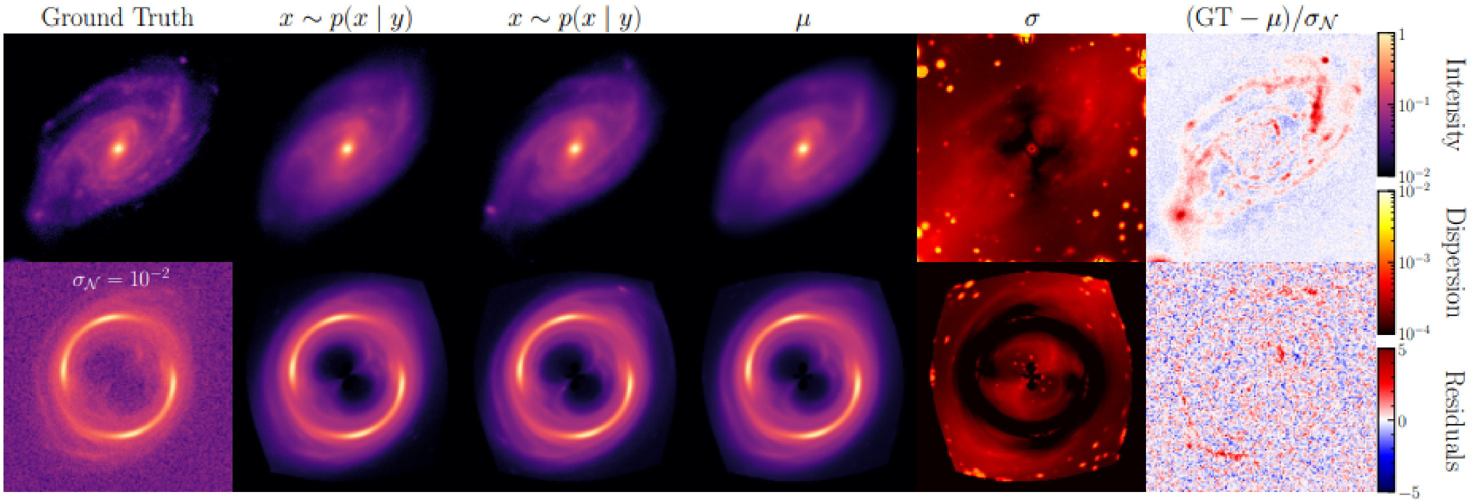
Illustrative applications



Diffusion models for **calorimeter shower simulation** (Mikuni and Nachman, 2022)

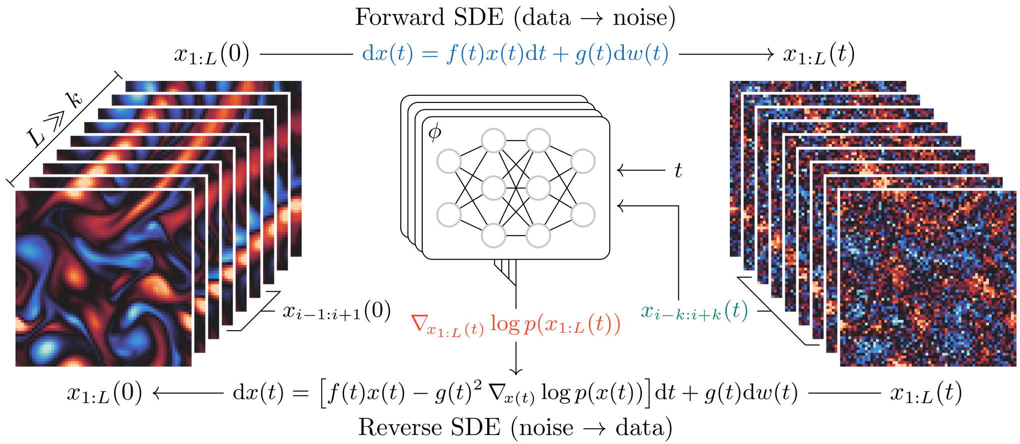
—

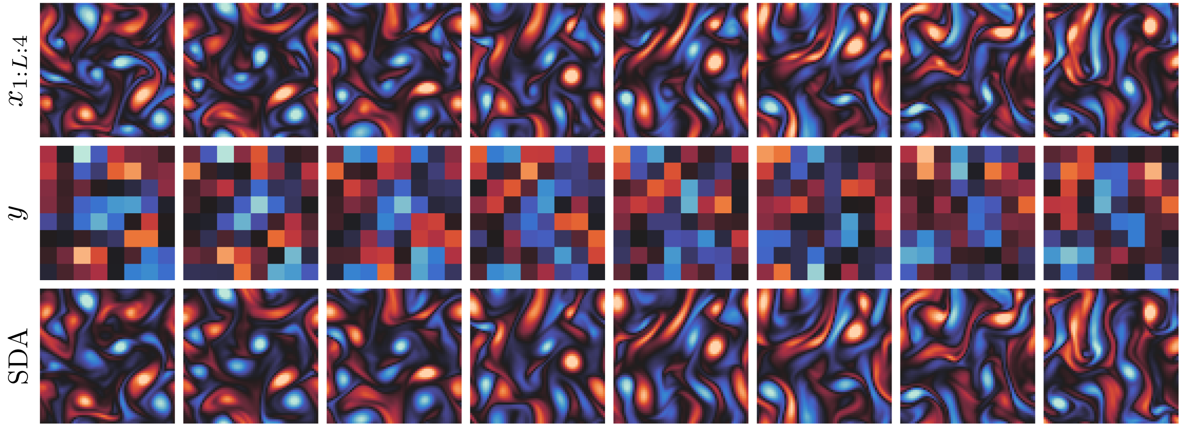
Credits: Mikuni and Nachman, 2022.



Posterior samples of **source galaxies in strong gravitational lenses** with score-based priors (Adam et al, 2022).

—
Credits: Adam et al, 2022.





Data assimilation in large-scale dynamical systems (Rozet and Louppe, 2023).

—

Credits: Rozet and Louppe, 2023.

Questions?

Ask me anything!

Latent diffusion models

Credits: Kreis, Gao, and Vahdat, 2023.

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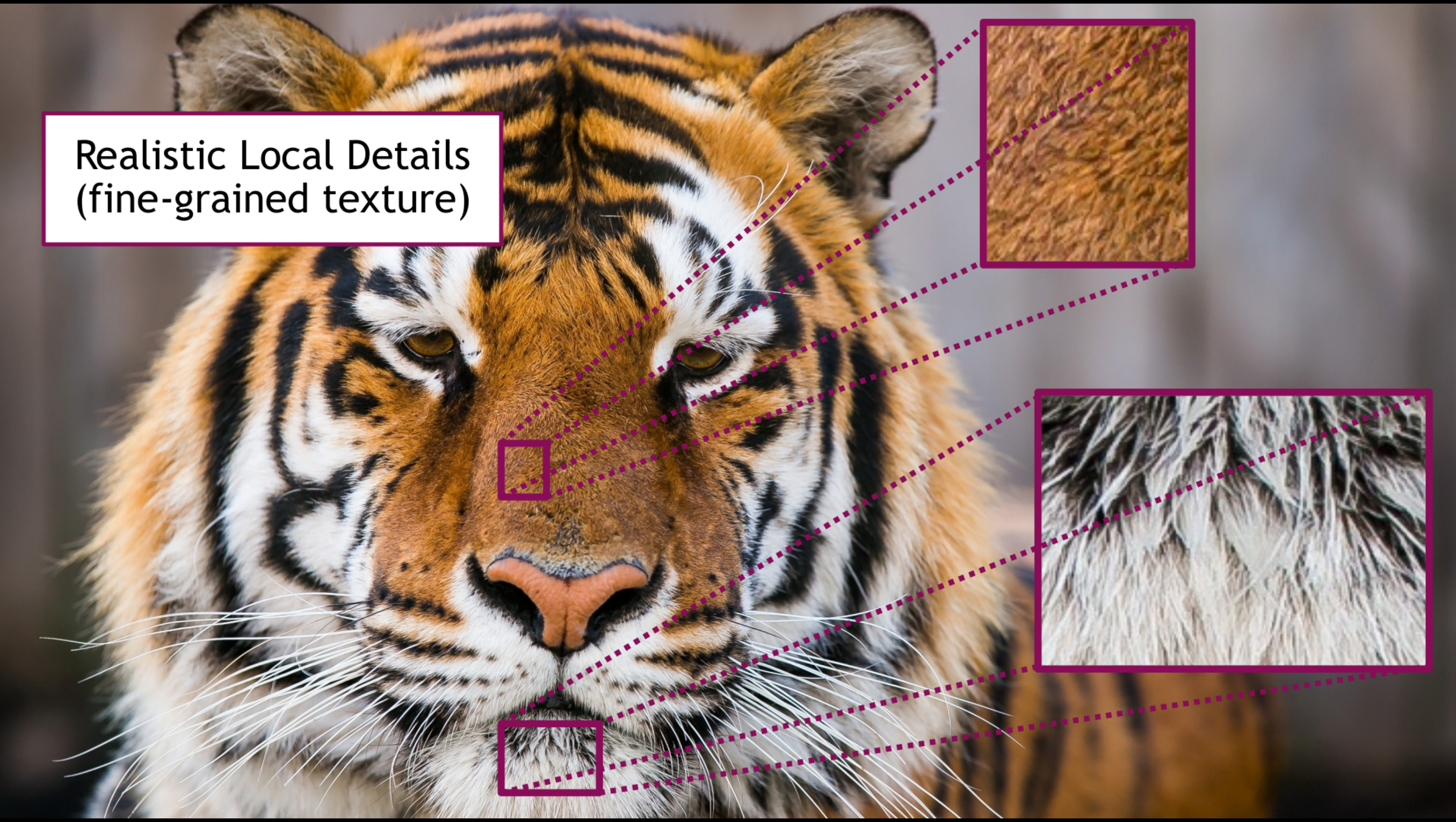
Credits: Kreis, Gao, and Vahdat, 2023.



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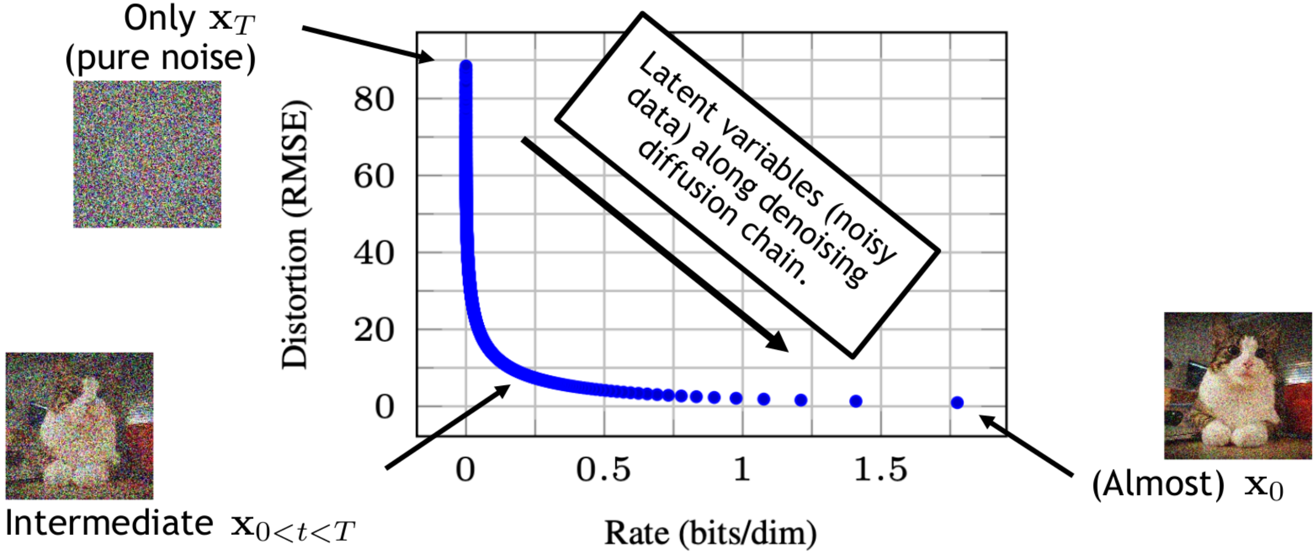
Credits: Kreis, Gao, and Vahdat, 2023.



Diffusion models encode images in their noisy latent space.

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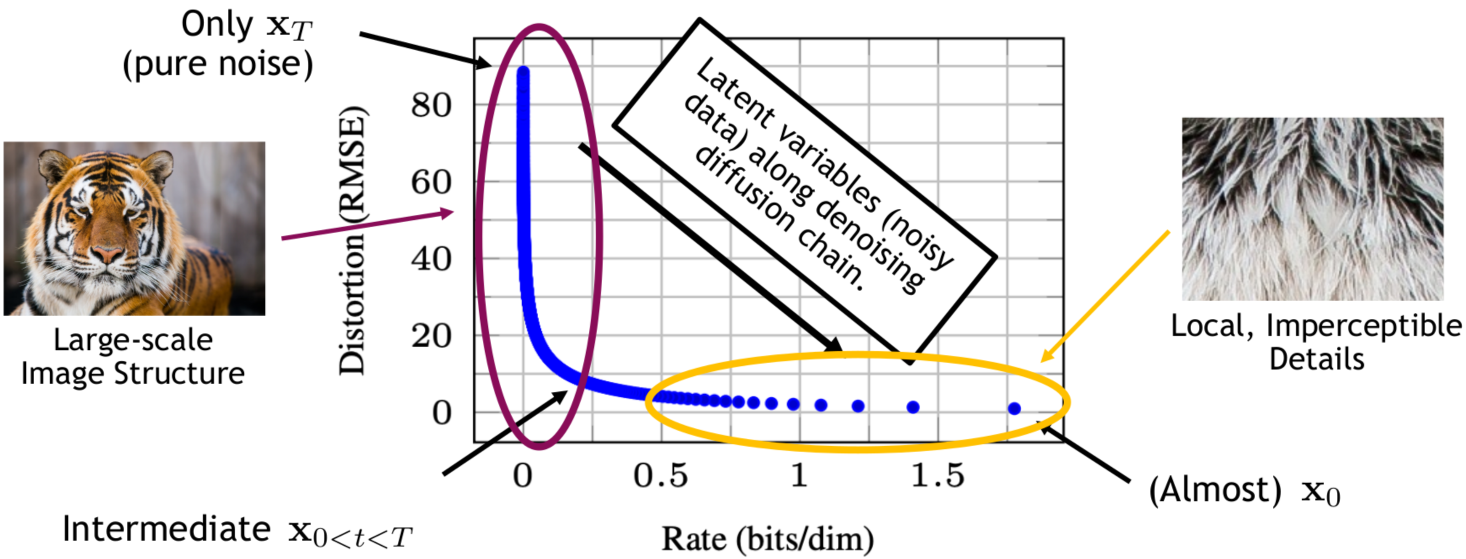
Credits: Kreis, Gao, and Vahdat, 2023.



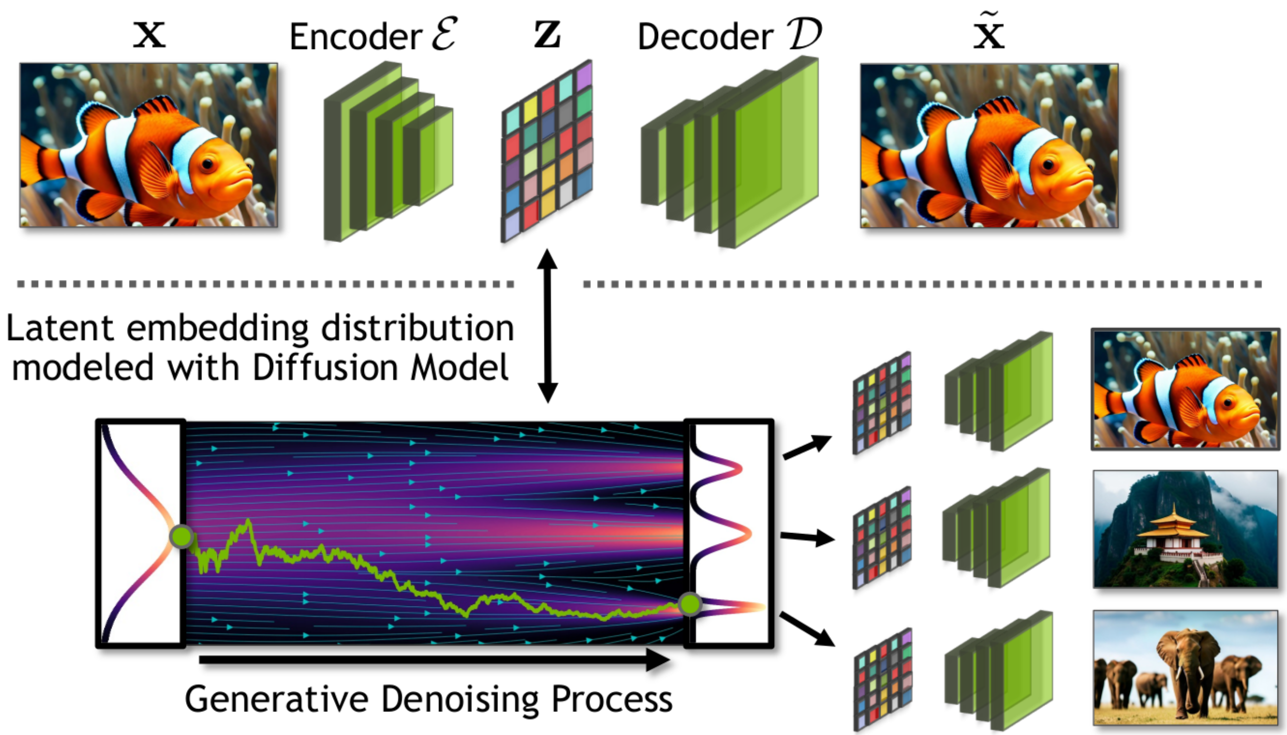
However, to encode each little detail, a lot of capacity is needed.

Credits: Kreis, Gao, and Vahdat, 2023.

Latent diffusion models

Latent diffusion models (LDMs) are made of two components:

- A strong auto-encoder ($\mathcal{E}$ and $\mathcal{D}$) that maps data to a latent space and back.
- An efficient diffusion model that generates data in the latent space.



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Credits: Kreis, Gao, and Vahdat, 2023.

The advantages of LDMs over diffusion models are:

- A **compressed latent space**. Training a diffusion model in a lower-dimensional latent space is computationally more efficient.
- A **regularized latent space**. The latent space is trained to be simple, making the diffusion process easier to reverse and faster to sample from.
- **Flexibility**. The auto-encoder can be tailored to data (images, text, graphs, point clouds, meshes, etc.) and the desired application.

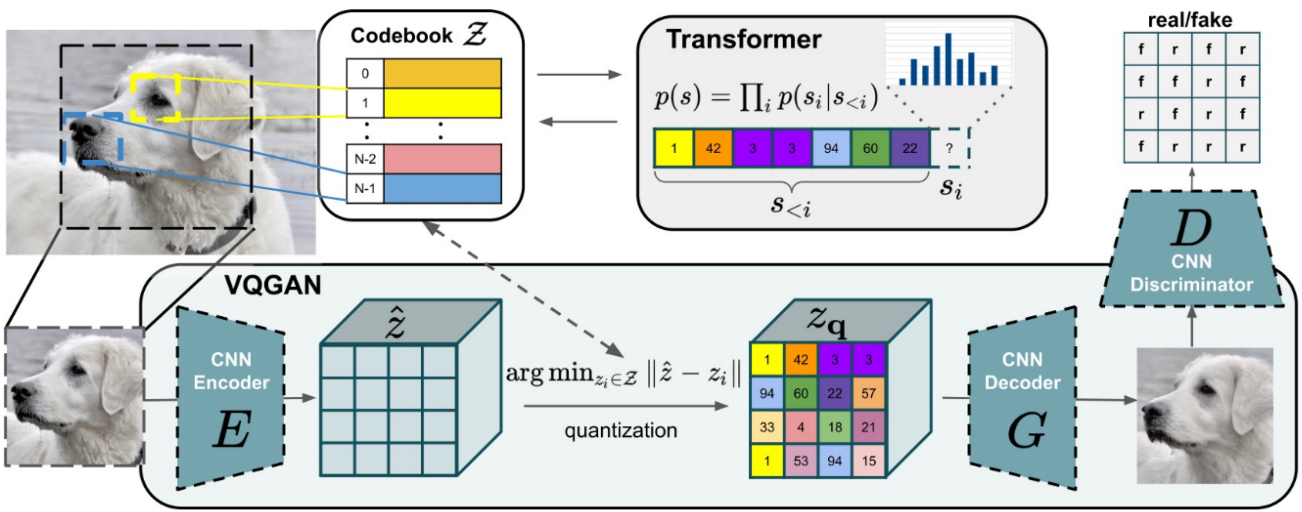
Latent space regularization

Option 1: KL regularization, as in VAEs.

- $q_{\mathcal{E}}(\mathbf{z}|\mathbf{x})$ is a Gaussian distribution.
- Prior matching penalty $\text{KL}(q_{\mathcal{E}}(\mathbf{z}|\mathbf{x})||\mathcal{N}(\mathbf{0},\mathbf{I}))$.

Option 2: Vector quantization regularization, as in VQ-VAEs.

- Discretize the latent space into a codebook.



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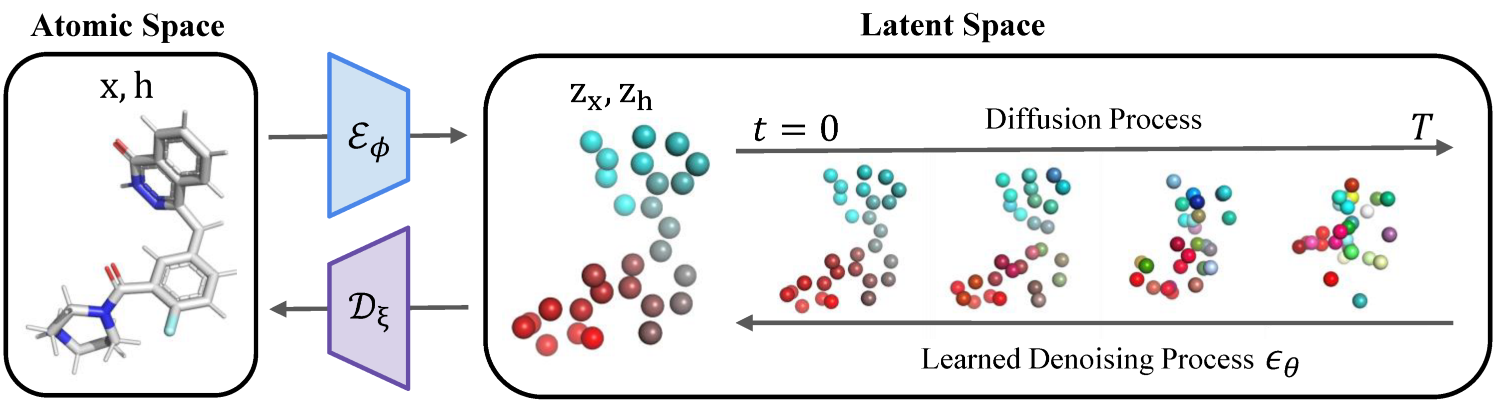
Credits: Kreis, Gao, and Vahdat, 2023.

Illustrative applications

Text-to-image generation with Emu (Dai et al, 2023).



Geometric latent diffusion models for **3d molecule generation** (Xu et al, 2023).

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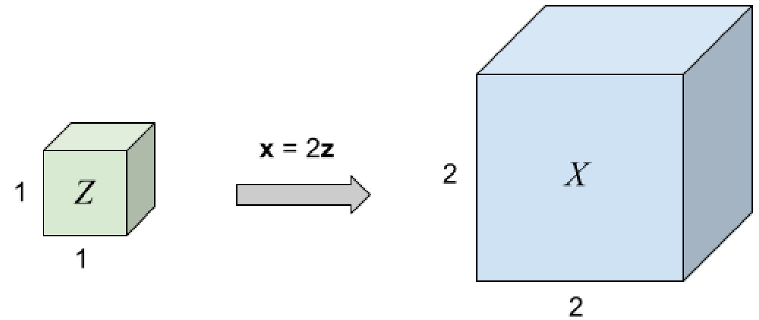
Credits: Xu et al, 2023.

Normalizing flows

Change of variables



Assume $p(\mathbf{z})$ is a uniformly distributed unit cube in $\mathbb{R}^3$ and $\mathbf{x} = f(\mathbf{z}) = 2\mathbf{z}$. Since the total probability mass must be conserved,

$$p(\mathbf{x}) = p(\mathbf{x} = f(\mathbf{z})) = p(\mathbf{z})\frac{V_{\mathbf{z}}}{V_{\mathbf{x}}} = p(\mathbf{z})\frac{1}{8},$$

where $\frac{1}{8} = \left|\det\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}\right|^{-1}$ represents the inverse determinant of the linear transformation f.

What if f is non-linear?

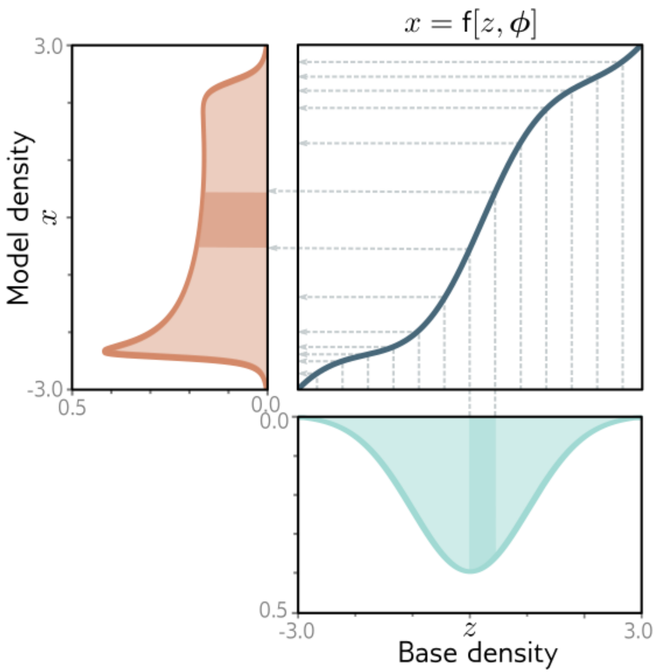


Figure 16.2 Transforming distributions. The base density (cyan, bottom) passes through a function (blue curve, top right) to create the model density (orange, left). Consider dividing the base density into equal intervals (gray vertical lines). The probability mass between adjacent lines must remain the same after transformation. The cyan-shaded region passes through a part of the function where the gradient is larger than one, so this region is stretched. Consequently, the height of the orange-shaded region must be lower so that it retains the same area as the cyan-shaded region. In other places (e.g., $z = -2$), the gradient is less than one, and the model density increases relative to the base density.

—

Image credits: Simon J.D. Prince, Understanding Deep Learning, 2023.

Change of variables theorem

If f is non-linear,

- the Jacobian $J_f(\mathbf{z})$ of $\mathbf{x} = f(\mathbf{z})$ represents the infinitesimal linear transformation in the neighborhood of $\mathbf{z}$;
- if the function is a bijective map, then the mass must be conserved locally.

Therefore, the local change of density yields

$$p(\mathbf{x} = f(\mathbf{z})) = p(\mathbf{z}) \left|\det J_f(\mathbf{z})\right|^{-1}.$$

Similarly, for $g = f^{-1}$, we have

$$p(\mathbf{x}) = p(\mathbf{z} = g(\mathbf{x})) \left|\det J_g(\mathbf{x})\right|.$$

Example: affine coupling layers

Assume $\mathbf{z} = (\mathbf{z}_a, \mathbf{z}_b)$ and $\mathbf{x} = (\mathbf{x}_a, \mathbf{x}_b)$. Then,

- Forward mapping $\mathbf{x} = f(\mathbf{z})$:

$$\mathbf{x}_a = \mathbf{z}_a, \quad \mathbf{x}_b = \mathbf{z}_b \odot \exp(s(\mathbf{z}_a)) + t(\mathbf{z}_a),$$

- Inverse mapping $\mathbf{z} = g(\mathbf{x})$:

$$\mathbf{z}_a = \mathbf{x}_a, \quad \mathbf{z}_b = (\mathbf{x}_b - t(\mathbf{x}_a)) \odot \exp(-s(\mathbf{x}_a)),$$

where s and t are arbitrary neural networks.

For $\mathbf{x} = (\mathbf{x}_a, \mathbf{x}_b)$, the log-likelihood is

$$\log p(\mathbf{x}) = \log p(\mathbf{z}) \left|\det J_f(\mathbf{z})\right|^{-1}$$

where the Jacobian $J_f(\mathbf{z}) = \frac{\partial \mathbf{x}}{\partial \mathbf{z}}$ is a lower triangular matrix

$$\begin{pmatrix} \mathbf{I} & 0 \\ \frac{\partial \mathbf{x}_b}{\partial \mathbf{z}_a} & \text{diag}(\exp(s(\mathbf{z}_a))) \end{pmatrix},$$

such that $\left|\det J_f(\mathbf{z})\right| = \prod_i \exp(s(\mathbf{z}_a))_i = \exp(\sum_i s(\mathbf{z}_a)_i)$.

Therefore, the log-likelihood is

$$\log p(\mathbf{x}) = \log p(\mathbf{z}) - \sum_i s(\mathbf{z}_a)_i$$

Normalizing flows

A normalizing flow is a change of variable f that transforms a base distribution $p(\mathbf{z})$ into $p(\mathbf{x})$ through a discrete sequence of invertible transformations.

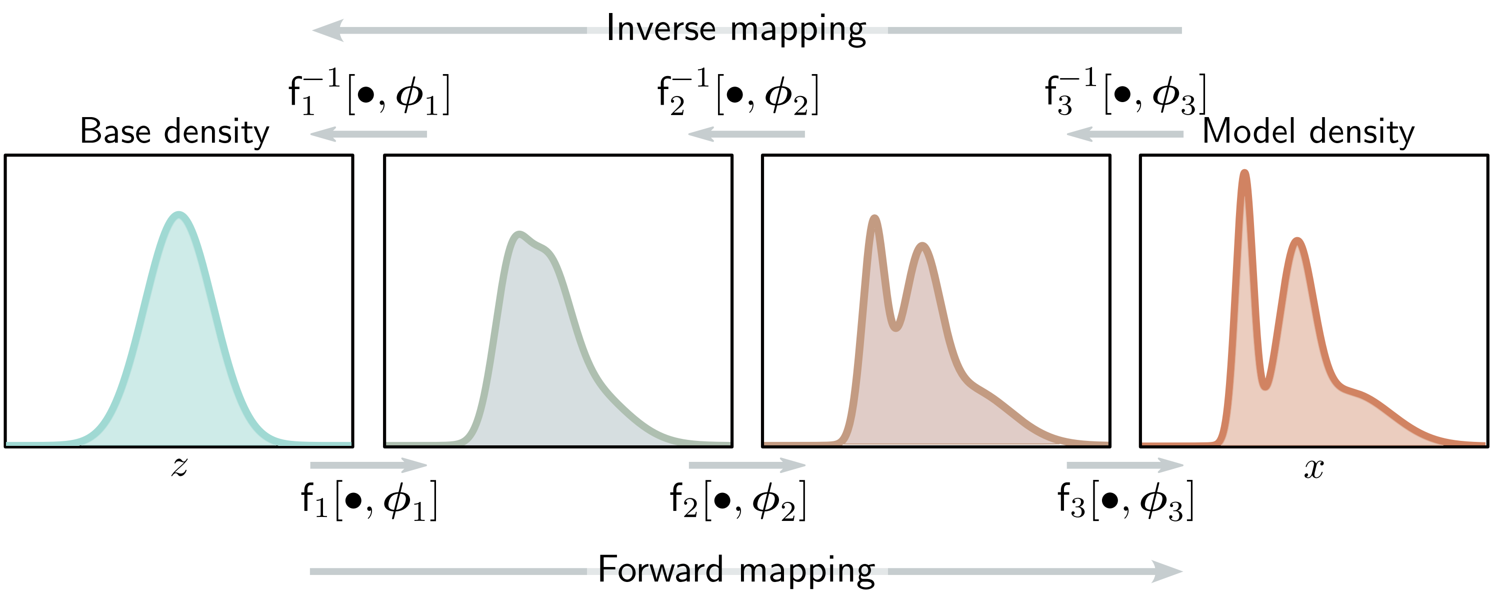


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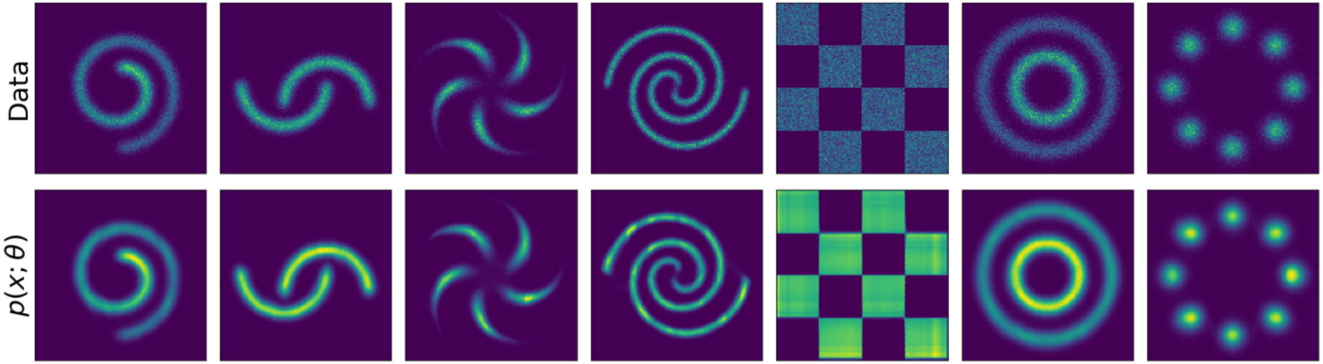
Image credits: Simon J.D. Prince, Understanding Deep Learning, 2023.

Formally,

$$
\begin{aligned}
\mathbf{z}_0 &\sim p(\mathbf{z}) \\
\mathbf{z}_k &= f_k(\mathbf{z}_{k-1}), \quad k = 1, ..., K \\
\mathbf{x} = \mathbf{z}_K &= f_K \circ ... \circ f_1(\mathbf{z}_0).
\end{aligned}
$$

The change of variable theorem yields

$$
\log p(\mathbf{x}) = \log p(\mathbf{z}_0) - \sum_{k=1}^{K} \log \left| \det J_{f_k}(\mathbf{z}_{k-1}) \right| .
$$



Normalizing flows can fit complex multimodal discontinuous densities.

—

Image credits: Wehenkel and Louppe, 2019.

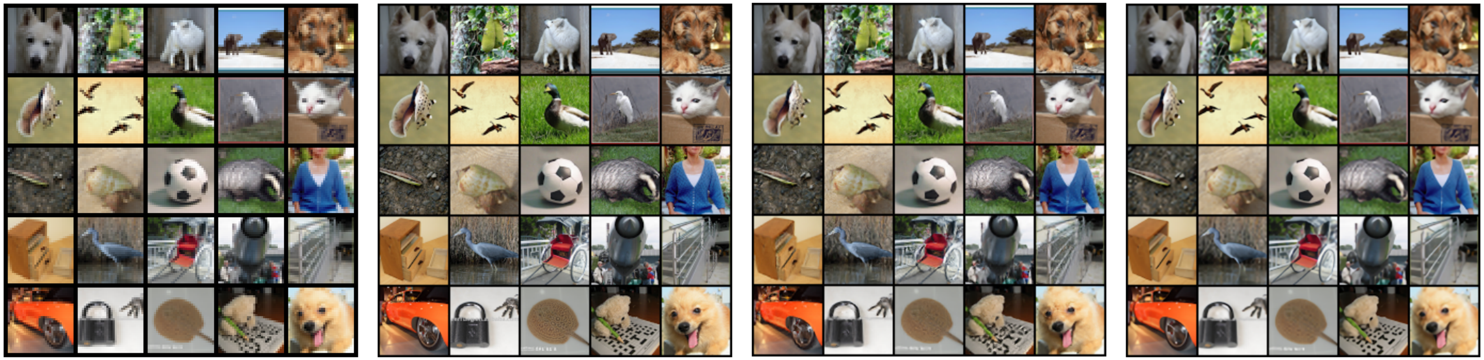
Note that a normalizing flow can be seen as a (degenerate) latent variable model where the conditional density $p(\mathbf{x}|\mathbf{z})$ is a Dirac distribution centered at $\mathbf{x} = f(\mathbf{z})$.

Conditional normalizing flows

Normalizing flows can also estimate densities $p(\mathbf{x}|c)$ conditioned on a context c
.

- Transformations are made conditional by taking c as an additional input. For example, in a coupling layer, the networks can be upgraded to $s(\mathbf{z}, c)$ and $t(\mathbf{z}, c)$.
- Optionally, the base distribution $p(\mathbf{z})$ can also be made conditional on c.

(Accordingly, aleatoric uncertainty of some output y conditioned on an input $\mathbf{x}$ can be modelled by a conditional normalizing flow $p(y|\mathbf{x})$ where the context c is the input $\mathbf{x}$.)



(a) *Low resolution* (b) *Ground truth* (b) *CNF sample* (c) *Baseline mode*

Figure 2: Super resolution results on the Imagenet64 test data. Samples are taken from the CNF $x_{hr} \sim p(x_{hr}|x_{lr})$ and the mode is visualized for the factorized baseline model. *Best viewed electronically.*

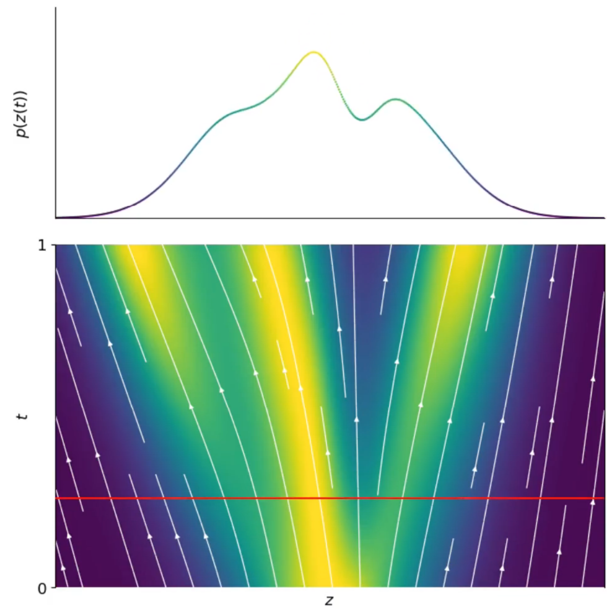
—

Image credits: Winkler et al, 2019.

Continuous-time normalizing flows

Replace the discrete sequence of transformations with a neural ODE with reversible dynamics such that

$$
\begin{aligned}
\mathbf{z}_0 &\sim p(\mathbf{z}) \\
\frac{d\mathbf{z}(t)}{dt} &= f(\mathbf{z}(t), t, \theta) \\
\mathbf{x} = \mathbf{z}(1) &= \mathbf{z}_0 + \int_0^1 f(\mathbf{z}(t), t) dt.
\end{aligned}
$$



The instantaneous change of variable yields

$$\log p(\mathbf{x}) = \log p(\mathbf{z}(0)) - \int_0^1 \mathrm{Tr}\left(\frac{\partial f(\mathbf{z}(t), t, \theta)}{\partial \mathbf{z}(t)}\right) dt.$$

—

Image credits: Grathwohl et al, 2018.

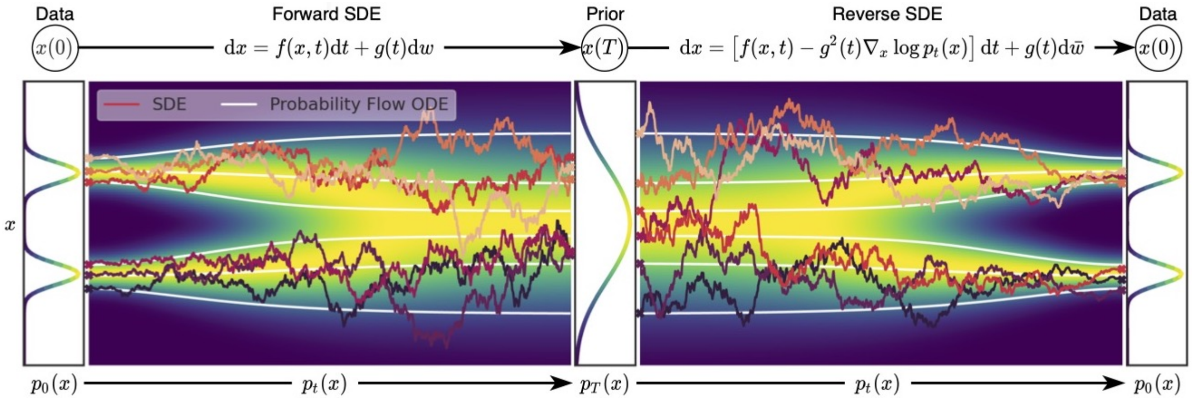
Probability flow ODE

Back to diffusion: For any diffusion process, there exists a corresponding deterministic process

$$\mathrm{d}\mathbf{x}_t = \left[\mathbf{f}(t, \mathbf{x}_t) - \frac{1}{2}g^2(t)\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t)\right] \mathrm{d}t$$

whose trajectories share the same marginal densities $p(\mathbf{x}_t)$.

Therefore, when $\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t)$ is replaced by its approximation $s_\theta(\mathbf{x}_t, t)$, the probability flow ODE becomes a special case of a neural ODE. In particular, it is an example of continuous-time normalizing flows!



The end.