Deep Learning

Diffusion Models and Normalizing Flows

11-785 - Fall 2023

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Open Question

1. Say we have a data distribution **p** that is a mixture of two 2D gaussians as shown below in red. We want to approximate this with one gaussian estimate **q** using KL-divergence. Which of the following three will result from optimizing $\mathbf{D}_{\mathrm{KL}}\,(p\,||\,q)$
2. and which from $\mathbf{D}_{\mathrm{KL}}\,(q\,||\,p)$?

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$\mathbf{D}_{\mathrm{KL}}\ (q\,||\,p)$ $\mathbf{D}_{\mathrm{KL}}\ (q\,||\,p)$ $\mathbf{D}_{\mathrm{KL}}\ (p\,||\,q)$

Background

1. Generative Models and Discriminative models
2. Autoencoders
3. Variational Autoencoders
    1. Reparameterization trick
    2. ELBO

Sandcastles

How to create a sandcastle:

Step 1: Take a sandcastle

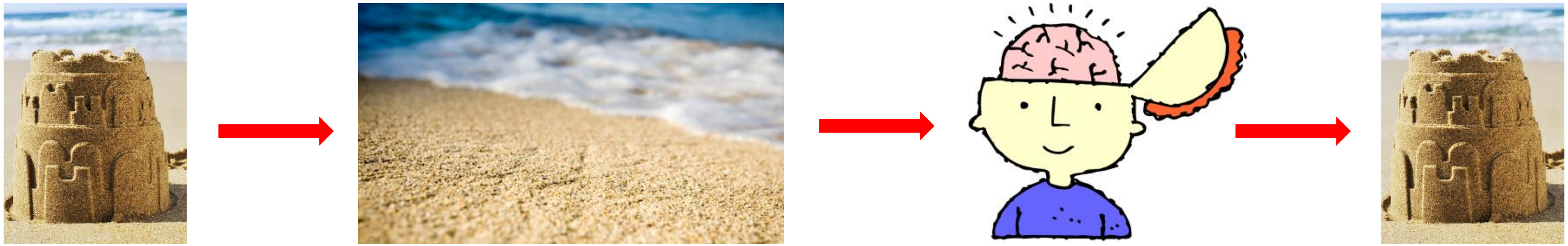
Step 2: Destroy the sandcastle

Step 3: Remember how you destroyed the sandcastle

Step 4: Reverse the process

Key Idea

Once you know how to reconstruct sandcastles, you can start with some different "sand", apply this process, and end up with a different "sandcastle"



Part 1

Diffusion Models

ELBO Recap

Why use ELBO?

Directly maximizing $p(x)$ is very difficult:

- it involves either marginalizing over the entire latent space $\boldsymbol{Z}$ (intractable for complex models) OR
- It involves having access to the ground truth latent encoder $p(z|x)$

ELBO:

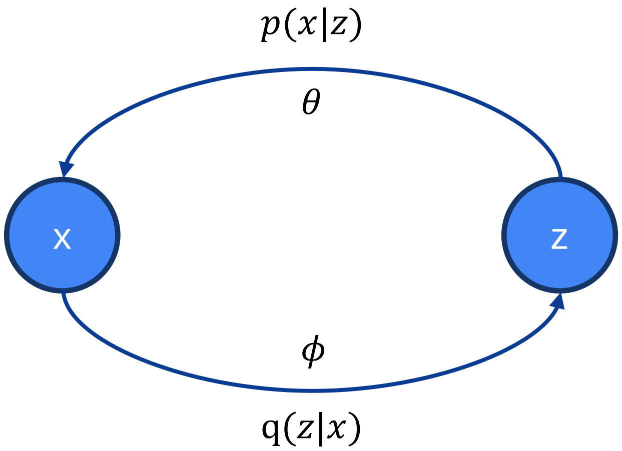
$$\log(p(x)) \geq \mathbb{E}_{q_\phi(z\,|\,x)}\left[\log \frac{p(x,z)}{q_\phi(z|x)}\right]$$

Question: Why does the $\geq$ show up here? → With the derivation in the appendix, we see a $D_{KL}(q_\phi(z|x)\,||\,p(z|x))$ term show up which is always ≥ 0.

Applying chain-rule of probabilities:

$$ELBO = \underbrace{\mathbb{E}_{q_\phi(z\,|\,x)}[\log p_\theta(x|z)]}_{\text{Reconstruction}} - \underbrace{D_{KL}(q_\phi(z\,|\,x)||\,p(z))}_{\text{Prior matching}}$$

Variational Autoencoder Recap



Latent variable sampling: $z \sim \mathcal{N}(z;\ \mu_\phi(x), \sigma_\phi^2(x))$

Reparameterization trick: $z = \mu_\phi(x) + \sigma_\phi(x)\ \odot \epsilon,\ \ \epsilon \sim \mathcal{N}(0, I)$

Training:

- Jointly optimize θ and ϕ
- Maximize **ELBO**

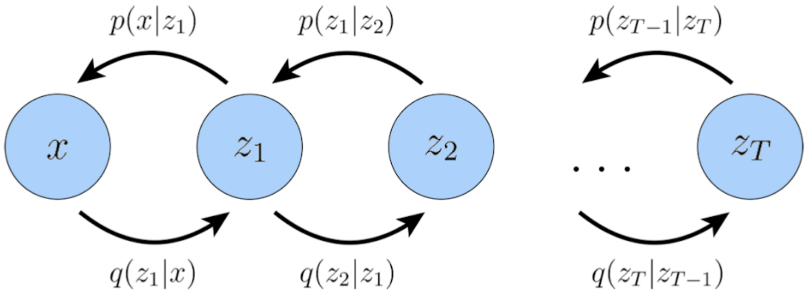
Empirically, we found that two things make VAEs work really well:

1. Increasing the depth of the networks
2. Introducing a hierarchy of latent variables (latent variables of latent variables)

$x \leftarrow z_1 \leftarrow z_2 \leftarrow\ \ldots \leftarrow z_T$, such that each latent is conditioned on all previous latents.

We are particularly interested in such HAVEs that where the process is a **Markovian chain - MHVAE**

Markovian Hierarchical Variational Autoencoder



Joint probability: $p(x, z_{1:T}) = p(z_T)p_\theta(x \mid z_1) \prod_{t=2}^{T} p_\theta(z_{t-1}|z_t)$

Posterior probability: $q_\phi(z_{1:T} \mid x) = q_\phi(z_1 | \, x) \prod_{t=2}^{T} q_\phi(z_t|z_{t-1})$

Updated ELBO:

$$\log\big(p(x)\big) \geq \mathbb{E}_{q_\phi(z_{1:T} \mid x)}\left[\log \frac{p(x, z_{1:T})}{q_\phi(z_{1:T} \mid x)}\right]$$

Diffusion Models

Diffusion models are essentially **MHVAEs** with **3 restrictions:**

1. Latent dimension is the same as the data dimension
2. The encoder has no parameters to be learnt. It is defined to be a linear gaussian such that the t^{th} gaussian is centered around the previous latent z_{t-1}
3. The parameters for the gaussians are scheduled such that the final latent is a standard gaussian.

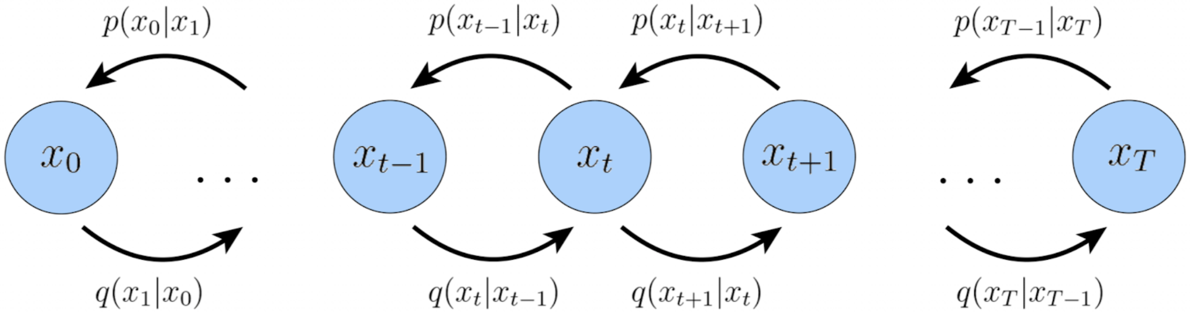
$$z_T \sim \mathcal{N}(z_T;\ 0, \boldsymbol{I})$$

The first restriction allows for some mild abuse of notation:

$$q_\phi(x_{1:T} \mid x_0) = \prod_{t=1}^{T} q_\phi(x_t | x_{t-1})$$

$$p(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1} | x_t)$$

Diffusion Models



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Diffusion Models – Diffusion Process

Following the second restriction, we now define the linear gaussian for the encoding (diffusion) process:

$$q(x_t|x_{t-1}) = \mathcal{N}(x_t; \mu_t(x_{t-1}), \Sigma_t \boldsymbol{I})$$

$$\mu_t(x_{t-1}) = \sqrt{1-\beta_t}x_{t-1}, \quad \Sigma_t = \beta_t$$

We additionally define $\alpha_t = 1 - \beta_t$.
β_t is defined to preserve variance across the diffusion steps.

We can now write

$$q(x_t|x_{t-1}) = \mathcal{N}\left(x_t; \sqrt{\alpha_t}x_{(t-1)}, (1-\alpha_t)\boldsymbol{I}\right)$$

Using the reparameterization trick:

$$x_t = \sqrt{\alpha_t}x_{(t-1)} + \left(\sqrt{1-\alpha_t}\right)\epsilon, \qquad \epsilon \sim \mathcal{N}(0, \boldsymbol{I})$$

$$= \sqrt{\alpha_t\alpha_{t-1}}x_{(t-2)} + \left(\sqrt{1-\alpha_t\alpha_{t-2}}\right)\epsilon$$

$$= \sqrt{\alpha_t\alpha_{t-1}\alpha_{t-2}}x_{(t-3)} + \left(\sqrt{1-\alpha_t\alpha_{t-2}\alpha_{t-3}}\right)\epsilon$$

$$= \sqrt{\alpha_t\alpha_{t-1} \ldots \alpha_1}x_{(0)} + \left(\sqrt{1-\alpha_t\alpha_{t-2} \ldots \alpha_1}\right)\epsilon$$

$$= \sqrt{\boldsymbol{\overline{\alpha_t}}}\boldsymbol{x_{(0)}} + \left(\sqrt{\boldsymbol{1-\overline{\alpha_t}}}\right)\boldsymbol{\epsilon}$$

This takes us from time step 0 to t in **one step!**

From the third restriction, we get

$$\alpha_T \to 0$$

Sum of two gaussians is another gaussian with mean as the sum of the two means and variance as the sum of the two variances.

$$(1-\alpha_t)\epsilon \to \mathcal{N}(\epsilon; 0, 1-\alpha_t\boldsymbol{I})$$

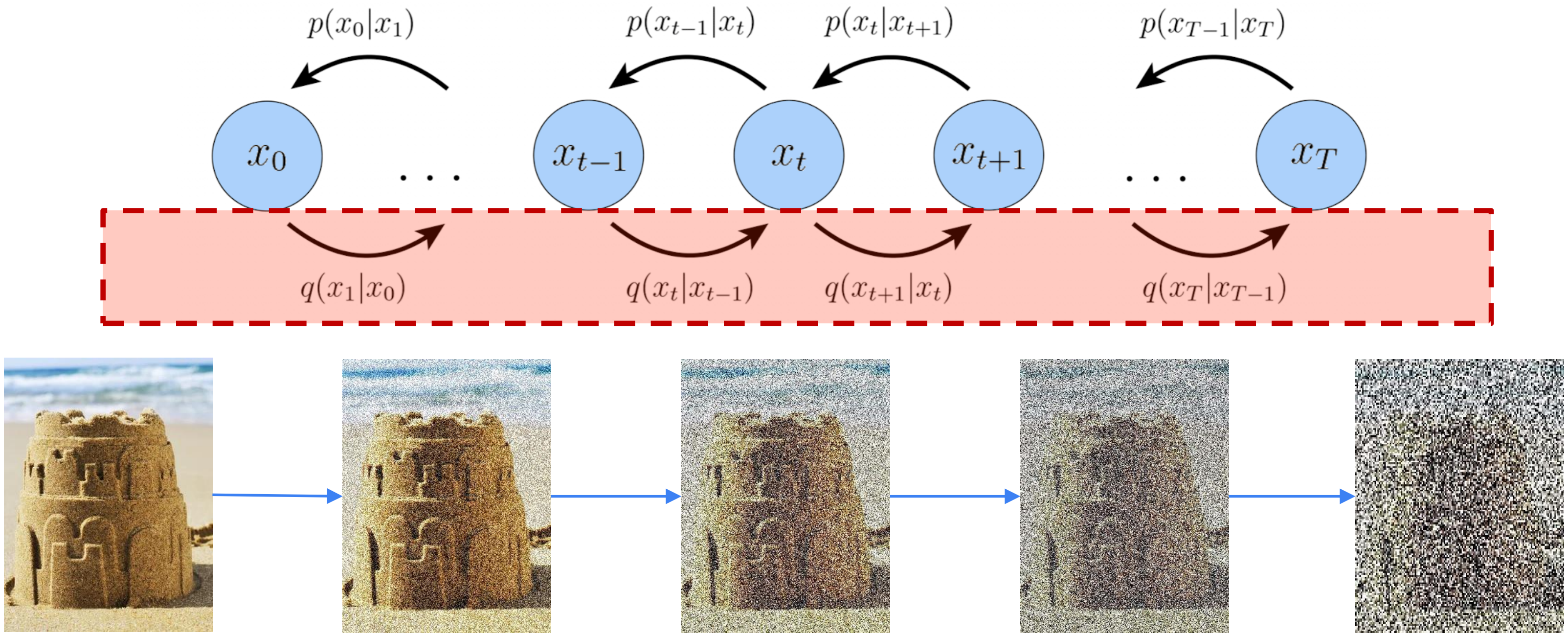
Define

$$\boldsymbol{\overline{\alpha_t}} = \prod_{s=1}^{t} \boldsymbol{\alpha_s}$$

Diffusion Models – Diffusion Process

$$q(x_t|x_{t-1}) = \sqrt{\alpha_t}x_{(t-1)} + \left(\sqrt{1-\alpha_t}\right)\epsilon, \qquad \epsilon \sim \mathcal{N}(0, \boldsymbol{I})$$

This formulation essentially paints a picture of this process to be incrementally adding noise till we reach x_T which is defined to be pure noise.



Diffusion Models – Generative Process

From the third assumption, we can write the exact prior on the final step x_T :

$$p(x_T) = \mathcal{N}(x_T; 0, \boldsymbol{I})$$

For all other steps, we can write a learned distribution:

$$p_\theta(x_{t-1}|x_t) \ = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_t \boldsymbol{I})$$

Exactly tractable
variance

Neural Network: **U-Net**
Denoising network

$$\boxed{p_\theta(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)}$$

Diffusion Models – Updated ELBO

*Derivation in appendix!

$$\log p(x) = \log \int p(x_{0:T}) dx_{0:T}$$

$$\ldots *$$

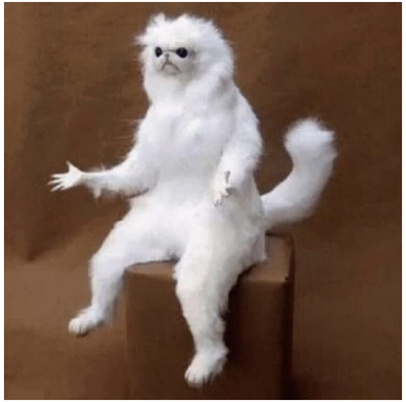
$$= \mathbb{E}_{q(x_1 \mid x_0)}[\log p_\theta(x_0|x_1)] - \mathbb{E}_{q(x_{T-1} \mid x_0)}[D_{KL}(q(x_T \mid x_{T-1})||p(x_T))]$$

$$- \sum_{t=1}^{T-1} \mathbb{E}_{q(x_{t-1}, x_{t+1} \mid x_0)}\left[D_{KL}\left(q(x_t \mid x_{t-1}) || p_\theta(x_t|x_{t+1})\right)\right]$$

This has **2** random variables for each **t**, this makes the computation slightly hard. We would prefer for there to be need for just **1**!

We can arbitrarily modify the diffusion process distribution to

$$q(x_t \mid x_{t-1}, x_0) = \frac{q(x_{t-1} \mid x_t, x_0) q(x_t|x_0)}{q(x_{t-1} \mid x_0)}$$



Diffusion Models – Updated ELBO

*Derivation in appendix!

$$\log p(x) = \log \int p(x_{0:T}) dx_{0:T}$$

$$\dots *$$

$$= \underbrace{\mathbb{E}_{q(x_1 \mid x_0)}[\log p_\theta(x_0|x_1)]}_{\text{Reconstruction}} - \underbrace{D_{KL}\left(q(x_T \mid x_0) || p(x_T)\right)}_{\text{Prior matching}} - \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(x_t \mid x_0)}\left[D_{KL}\left(q(x_{t-1}| x_t, x_0) || p_\theta(x_{t-1}|x_t)\right)\right]}_{\text{Denoising}}$$

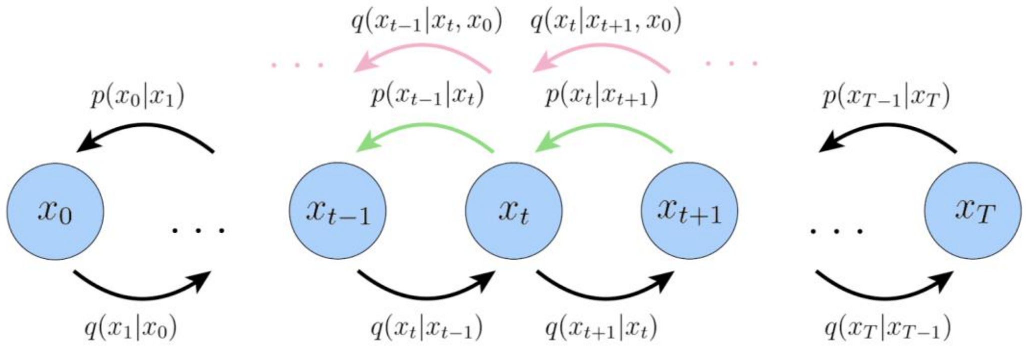
- Reconstruction: Reconstruction from least noisy version **(hyperparameter choice can make this arbitrarily small)**
- Prior matching: Moving the posterior closer to the true prior on the final noisy step **(0 for diffusion models)**
- Denoising: Divergence between approximate denoising (p_θ) and true denoising (q) steps

$q(x_{t-1}| x_t, x_0)$ is **tractable** and can be calculated **exactly** without any approximation:

$$q(x_{t-1}| x_t, x_0) = \mathcal{N}(x_{t-1}; \bar{\mu}_t, \Sigma_t \boldsymbol{I})$$

$$\bar{\mu}_t = \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})x_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)x_0}{1-\overline{\alpha_t}}, \qquad \Sigma_t = \frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\overline{\alpha_t}}$$

Diffusion Models – Loss formulation



Loss can focus on the denoising term. Decomposing for each timestep, we can have the t[th] loss term:

$$L_t = D_{KL}\left(q(x_{t-1}|\, x_t, x_0)\ ||p_\theta(x_{t-1}|x_t)\right) + C$$

Since both inputs of the divergence are gaussians, this further simplifies to:

$$\mathrm{L_t} = \mathbb{E}_q\left[\frac{1}{2\Sigma_t}||\bar{\mu}_t - \mu_\theta(\mathrm{x}_t, t)||^2\right] + \mathrm{C}$$

Diffusion Models – Loss formulation

Further, we have $x_t = \sqrt{\alpha_t} x_{(t-1)} + \left(\sqrt{1-\alpha_t}\right)\epsilon,\ \epsilon \sim \mathcal{N}(0, \boldsymbol{I})$ from definition

This lets us rewrite the true mean of the denoising process as:

$$\bar{\mu}_t = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{(1-\alpha_t)}{\sqrt{1 - \bar{\alpha}_t}}\epsilon\right)$$

We can also write the predicted mean as:

$$\mu_\theta(x_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{(1-\alpha_t)}{\sqrt{1 - \bar{\alpha}_t}}\epsilon_\theta(x_t, t)\right)$$

This lets us reformulate the loss to present a noise prediction problem:

$$L_{t-1} = \mathbb{E}_{x_0,\epsilon}\left[\frac{(1-\alpha_t)^2}{2\Sigma_t \alpha_t (1 - \bar{\alpha}_t)} ||\epsilon - \epsilon_\theta(x_t, t)||^2\right] + C$$

Diffusion Models – Training and Inference

Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
  $$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta\big(\overbrace{\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}}^{x_t}, t\big) \right\|^2$$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \ldots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

How do we tell the model what timestep we are on?

Temporal encodings in the form or sinusoids (or anything, really)

Diffusion models - Summary

- Diffusion models are **Markovian Hierarchical VAEs** with extra restrictions
- The loss is the vanilla VAE ELBO loss with an added denoising term
- The encoder has **0 parameters**
- The true denoising posterior can be **exactly calculated**
- The problem can be reformulated as a noise prediction problem
- There’s a ton of math underlying a rather simple intuition

Part 2

Normalizing Flows

Sandcastles

How to create a sandcastle:

Step 1: Take a sandcastle

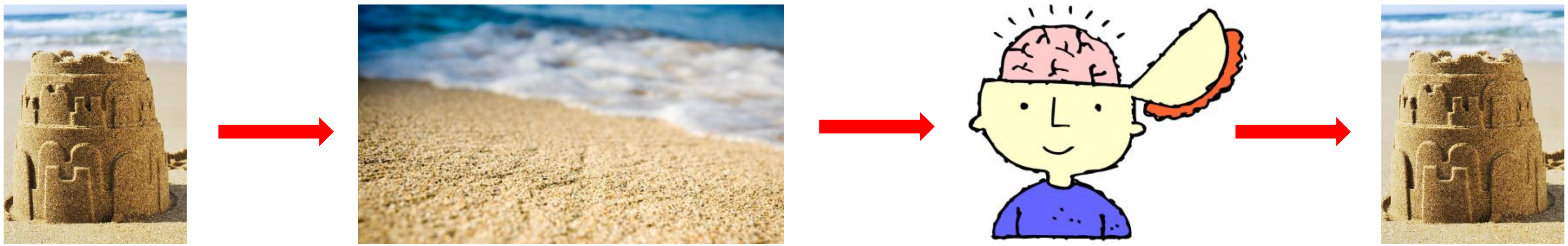
Step 2: Destroy the sandcastle

Step 3: Remember how you destroyed the sandcastle

Step 4: Reverse the process

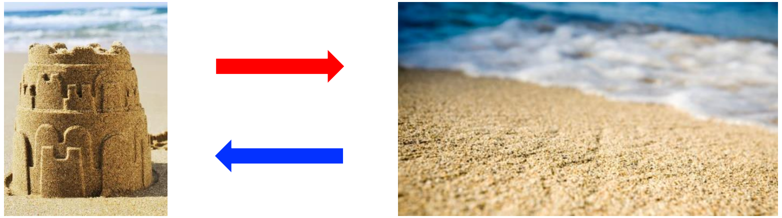
Key Idea

Once you know how to reconstruct sandcastles, you can start with some different “sand”, apply this process, and end up with a different “sandcastle”

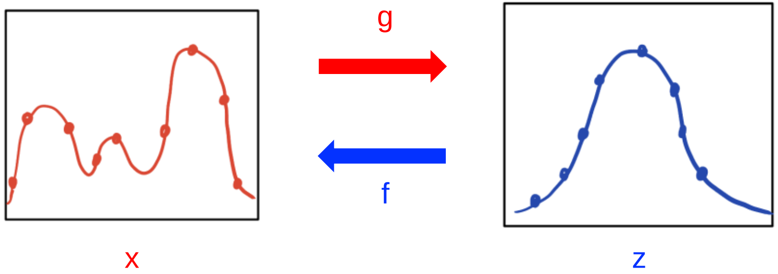


Normalizing Flows – Motivation

- In VAEs we are faced with an intractable likelihood calculation
- We use an ELBO instead as a surrogate objective to MLE
- What if we wanted to do MLE exactly?
- That would require us to go from sandcastle to sand, and back, without any approximation or estimation!



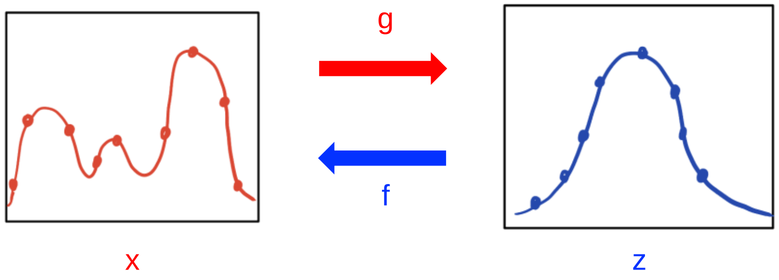
We would need for all the steps we do to be **invertible!**



It follows that

$\mathbf{f^{-1} = g}$

Normalizing Flows – Log likelihood



Bijection (and invertibility) allow us to directly compute the likelihood:

$$\int p_x(x)dx = \int p_z(g(x))dz$$

In multiple dimensions, we generalize to the determinant of the Jacobian

$$p_x(x) = p_z(g(x))\left|\frac{dg(x)}{dx}\right| \rightarrow p_z(g(x))|det.J(g(x))|$$

$$\log p_x(x) = \log p_z(g(x)) + \log|det.J(g(x))|$$

Intuitively

z = g(x) determines where a point in x-space maps to z-space (where to move grains of sand)

|det. J(g(x))| describes how much probability mass (sand) gets moved in a local neighborhood.

Normalizing Flows – Closer look at the Jacobian

$$z = g(x) = f^{-1}(x)$$

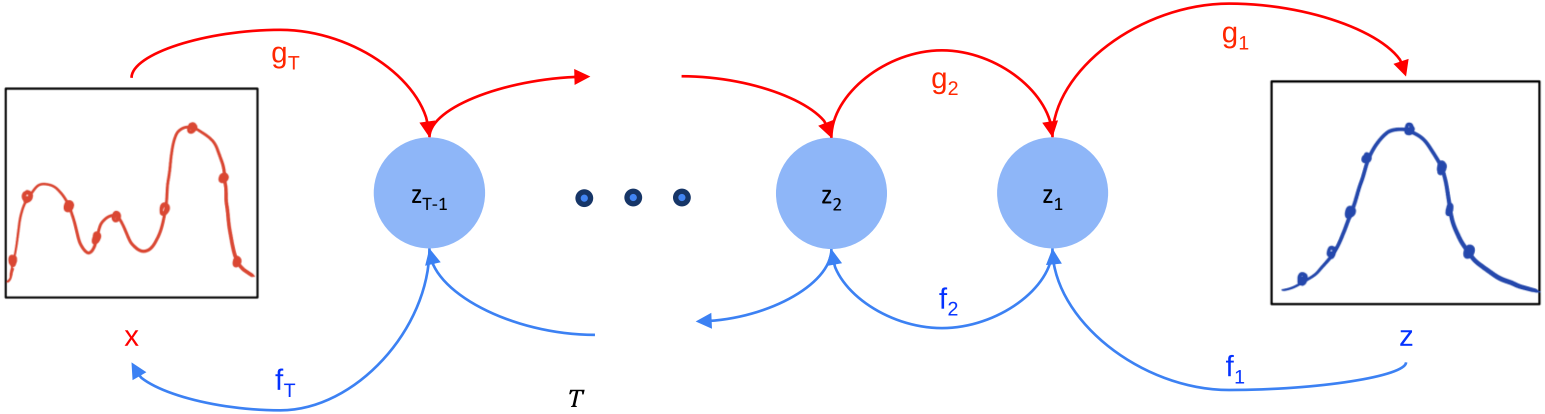
$$J_x\, g(x) = \begin{bmatrix} \frac{\partial z_1}{\partial x_1} & \cdots & \frac{\partial z_1}{\partial x_k} \\ \vdots & & \vdots \\ \frac{\partial z_k}{\partial x_1} & \cdots & \frac{\partial z_k}{\partial x_k} \end{bmatrix}$$

Normalizing Flows – Compositions

Bijections allow for composing several functions together!

This follows that we can now define:

$$z \sim p(z)$$
$$x = f_T \circ f_{T-1} \circ \cdots \circ f_1\,(z)$$



$$\log p_x(x) = \log p_z(z_0) + \sum_{t=1}^{T} \log\left|det.J_{z_t}\big(g(z_{t-1})\big)\right|, \qquad z_T = x,\ z_0 = z$$

Inverse: $z = g_1 \circ g_2 \circ \cdots \circ g_T(x)$

Normalizing Flows – Characteristics

For a good (efficient) flow, we must have functions (steps) that are:

1. Expressive
2. Invertible
3. Offer cheap to compute Jacobian determinants

Computing a determinant is a **cubic** operation, but some special cases of matrices can make it very cheap.
Especially, **diagonal** matrices:

For a diagonal matrix, the determinant is simply the product of its diagonal elements. Same applies for any triangular matrix!

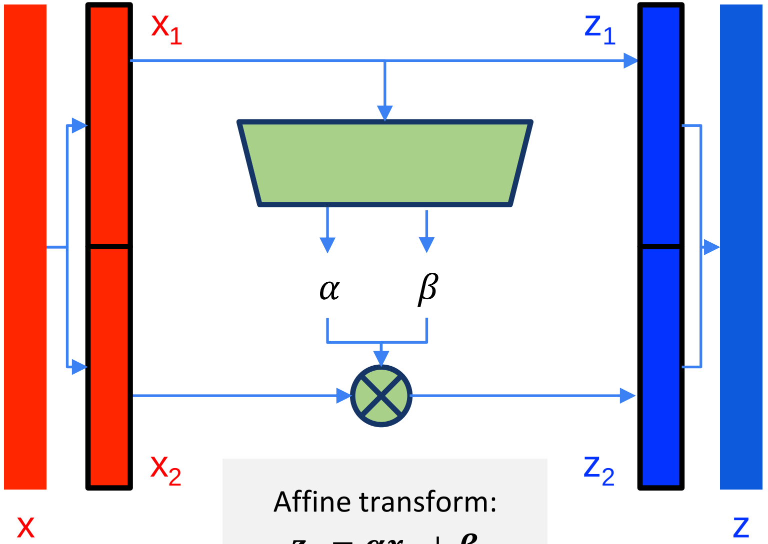
In linear algebra, a **diagonal matrix** is a matrix (usually a square matrix) in which the entries outside the main diagonal (↘) are all zero. The diagonal entries themselves may or may not be zero. Thus, the matrix $D = (d_{i,j})$ with n columns and n rows is diagonal if:

$$d_{i,j} = 0 \text{ if } i \neq j \ \forall i, j \in \{1, 2, \ldots, n\}$$

For example, the following matrix is diagonal:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$

Normalizing Flows – Construction

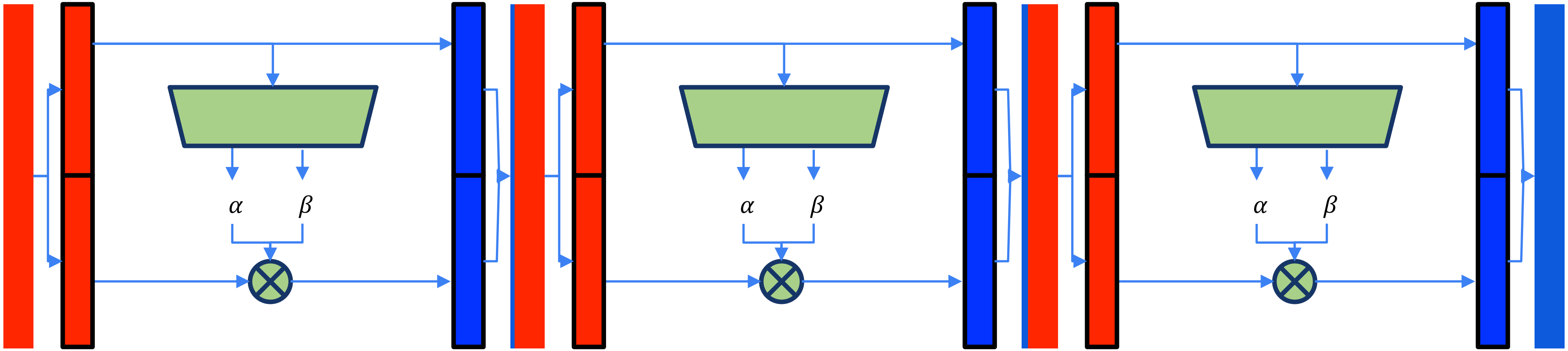


Affine transform:

$$z_2 = \alpha x_2 + \beta$$

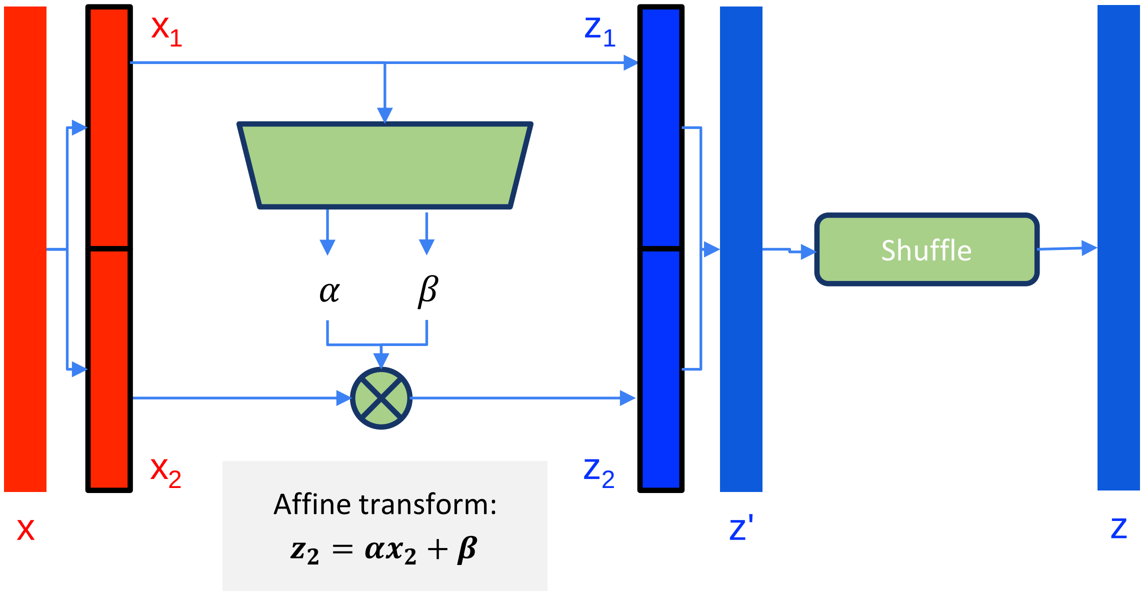
$$J_x(z) \quad \begin{array}{cc} & \begin{array}{cc} x_1 & \quad x_2 \end{array} \\ \begin{array}{c} z_1 \\ z_2 \end{array} & \left[\begin{array}{c|c} I & 0 \\ \hline ? & \alpha I \end{array}\right] \end{array}$$

Normalizing Flows – Composition



Is there a problem here?

Normalizing Flows – Construction with a shuffle



This the most popular type of flow called as **Coupling Flow** – Used in implementations such as NICE and GLOW

Normalizing Flows – In practice for images

- Multiscale architecture
- Split along channels
- Employ CNNs
- Perform permutations using 1x1 Conv layers

GLOW!

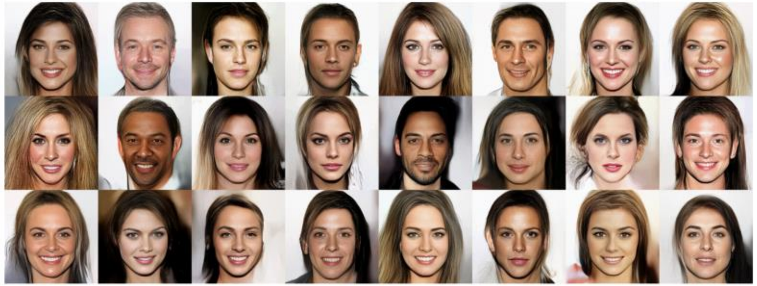


Figure 4: Random samples from the model, with temperature 0.7.

Figure 5: Linear interpolation in latent space between real images.

References

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- Hans van Gorp's lecture, https://www.youtube.com/watch?v=yxVcnuRrKqQ&t=17s
- Tim Salimans' lecture, https://www.youtube.com/watch?v=pea3sH6orMc

Appendix

Vanilla VAE ELBO optimization derivation

The KL divergence term that shows up tries to match the learned posterior ***q*** to the true posterior ***p***.

Since KL divergence is always positive, we can ignore that term and replace the equality with the inequality.

$$
\begin{aligned}
\log p(\boldsymbol{x}) &= \log p(\boldsymbol{x}) \int q_{\phi}(\boldsymbol{z}|\boldsymbol{x}) dz && \left(\text{Multiply by } 1 = \int q_{\phi}(\boldsymbol{z}|\boldsymbol{x}) d\boldsymbol{z}\right) \\
&= \int q_{\phi}(\boldsymbol{z}|\boldsymbol{x})(\log p(\boldsymbol{x})) dz && (\text{Bring evidence into integral}) \\
&= \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\left[\log p(\boldsymbol{x})\right] && (\text{Definition of Expectation}) \\
&= \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{p(\boldsymbol{z}|\boldsymbol{x})}\right] && (\text{Apply Equation 2}) \\
&= \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}) q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}{p(\boldsymbol{z}|\boldsymbol{x}) q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\right] && \left(\text{Multiply by } 1 = \frac{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\right) \\
&= \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\right] + \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}{p(\boldsymbol{z}|\boldsymbol{x})}\right] && (\text{Split the Expectation}) \\
&= \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\right] + D_{\mathrm{KL}}(q_{\phi}(\boldsymbol{z}|\boldsymbol{x}) \parallel p(\boldsymbol{z}|\boldsymbol{x})) && (\text{Definition of KL Divergence}) \\
&\geq \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\right] && (\text{KL Divergence always} \geq 0)
\end{aligned}
$$

Initial ELBO optimization derivation for diffusion models

Ends up with expectation calculation over multiple random variables

$$
\begin{aligned}
\log p(\boldsymbol{x}) &= \log \int p(\boldsymbol{x}_{0:T}) d\boldsymbol{x}_{1:T} \\
&= \log \int \frac{p(\boldsymbol{x}_{0:T}) q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} d\boldsymbol{x}_{1:T} \\
&= \log \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \right] \\
&\geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T) \prod_{t=1}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\prod_{t=1}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T) p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1) \prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_T|\boldsymbol{x}_{T-1}) \prod_{t=1}^{T-1} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T) p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1) \prod_{t=1}^{T-1} p_{\boldsymbol{\theta}}(\boldsymbol{x}_t|\boldsymbol{x}_{t+1})}{q(\boldsymbol{x}_T|\boldsymbol{x}_{T-1}) \prod_{t=1}^{T-1} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T) p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_T|\boldsymbol{x}_{T-1})} \right] + \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \prod_{t=1}^{T-1} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_t|\boldsymbol{x}_{t+1})}{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1) \right] + \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T|\boldsymbol{x}_{T-1})} \right] + \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\sum_{t=1}^{T-1} \log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_t|\boldsymbol{x}_{t+1})}{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1) \right] + \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T|\boldsymbol{x}_{T-1})} \right] + \sum_{t=1}^{T-1} \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_t|\boldsymbol{x}_{t+1})}{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} \left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1) \right] + \mathbb{E}_{q(\boldsymbol{x}_{T-1}, \boldsymbol{x}_T|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T|\boldsymbol{x}_{T-1})} \right] + \sum_{t=1}^{T-1} \mathbb{E}_{q(\boldsymbol{x}_{t-1}, \boldsymbol{x}_t, \boldsymbol{x}_{t+1}|\boldsymbol{x}_0)} \left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_t|\boldsymbol{x}_{t+1})}{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})} \right] \\
&= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} \left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1) \right]}_{\text{reconstruction term}} - \underbrace{\mathbb{E}_{q(\boldsymbol{x}_{T-1}|\boldsymbol{x}_0)} \left[D_{\mathrm{KL}}(q(\boldsymbol{x}_T|\boldsymbol{x}_{T-1}) \parallel p(\boldsymbol{x}_T)) \right]}_{\text{prior matching term}} \\
&\quad - \sum_{t=1}^{T-1} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_{t-1}, \boldsymbol{x}_{t+1}|\boldsymbol{x}_0)} \left[D_{\mathrm{KL}}(q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) \parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_t|\boldsymbol{x}_{t+1})) \right]}_{\text{consistency term}}
\end{aligned}
$$

Modified ELBO optimization derivation for diffusion models

Only involves one random variable per expectation term!

$$
\begin{aligned}
\log p(\boldsymbol{x}) &\geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)\prod_{t=1}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\prod_{t=1}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)\prod_{t=2}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)\prod_{t=2}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1},\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1},\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)q(\boldsymbol{x}_t|\boldsymbol{x}_0)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\cancel{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}}{\cancel{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}}}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{\cancel{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}} + \log \frac{\cancel{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)} + \sum_{t=2}^{T} \log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\right] + \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)}\right] + \sum_{t=2}^{T} \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\right] + \mathbb{E}_{q(\boldsymbol{x}_T|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)}\right] + \sum_{t=2}^{T} \mathbb{E}_{q(\boldsymbol{x}_t,\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\right]}_{\text{reconstruction term}} - \underbrace{D_{\mathrm{KL}}(q(\boldsymbol{x}_T|\boldsymbol{x}_0)\parallel p(\boldsymbol{x}_T))}_{\text{prior matching term}} - \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}\left[D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t))\right]}_{\text{denoising matching term}}
\end{aligned}
$$