CSC 412/2506:
Probabilistic Learning and Reasoning
Week 12 - 2/2: Diffusion Models

Murat A. Erdogdu

University of Toronto

These slides are based on:

- CVPR 2022 Tutorial: Denoising Diffusion-based Generative Modeling: Foundations and Applications, by Kreis, Gao, and Vahdat
- Lilian Weng's blogpost: What are diffusion models?

Generative Modeling

Common methods:

- Variational Autoencoders
- Generative Adversarial Networks (GAN)
- Flow-based models
- Today: Diffusion Models

Diffusion Models: Text-to-Image Generation and More

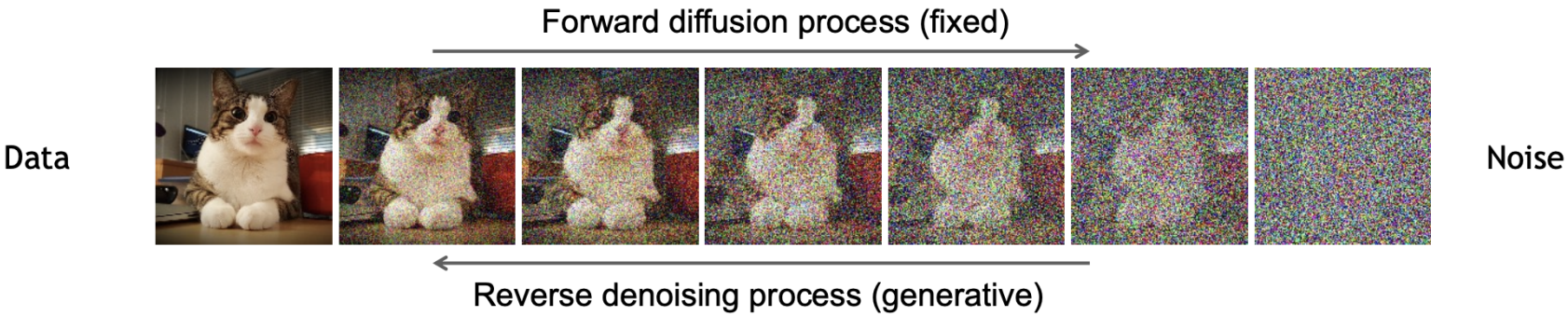
DALL·E 3, prompt: Tiny potato kings wearing majestic crowns, sitting on thrones, overseeing their vast potato kingdom filled with potato subjects and potato castles.

Stable Diffusion 3, prompt: Frog sitting in a 1950s diner wearing a leather jacket and a top hat. On the table is a giant burger and a small sign that says “froggy fridays”.

Diffusion Models

Diffusion models use two processes:

- A *forward process*, start from image and keep adding noise.
- A *reverse process*, start from noise and keep *denoising* it to recover an image.



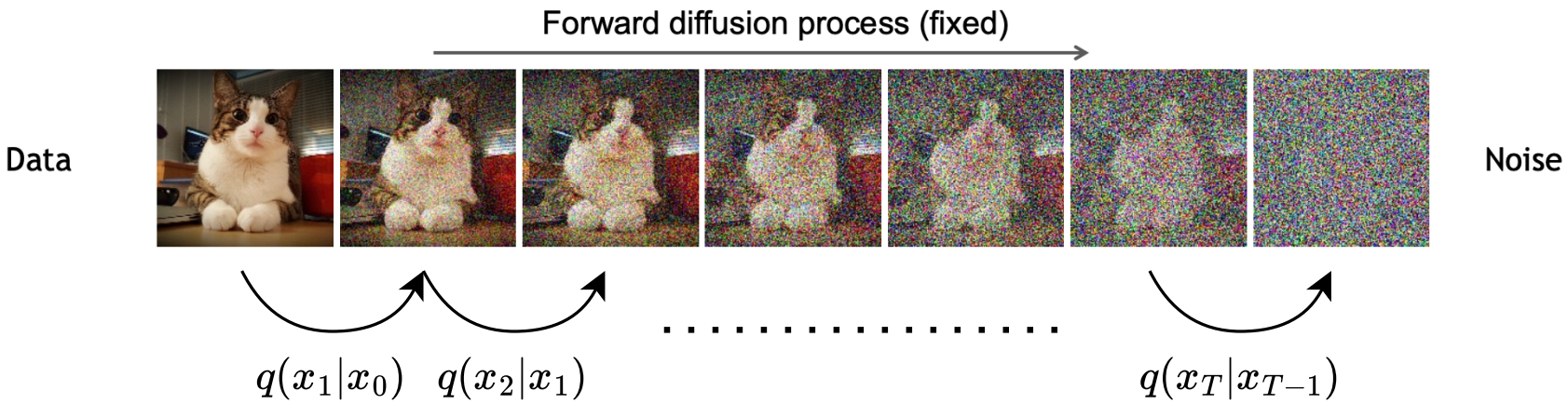
Forward Process

- The forward process is a Markov chain: $q(x_{1:T}|x_0) = \prod_{t=1}^{T} q(x_t|x_{t-1})$
- Each step adds Gaussian noise:

$$q(x_t|x_{t-1}) = \mathcal{N}(\sqrt{1-\beta_t}x_{t-1}, \beta_t I),$$

Or equivalently,

$$x_t = \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}\epsilon_{t-1}, \quad \epsilon_{t-1} \sim \mathcal{N}(0, I).$$



Forward Process

Let $\alpha_t := 1 - \beta_t$ and $\bar{\alpha}_t := \prod_{i=1}^{t} \alpha_i$.

$$\begin{aligned} x_t &= \sqrt{\alpha_t} x_{t-1} + \sqrt{1-\alpha_t}\epsilon_{t-1} \\ &= \sqrt{\alpha_t\alpha_{t-1}} x_{t-2} + \sqrt{\alpha_t(1-\alpha_{t-1})}\epsilon_{t-2} + \sqrt{1-\alpha_t}\epsilon_{t-1} \\ &\overset{(d)}{=} \sqrt{\alpha_t\alpha_{t-1}} x_{t-2} + \sqrt{1-\alpha_t\alpha_{t-1}}\epsilon, \quad \epsilon \sim \mathcal{N}(0, I). \end{aligned}$$

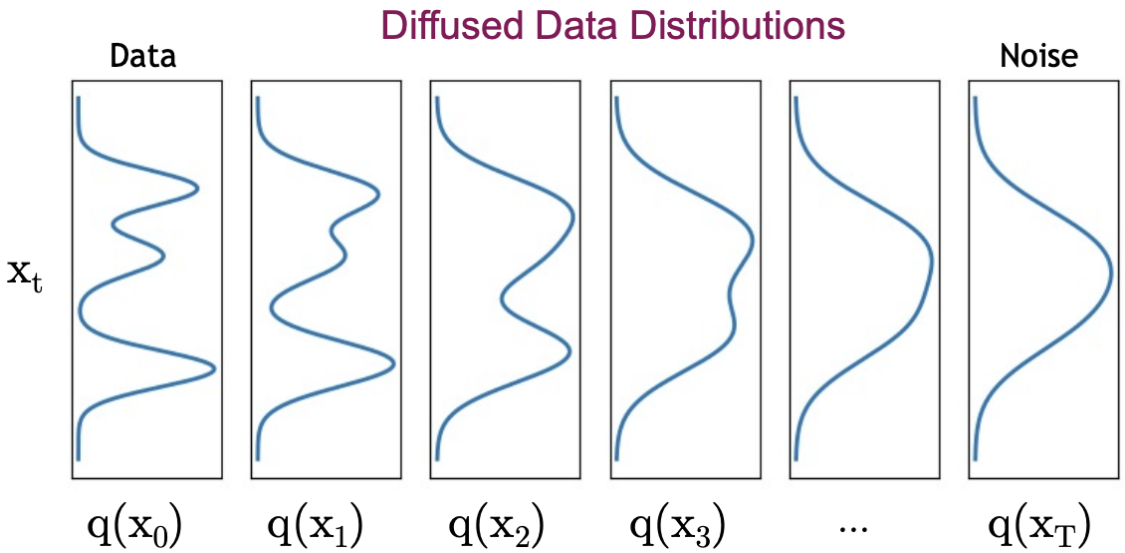
Therefore

$$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, \quad \epsilon \sim \mathcal{N}(0, I).$$

Forward Process and White Noise

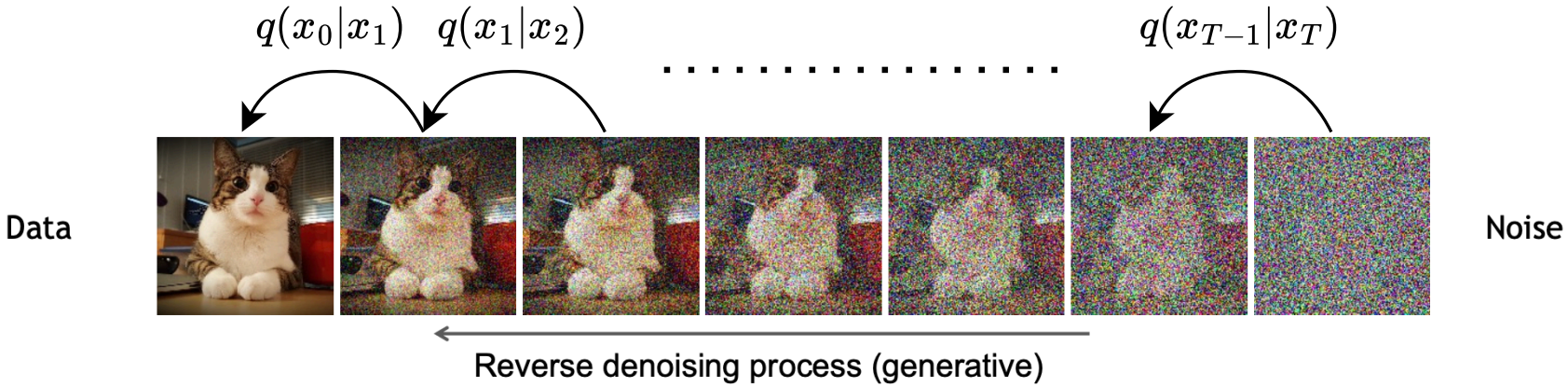
$$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t}\epsilon, \quad \epsilon \sim \mathcal{N}(0, I).$$

$(\beta_t)_{t=1}^T$ is chosen such that $\bar{\alpha}_T \to 0$, thus x_T converges to a standard normal random vector.



Reverse Process

- Ideally, to generate a sample:
  1. $x_T \sim \mathcal{N}(0, I) \approx q(X_T)$.
  2. $x_{t-1} \sim q(x_{t-1}|x_t)$ for $t = T, \ldots, 1$.
- But $q(x_{t-1}|x_t)$ is intractable.



Reverse Process

- $q(x_{t-1}|x_t)$ is approximately normal if β_t is small.
- We approximate it with

$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(\mu_\theta(x_t, t), \sigma_t^2).$$

- μ_θ comes from a trainable architecture (e.g. neural network) with parameter θ.
- For the reverse process

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

- To make $p_\theta(x_{1:T}|x_0)$ close to $q(x_{1:T}|x_0)$, we will use ideas from Variational Inference.

Evidence Lower Bound: ELBO

- Recall the ELBO:

$$KL(q(x_{1:T}|x_0)||p_\theta(x_{1:T}|x_0)) + \mathbb{E}_{x_{1:T}\sim q}\left[\log \frac{p_\theta(x_{0:T})}{q(x_{1:T}|x_0)}\right] = \log p_\theta(x_0)$$

$$\implies \text{Minimize} \quad \mathbb{E}_{x_{0:T}\sim q}\left[\log \frac{q(x_{1:T}|x_0)}{p_\theta(x_{0:T})}\right] =: L.$$

- Our goal becomes minimizing L.

Variational Upper Bound

- While expressing $q(x_{t-1}|x_t)$ is difficult. By Bayes rule, expressing $q(x_{t-1}|x_t, x_0)$ is easy:

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

$$\implies q(x_t|x_{t-1}) = \frac{q(x_t|x_0)q(x_{t-1}|x_t, x_0)}{q(x_{t-1}|x_0)}. \qquad (*)$$

Variational Upper Bound

$$
\begin{aligned}
L &= \mathbb{E}_{x_{0:T}\sim q}\left[\log \frac{q(x_{1:T}|x_0)}{p_\theta(x_{0:T})}\right] \\
&= \mathbb{E}_{x_{0:T}\sim q}\left[\log \frac{\prod_{t=1}^{T} q(x_t|x_{t-1})}{p_\theta(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)}\right] \\
&= \mathbb{E}_{x_{0:T}\sim q}\left[\log \frac{q(x_T|x_0)\prod_{t=2}^{T} q(x_{t-1}|x_t,x_0)}{p_\theta(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)}\right] \quad \text{By } (*) \\
&= \mathbb{E}_{x_{0:T}\sim q}\Bigg[\underbrace{KL(q(x_T|x_0)||p_\theta(x_T))}_{l_T} + \sum_{t=2}^{T}\underbrace{KL(q(x_{t-1}|x_t,x_0)||p_\theta(x_{t-1}|x_t))}_{l_{t-1}} \\
&\quad + \underbrace{-\log p_\theta(x_0|x_1)}_{l_0}\Bigg]
\end{aligned}
$$

Variational Upper Bound

- Let $L_t = \mathbb{E}_q[l_t]$ for $t = 0, \ldots, T$.
- L_T is constant because x_T is just the standard normal random vector.
- To compute L_t for $t = 1, \ldots, T-1$, we first show $q(x_{t-1}|x_t, x_0)$ is Gaussian.

$$
\begin{aligned}
q(x_{t-1}|x_t, x_0) &\propto q(x_t|x_{t-1})q(x_{t-1}|x_0) \\
&\propto \exp\left(-\frac{\|x_t - \sqrt{\alpha_t}x_{t-1}\|^2}{2\beta_t} - \frac{\|x_{t-1} - \sqrt{\bar{\alpha}_{t-1}}x_0\|^2}{2(1-\bar{\alpha}_{t-1})}\right) \\
&\propto \exp\left(-\frac{\|x_{t-1} - \tilde{\mu}(x_t, x_0)\|^2}{2\tilde{\beta}_t}\right),
\end{aligned}
$$

Variational Upper Bound

- Therefore, $q(x_{t-1}|x_t, x_0) = \mathcal{N}(\tilde{\mu}(x_t, x_0), \tilde{\beta}_t I)$.
- Basic algebra shows

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

$$\tilde{\beta}_t = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t.$$

- Computing KL between two Gaussians is straightforward:

$$\begin{aligned} L_{t-1} &= \mathbb{E}_q \left[KL(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t)) \right] \\ &= \mathbb{E}_q \left[\frac{\|\tilde{\mu}(x_t, x_0) - \mu_\theta(x_t, t)\|^2}{2\sigma_t^2} \right] + \text{ const.} \end{aligned}$$

Parameterizing the Mean

- Recall $x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, \quad \epsilon \sim \mathcal{N}(0, I)$.
- By plugging in x_0 in terms of x_t and ϵ:

$$\tilde{\mu}(x_t, x_0) = \frac{1}{\sqrt{\alpha_t}} \left(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}} \epsilon \right).$$

- As a result, we parameterize $\mu_\theta(x_t)$ to try to predict the noise using a neural network $\epsilon_\theta(x_t, t)$,

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

Training Objective

- The loss thus becomes

$$L_{t-1} = \underbrace{\frac{\beta_t^2}{2\sigma_t^2\alpha_t(1-\alpha_t)}}_{\lambda_t} \mathbb{E}_{x_0\sim q,\epsilon\sim\mathcal{N}(0,I)}\left[\|\epsilon_\theta(x_t,t)-\epsilon\|^2\right],$$

  where $x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon$.
- Ho et al. [2020] observed that the performance improves if we simply choose $\lambda_t = 1$.
- The simplified loss is thus

$$L_{t-1}^{\text{simple}} = \mathbb{E}_{x_0\sim q,\epsilon\sim\mathcal{N}(0,I)}\left[\|\epsilon_\theta\left(\sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t\right)-\epsilon\|^2\right].$$

Test-Time Sample Generation

- Start from $x_T \sim \mathcal{N}(0, I)$.
- For $t = T, \ldots, 1$, sample $x_{t-1} \sim p_\theta(x_{t-1}|x_t)$
  - Recall $p_\theta(x_{t-1}|x_t) = \mathcal{N}(\mu_\theta(x_t, t), \sigma_t^2)$.
  - As a result

$$x_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(x_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \epsilon_\theta(x_t, t) \right) + \sigma_t z, \quad z \sim \mathcal{N}(0, I).$$

Summary

Algorithm 1 Training

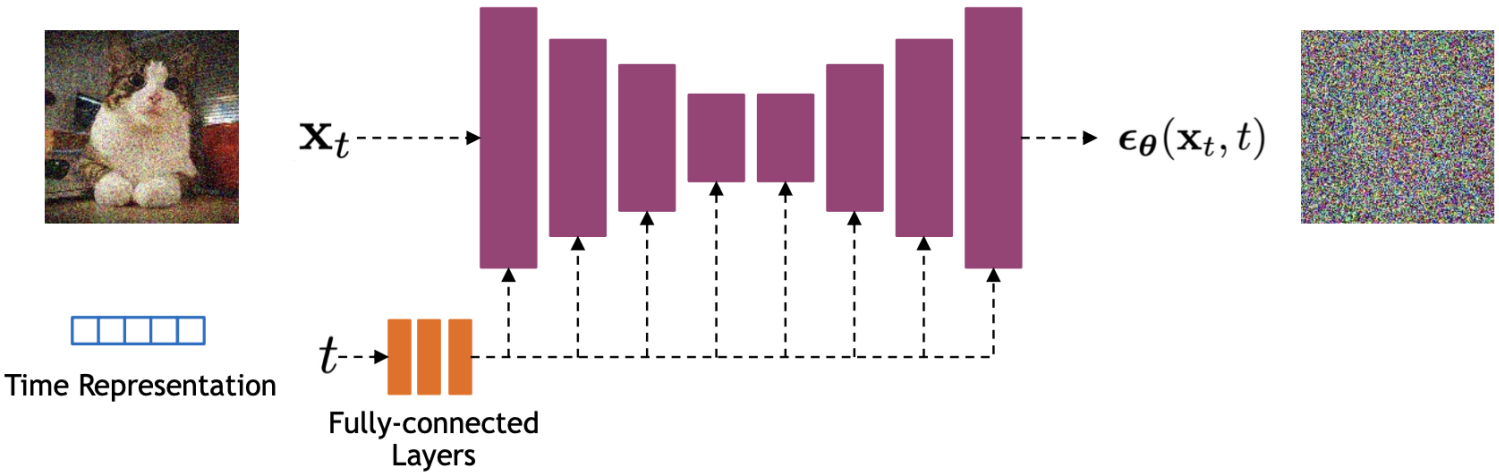
repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \text{Uniform}(\{1, \dots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
    $$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0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

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \dots, 1$ **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 $\mathbf{x}_0$

Design Choices: Architecture

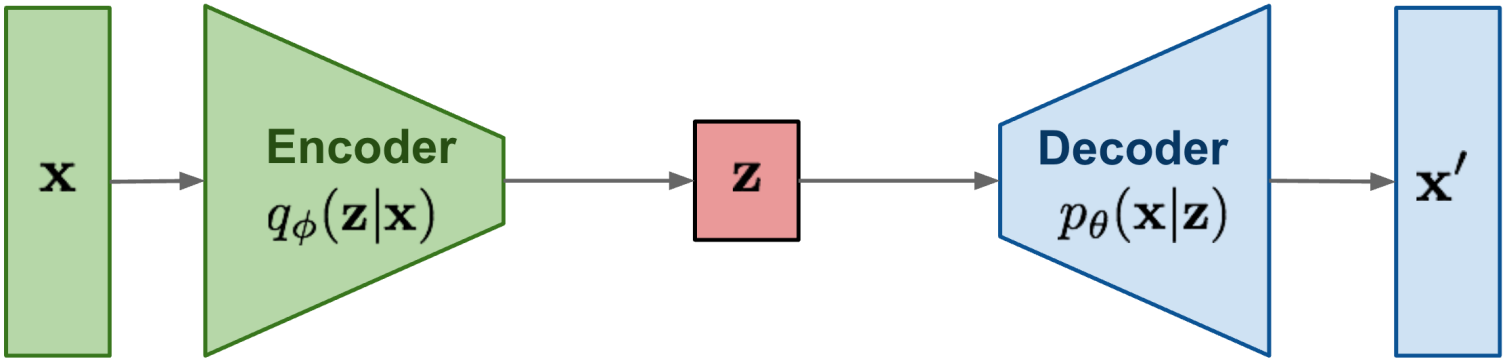
- $\epsilon_\theta(x_t, t)$ is implemented using a **U-Net** architecture, with **residual blocks** and **self-attention** layers.
- Weights are shared across time.



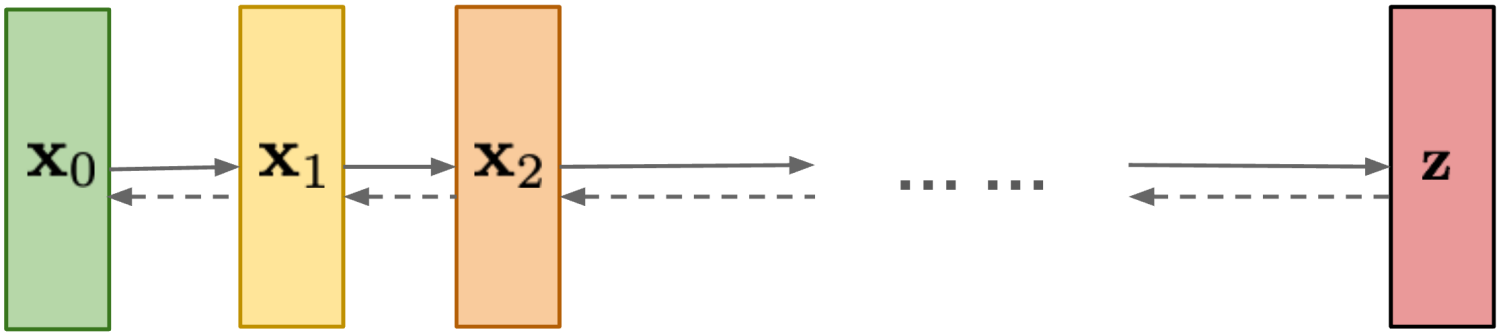
Design Choices: Hyperparameters

- β_t and σ_t control the variance of the forward and reverse process respectively.
- β_t is chosen linearly between $\beta_1 = 10^{-4}$ and $\beta_T = 0.02$.
- $\sigma_t^2 = \beta_t$. We could instead consider a trainable full covariance matrix, i.e. $\Sigma_\theta(x_t, t)$.
- $T = 1000$ steps are taken.
- Fancier β_t schedules can further reduce loss [Nichol and Dhariwal, 2021].

Comparison with Variational Autoencoders (VAE)



VAE



Diffusion Model

Comparison with VAEs

- Diffusion models and VAEs both map to isotropic Gaussian.
- The latent space has the same dimension as the input space in DMs. In VAEs, it is smaller dimensional.
- The forward process is the encoder, which is **fixed**. This is trained in VAEs.
- The reverse process is the decoder, which is **trained**, similar to the VAEs.

Conditional Generation

- The original examples we saw were images generated conditioned on a text caption. More examples:

Midjourney, prompt: A close-up profile of a cute green-eyed kitten with a black nose and light cheeks sitting on top of a wooden floor under bright daylight.

DALL·E 3, prompt: Illustration of a chic chair with a design reminiscent of a pumpkin's form, with deep orange cushioning, in a stylish loft setting.

- But the diffusion model we learned about can only generate unconditioned images.

Conditional Generation: General Formulation

- Suppose we want to condition on y (e.g. class label or describing caption).
- The training data are pairs of (x_0, y).
- Conditional reverse process:

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

- We still model the transition probabilities as Gaussian:

$$p_\theta(x_{t-1}|x_t, y) = \mathcal{N}(\mu_\theta(x_t, t, c), \Sigma_\theta(x_t, t, y)).$$

Conditional Generation

- The new loss:

$$L = \mathbb{E}_q \left[l_T + \sum_{t \geq 2} KL(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t, y)) - \log p_\theta(x_0|x_1, y\ ) \right]$$

- How to incorporate y into the U-Net architecture?
  - Different techniques for different types of conditioning (labels, images, captions, ...)

Classifier Guidance

- To further strengthen conditioning, we can train a classifier $p_\phi(y|x)$ and incorporate its log-gradient into score with a scale s.
- [Nichol and Dhariwal, 2021]

Algorithm 1 Classifier guided diffusion sampling, given a diffusion model $(\mu_\theta(x_t), \Sigma_\theta(x_t))$, classifier $p_\phi(y|x_t)$, and gradient scale s.

Input: class label y, gradient scale s
$x_T \leftarrow$ sample from $\mathcal{N}(0, \mathbf{I})$
for all t from T to 1 **do**
  $\mu, \Sigma \leftarrow \mu_\theta(x_t), \Sigma_\theta(x_t)$
  $x_{t-1} \leftarrow$ sample from $\mathcal{N}(\mu + s\Sigma \nabla_{x_t} \log p_\phi(y|x_t), \Sigma)$
end for
return x_0

Classifier-Free Guidance

- Instead of training a separate classifier, simultaneously train a conditional and an unconditional diffusion model.
- We have an implicit classifier by Bayes rule,

$$p(y|x_t) \propto_y \frac{p(x_t|y)}{p(x_t)}.$$

- We can simply use

$$\nabla_{x_t} \log p(y|x_t) = \nabla_{x_t} \log p(x_t|y) - \nabla_{x_t} \log p(x_t).$$

Tradeoff: Sample Quality vs Diversity

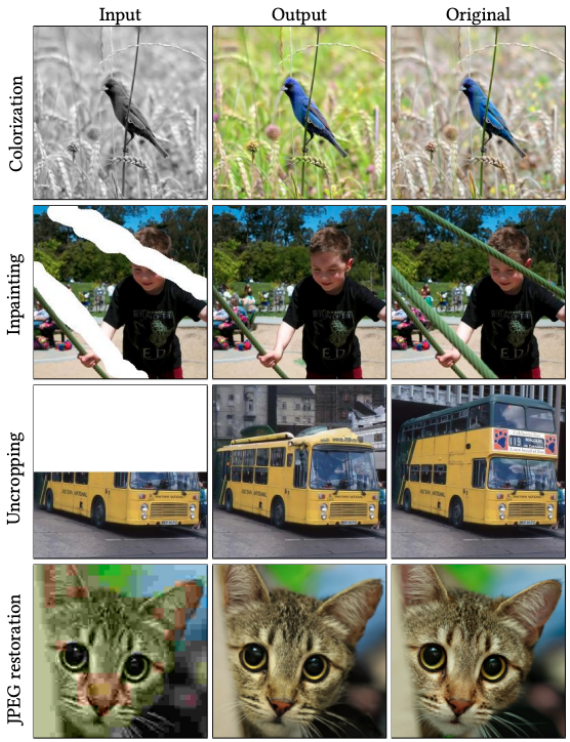
s = 0

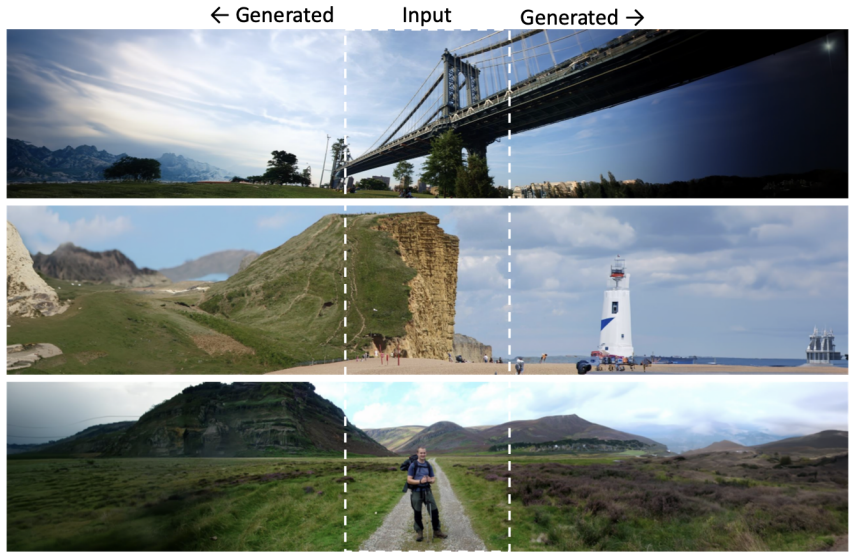
s = 1

s = 3

Conditioning Applications

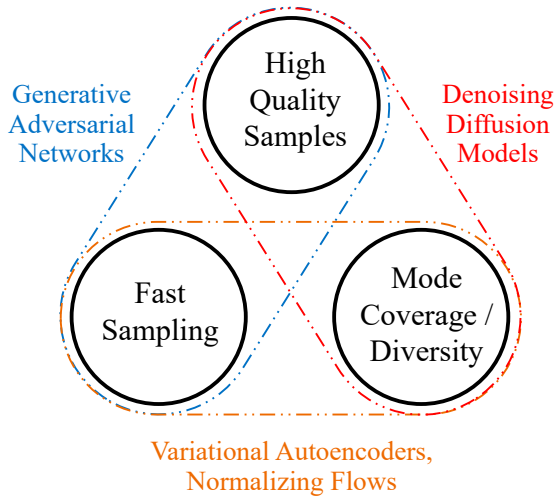
Conditioning is not always on captions.





[Saharia et al., 2022]

Tradeoffs in Generative Modeling



[Xiao et al., 2021]

- Accelerating diffusion models can overcome the above trilemma.

Summary

- Diffusion Models: Forward and Reverse Processes
- Training via Variational Upper Bounds
- Conditional Generation
- Tradeoffs

Topics for Further Reading

- Denoising Score Matching [Song et al., 2021]
- Probability Flow ODE [Song et al., 2021]

References I

Jonathan Ho, Ajay Jain, and Pieter Abbeel. Denoising diffusion probabilistic models. *Advances in neural information processing systems*, 33:6840–6851, 2020.

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