Machine Learning Department
School of Computer Science
Carnegie Mellon University

Diffusion Models
+
Variational Autoencoders (VAEs)

Matt Gormley & Aran Nayebi
Lecture 8
Sep. 22, 2025

Reminders

- **Homework 1: Generative Models of Text**
  - Out: Mon, Sep 8
  - Due: Mon, Sep 22 at 11:59pm
- **Quiz 2:**
  - In-class: Wed, Sep 24
  - Lectures 5-8
- **Homework 2: Generative Models of Images**
  - Out: Mon, Sep 22
  - Due: Sat, Oct 4 at 11:59pm

Recap of…

DIFFUSION MODELS

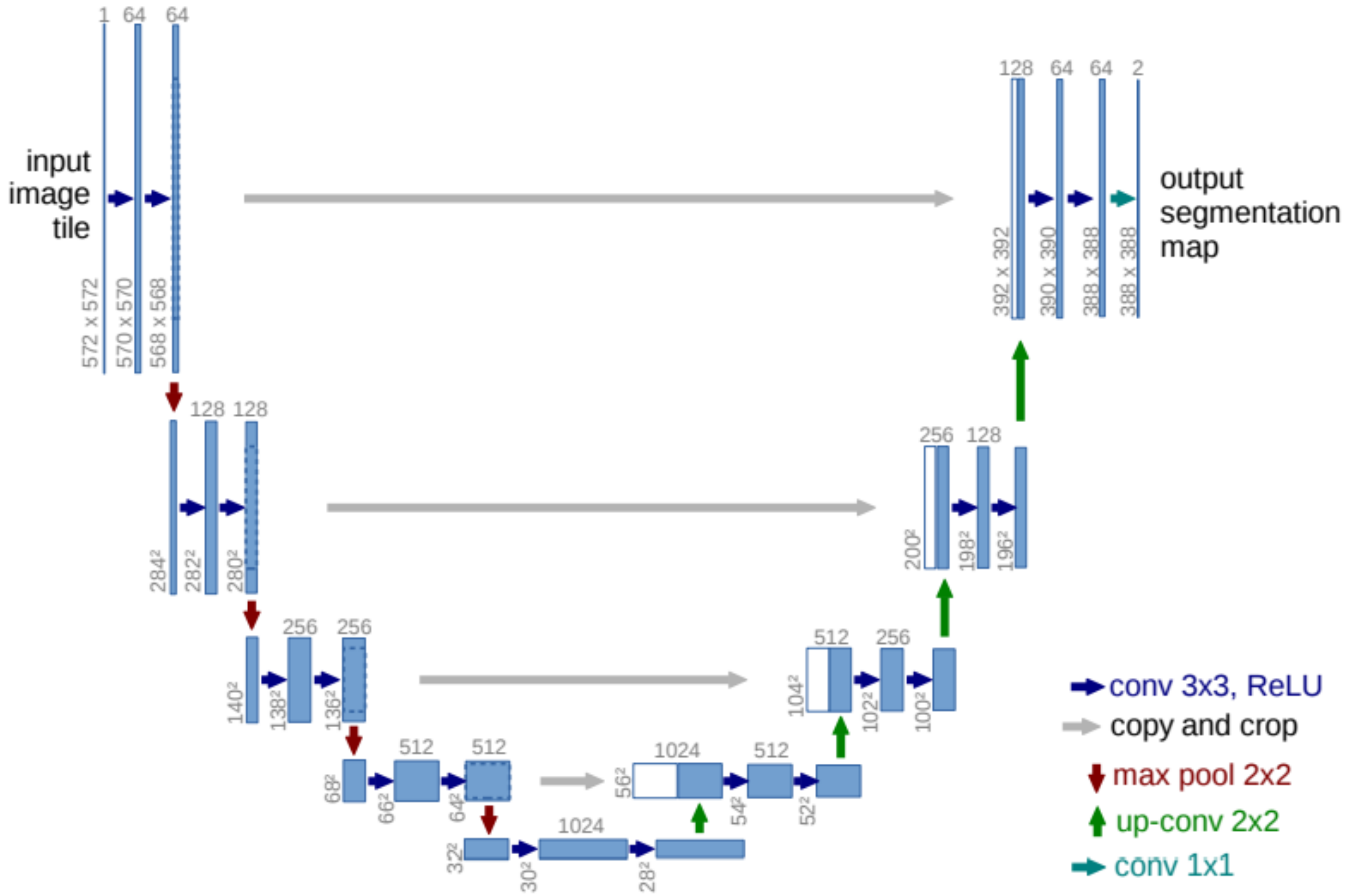
U-Net

Contracting path

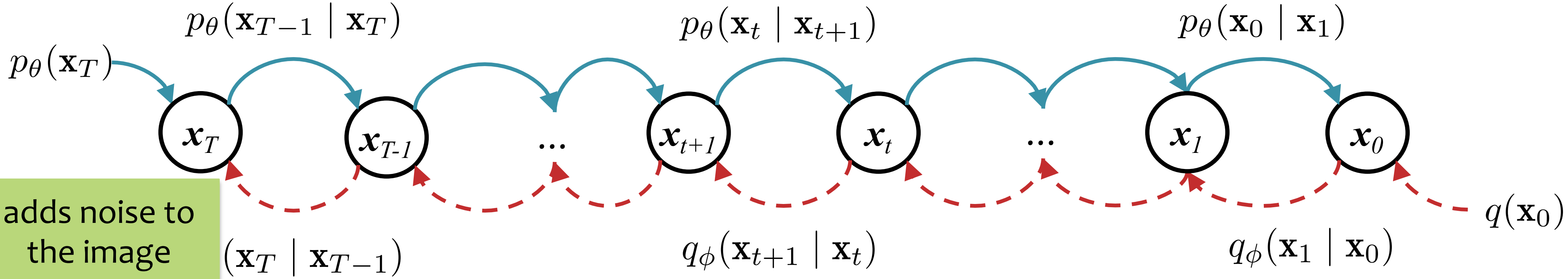
- block consists of:
  - 3x3 convolution
  - 3x3 convolution
  - ReLU
  - max-pooling with stride of 2 (downsample)
- repeat the block N times, doubling number of channels

Expanding path

- block consists of:
  - 2x2 convolution (upsampling)
  - concatenation with contracting path features
  - 3x3 convolution
  - 3x3 convolution
  - ReLU
- repeat the block N times, halving the number of channels



Diffusion Model



adds noise to the image

Forward Process:

if we could sample from this we'd be done

$$q_\phi(\mathbf{x}_{0:T}) = \boxed{q(\mathbf{x}_0)} \prod_{t=1}^{T} q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1})$$

(Learned) Reverse Process:

removes noise

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

goal is to learn this

(Exact) Reverse Process:

$$q_\phi(\mathbf{x}_{0:T}) = q_\phi(\mathbf{x}_T) \prod_{t=1}^{T} q_\phi(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$$

The *exact* reverse process requires inference. And, even though $q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1})$ is simple, computing $q_\phi(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$ is intractable! Why? Because $q(\mathbf{x}_0)$ might be not-so-simple.

$$q_\phi(\mathbf{x}_{t-1} \mid \mathbf{x}_t) = \frac{\int_{\mathbf{x}_{0:t-2,t+1:T}} q_\phi(\mathbf{x}_{0:T}) d\mathbf{x}_{0:t-2,t+1:T}}{\int_{\mathbf{x}_{0:t-2,t:T}} q_\phi(\mathbf{x}_{0:T}) d\mathbf{x}_{0:t-2,t:T}}$$

Diffusion Model

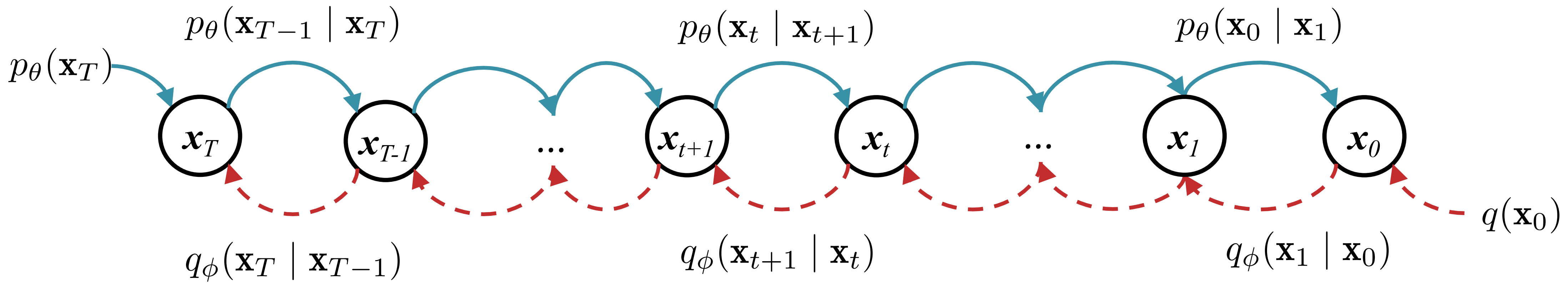
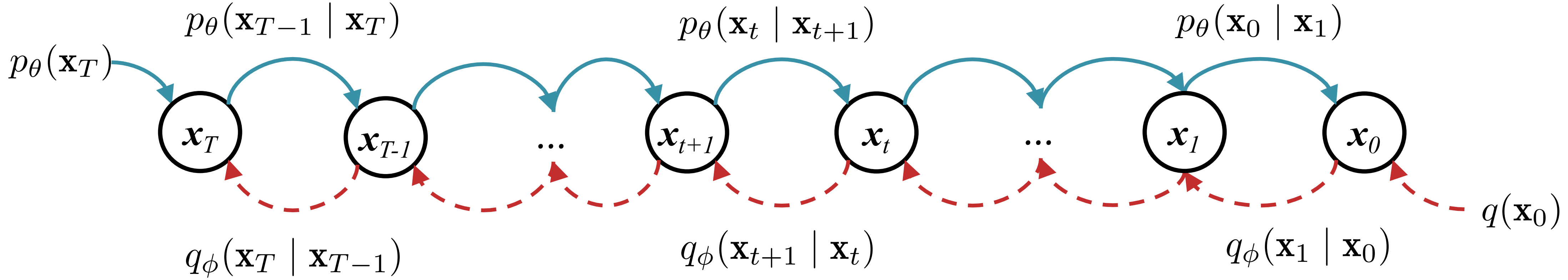


Figure from Ho et al. (2020)

Denoising Diffusion Probabilistic Model (DDPM)



Forward Process:

$$q_\phi(\mathbf{x}_{0:T}) = q(\mathbf{x}_0) \prod_{t=1}^{T} q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1})$$

$$q(\mathbf{x}_0) = \text{data distribution}$$

$$q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1}) \sim \mathcal{N}(\sqrt{\alpha_t}\mathbf{x}_{t-1}, (1-\alpha_t)\mathbf{I})$$

(Learned) Reverse Process:

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

$$p_\theta(\mathbf{x}_T) \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

$$p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t) \sim \mathcal{N}(\mu_\theta(\mathbf{x}_t, t), \mathbf{\Sigma}_\theta(\mathbf{x}_t, t))$$

Gaussians (an aside)

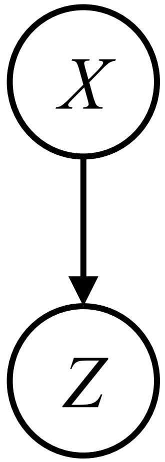
Let $X \sim \mathcal{N}(\mu_x, \sigma_x^2)$ and $Y \sim \mathcal{N}(\mu_y, \sigma_y^2)$

1. Sum of two Gaussians is a Gaussian. $X+Y \sim \mathcal{N}(\mu_x+\mu_y, \sigma_x^2+\sigma_y^2)$
2. Difference of two Gaussians is a Gaussian. $X-Y \sim \mathcal{N}(\mu_x-\mu_y, \sigma_x^2+\sigma_y^2)$

Let $Z \mid X \sim \mathcal{N}(\mu_z = g(X), \sigma_z^2)$

3. Gaussian with a Gaussian mean passed through a *linear/affine* function $g(\cdot)$ has a Gaussian marginal,

$p_Z(z) = \int_x p_{Z|X}(z|x) p_X(x)\, dx$ is a Gaussian density



Defining the Forward Process

Forward Process:

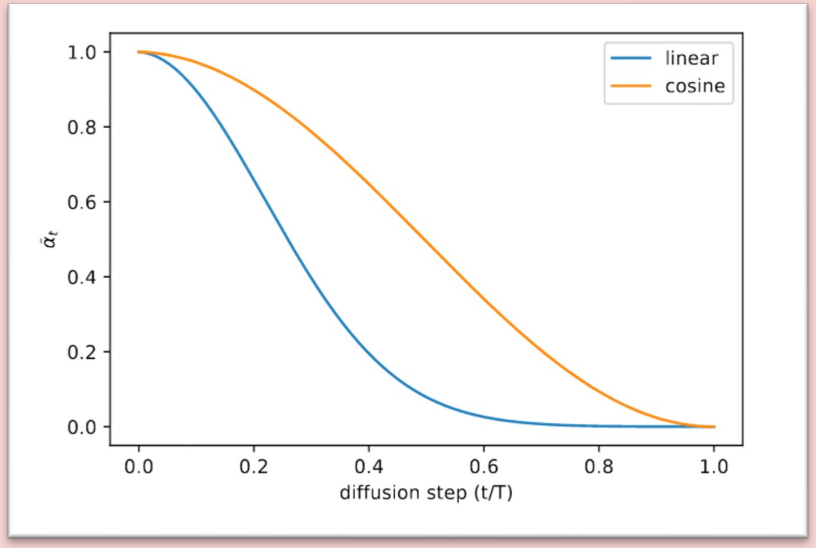
$$q_\phi(\mathbf{x}_{0:T}) = q(\mathbf{x}_0) \prod_{t=1}^{T} q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1})$$

$$q(\mathbf{x}_0) = \text{data distribution}$$

$$q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1}) \sim \mathcal{N}(\sqrt{\alpha_t}\mathbf{x}_{t-1}, (1-\alpha_t)\mathbf{I})$$

Noise schedule:

We choose α_t to follow a fixed schedule s.t. $q_\phi(\mathbf{x}_T) \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$, just like $p_\theta(\mathbf{x}_T)$.



Property #1:

$$q(\mathbf{x}_t \mid \mathbf{x}_0) \sim \mathcal{N}(\sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$$

$$\text{where } \bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$$

Q: So what is $q_\phi(\mathbf{x}_T \mid \mathbf{x}_0)$? Note the *capital* T in the subscript.

A:

$$q(\mathbf{x}_T \mid \mathbf{x}_0) \sim \mathcal{N}(\boldsymbol{\mu} \approx \mathbf{0}, \boldsymbol{\Sigma} \approx \mathbf{I})$$

Gaussians (an aside)

Let $X \sim \mathcal{N}(\mu_x, \sigma_x^2)$ and $Y \sim \mathcal{N}(\mu_y, \sigma_y^2)$

1. Sum of two Gaussians is a Gaussian. $X + Y \sim \mathcal{N}(\mu_x + \mu_y, \sigma_x^2 + \sigma_y^2)$
2. Difference of two Gaussians is a Gaussian. $X - Y \sim \mathcal{N}(\mu_x - \mu_y, \sigma_x^2 + \sigma_y^2)$

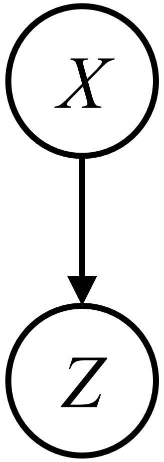
Let $Z \mid X \sim \mathcal{N}(\mu_z = g(X), \sigma_z^2)$

3. Gaussian with a Gaussian mean passed through a *linear/affine* function $g(\cdot)$ has a Gaussian marginal,

   $p_Z(z) = \int_x p_{Z|X}(z|x) p_X(x)\, dx$ is a Gaussian density

   and a Gaussian posterior.

   $p_{X|Z}(x \mid z) = p_{Z|X}(z|x) p_X(x) / p_Z(z)$ is a Gaussian density



Parameterizing the *learned* reverse process

Recall: $p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t) \sim \mathcal{N}(\mu_\theta(\mathbf{x}_t, t), \mathbf{\Sigma}_\theta(\mathbf{x}_t, t))$

Later we will show that given a training sample $\mathbf{x}_0$, we want

$$p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$$

to be as close as possible to

$$q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)$$

Intuitively, this makes sense: if the *learned* reverse process is supposed to subtract away the noise, then whenever we're working with a specific $\mathbf{x}_0$ it should subtract it away exactly as *exact* reverse process would have.

Properties of forward and *exact* reverse processes

Property #1:

$$q(\mathbf{x}_t \mid \mathbf{x}_0) \sim \mathcal{N}(\sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$$

$$\text{where } \bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$$

$\Rightarrow$ we can sample $\mathbf{x}_t$ from $\mathbf{x}_0$ at any timestep t efficiently in closed form

$\Rightarrow$ $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}$ where $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

Property #2: Estimating $q(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$ is intractable because of its dependence on $q(\mathbf{x}_0)$. However, conditioning on $\mathbf{x}_0$ we can efficiently work with:

$$q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0), \sigma_t^2\mathbf{I})$$

$$\begin{aligned}
\text{where } \tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0) &= \frac{\sqrt{\bar{\alpha}_t}(1-\alpha_t)}{1-\bar{\alpha}_t}\mathbf{x}_0 + \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_t)}{1-\bar{\alpha}_t}\mathbf{x}_t \\
&= \alpha_t^{(0)}\mathbf{x}_0 + \alpha_t^{(t)}\mathbf{x}_t \\
\sigma_t^2 &= \frac{(1-\bar{\alpha}_{t-1})(1-\alpha_t)}{1-\bar{\alpha}_t}
\end{aligned}$$

Property #3: Combining the two previous properties, we can obtain a different parameterization of $\tilde{\mu}_q$ which has been shown empirically to help in learning p_θ.

Rearranging $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}$ we have that:

$$\mathbf{x}_0 = \left(\mathbf{x}_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}\right) / \sqrt{\bar{\alpha}_t}$$

Substituting this definition of $\mathbf{x}_0$ into property #2's definition of $\tilde{\mu}_q$ gives:

$$\begin{aligned}
\tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0) &= \alpha_t^{(0)}\mathbf{x}_0 + \alpha_t^{(t)}\mathbf{x}_t \\
&= \alpha_t^{(0)}\left(\left(\mathbf{x}_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}\right) / \sqrt{\bar{\alpha}_t}\right) + \alpha_t^{(t)}\mathbf{x}_t \\
&= \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{(1-\alpha_t)}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}\right)
\end{aligned}$$

Parameterizing the *learned* reverse process

Recall: $p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t) \sim \mathcal{N}(\mu_\theta(\mathbf{x}_t, t), \mathbf{\Sigma}_\theta(\mathbf{x}_t, t))$

Idea #1: Rather than learn $\Sigma_\theta(\mathbf{x}_t, t)$ just use what we know about $q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) \sim \mathcal{N}(\tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0), \sigma_t^2 \mathbf{I})$:

$$\Sigma_\theta(\mathbf{x}_t, t) = \sigma_t^2 \mathbf{I}$$

Idea #2: Choose μ_θ based on $q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)$, i.e. we want $\mu_\theta(\mathbf{x}_t, t)$ to be close to $\tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0)$. Here are three ways we could parameterize this:

Option A: Learn a network that approximates $\tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0)$ directly from $\mathbf{x}_t$ and t:

$$\mu_\theta(\mathbf{x}_t, t) = \text{UNet}_\theta(\mathbf{x}_t, t)$$

where t is treated as an extra feature in UNet

Option B: Learn a network that approximates the real $\mathbf{x}_0$ from only $\mathbf{x}_t$ and t:

$$\mu_\theta(\mathbf{x}_t, t) = \alpha_t^{(0)} \mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) + \alpha_t^{(t)} \mathbf{x}_t$$

where $\mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) = \text{UNet}_\theta(\mathbf{x}_t, t)$

Option C: Learn a network that approximates the ϵ that gave rise to $\mathbf{x}_t$ from $\mathbf{x}_0$ in the forward process from $\mathbf{x}_t$ and t:

$$\mu_\theta(\mathbf{x}_t, t) = \alpha_t^{(0)} \mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) + \alpha_t^{(t)} \mathbf{x}_t$$

where $\mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) = \left(\mathbf{x}_t - \sqrt{1 - \bar{\alpha}_t}\,\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) / \sqrt{\bar{\alpha}_t}$

where $\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) = \text{UNet}_\theta(\mathbf{x}_t, t)$

Gaussians (an aside)

Let $X \sim \mathcal{N}(\mu_x, \sigma_x^2)$ and $Y \sim \mathcal{N}(\mu_y, \sigma_y^2)$

1. Sum of two Gaussians is a Gaussian. $X+Y \sim \mathcal{N}(\mu_x+\mu_y, \sigma_x^2+\sigma_y^2)$
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   and a Gaussian posterior.

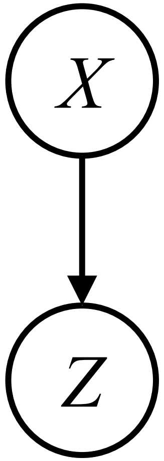
   $p_{X|Z}(x \mid z) = p_{Z|X}(z|x) p_X(x) / p_Z(z)$ is a Gaussian density

4. Gaussian with a Gaussian mean passed through a *nonlinear* function $g(\cdot)$ does not have a Gaussian marginal,

   $p_Z(z) = \int_x p_{Z|X}(z|x) p_X(x)\, dx$ is **not** a Gaussian density in general

   nor a Gaussian posterior.

   $p_{X|Z}(x \mid z) = p_{Z|X}(z|x) p_X(x) / p_Z(z)$ is **not** a Gaussian density in general



DIFFUSION MODEL TRAINING

Learning the Reverse Process

Recall: given a training sample $\mathbf{x}_0$, we want

$$p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$$

to be as close as possible to

$$q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)$$

Depending on which of the options for parameterization we pick, we get a different training algorithm.

Algorithm 1 Training (Option A, all timesteps)

initialize θ
for $e \in \{1, \ldots, E\}$ **do**
    for $x_0 \in \mathcal{D}$ **do**
        for $t \in \{1, \ldots, T\}$ **do**
            $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
            $\mathbf{x}_t \leftarrow \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}$
            $\tilde{\mu}_q \leftarrow \alpha_t^{(0)}\mathbf{x}_0 + \alpha_t^{(t)}\mathbf{x}_t$
            $\ell_t(\theta) \leftarrow \|\tilde{\mu}_q - \mu_\theta(\mathbf{x}_t, t)\|^2$
        $\theta \leftarrow \theta - \nabla_\theta \sum_{t=1}^{T} \ell_t(\theta)$

Option A: Learn a network that approximates $\tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0)$ directly from $\mathbf{x}_t$ and t:

$$\mu_\theta(\mathbf{x}_t, t) = \text{UNet}_\theta(\mathbf{x}_t, t)$$

where t is treated as an extra feature in UNet

Learning the Reverse Process

Recall: given a training sample $\mathbf{x}_0$, we want

$$p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$$

to be as close as possible to

$$q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)$$

Depending on which of the options for parameterization we pick, we get a different training algorithm.

Algorithm 1 Training (Option A)

1: initialize θ
2: **for** $e \in \{1, \ldots, E\}$ **do**
3: **for** $x_0 \in \mathcal{D}$ **do**
4: $t \sim$ Uniform$(1, \ldots, T)$
5: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
6: $\mathbf{x}_t \leftarrow \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}$
7: $\tilde{\mu}_q \leftarrow \alpha_t^{(0)}\mathbf{x}_0 + \alpha_t^{(t)}\mathbf{x}_t$
8: $\ell_t(\theta) \leftarrow \|\tilde{\mu}_q - \mu_\theta(\mathbf{x}_t, t)\|^2$
9: $\theta \leftarrow \theta - \nabla_\theta \ell_t(\theta)$

Option A: Learn a network that approximates $\tilde{\mu}_q(\mathbf{x}_t, \mathbf{x}_0)$ directly from $\mathbf{x}_t$ and t:

$$\mu_\theta(\mathbf{x}_t, t) = \text{UNet}_\theta(\mathbf{x}_t, t)$$

where t is treated as an extra feature in UNet

Learning the Reverse Process

Recall: given a training sample $\mathbf{x}_0$, we want

$$p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$$

to be as close as possible to

$$q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)$$

Depending on which of the options for parameterization we pick, we get a different training algorithm.

Algorithm 1 Training (Option B)

initialize θ
for $e \in \{1, \dots, E\}$ **do**
  for $x_0 \in \mathcal{D}$ **do**
    $t \sim$ Uniform$(1, \dots, T)$
    $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
    $\mathbf{x}_t \leftarrow \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}$
    $\ell_t(\theta) \leftarrow \|\mathbf{x}_0 - \mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t)\|^2$
    $\theta \leftarrow \theta - \nabla_\theta \ell_t(\theta)$

Option B: Learn a network that approximates the real $\mathbf{x}_0$ from only $\mathbf{x}_t$ and t:

$$\mu_\theta(\mathbf{x}_t, t) = \alpha_t^{(0)}\mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) + \alpha_t^{(t)}\mathbf{x}_t$$

where $\mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) = \text{UNet}_\theta(\mathbf{x}_t, t)$

Learning the Reverse Process

Recall: given a training sample $\mathbf{x}_0$, we want

$$p_\theta(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$$

to be as close as possible to

$$q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)$$

Depending on which of the options for parameterization we pick, we get a different training algorithm.

Option C is the best empirically

Algorithm 1 Training (Option C)

1: initialize θ
2: **for** $e \in \{1, \ldots, E\}$ **do**
3:     **for** $x_0 \in \mathcal{D}$ **do**
4:         $t \sim \text{Uniform}(1, \ldots, T)$
5:         $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
6:         $\mathbf{x}_t \leftarrow \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}$
7:         $\ell_t(\theta) \leftarrow \|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\|^2$
8:         $\theta \leftarrow \theta - \nabla_\theta \ell_t(\theta)$

Option C: Learn a network that approximates the ϵ that gave rise to $\mathbf{x}_t$ from $\mathbf{x}_0$ in the forward process from $\mathbf{x}_t$ and t:

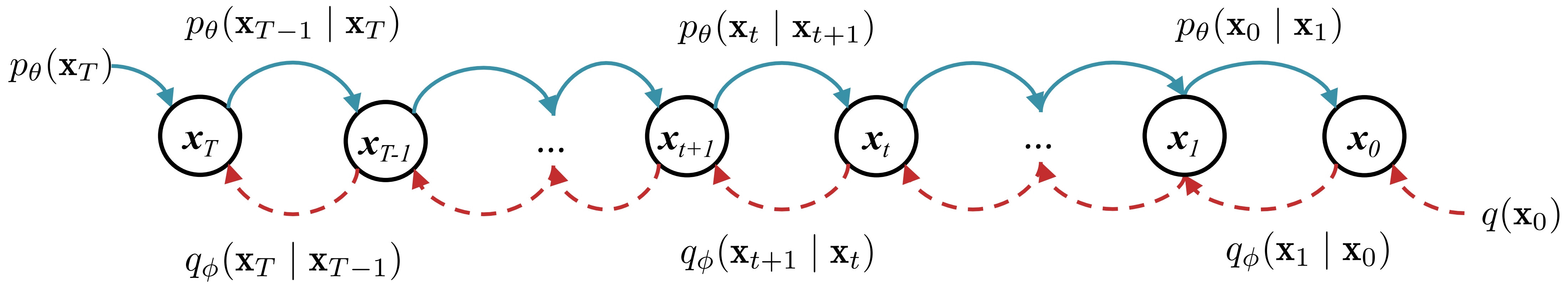
$$\mu_\theta(\mathbf{x}_t, t) = \alpha_t^{(0)} \mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) + \alpha_t^{(t)} \mathbf{x}_t$$

where $\mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) = \left(\mathbf{x}_t - \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) / \sqrt{\bar{\alpha}_t}$

where $\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) = \text{UNet}_\theta(\mathbf{x}_t, t)$

Training (Computation Graph)

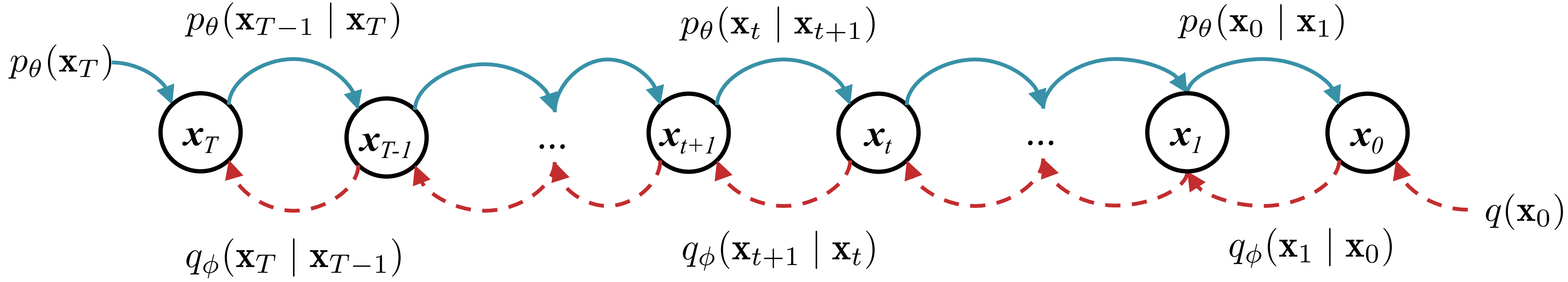
Sampling from the *learned* reverse process



Algorithm 1 Sampling

1: $\mathbf{x}_T \sim p_\theta(\mathbf{x}_T)$
2: **for** $t \in \{T, \dots, 1\}$ **do**
3: $\quad \mathbf{x}_{t-1} \sim p(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$
4: **return** $\mathbf{x}_0$

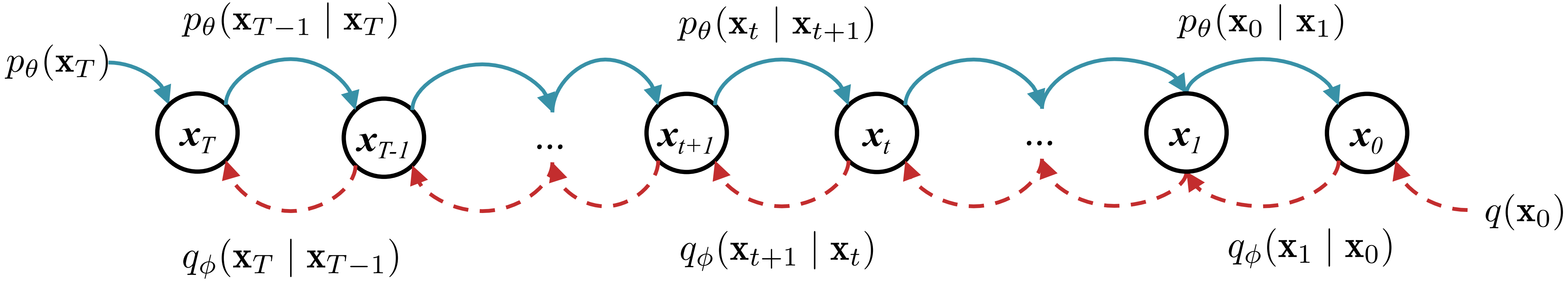
Sampling from the *learned* reverse process



Algorithm 1 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t \in \{T, \dots, 1\}$ **do**
    $\mathbf{x}_{t-1} \sim \mathcal{N}(\mu_\theta(\mathbf{x}_t, t), \mathbf{\Sigma}_\theta(\mathbf{x}_t, t))$
return $\mathbf{x}_0$

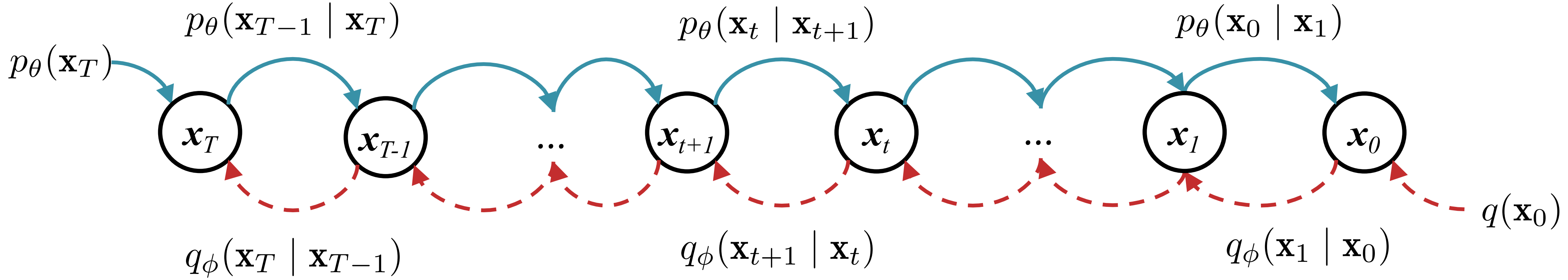
Sampling from the *learned* reverse process



Algorithm 1 Sampling (Option A)

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t \in \{T, \ldots, 1\}$ **do**
3: $\quad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
4: $\quad \mathbf{x}_{t-1} \leftarrow \mu_\theta(\mathbf{x}_t, t) + \sigma_t \boldsymbol{\epsilon}$
5: **return** $\mathbf{x}_0$

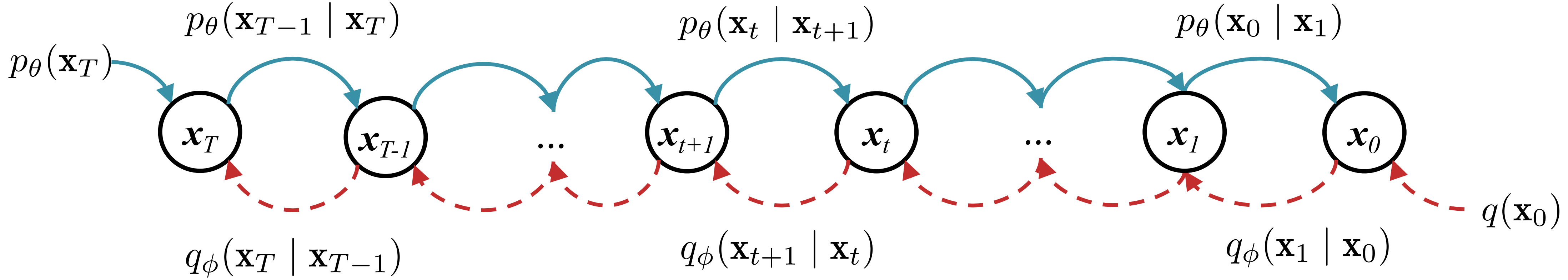
Sampling from the *learned* reverse process



Algorithm 1 Sampling (Option B)

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t \in \{T, \ldots, 1\}$ **do**
3: $\quad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
4: $\quad \hat{\boldsymbol{\mu}}_t \leftarrow \alpha_t^{(0)} \mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) + \alpha_t^{(t)} \mathbf{x}_t$
5: $\quad \mathbf{x}_{t-1} \leftarrow \hat{\boldsymbol{\mu}}_t + \sigma_t \boldsymbol{\epsilon}$
6: **return** $\mathbf{x}_0$

Sampling from the *learned* reverse process



Algorithm 1 Sampling (Option C)

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t \in \{T, \ldots, 1\}$ **do**
3: $\quad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
4: $\quad \hat{\mathbf{x}}_0 \leftarrow \left(\mathbf{x}_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) / \sqrt{\bar{\alpha}_t}$
5: $\quad \hat{\boldsymbol{\mu}}_t \leftarrow \alpha_t^{(0)} \hat{\mathbf{x}}_0 + \alpha_t^{(t)} \mathbf{x}_t$
6: $\quad \mathbf{x}_{t-1} \leftarrow \hat{\boldsymbol{\mu}}_t + \sigma_t \boldsymbol{\epsilon}$
7: **return** $\mathbf{x}_0$

Unsupervised Learning

Assumptions:

1. our data comes from some distribution $p^*(\mathbf{x}_0)$
2. we choose a distribution $p_\theta(\mathbf{x}_0)$ for which sampling $x_0 \sim p_\theta(\mathbf{x}_0)$ is tractable

Goal: learn θ s.t. $p_\theta(\mathbf{x}_0) \approx p^*(\mathbf{x}_0)$

Example: Diffusion Models

- true $p^*(\mathbf{x}_0)$ is distribution over photos taken and posted to Flikr
- choose $p_\theta(\mathbf{x}_0)$ to be an expressive model (e.g. noise fed into inverted CNN) that can generate images
  - sampling is will be easy
- learn by finding $\theta \approx \mathrm{argmax}_\theta \log(p_\theta(\mathbf{x}_0))$?
  - Sort of! We can't compute the gradient $\nabla_\theta \log(p_\theta(\mathbf{x}_0))$
  - So we instead optimize a variational lower bound (more on that later)

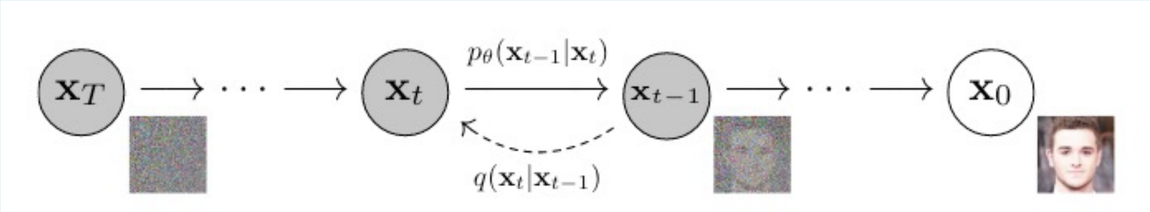


Figure from Ho et al. (2020)

DDPM Objective Function

$$\mathbb{E}\left[-\log p_\theta(\mathbf{x}_0)\right] \leq \mathbb{E}_q\left[-\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right] = \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t\geq 1} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}\right] =: L$$

$$L = \mathbb{E}_q\left[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \parallel p(\mathbf{x}_T))}_{L_T} + \sum_{t>1} \underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} \underbrace{- \log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0}\right]$$

This KL divergence term L_{t-1} wants the two conditional distributions to be as close as possible.

Equations from Ho et al. (2020)

VARIATIONAL AUTOENCODERS

GAN → VAE → Diffusion

(in 5 minutes)

GANs

$p_\theta(\mathbf{z}) \sim \mathcal{N}(0, \mathbf{I})$

$p_\theta(\mathbf{x} \mid \mathbf{z})$ = point mass on $G_\theta(\mathbf{z})$

Model:

MLE?: $\hat{\theta} = \arg\max_\theta \sum_{i=1}^{N} \log p(\mathbf{x}^{(i)})$ NOPE!

$p(\mathbf{x}) = \int_{\mathbf{z}} p(\mathbf{x} \mid \mathbf{z})\, p(\mathbf{z})\, d\mathbf{z}$

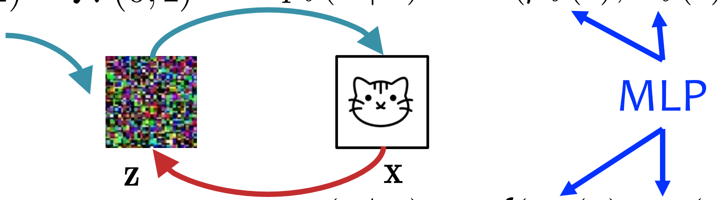
Learn: minimax game

VAEs

$p_\theta(\mathbf{z}) \sim \mathcal{N}(0, \mathbf{I})$

$p_\theta(\mathbf{x} \mid \mathbf{z}) \sim \mathcal{N}(\mu_\theta(\mathbf{z}), \Sigma_\theta(\mathbf{z}))$

Model:



$q_\phi(\mathbf{z} \mid \mathbf{x}) \sim \mathcal{N}(\mu_\phi(\mathbf{x}), \Sigma_\phi(\mathbf{x}))$

$h = \tanh(\mathbf{W}_1 \mathbf{z} + \mathbf{b}_1)$

$\mu_\theta(\mathbf{z}) = \mathbf{W}_2 h + \mathbf{b}_2$

$\Sigma_\theta(\mathbf{z}) = (\mathbf{W}_3 h + \mathbf{b}_3)\mathbf{I}$

MLE?: $\hat{\theta} = \arg\max_\theta \sum_{i=1}^{N} \log p(\mathbf{x}^{(i)})$ NOPE!

$p(\mathbf{x}) = \int_{\mathbf{z}} p(\mathbf{x} \mid \mathbf{z})\, p(\mathbf{z})\, d\mathbf{z}$

Learn: $\theta, \phi = \underset{\theta,\phi}{\arg\min}\ \mathrm{KL}(q_\phi(\mathbf{z} \mid \mathbf{x}) \,\|\, p_\theta(\mathbf{z} \mid \mathbf{x}))$

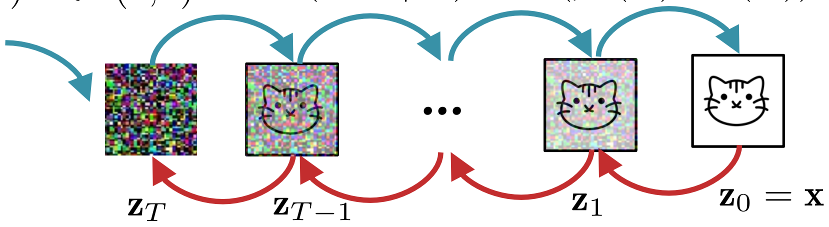
where $p_\theta(\mathbf{z} \mid \mathbf{x})$ is true posterior of $p(\mathbf{x} \mid \mathbf{z})\, p(\mathbf{z})$

Diffusion

$p_\theta(\mathbf{z}) \sim \mathcal{N}(0, \mathbf{I})$

$p_\theta(\mathbf{z}_{t-1} \mid \mathbf{z}_t) \sim \mathcal{N}(\mu_\theta(\mathbf{z}_t), \Sigma_\theta(\mathbf{z}_t))$

Model:



$q(\mathbf{z}_t \mid \mathbf{z}_{t-1}) \sim \mathcal{N}(\mu_\phi(\mathbf{z}_{t-1}), \Sigma_\phi(\mathbf{z}_{t-1}))$ $q(\mathbf{z}_0)$ = data dist.

Learn: $\theta = \underset{\theta}{\arg\min}\ \mathrm{KL}(q(\mathbf{z}_{1:T} \mid \mathbf{x}) \,\|\, p_\theta(\mathbf{z}_{1:T} \mid \mathbf{x}))$

where $p_\theta(\mathbf{z}_{1:T} \mid \mathbf{x})$ is true posterior of $p(\mathbf{x} \mid \mathbf{z}_1) \cdots p(\mathbf{z}_{T-1} \mid \mathbf{z}_T) p(\mathbf{z}_T)$

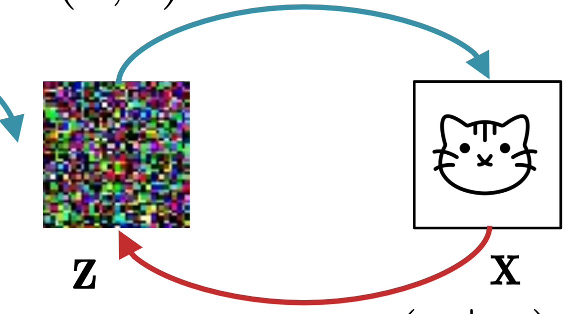
MLE?: NOPE!

Variational Autoencoder

VAEs

Model:

$p_\theta(\mathbf{z}) \sim \mathcal{N}(0, \mathbf{I})$ $\qquad$ $p_\theta(\mathbf{x} \mid \mathbf{z}) \sim \mathcal{N}(\mu_\theta(\mathbf{z}), \Sigma_\theta(\mathbf{z}))$



$q_\phi(\mathbf{z} \mid \mathbf{x}) \sim \mathcal{N}(\mu_\phi(\mathbf{x}), \Sigma_\phi(\mathbf{x}))$

MLP

$h = \tanh(\mathbf{W}_1 \mathbf{z} + \mathbf{b}_1)$

$\mu_\theta(\mathbf{z}) = \mathbf{W}_2 h + \mathbf{b}_2$

$\Sigma_\theta(\mathbf{z}) = (\mathbf{W}_3 h + \mathbf{b}_3)\mathbf{I}$

MLE?: $\hat{\theta} = \arg\max_\theta \sum_{i=1}^N \log p(\mathbf{x}^{(i)})$ NOPE!

$$p(\mathbf{x}) = \int_{\mathbf{z}} p(\mathbf{x} \mid \mathbf{z})\, p(\mathbf{z})\, d\mathbf{z}$$

Learn: $\theta, \phi = \arg\min_{\theta,\phi} \mathrm{KL}(q_\phi(\mathbf{z} \mid \mathbf{x}) \,\|\, p_\theta(\mathbf{z} \mid \mathbf{x}))$

where $p_\theta(\mathbf{z} \mid \mathbf{x})$ is true posterior of $p(\mathbf{x} \mid \mathbf{z})\, p(\mathbf{z})$

Background for Variational Autoencoders (VAEs)

To talk about VAEs we need to lay some groundwork:

1. Autoencoders (not the variational kind)
2. KL divergence
3. Variational inference (using KL as an objective)
4. Monte Carlo estimation (for approximating expectations)
5. (Score function trick)
6. Reparameterization trick (for variance reduction)
7. Stochastic Gradient Variational Bayes