Machine Learning Department
School of Computer Science
Carnegie Mellon University

Diffusion Models
+
Variational Autoencoders (VAEs)

Matt Gormley & Pat Virtue
Lecture 8
Feb. 10, 2025

Reminders

- Homework 1: Generative Models of Text
  - Out: Mon, Jan 27
  - Due: Mon, Feb 10 at 11:59pm
- Quiz 2:
  - In-class: Mon, Feb 17
  - Lectures 5-8
- Homework 2: Generative Models of Images
  - Out: Mon, Feb 10
  - Due: Sat, Feb 22 at 11:59pm

Recap of…

DIFFUSION MODELS

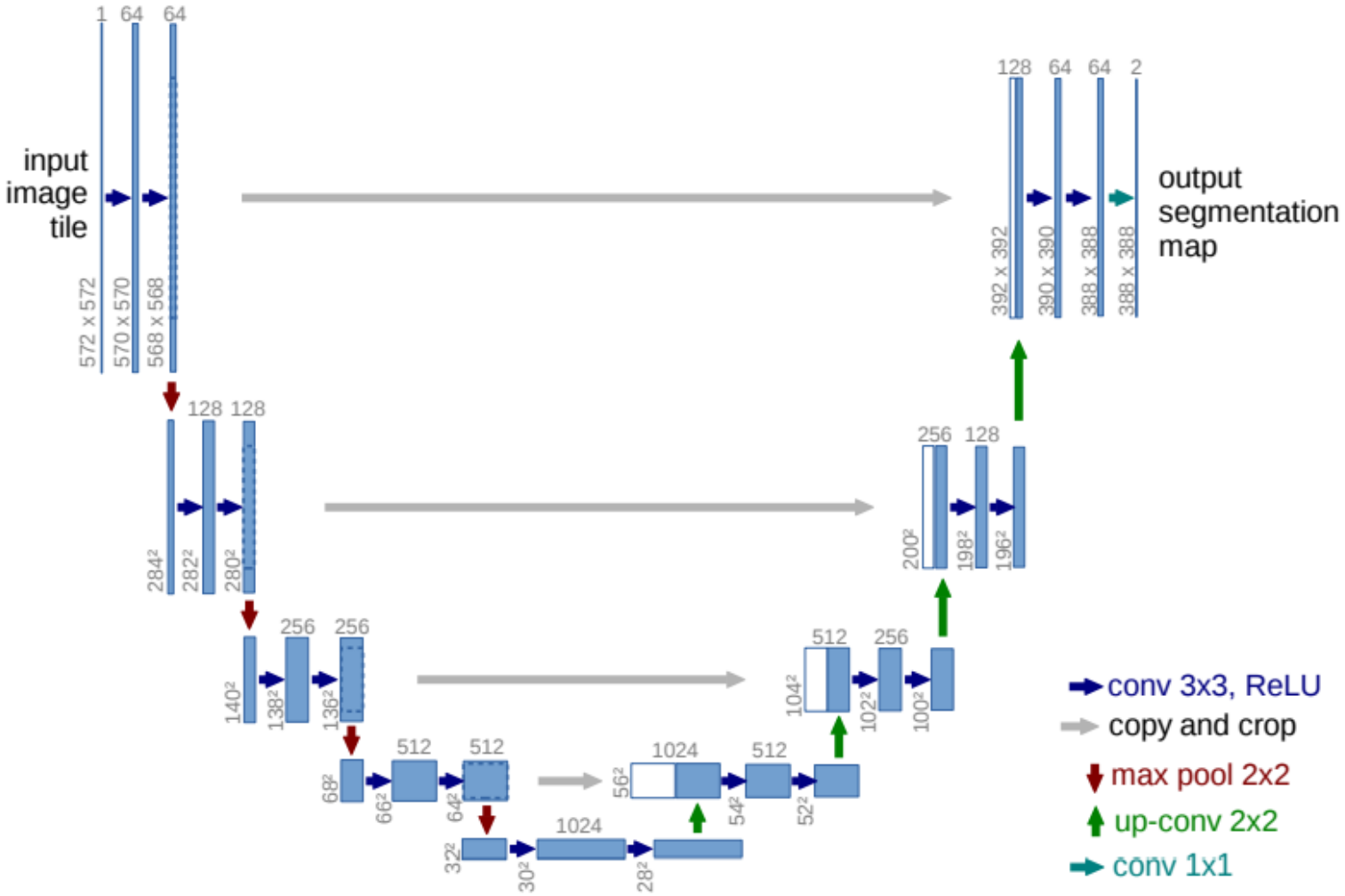
U-Net

Contracting path

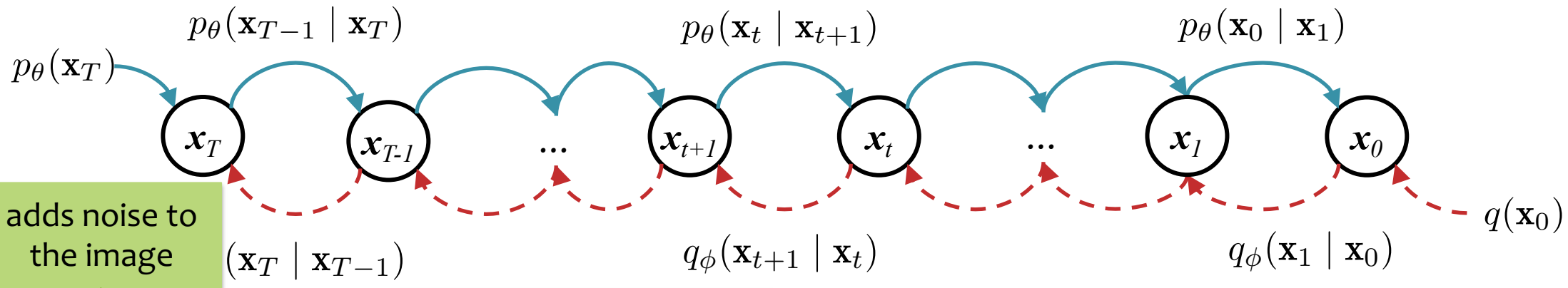
- block consists of:
  - 3x3 convolution
  - 3x3 convolution
  - ReLU
  - max-pooling with stride of 2 (downsample)
- repeat the block N times, doubling number of channels

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

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

(Learned) Reverse Process:

removes noise

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

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

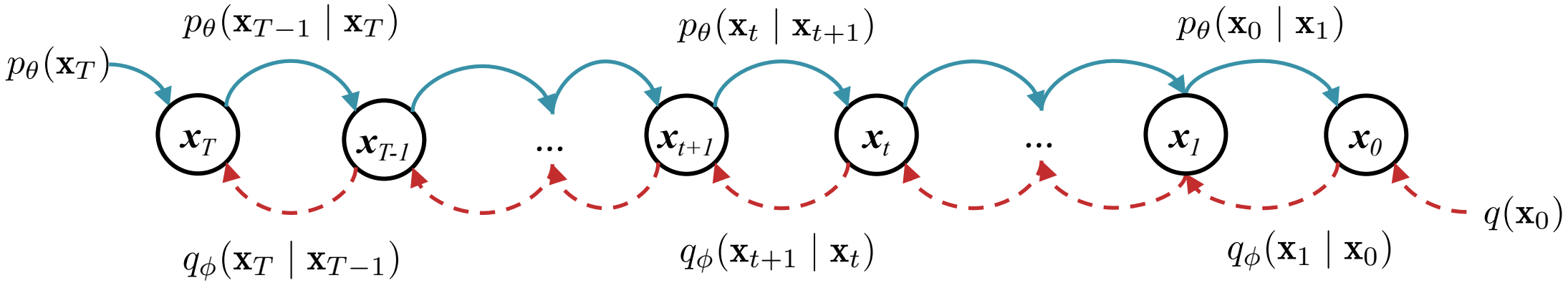
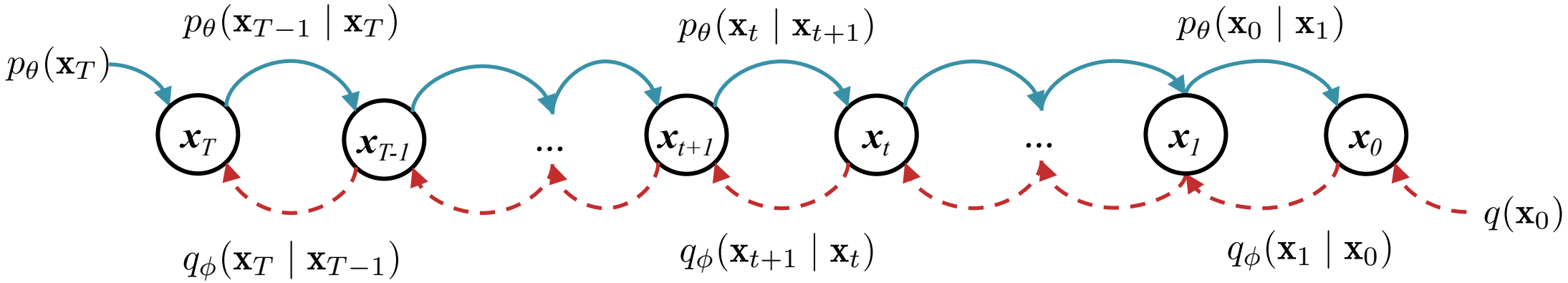


Figure from Ho et al. (2020)

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:

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

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

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

Gaussian (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

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

3. Gaussian with a Gaussian mean has a Gaussian Conditional

$$Z \sim \mathcal{N}(\mu_z = X, \sigma_z^2) \Rightarrow P(Z \mid X) \sim \mathcal{N}(\cdot, \cdot)$$

Defining the Forward Process

Forward Process:

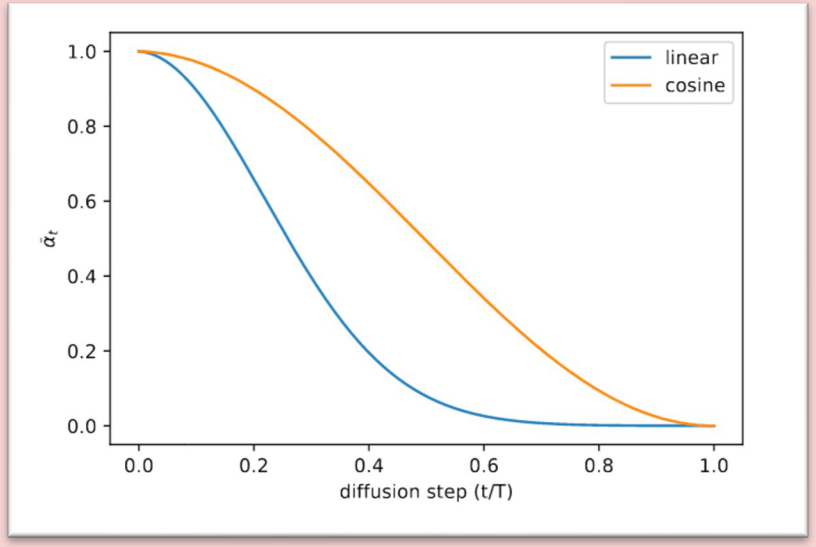
$$q_\phi(\mathbf{x}_{0:T}) = q(\mathbf{x}_0) \prod_{t=1}^{T} q_\phi(\mathbf{x}_t \mid \mathbf{x}_{t-1})$$

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

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

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:

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

Gaussian (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

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

3. Gaussian with a Gaussian mean has a Gaussian Conditional

$$Z \sim \mathcal{N}(\mu_z = X, \sigma_z^2) \Rightarrow P(Z \mid X) \sim \mathcal{N}(\cdot, \cdot)$$

4. But #3 does not hold if X is passed through a nonlinear function f

$$W \sim \mathcal{N}(\mu_z = f(X), \sigma_w^2) \not\Rightarrow P(W \mid X) \sim \mathcal{N}(\cdot, \cdot)$$

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:

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

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

$$\sigma_t^2 = \frac{(1-\bar{\alpha}_{t-1})(1-\alpha_t)}{1-\bar{\alpha}_t}$$

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

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

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 $e \in \{1, \dots, E\}$ **do**
  for $x_0 \in \mathcal{D}$ **do**
    for $t \in \{1, \dots, T\}$ **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: $t \sim \text{Uniform}(1, \ldots, T)$
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: $\tilde{\mu}_q \leftarrow \alpha_t^{(0)}\mathbf{x}_0 + \alpha_t^{(t)}\mathbf{x}_t$
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)

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: $\ell_t(\theta) \leftarrow \|\mathbf{x}_0 - \mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t)\|^2$
8: $\theta \leftarrow \theta - \nabla_\theta \ell_t(\theta)$

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:

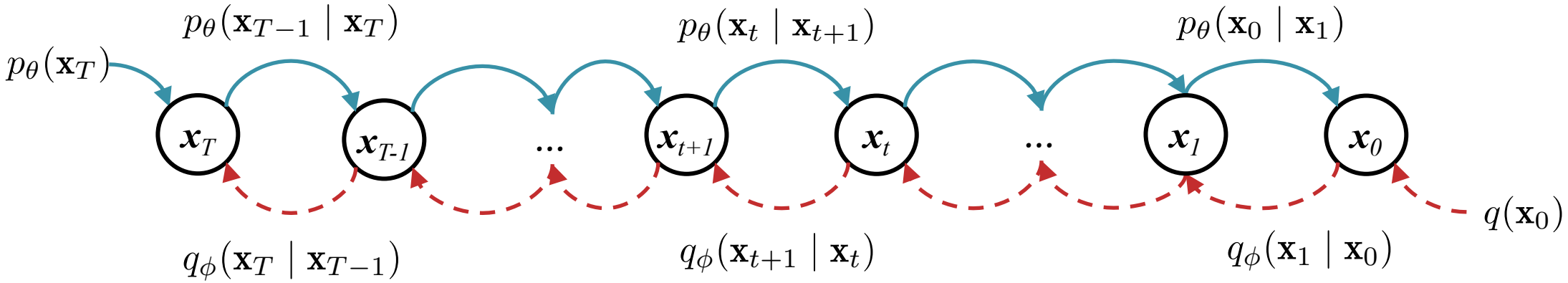
$$\mu_\theta(\mathbf{x}_t, t) = \alpha_t^{(0)}\mathbf{x}_\theta^{(0)}(\mathbf{x}_t, t) + \alpha_t^{(t)}\mathbf{x}_t$$

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)

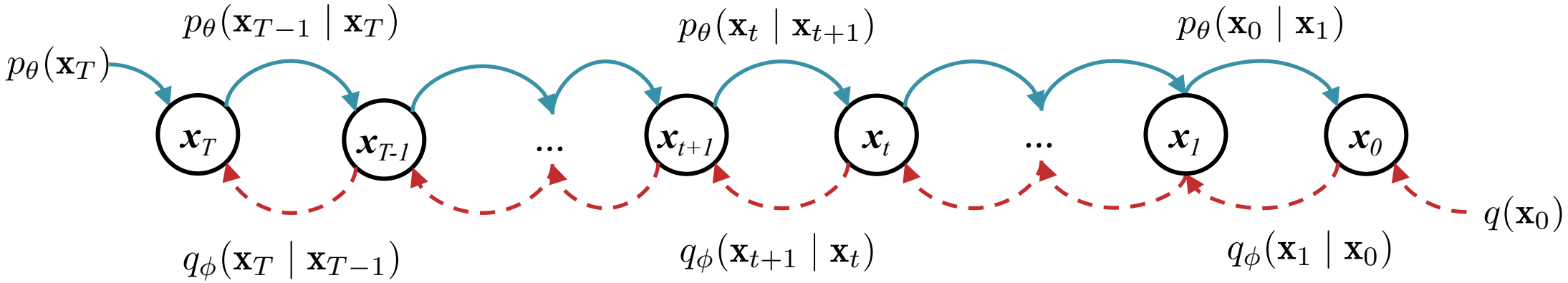
Sampling from the *learned* reverse process



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** $\mathbf{x}_0$

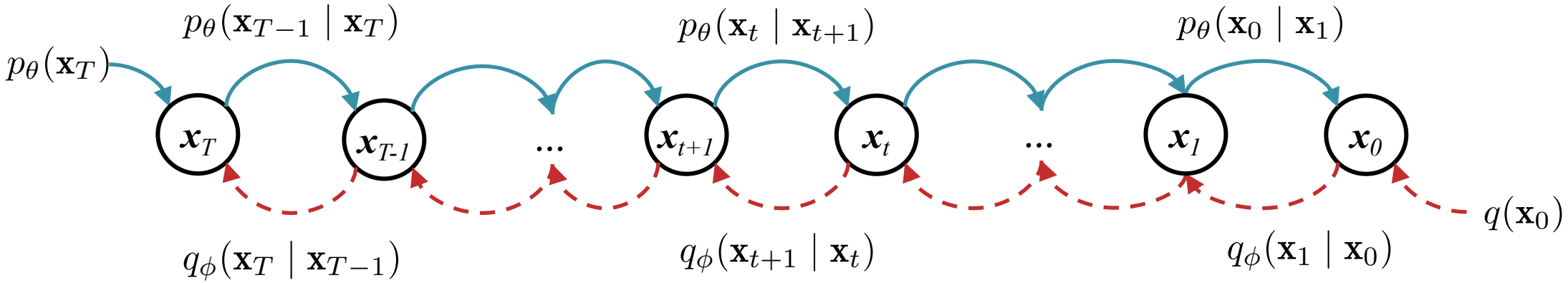
Sampling from the *learned* reverse process



Algorithm 1 Sampling

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

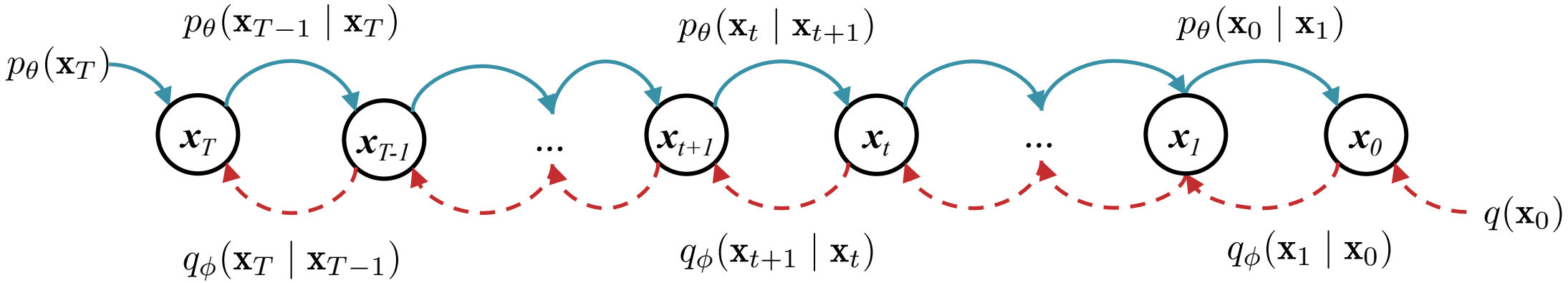
Sampling from the *learned* reverse process



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: $\quad \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
4: $\quad \mathbf{x}_{t-1} \leftarrow \mu_\theta(\mathbf{x}_t, t) + \sigma_t \epsilon$
5: **return** $\mathbf{x}_0$

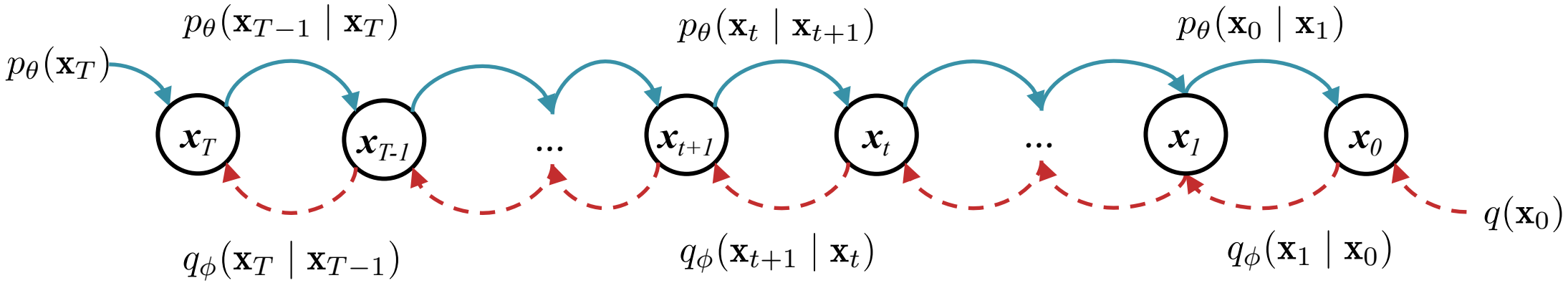
Sampling from the *learned* reverse process



Algorithm 1 Sampling (Option B)

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t \in \{T, \dots, 1\}$ **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 $p^*(\mathbf{x}_o)$
2. we choose a distribution $p_\theta(\mathbf{x}_o)$ for which sampling $x_o \sim p_\theta(\mathbf{x}_o)$ is tractable

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

Example: Diffusion Models

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

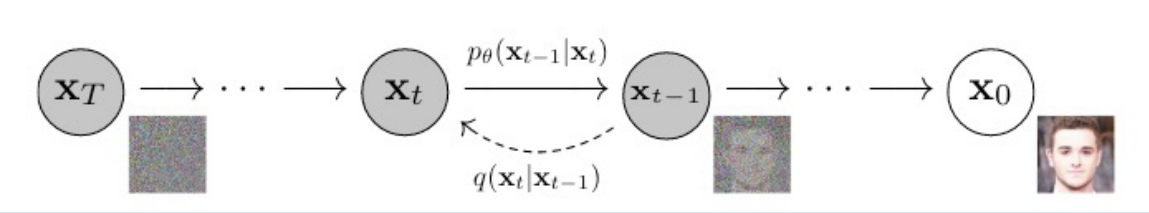


Figure from Ho et al. (2020)

DDPM Objective Function

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

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

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

Unsupervised Learning

Assumptions:

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

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

Example: VAEs / Diffusion Models

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

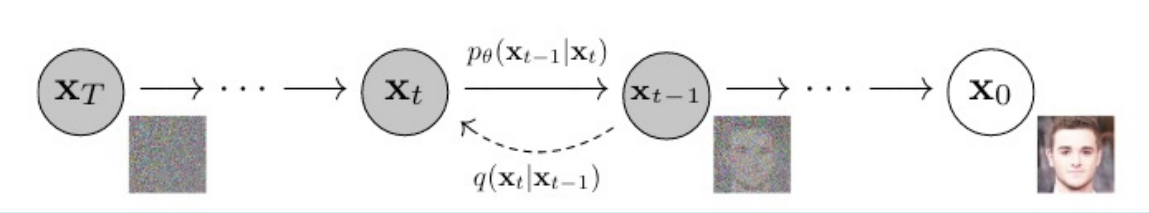


Figure from Ho et al. (2020)

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Figure from Ho et al. (2020)

Variational Autoencoders

Outline

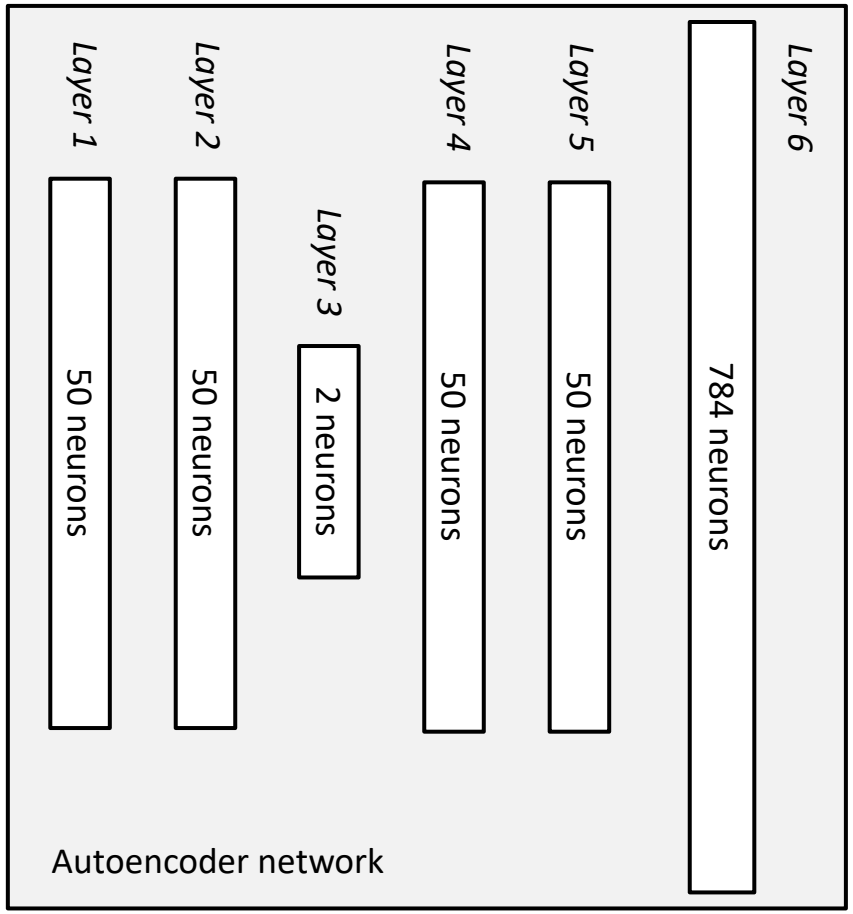
- Autoencoders
- Sampling from Autoencoders???
- Autoencoders → Variational Autoencoders
- KL Divergence diversion ☺
- Variational Inverence
  - ELBO (Evidence Lower BOund)

Autoencoders

Force dimensionality reduction bottleneck,

then try to reconstruct input image

Input
28x28 = 784 pixels



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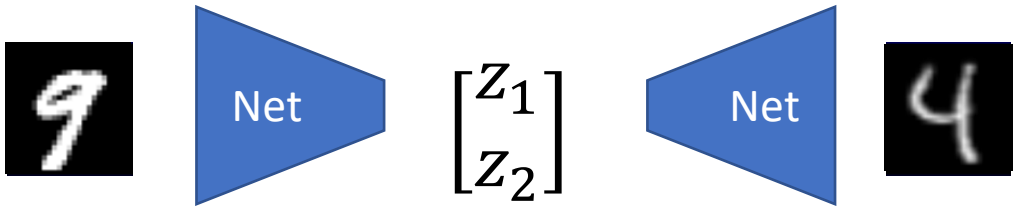
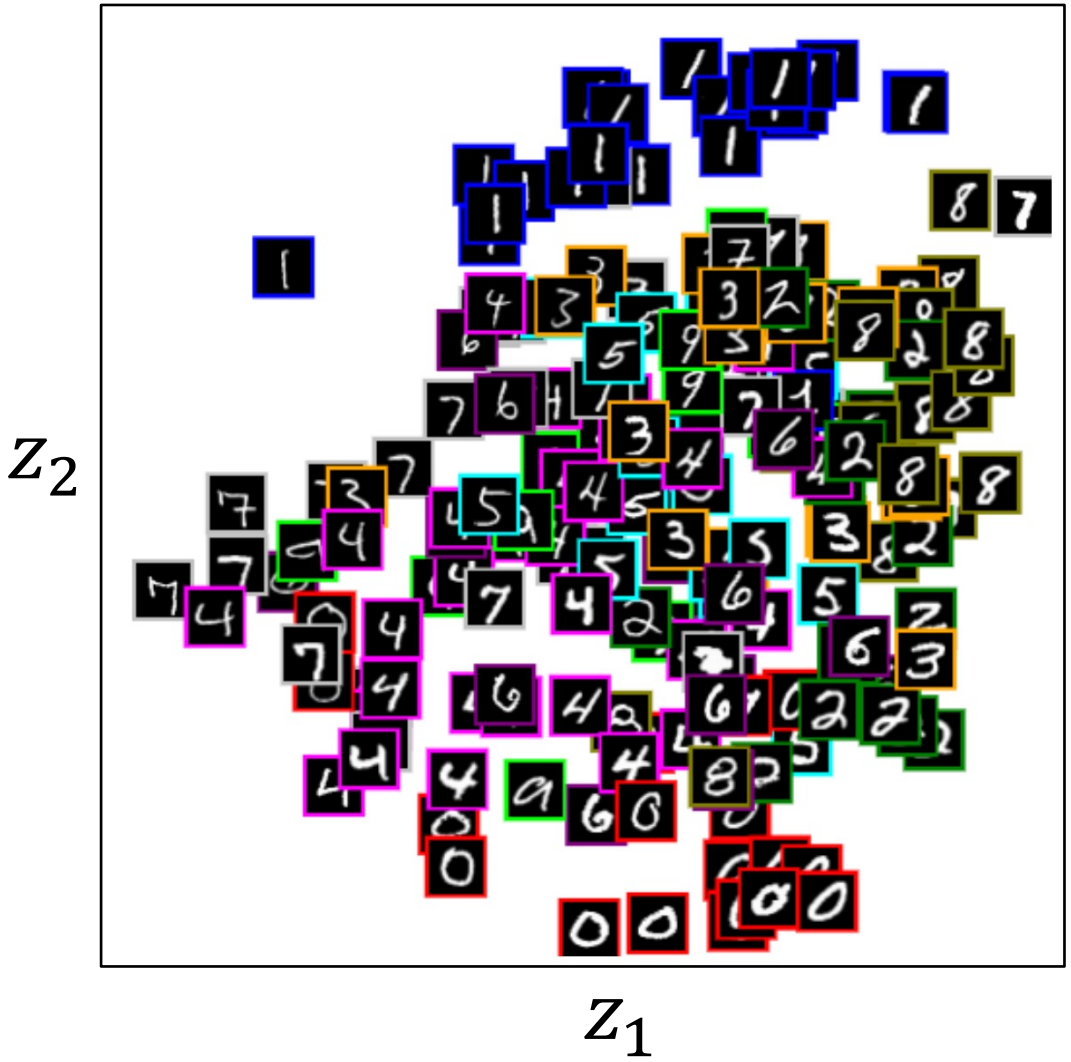
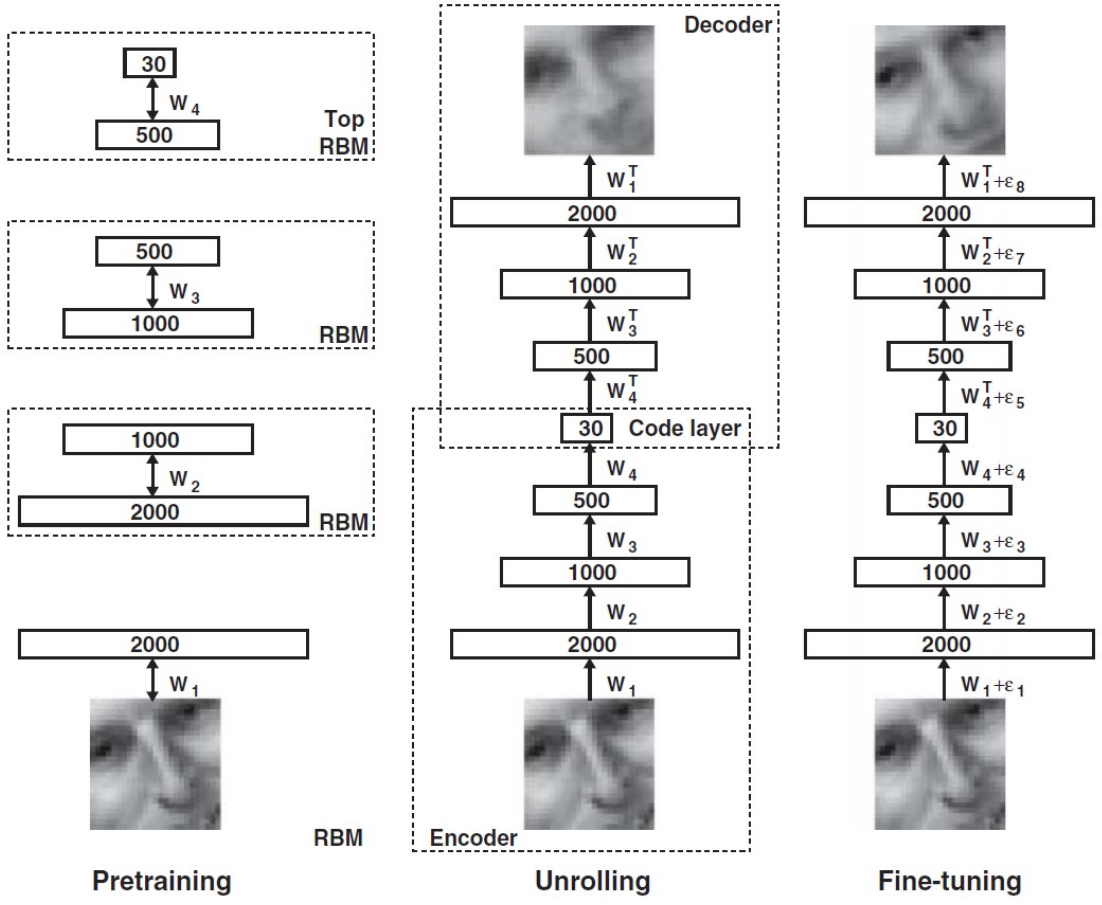




https://cs.stanford.edu/people/karpathy/convnetjs/demo/autoencoder.html

Dimensionality Reduction with Deep Learning

- Hinton, Geoffrey E., and Ruslan R. Salakhutdinov.
- "Reducing the dimensionality of data with neural networks."
- *Science* 313.5786 (2006): 504-507.



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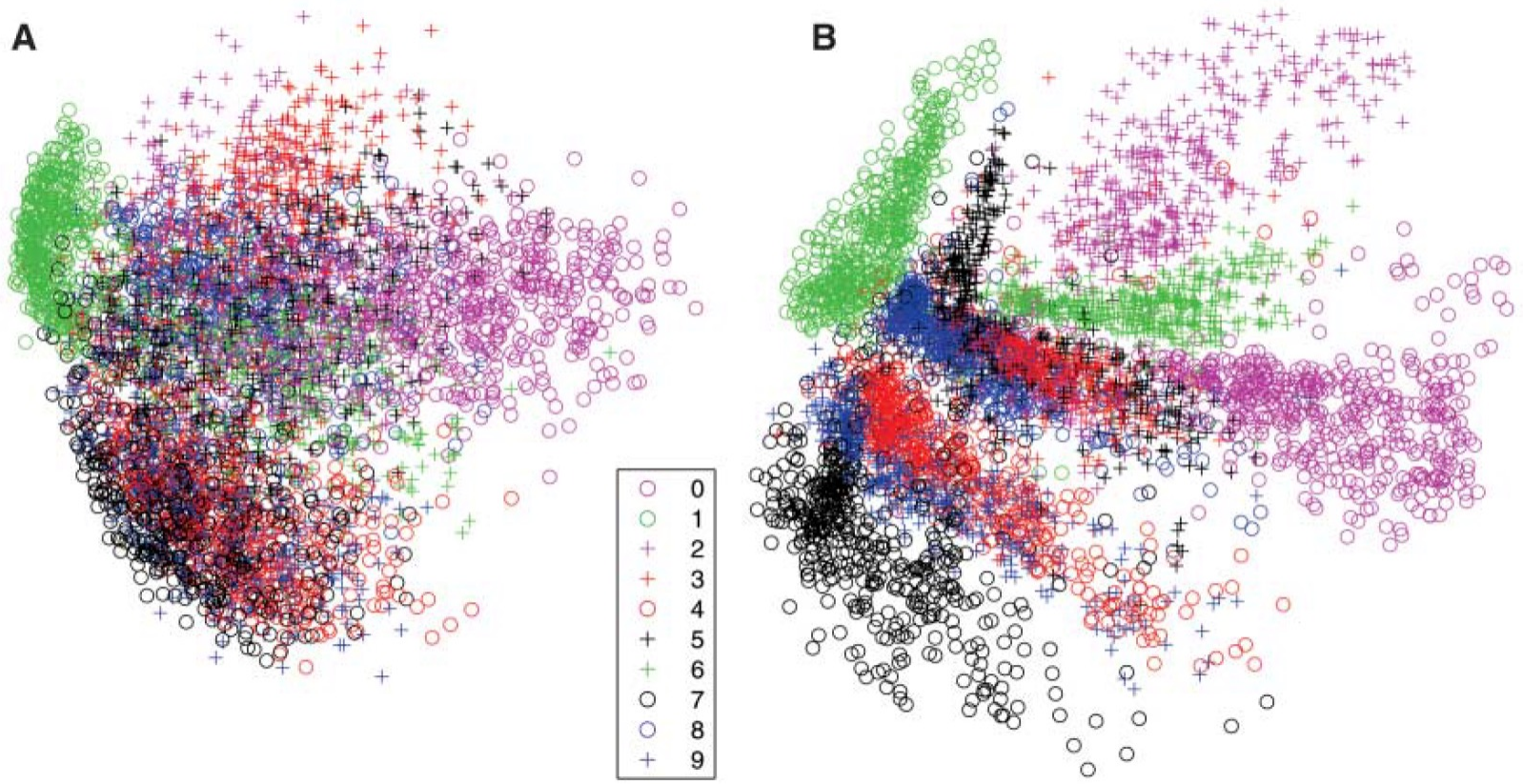
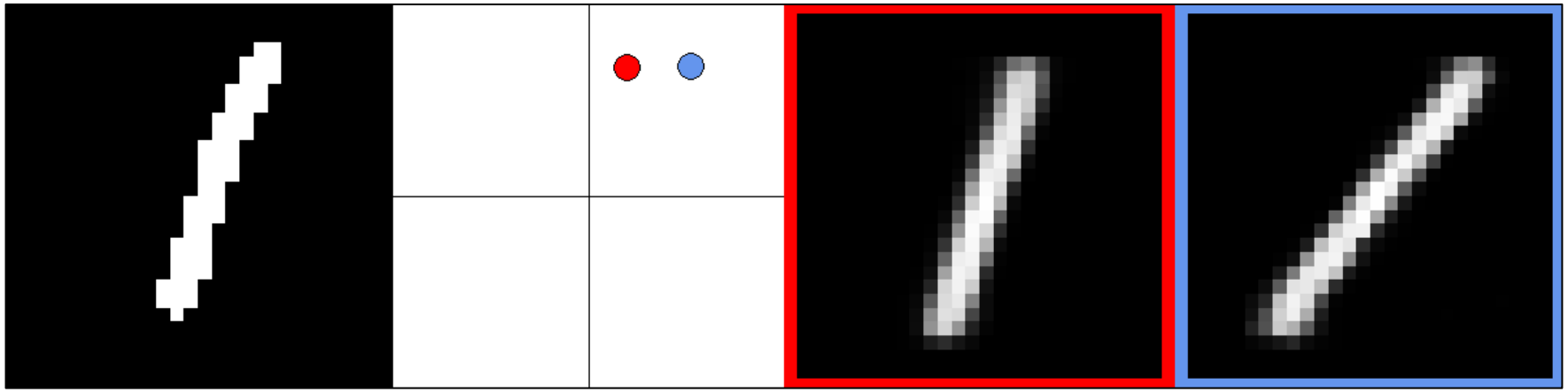
PCA



Neural Network

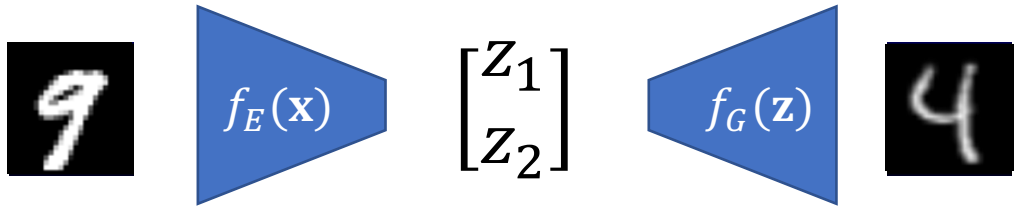
Digit Autoencoder

- Demo: Using a learned feature space



Autoencoder Learning

Objective



Sampling p(x) from Autoencoder

How do we sample a new image?

From Autoencoders to VAE