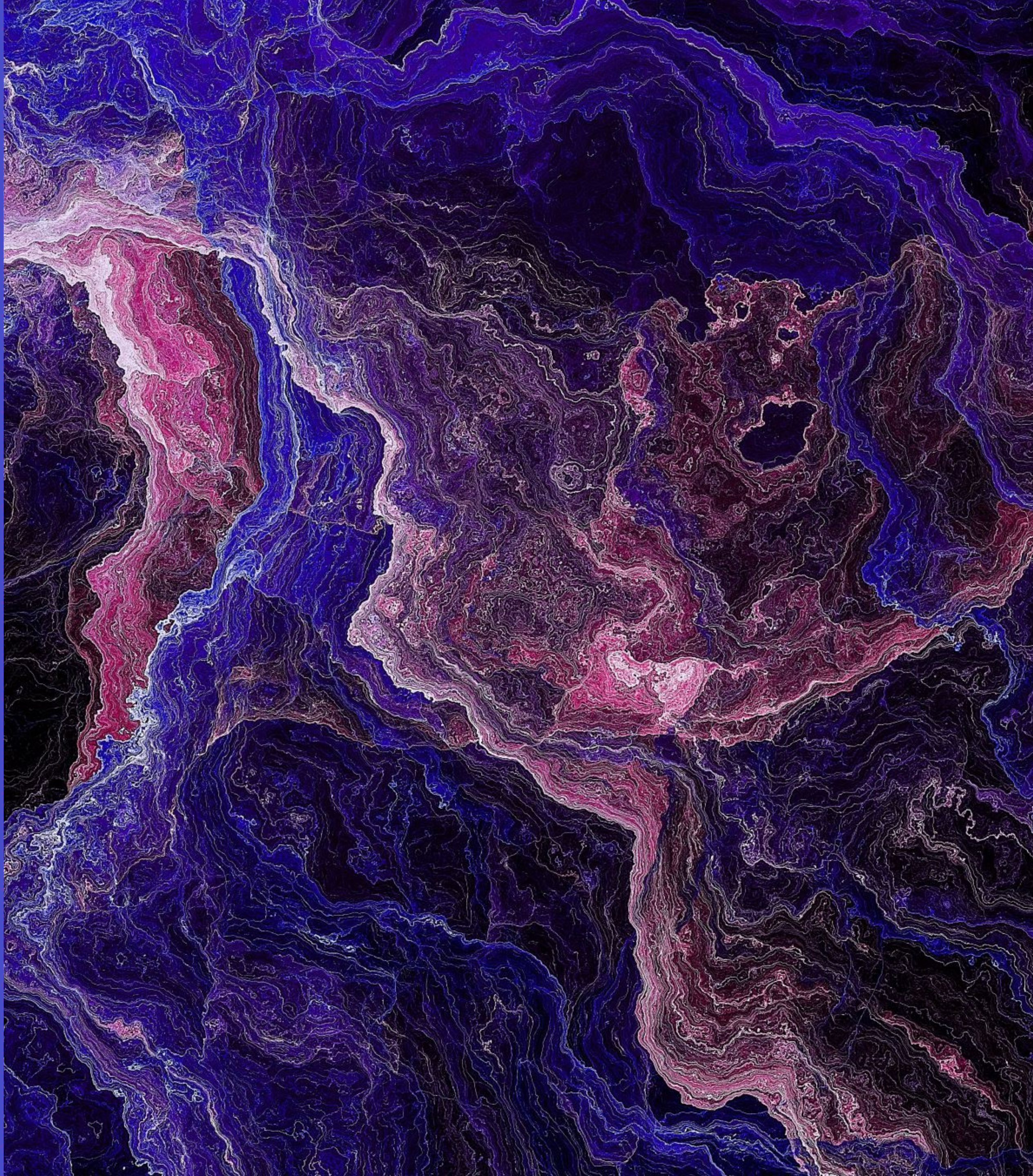
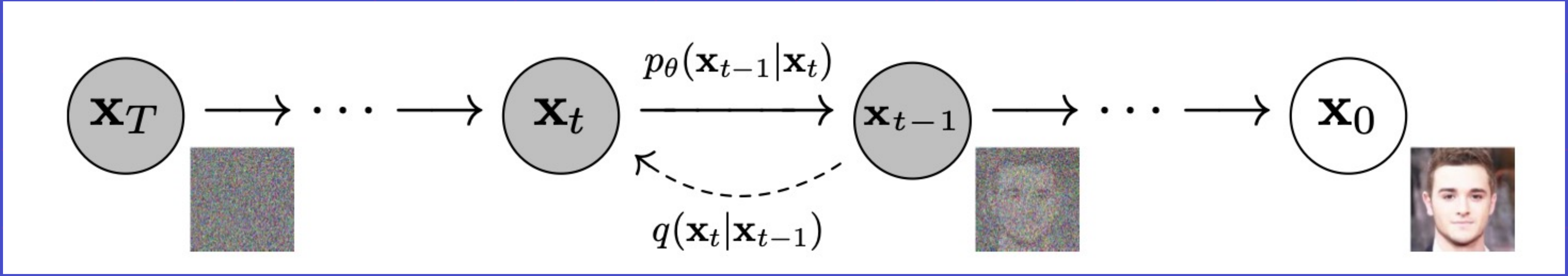
Diffusion models

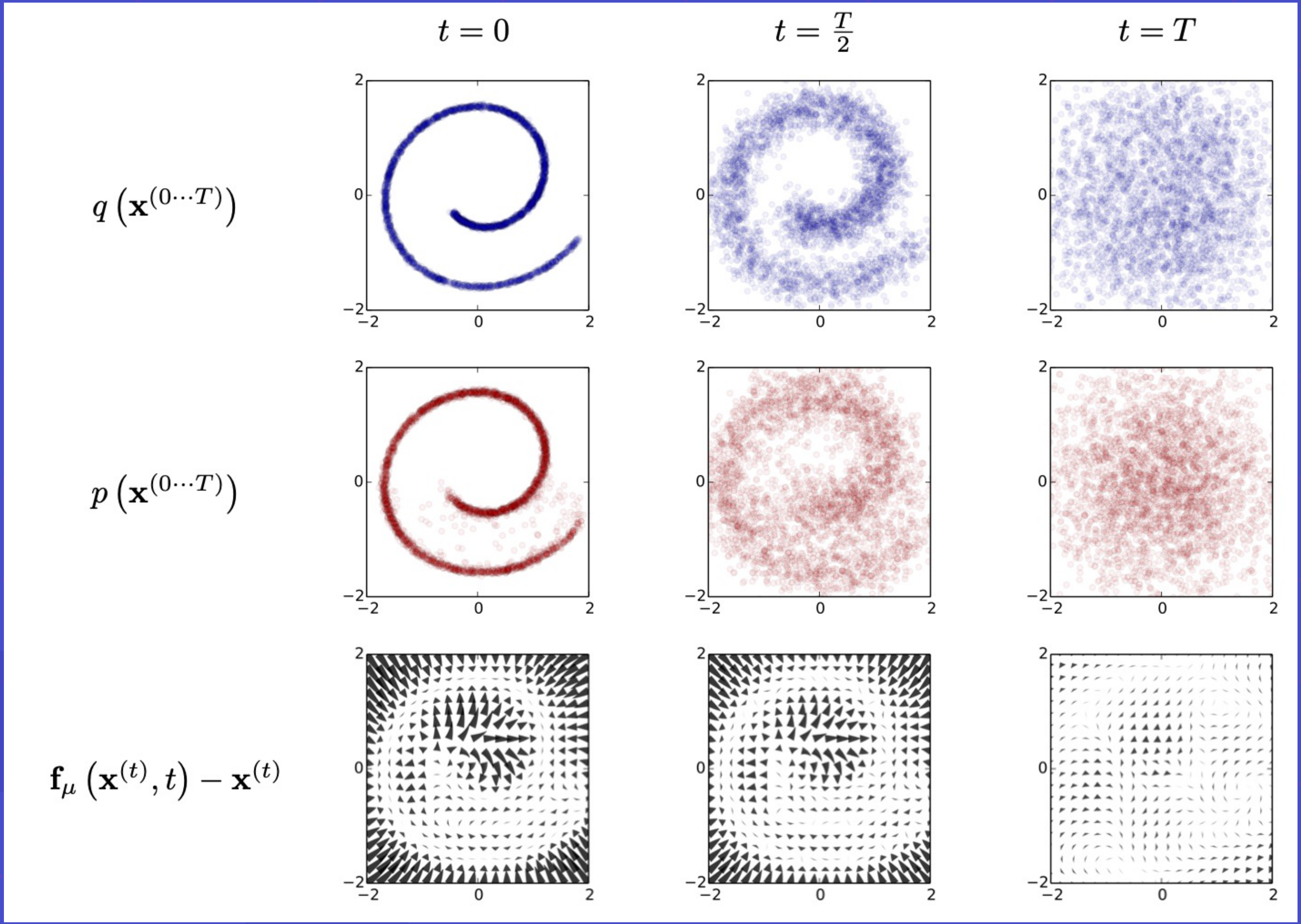


The markov chain


$\mathbf{x}_T$
$\mathbf{x}_t$
$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$
$\mathbf{x}_{t-1}$
$q(\mathbf{x}_t|\mathbf{x}_{t-1})$
$\mathbf{x}_0$

Source: https://arxiv.org/abs/2006.11239

An example of this process



Forward process (adding noise)

Reverse process

The 'dynamics' / difference

Source: https://arxiv.org/abs/1503.03585

Another example

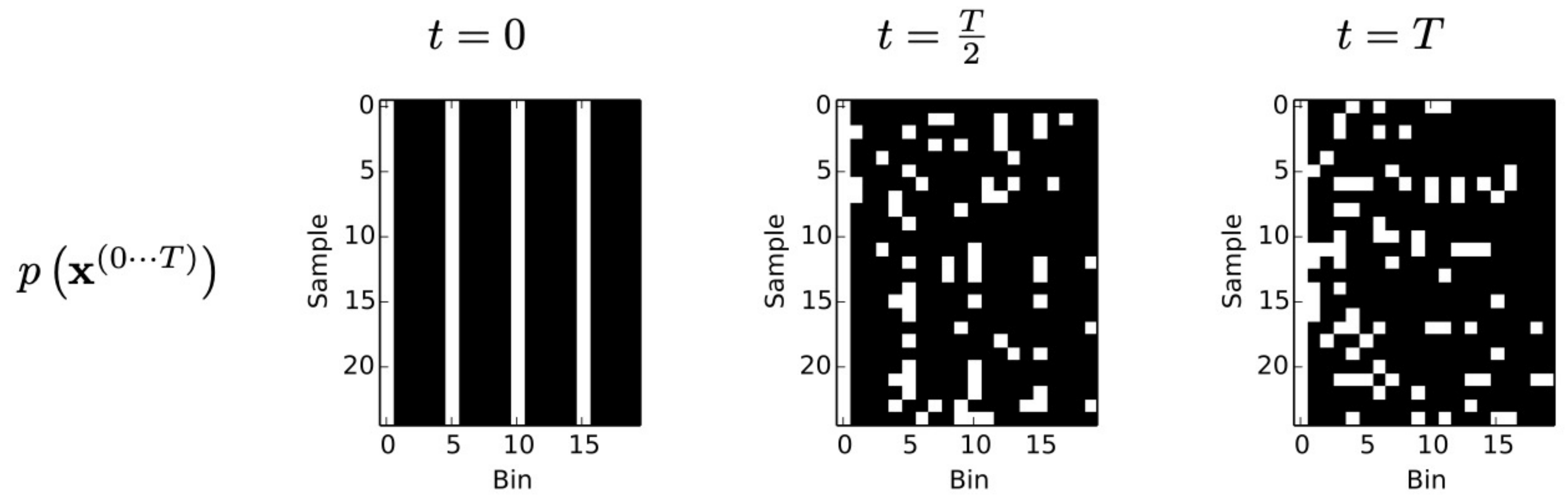
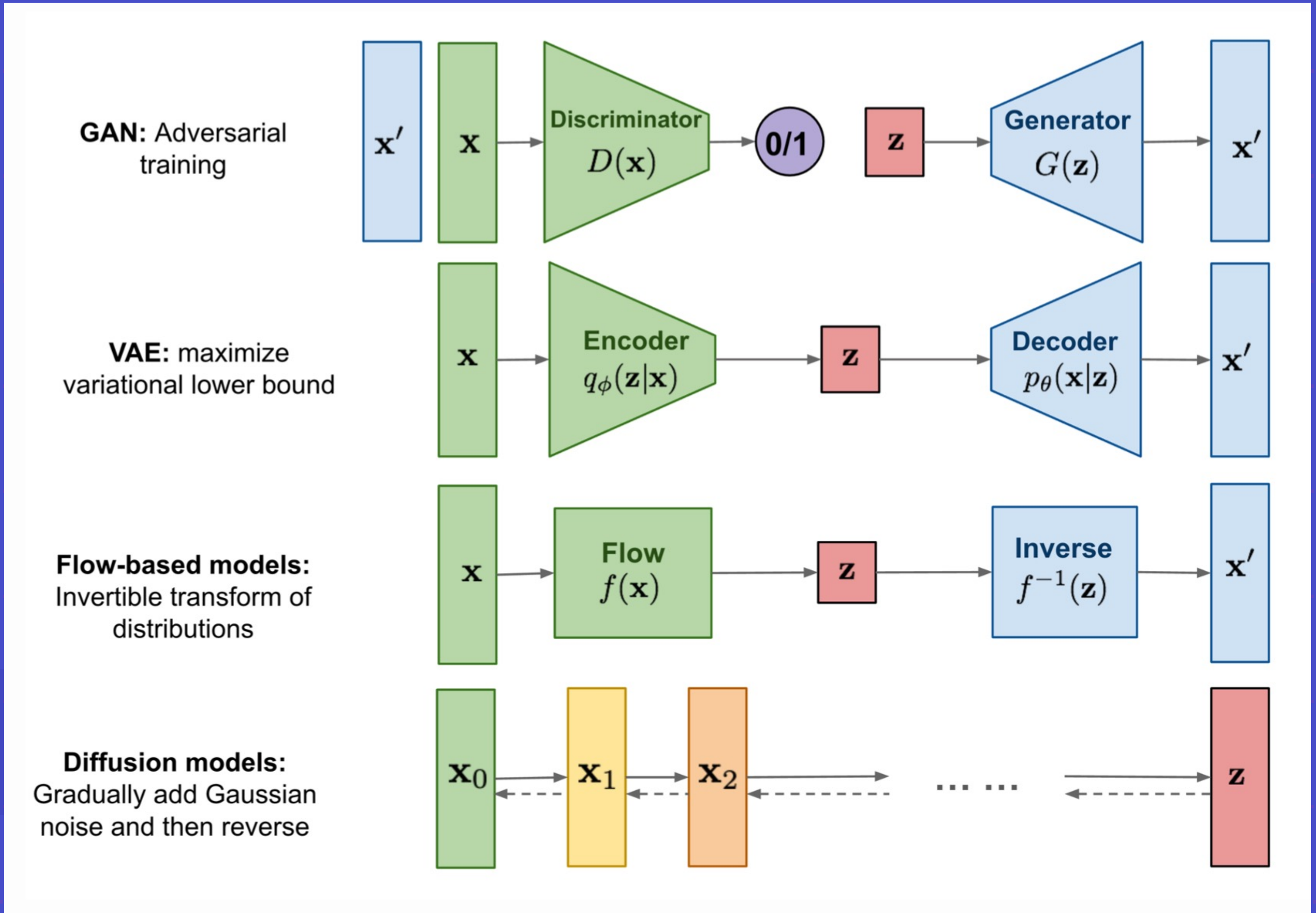


Figure 2. Binary sequence learning via binomial diffusion. A binomial diffusion model was trained on binary 'heartbeat' data, where a pulse occurs every 5th bin. Generated samples (left) are identical to the training data. The sampling procedure consists of initialization at independent binomial noise (right), which is then transformed into the data distribution by a binomial diffusion process, with trained bit flip probabilities. Each row contains an independent sample. For ease of visualization, all samples have been shifted so that a pulse occurs in the first column. In the raw sequence data, the first pulse is uniformly distributed over the first five bins.

Source: https://arxiv.org/abs/1503.03585

Similarities with other generative models

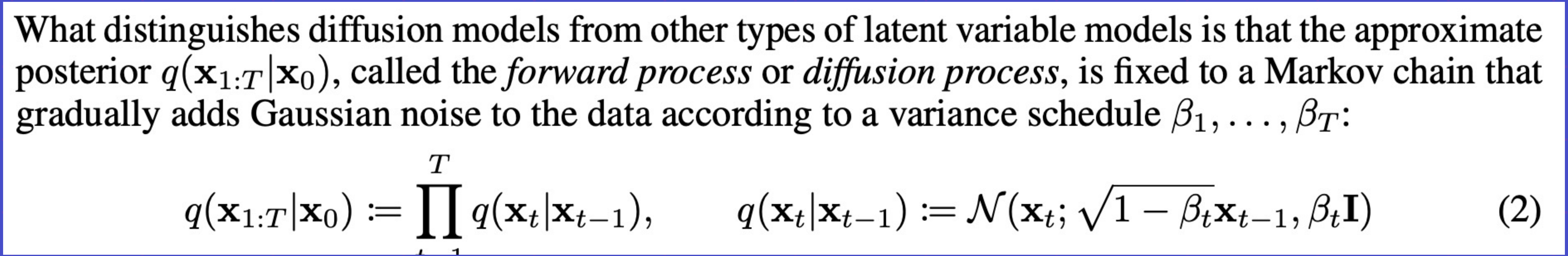


GAN: Adversarial training
$\mathbf{x}'$
$\mathbf{x}$
Discriminator $D(\mathbf{x})$
0/1
$\mathbf{z}$
Generator $G(\mathbf{z})$
$\mathbf{x}'$
VAE: maximize variational lower bound
$\mathbf{x}$
Encoder $q_\phi(\mathbf{z}|\mathbf{x})$
$\mathbf{z}$
Decoder $p_\theta(\mathbf{x}|\mathbf{z})$
$\mathbf{x}'$
Flow-based models: Invertible transform of distributions
$\mathbf{x}$
Flow $f(\mathbf{x})$
$\mathbf{z}$
Inverse $f^{-1}(\mathbf{z})$
$\mathbf{x}'$
Diffusion models: Gradually add Gaussian noise and then reverse
$\mathbf{x}_0$
$\mathbf{x}_1$
$\mathbf{x}_2$
... ...
$\mathbf{z}$

Fig. 1. Overview of different types of generative models.

Source: https://lilianweng.github.io/lil-log/2021/07/11/diffusion-models.html

Mathematically

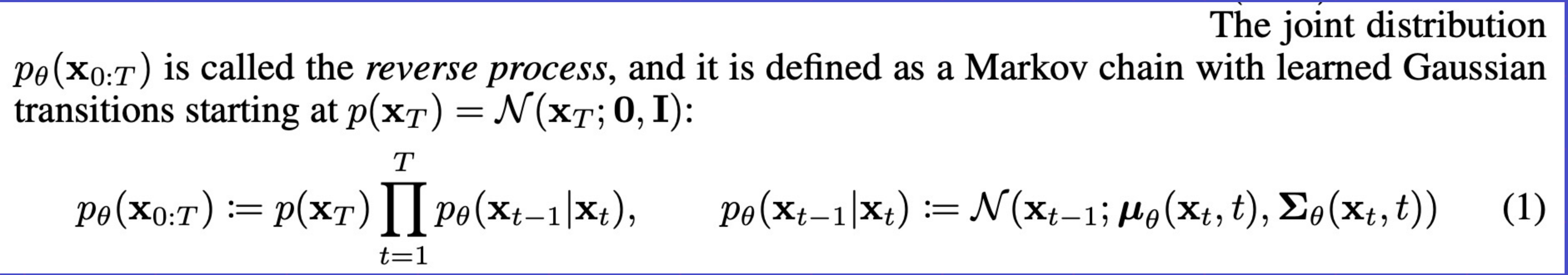


What distinguishes diffusion models from other types of latent variable models is that the approximate posterior $q(\mathbf{x}_{1:T}|\mathbf{x}_0)$, called the *forward process* or *diffusion process*, is fixed to a Markov chain that gradually adds Gaussian noise to the data according to a variance schedule $\beta_1, \ldots, \beta_T$:

$$q(\mathbf{x}_{1:T}|\mathbf{x}_0) := \prod^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1}), \qquad q(\mathbf{x}_t|\mathbf{x}_{t-1}) := \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I}) \tag{2}$$

Source: https://arxiv.org/abs/2006.11239

Mathematically

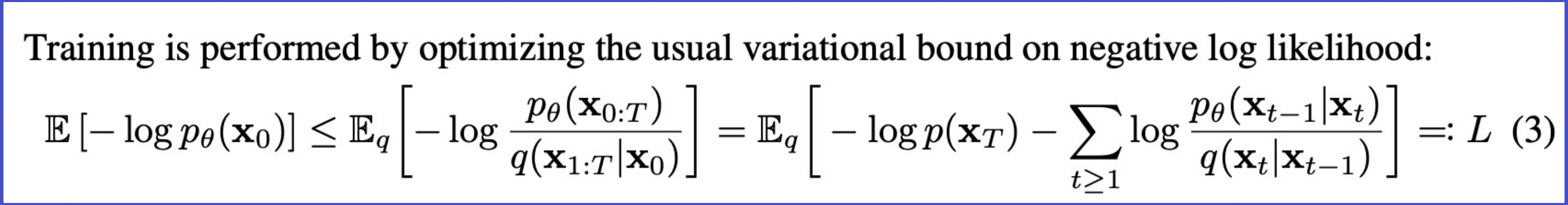


The joint distribution $p_\theta(\mathbf{x}_{0:T})$ is called the *reverse process*, and it is defined as a Markov chain with learned Gaussian transitions starting at $p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$:

$$p_\theta(\mathbf{x}_{0:T}) := p(\mathbf{x}_T) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t), \qquad p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) := \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t)) \qquad (1)$$

Source: https://arxiv.org/abs/2006.11239

Mathematically

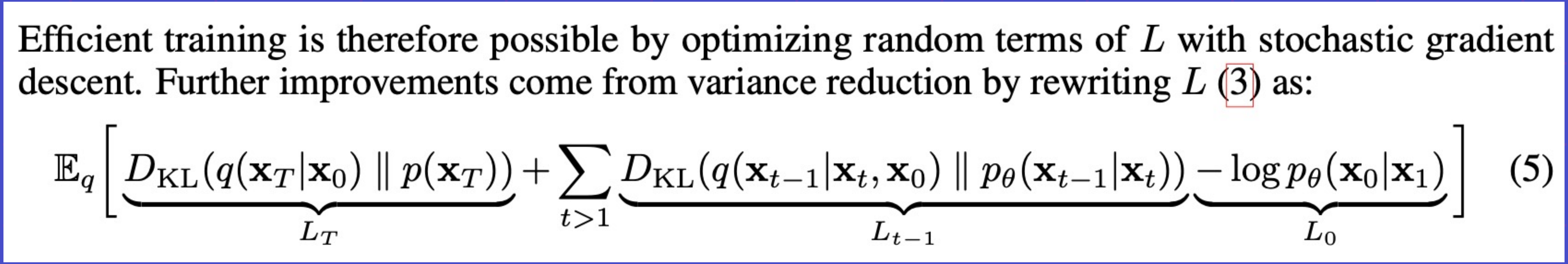


Training is performed by optimizing the usual variational bound on negative log likelihood:

$$\mathbb{E}\left[-\log p_\theta(\mathbf{x}_0)\right] \leq \mathbb{E}_q\left[-\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right] = \mathbb{E}_q\left[-\log p(\mathbf{x}_T) - \sum_{t\geq 1} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})}\right] =: L \quad (3)$$

Source: https://arxiv.org/abs/2006.11239

Mathematically



Efficient training is therefore possible by optimizing random terms of L with stochastic gradient descent. Further improvements come from variance reduction by rewriting L (3) as:

$$\mathbb{E}_q \Big[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \parallel p(\mathbf{x}_T))}_{L_T} + \sum_{t>1} \underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} \underbrace{- \log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0} \Big] \quad (5)$$

Source: https://arxiv.org/abs/2006.11239

Mathematically

However, we found it beneficial to sample quality (and simpler to implement) to train on the following variant of the variational bound:

$$L_{\text{simple}}(\theta) := \mathbb{E}_{t,\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\left\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t)\right\|^2\right] \tag{14}$$

$\alpha_t := 1 - \beta_t$ and $\bar{\alpha}_t := \prod_{s=1}^{t} \alpha_s$,

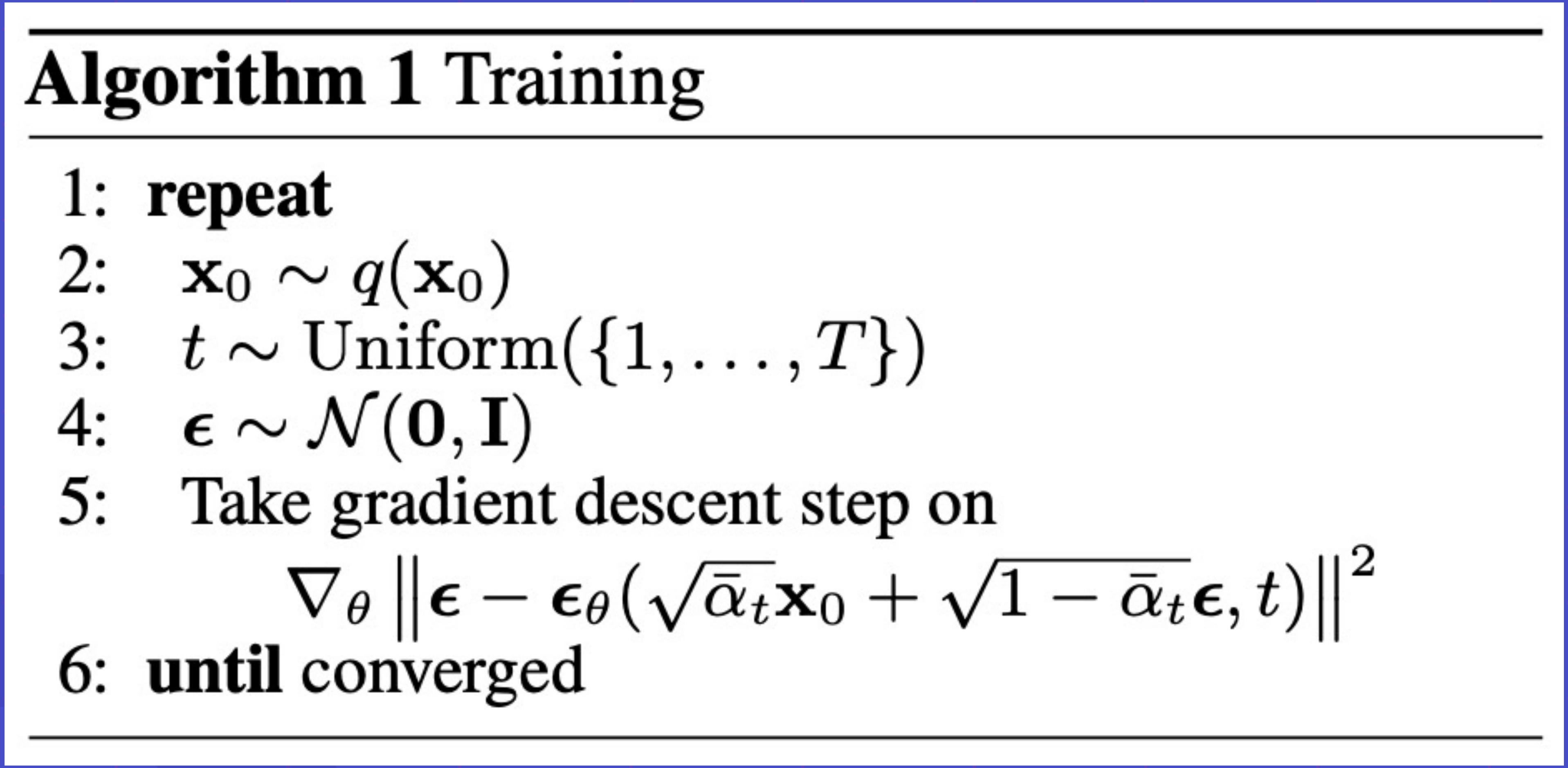
The forward process variances β_t can be learned by reparameterization [33] or held constant as hyperparameters

$\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

$\boldsymbol{\epsilon}_\theta$ as a learned gradient of the data density.

Source: https://arxiv.org/abs/2006.11239

Algorithm: training

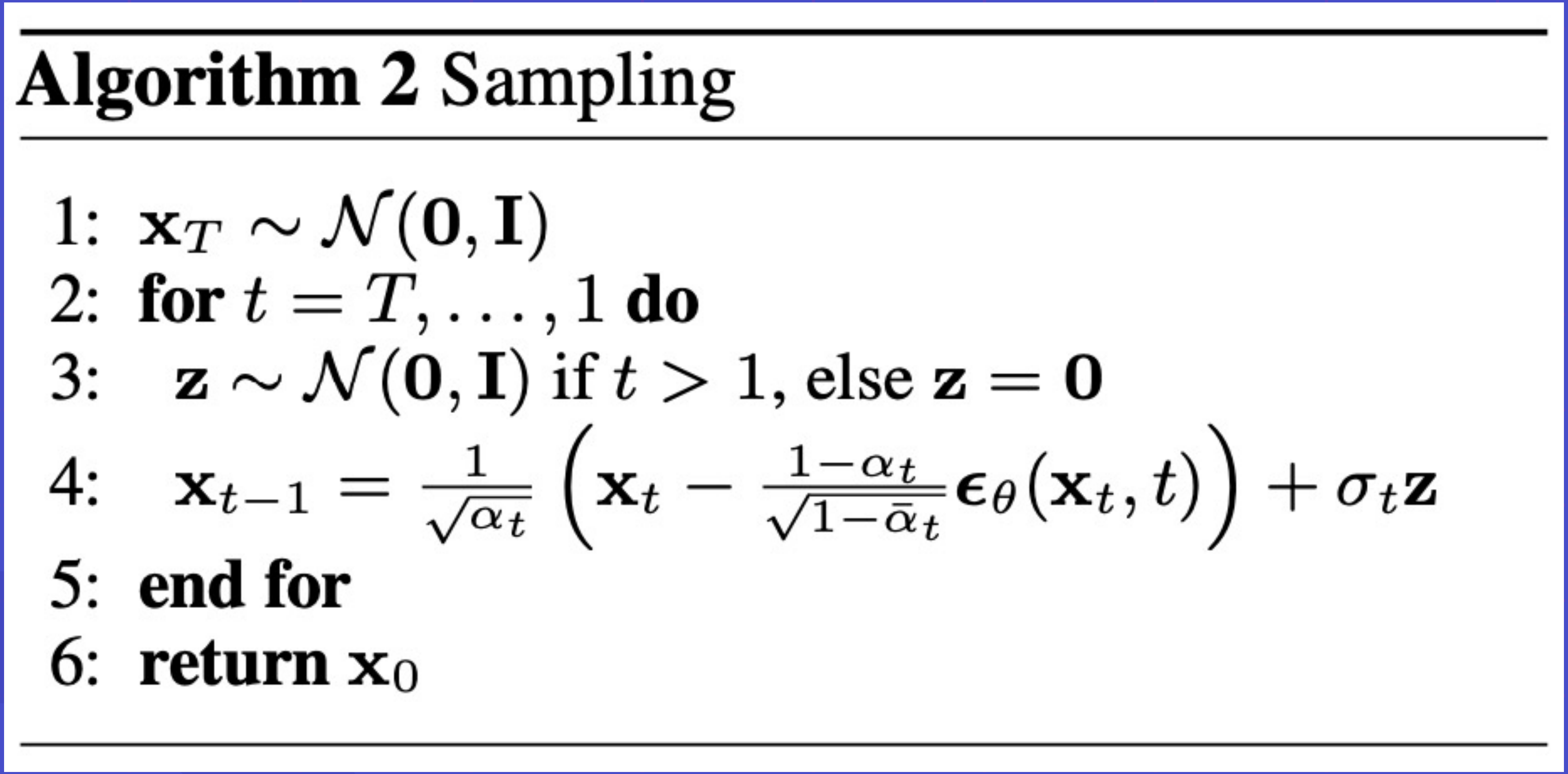


Algorithm 1 Training

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

Source: https://arxiv.org/abs/2006.11239

Algorithm: sampling



Algorithm 2 Sampling

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

Source: https://arxiv.org/abs/2006.11239

Unconditional sampling results

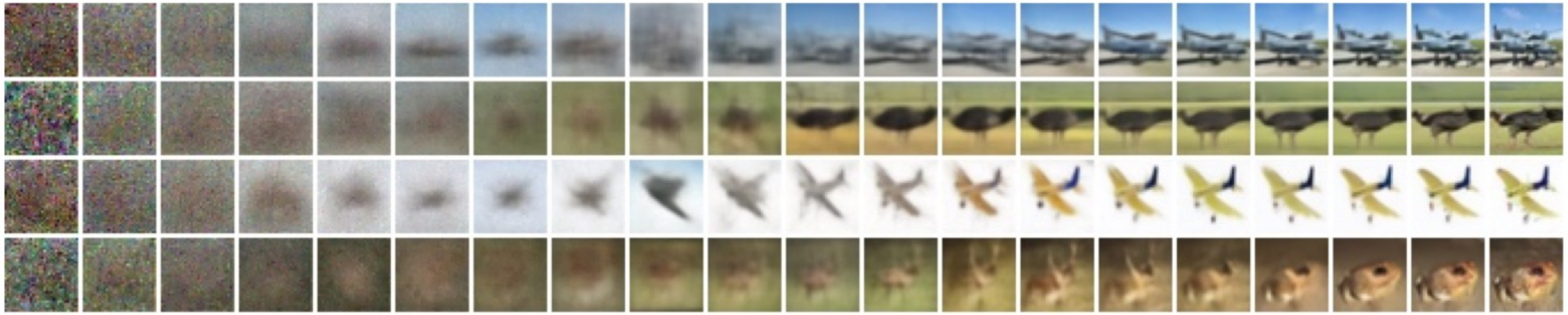


Figure 6: Unconditional CIFAR10 progressive generation ($\hat{\mathbf{x}}_0$ over time, from left to right). Extended samples and sample quality metrics over time in the appendix (Figs. 10 and 14).

Source: https://arxiv.org/abs/2006.11239

Conditional sampling results

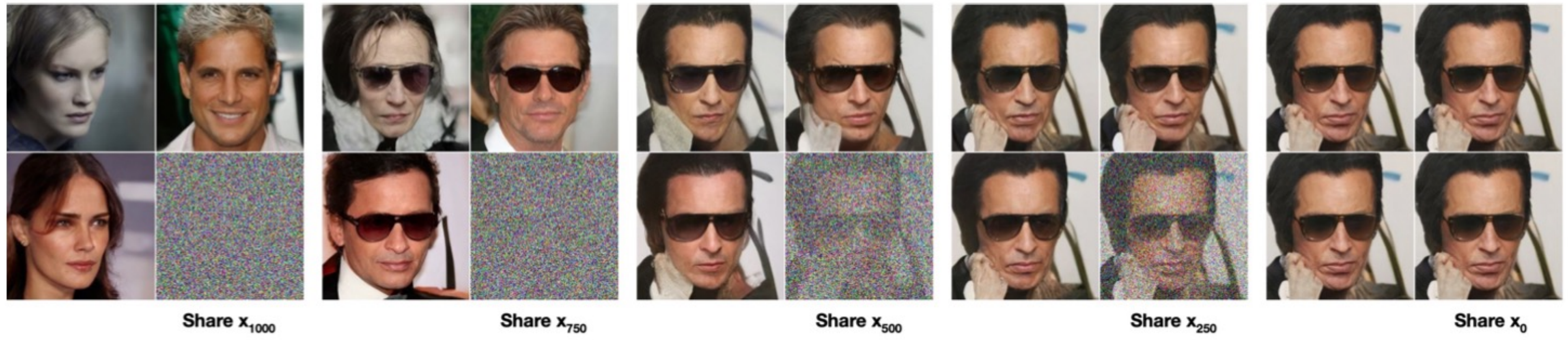


Figure 7: When conditioned on the same latent, CelebA-HQ 256×256 samples share high-level attributes. Bottom-right quadrants are $\mathbf{x}_t$, and other quadrants are samples from $p_\theta(\mathbf{x}_0|\mathbf{x}_t)$.

Source: https://arxiv.org/abs/2006.11239

Interpolations

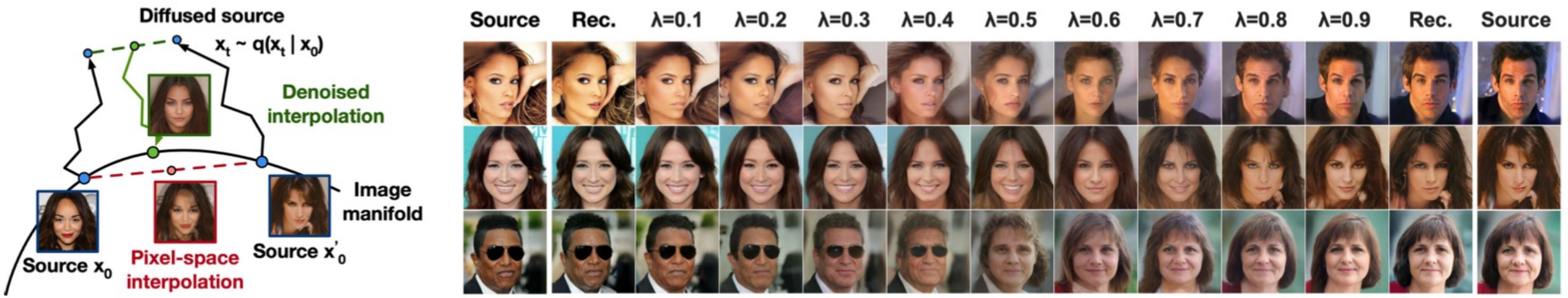
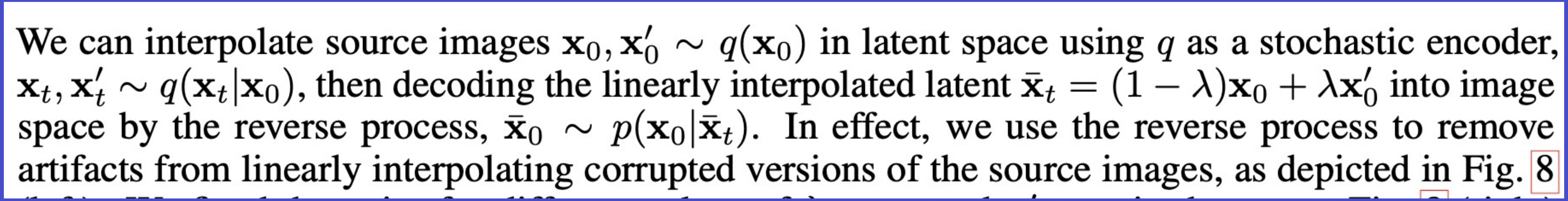


Figure 8: Interpolations of CelebA-HQ 256x256 images with 500 timesteps of diffusion.

Source: https://arxiv.org/abs/2006.11239

Interpolations: math



We can interpolate source images $\mathbf{x}_0, \mathbf{x}'_0 \sim q(\mathbf{x}_0)$ in latent space using q as a stochastic encoder, $\mathbf{x}_t, \mathbf{x}'_t \sim q(\mathbf{x}_t|\mathbf{x}_0)$, then decoding the linearly interpolated latent $\bar{\mathbf{x}}_t = (1 - \lambda)\mathbf{x}_0 + \lambda\mathbf{x}'_0$ into image space by the reverse process, $\bar{\mathbf{x}}_0 \sim p(\mathbf{x}_0|\bar{\mathbf{x}}_t)$. In effect, we use the reverse process to remove artifacts from linearly interpolating corrupted versions of the source images, as depicted in Fig. 8

Source: https://arxiv.org/abs/2006.11239

Questions