Denoising Diffusion Probabilistic Models

Горохов Антон, БПМИ212

Table of contents

1. Intro – Image generation

”Dataset of faces”

1. Intro – Known solutions

Generative adversarial networks (GANs)

autoregressive models

flows

variational autoencoders (VAEs)

2. Diffusion Process as a Markov chain

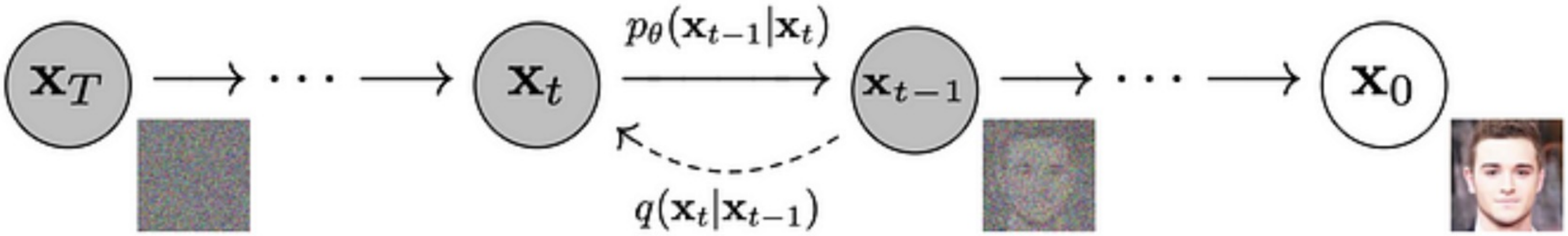


Image from paper Denoising Diffusion Probabilistic Models, page 2

2. Diffusion Process forward step

$$q(x_t|x_{t-1}) = \overbrace{\mathcal{N}}^{\text{normal distribution}}(\underbrace{x_t}_{\text{output}}, \overbrace{\sqrt{1-\beta_t}x_{t-1}}^{\text{mean}}, \underbrace{\beta_t I}_{\text{variance}})$$

3. Background

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

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

Difficulties with generating high quality samples

4. Model – loss function improvement

VLB loss $\mathbb{E}[-\log p_\theta(\mathbf{x}_0)] \leq \mathbb{E}_q\left[L_T + \sum_{t>1} D_{\mathrm{KL}}\left(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)\right) + L_0\right]$

$$\downarrow$$

DSM loss $\text{constant} * \left\|\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t)\right\|^2$

This is the final loss function we use to train DDPMs, which is just a "Mean Squared Error" between the noise added in the forward process and the noise predicted by the model. This is the most impactful contribution of the paper Denoising Diffusion Probabilistic Models.

4. Model

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

$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$

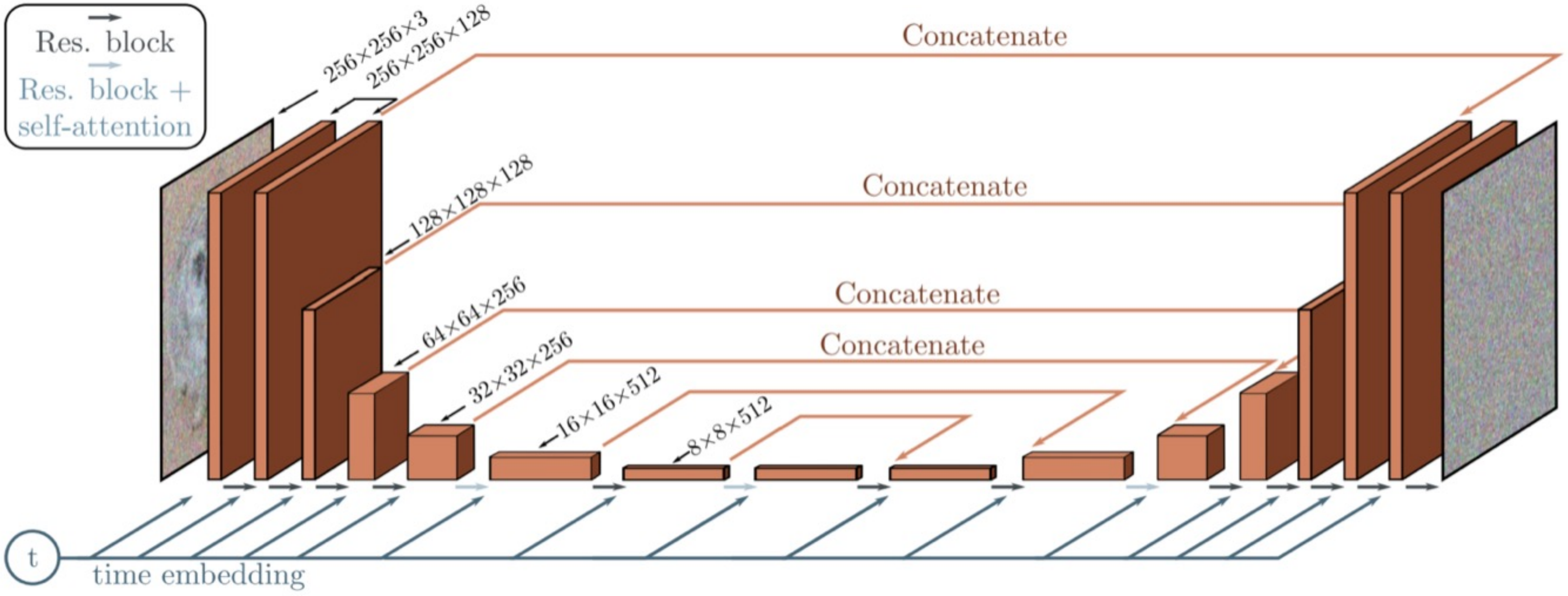
6: **until** converged

4. Model

Algorithm 2 Sampling

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

4. Model architecture



The U-Net architecture used in DDPMs

5. Experiments and results

- $T = 1000$
- Constant variances of Gaussian noise on each step (works better than predictable) from $\beta_1 = 10^{-4}$ to $\beta_T = 2 * 10^{-2}$

5. Experiments and results

Table 1: CIFAR10 results. NLL measured in bits/dim.

Model	IS	FID	NLL Test (Train)
Conditional			
EBM [11]	8.30	37.9	
JEM [17]	8.76	38.4	
BigGAN [3]	9.22	14.73	
StyleGAN2 + ADA (v1) [29]	**10.06**	**2.67**	
Unconditional			
Diffusion (original) [53]			≤ 5.40
Gated PixelCNN [59]	4.60	65.93	3.03 (2.90)
Sparse Transformer [7]			**2.80**
PixelIQN [43]	5.29	49.46	
EBM [11]	6.78	38.2	
NCSNv2 [56]		31.75	
NCSN [55]	8.87±0.12	25.32	
SNGAN [39]	8.22±0.05	21.7	
SNGAN-DDLS [4]	9.09±0.10	15.42	
StyleGAN2 + ADA (v1) [29]	$\mathbf{9.74} \pm 0.05$	3.26	
Ours (L, fixed isotropic $\mathbf{\Sigma}$)	7.67±0.13	13.51	≤ 3.70 (3.69)
Ours (L_{simple})	9.46±0.11	**3.17**	≤ 3.75 (3.72)

5. Experiments and results

Table 2: Unconditional CIFAR10 reverse process parameterization and training objective ablation. Blank entries were unstable to train and generated poor samples with out-of-range scores.

Objective	IS	FID
$\tilde{\boldsymbol{\mu}}$ prediction (baseline)		
L, learned diagonal $\boldsymbol{\Sigma}$	7.28 ± 0.10	23.69
L, fixed isotropic $\boldsymbol{\Sigma}$	8.06 ± 0.09	13.22
$\lVert \tilde{\boldsymbol{\mu}} - \tilde{\boldsymbol{\mu}}_\theta \rVert^2$	–	–
$\boldsymbol{\epsilon}$ prediction (ours)		
L, learned diagonal $\boldsymbol{\Sigma}$	–	–
L, fixed isotropic $\boldsymbol{\Sigma}$	7.67 ± 0.13	13.51
$\lVert \tilde{\boldsymbol{\epsilon}} - \boldsymbol{\epsilon}_\theta \rVert^2$ (L_{simple})	$\mathbf{9.46 \pm 0.11}$	$\mathbf{3.17}$

5. Experiments and results

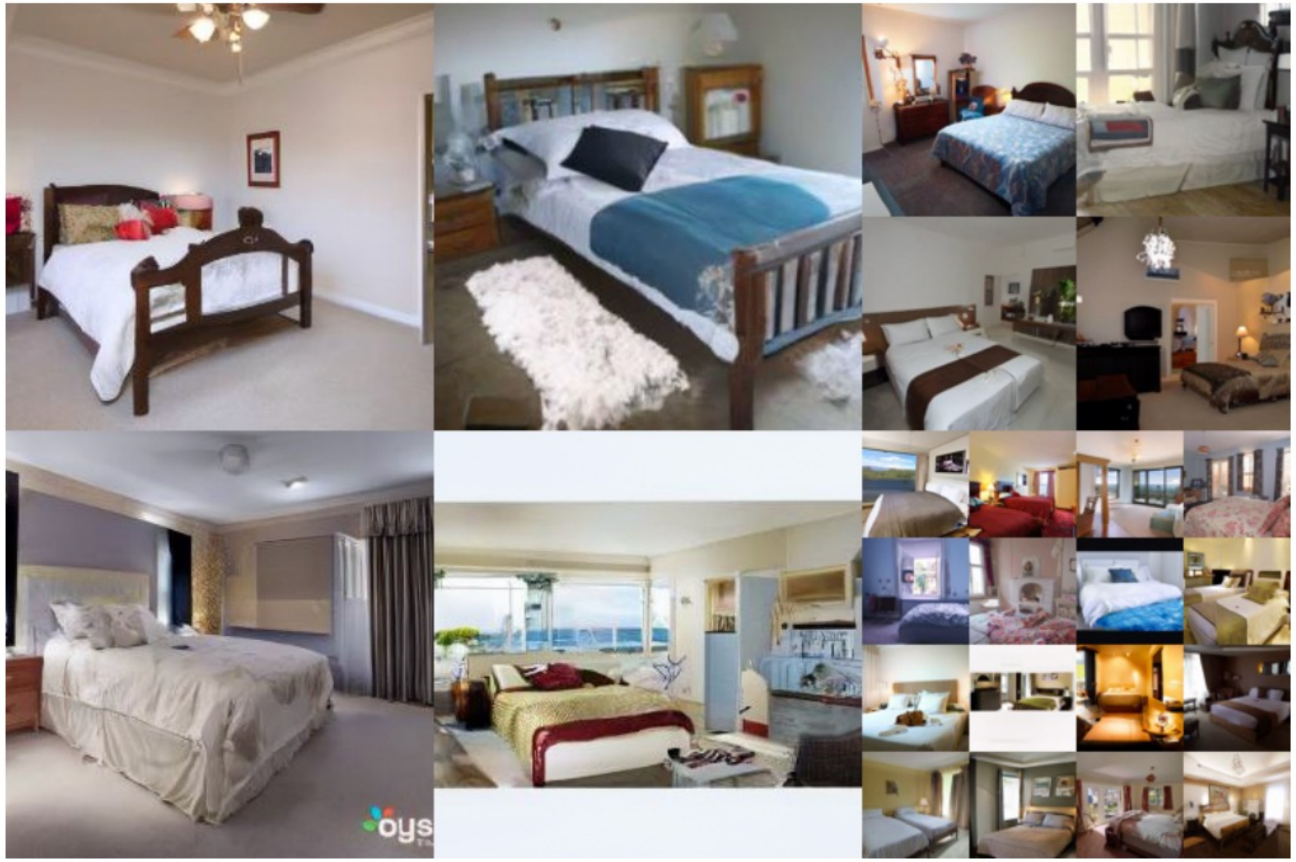
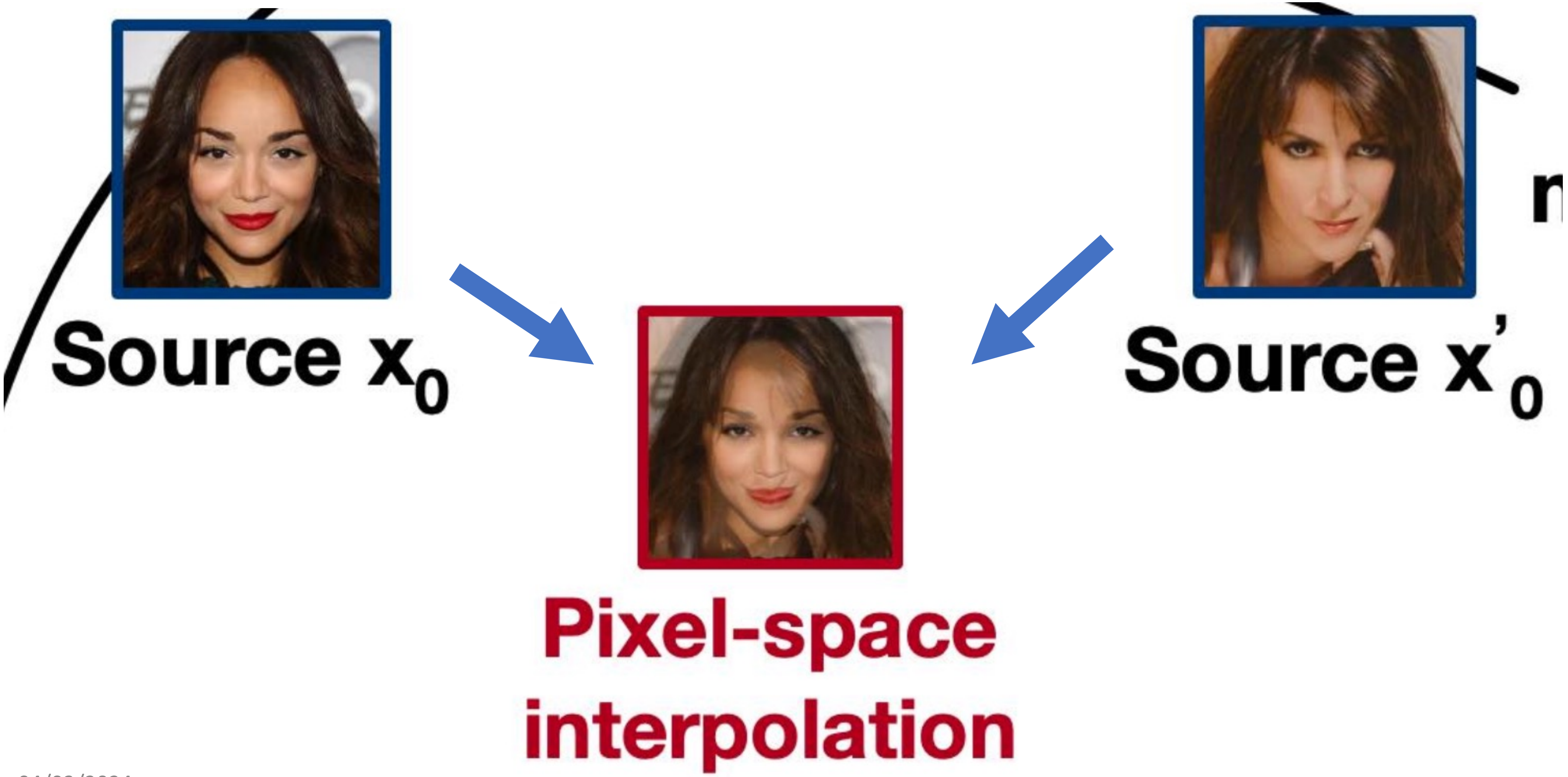


Figure 4: LSUN Bedroom samples. FID=4.90

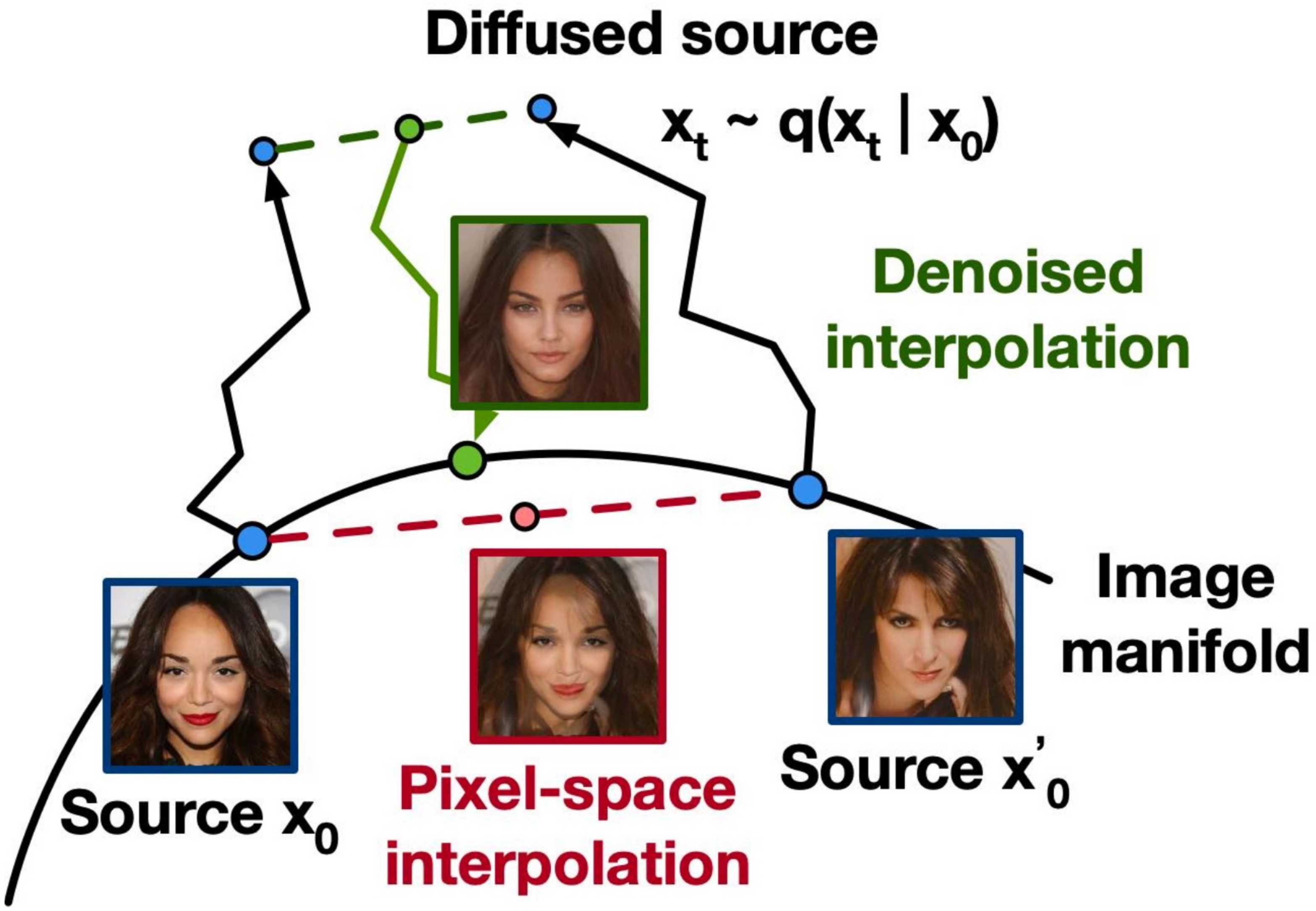
5. Experiments and results

Figure 3: LSUN Church samples. FID=7.89

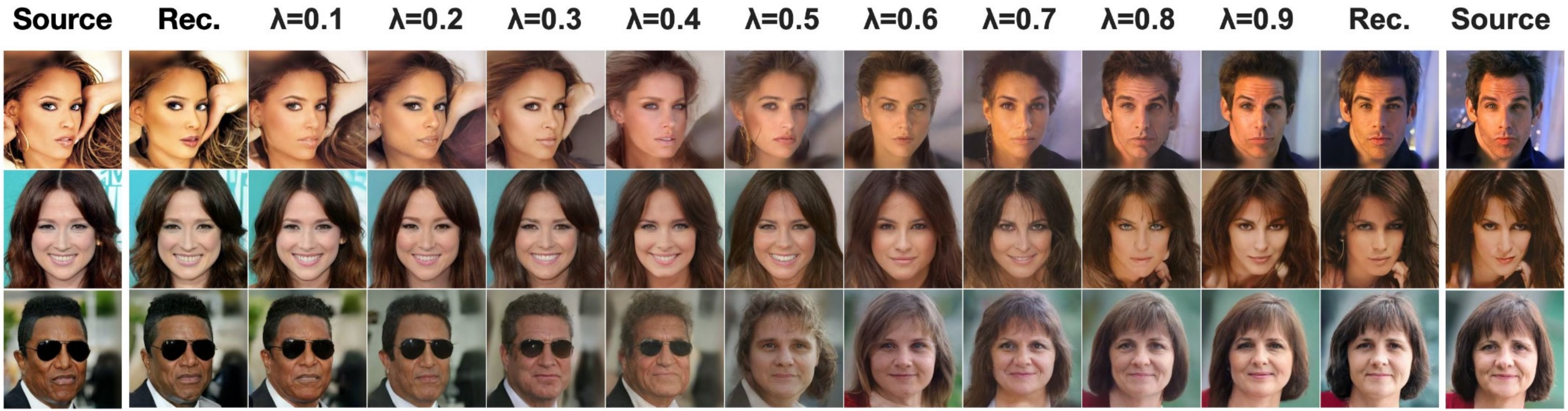
6. Image interpolation



6. Image interpolation



6. Image interpolation



7. Conclusion

- Great potential shown
- Appliances in data compression
- Possible risks of malicious usage