Диффузионные модели

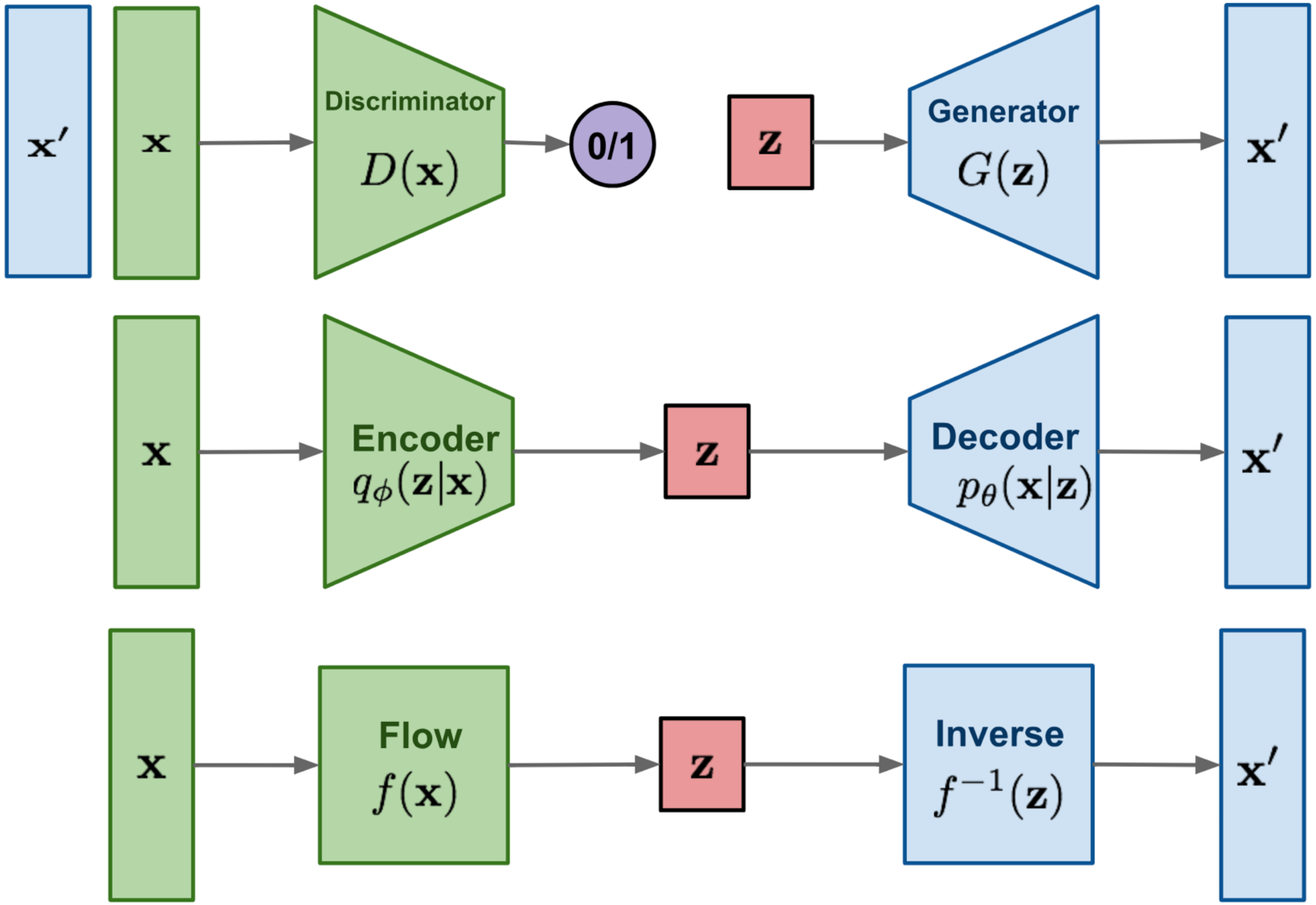
НАЦИОНАЛЬНЫЙ ИССЛЕДОВАТЕЛЬСКИЙ УНИВЕРСИТЕТ

Что мы уже знаем

GAN: minimax the classification error loss.

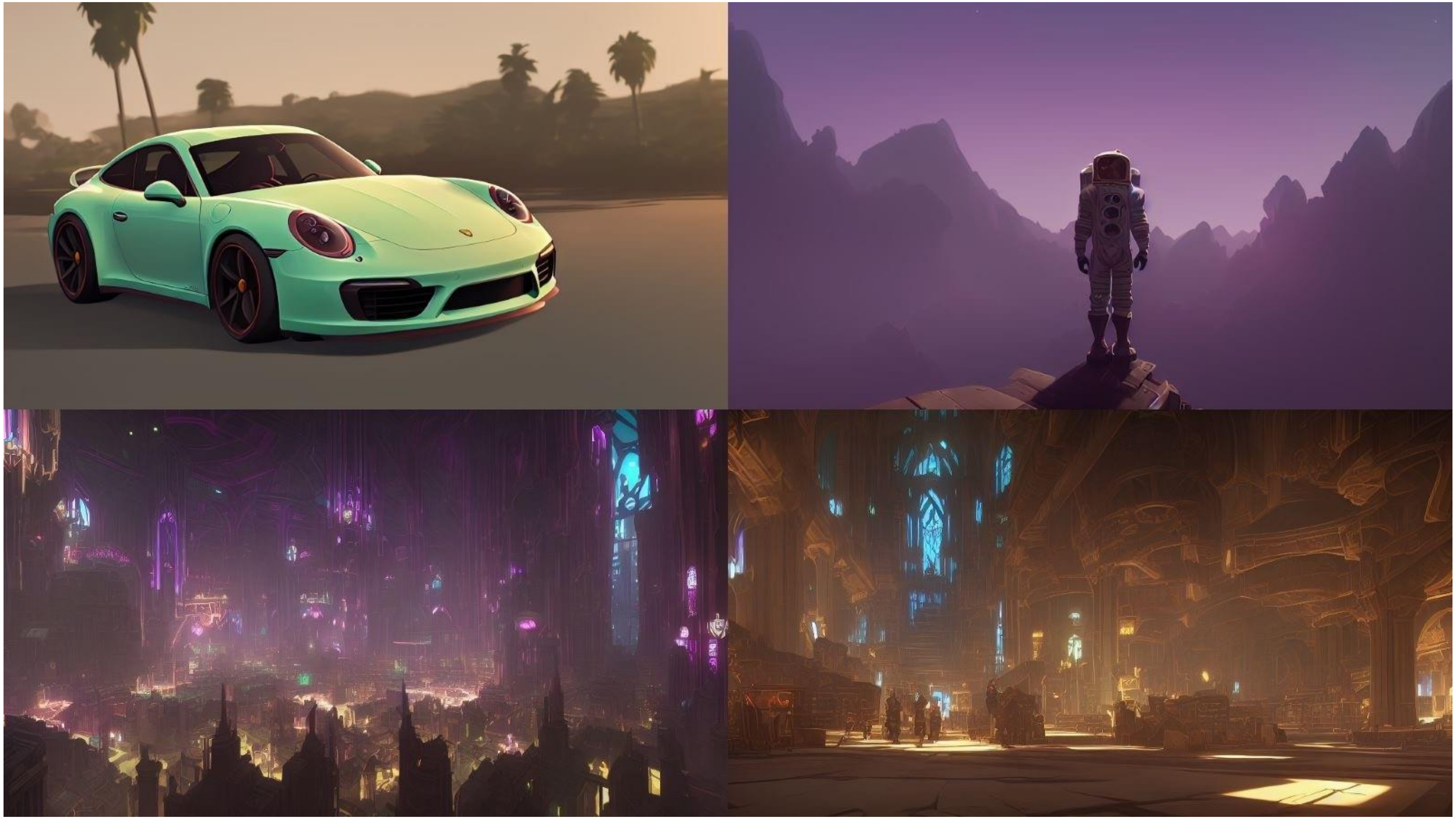
VAE: maximize ELBO.

Flow-based generative models: minimize the negative log-likelihood



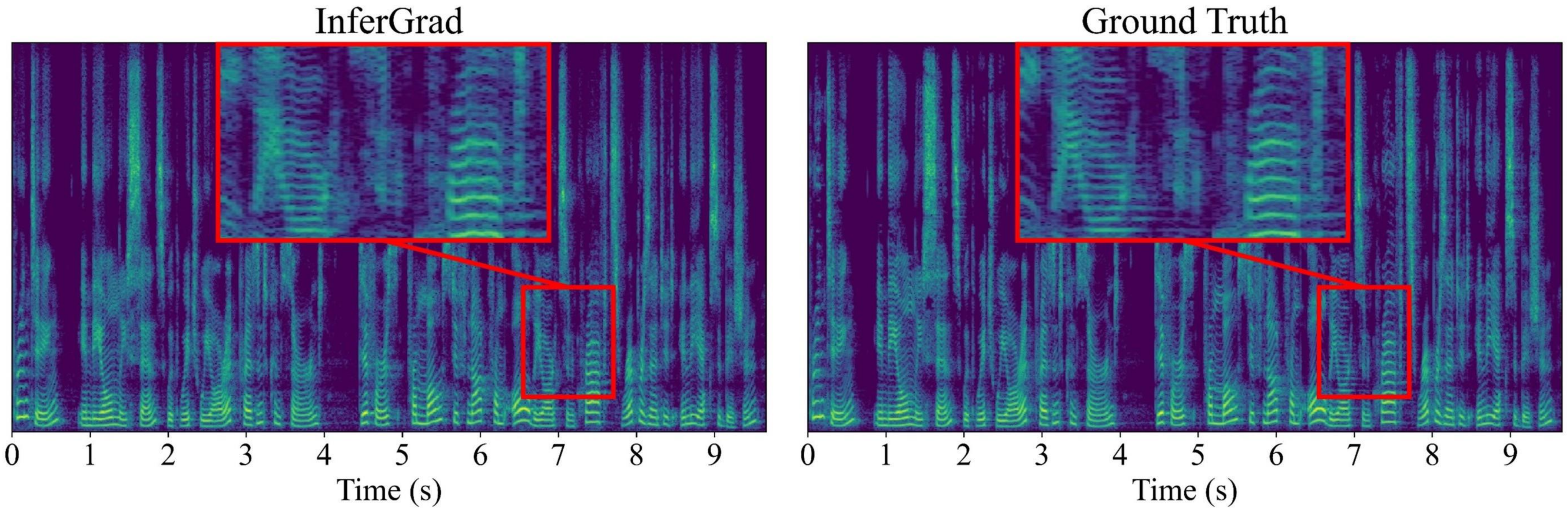
Приложения

Stable Diffusion (StabilityAI)



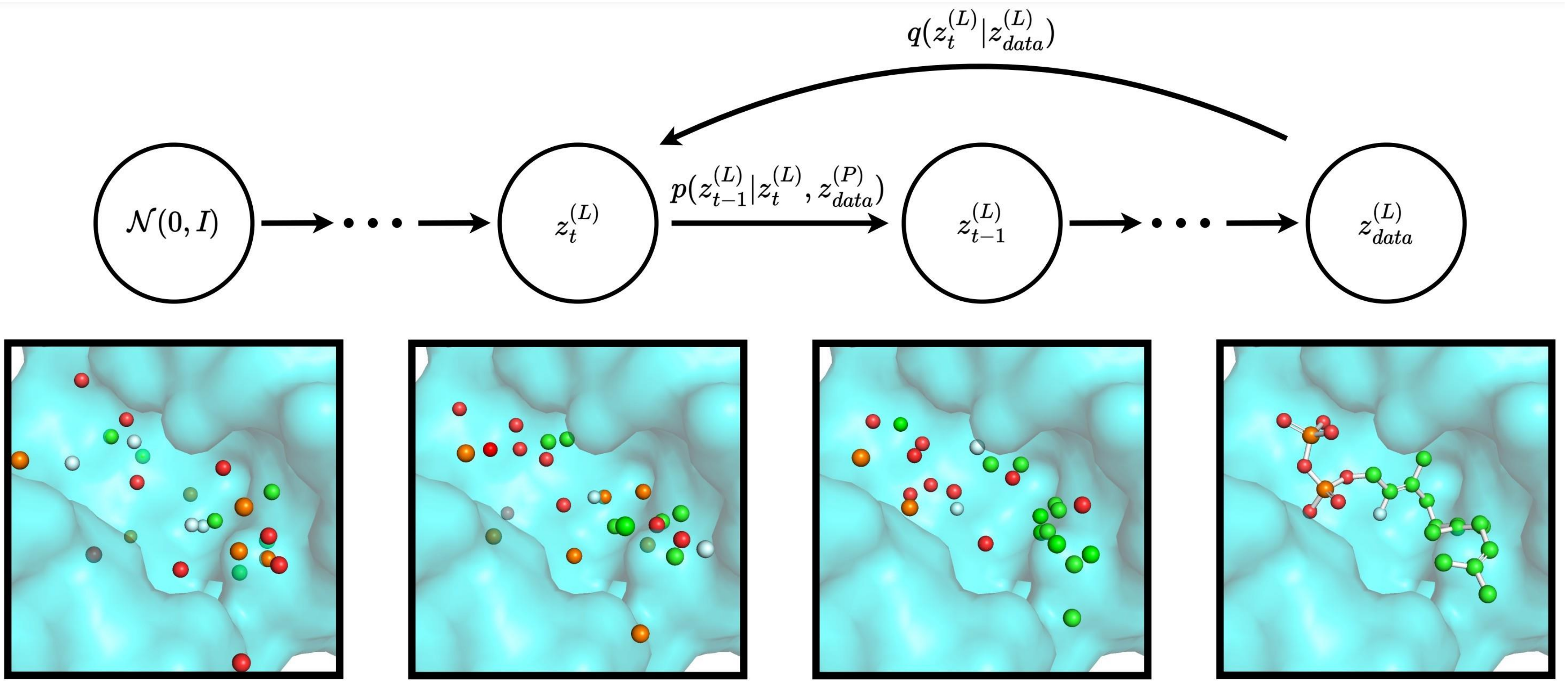
Source: https://learnopencv.com/image-generation-using-diffusion-models/

Text-to-speech generation



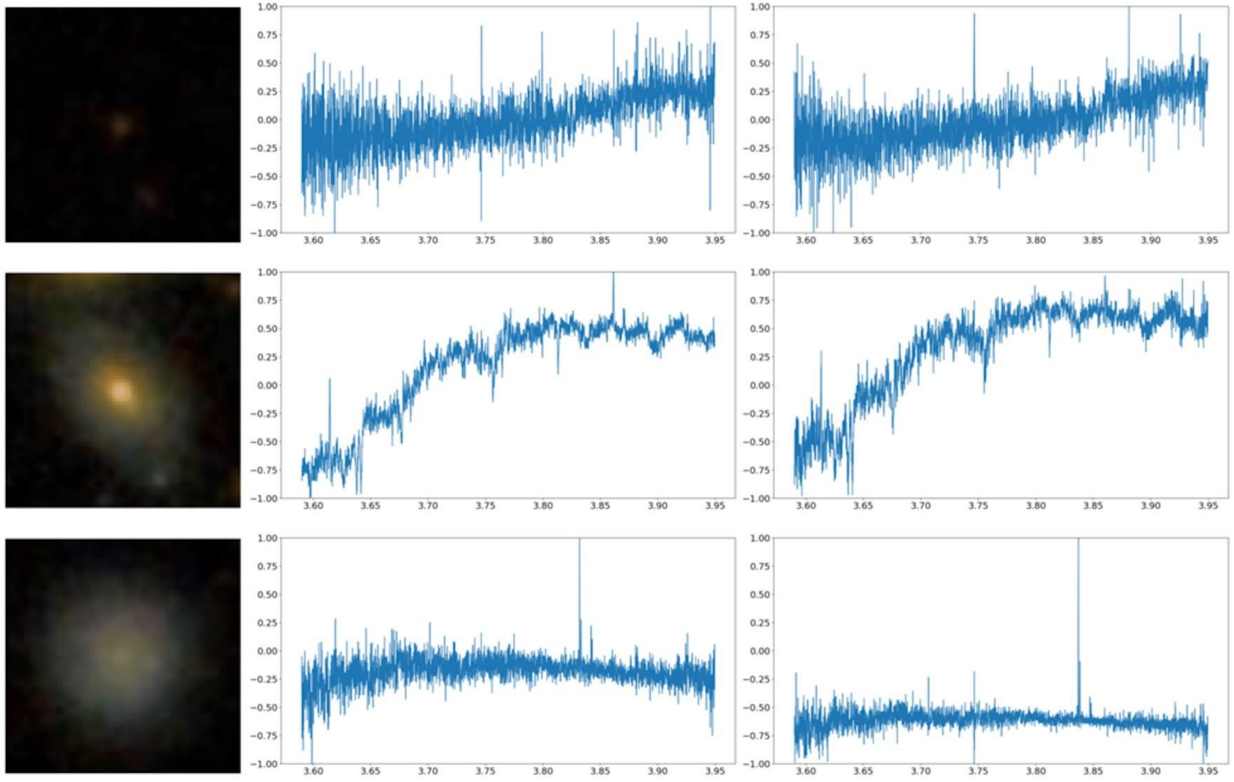
Source: https://github.com/heejkoo/Awesome-Diffusion-Models#text-to-speech

Molecular and material generation



Source: https://github.com/heejkoo/Awesome-Diffusion-Models#molecular-and-material-generation

Astronomical spectra generation



(a) (b) (c)

Figure 3: Generated spectra for the images in (a). In (b) we show the real spectra, in (c) the best match according to our contrastive model, out of 25 samples.

Source: https://ml4physicalsciences.github.io/2022/files/NeurIPS_ML4PS_2022_78.pdf

Dark matter density modelling

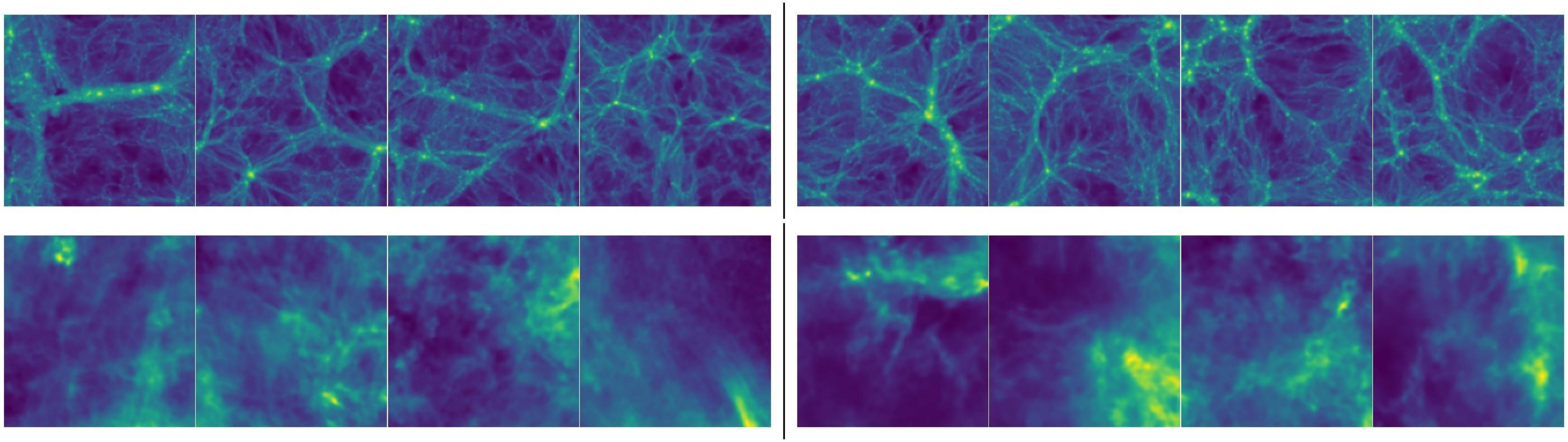
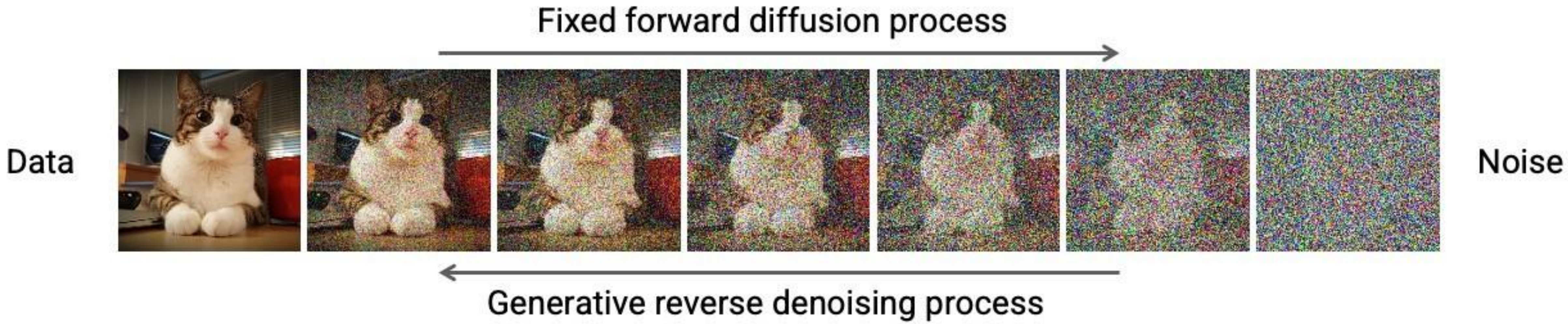


Figure 1: Four log cold dark matter mass density fields from the training data (top left) and from the sampled model (top right) at 128x128. Four samples of dust from the training data (bottom left) and from the trained model (bottom right).

Source: https://ml4physicalsciences.github.io/2022/files/NeurIPS_ML4PS_2022_25.pdf

Интуиция

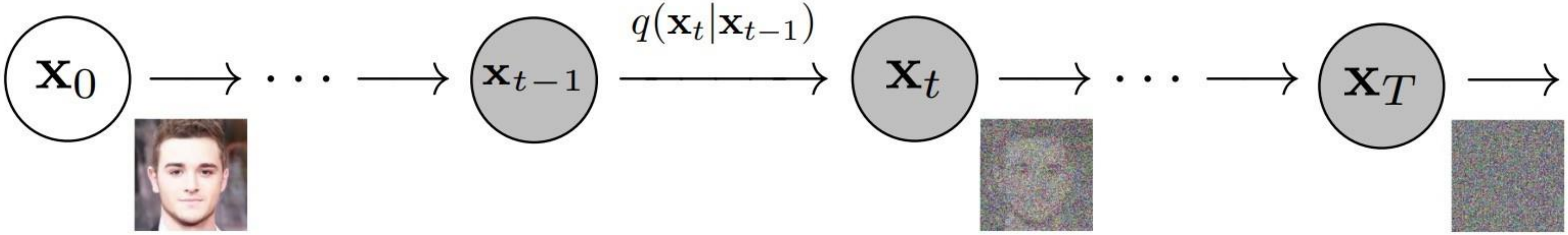
Общая идея диффузионных моделей



Источник: https://cvpr2022-tutorial-diffusion-models.github.io/

Процесс диффузии (зашумления)

Мы сами задаем как будем добавлять шум



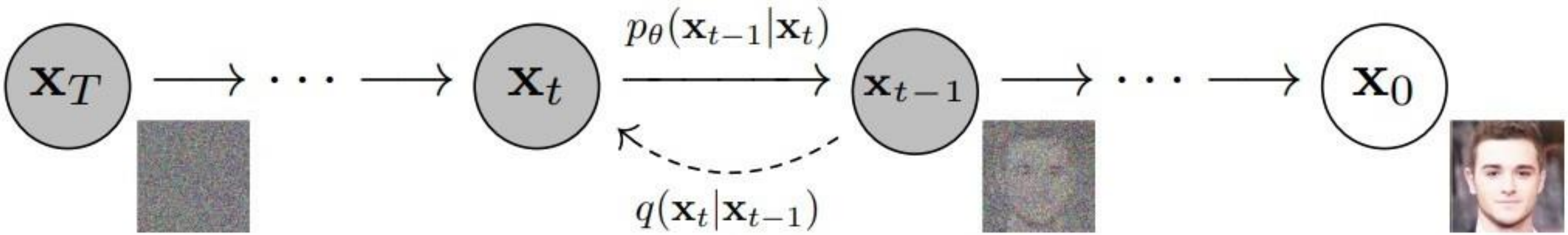
$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \boldsymbol{\mu}_t = \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \boldsymbol{\Sigma}_t = \beta_t\mathbf{I})$$

Константа

Источник: https://www.assemblyai.com/blog/diffusion-models-for-machine-learning-introduction/

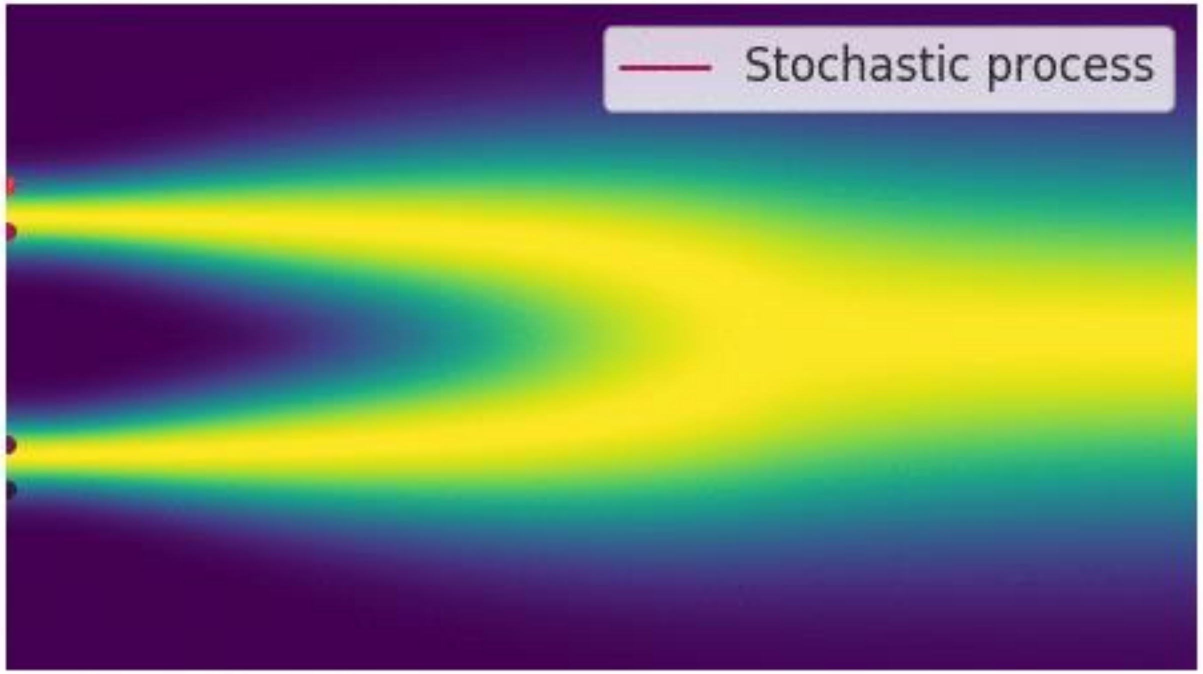
Обратный процесс

Учим с помощью нейронной сети



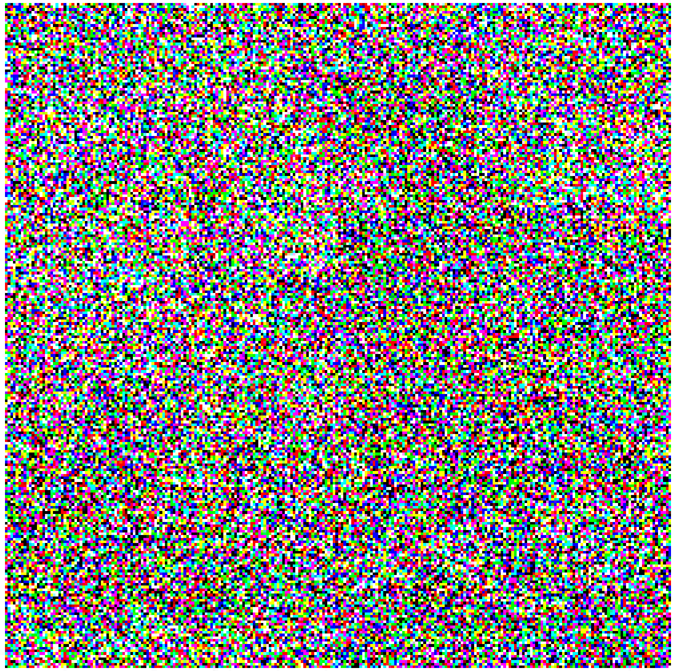
Источник: https://www.assemblyai.com/blog/diffusion-models-for-machine-learning-introduction/

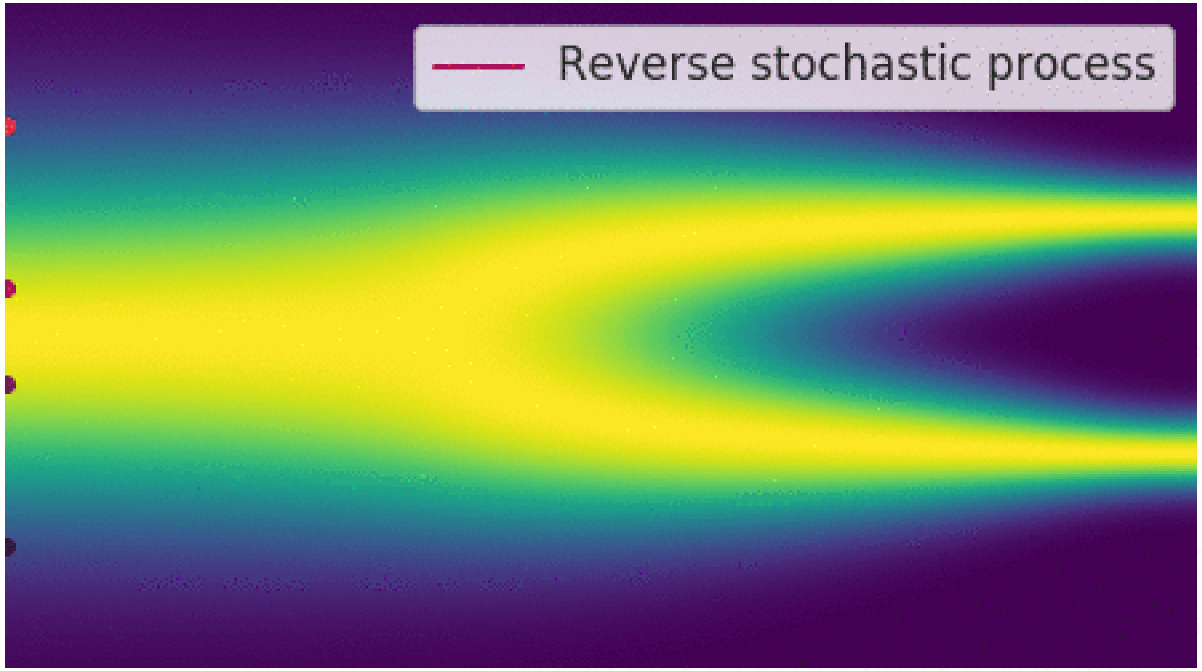
Демо: диффузия



Источник: https://yang-song.net/blog/2021/score/

Демо: обратный процесс

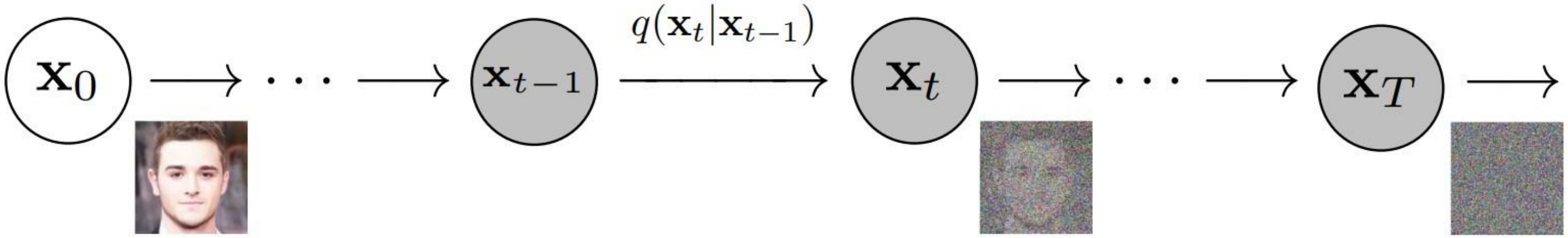




Источник: https://yang-song.net/blog/2021/score/

Диффузионные модели

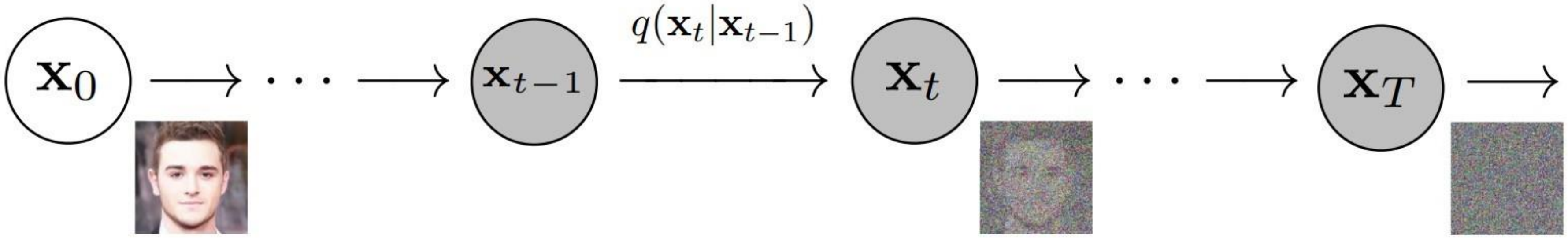
Процесс диффузии (зашумления)



- $x_t = \sqrt{\alpha_t} x_{t-1} + \sqrt{1 - \alpha_t} \epsilon_t$ $\qquad$ $\epsilon_t \sim N(0, I), \;\; \alpha_t = 1 - \beta_t$

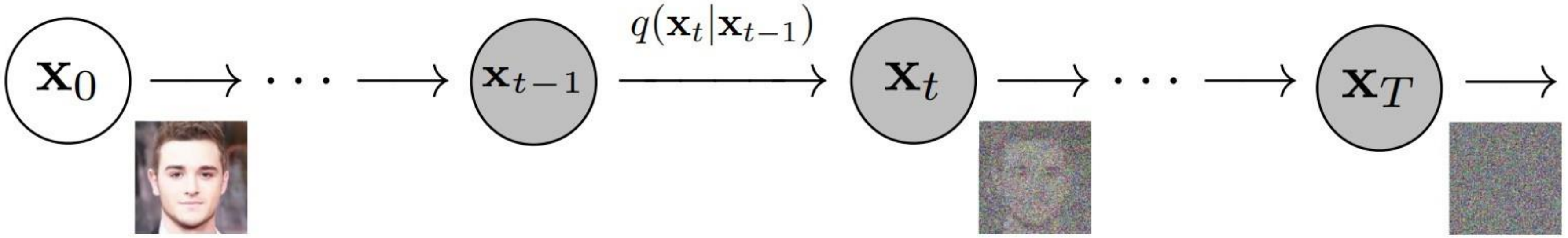
Мы сами так задали процесс

Процесс диффузии (зашумления)



- $x_t = \sqrt{\alpha_t} x_{t-1} + \sqrt{1 - \alpha_t} \epsilon_t$ $\quad$ $\epsilon_t \sim N(0, I), \quad \alpha_t = 1 - \beta_t$
- $x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon$ $\quad$ $\epsilon \sim N(0, I), \quad \bar{\alpha}_t = \prod_{i=1}^{t} \alpha_t$

Процесс диффузии (зашумления)

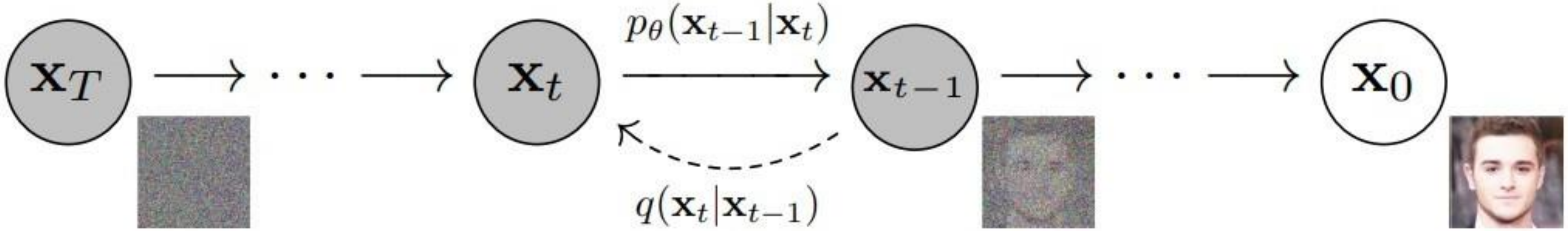


$$x_t = \sqrt{\alpha_t} x_{t-1} + \sqrt{1-\alpha_t}\epsilon_t \qquad \epsilon_t \sim N(0, I), \quad \alpha_t = 1 - \beta_t$$

$$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon \qquad \epsilon \sim N(0, I), \quad \bar{\alpha}_t = \prod_{i=1}^{t} \alpha_t$$

$$x_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon\right) + \tilde{\beta}_t z \qquad z \sim N(0, I), \quad \tilde{\beta}_t = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t$$

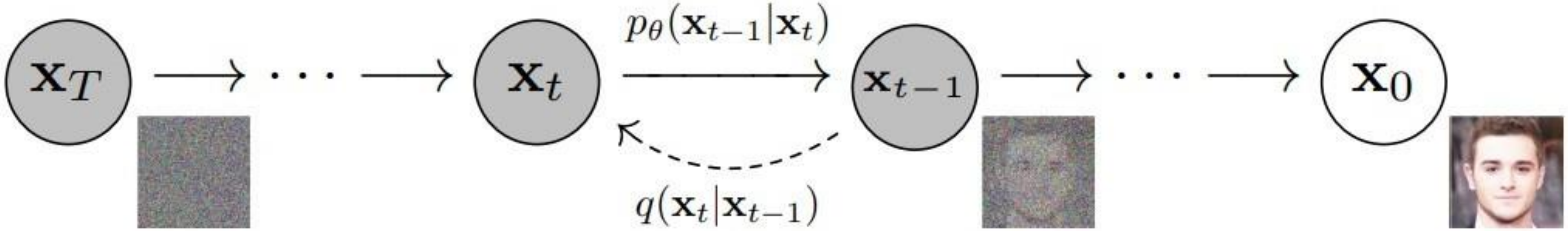
Обратный процесс



- $\hat{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(x_t, t)\right) + \sigma_t z \qquad z \sim N(0, I), \quad \sigma_t = const$

Предсказываем нейронной сетью

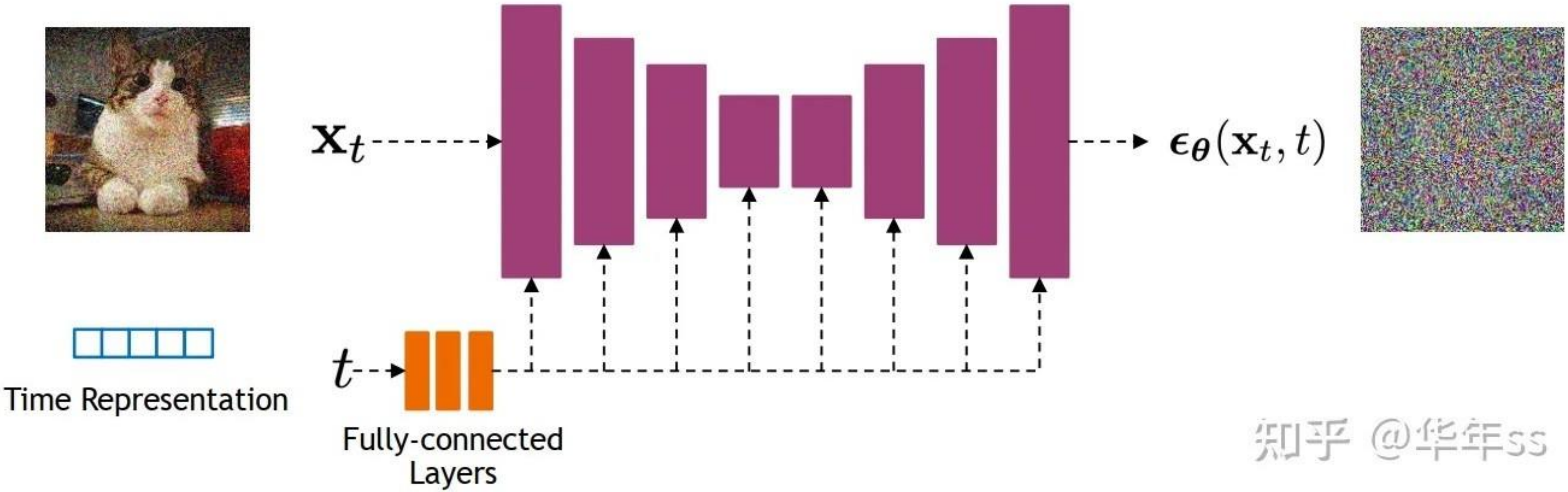
Обратный процесс



- $\hat{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(x_t, t)\right) + \sigma_t z \qquad z \sim N(0, I), \quad \sigma_t = const$
- Функция потерь для обучения:

$$L_t = \|x_{t-1} - \hat{x}_{t-1}\|_2^2 \propto \|\epsilon - \epsilon_\theta(x_t, t)\|_2^2 \to \min_\theta$$

Архитектура нейронной сети



Источник: https://www.zhihu.com/question/536012286/answer/2683123893

Алгоритм обучения

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

Источник: https://arxiv.org/pdf/2006.11239.pdf

Алгоритм генерации

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** $\mathbf{x}_0$

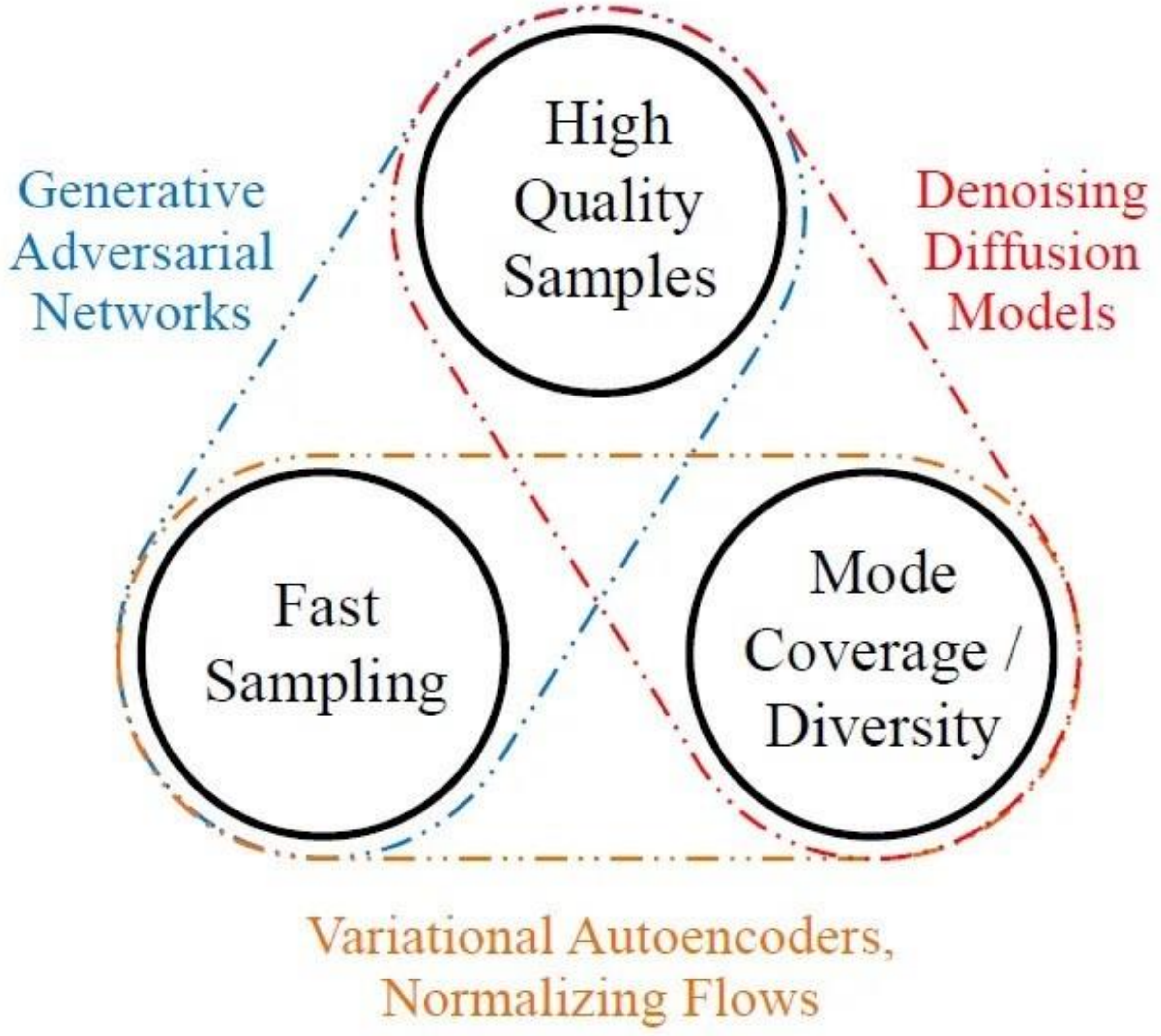
Источник: https://arxiv.org/pdf/2006.11239.pdf

Значения гиперпараметров

- $T = 1000$
- $\beta_1 < \beta_2 < \cdots < \beta_t < \cdots < \beta_T$
- $\beta_1 = 0.0001, \beta_T = 0.02$
- $\sigma^2 = \beta_t$

Заключение

Generative learning trilemma



Source: https://zhuanlan.zhihu.com/p/503932823

Заключение

GAN: minimax the classification error loss.

VAE: maximize ELBO.

Flow-based generative models: minimize the negative log-likelihood

Diffusion models: Gradually add Gaussian noise and then reverse