Diffusion Models

Naeemullah Khan
naeemullah.khan@kaust.edu.sa

جامعة الملك عبدالله
للعلوم والتقنية
King Abdullah University of
Science and Technology

KAUST Academy
King Abdullah University of Science and Technology

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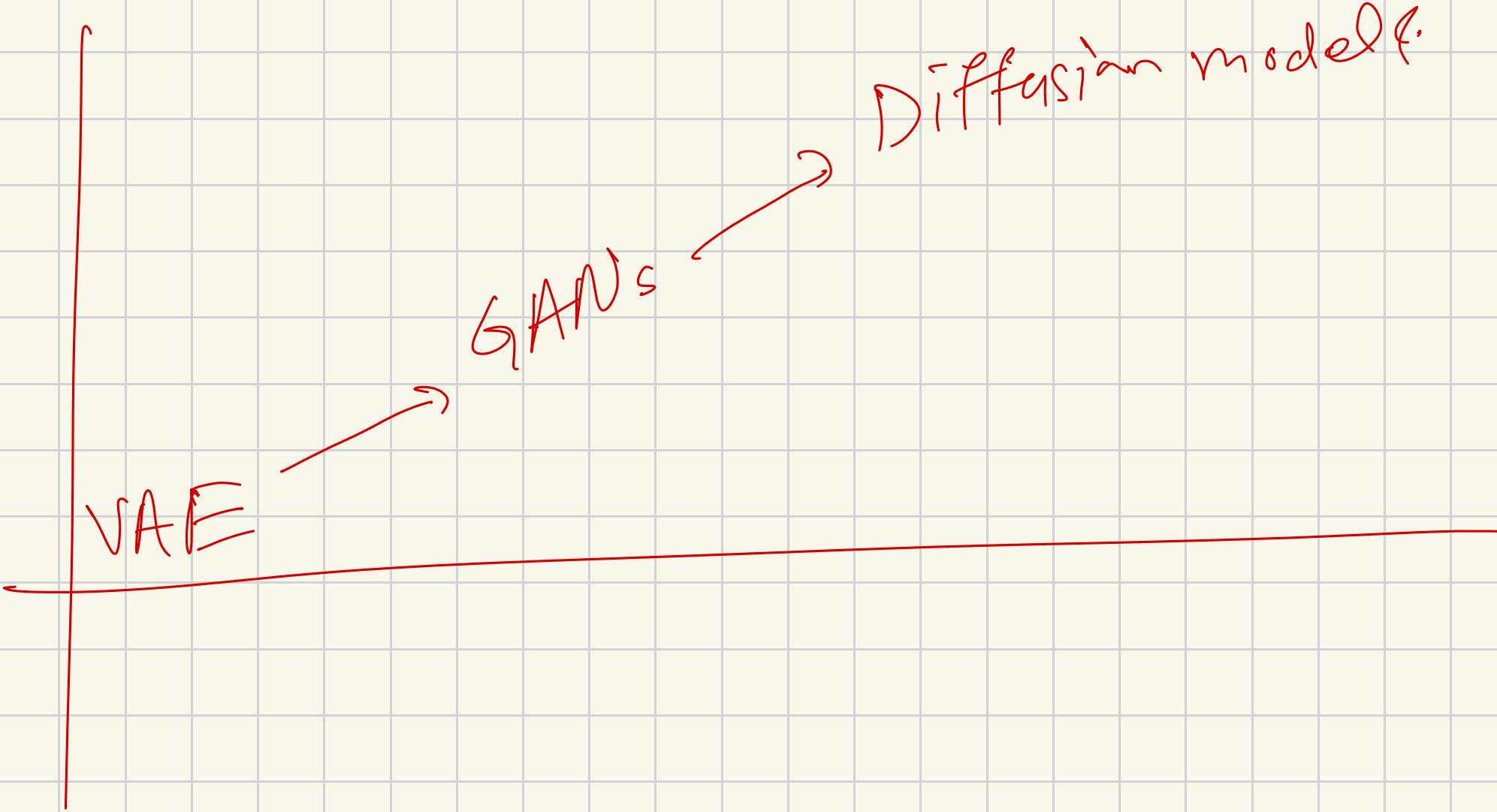
VAE
GANs
Diffusion models

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Table of Contents (cont.)

GANs: Recap

We have previously discussed Generative Adversarial Networks (GANs), which are a powerful class of generative models. Here are some key points to remember:

- Instead of explicitly modeling the data probability distribution, GANs learn it implicitly.
- Two networks are trained jointly: the **generator** creates fake samples to fool the **discriminator**, while the discriminator tries to distinguish between real and fake samples.
- GANs have been state-of-the-art in image generation due to the high quality of their outputs.

Diffusion Models: Motivation

- **The Journey of Generative Modeling:**
  - Early successes: GANs and VAEs enabled impressive image synthesis and data generation.
  - Drawbacks:
    - GANs: Training instability, mode collapse, and sensitivity to hyperparameters.
    - VAEs: Blurry outputs and limited expressiveness.
  - Key Challenge: Achieving both high sample quality and stable, reliable training.
- **Where do we go from here?**
  - Need for models that are robust, interpretable, and capable of generating diverse, high-fidelity samples.

Diffusion Models: Motivation (cont.)

- **Enter Diffusion Models:**
  - Inspired by thermodynamics, diffusion models gradually transform noise into data.
  - Highlights:
    - Simple training objective
    - Stable optimization
    - State-of-the-art sample quality
    - Probabilistic and interpretable framework

Diffusion Models: Learning Outcomes

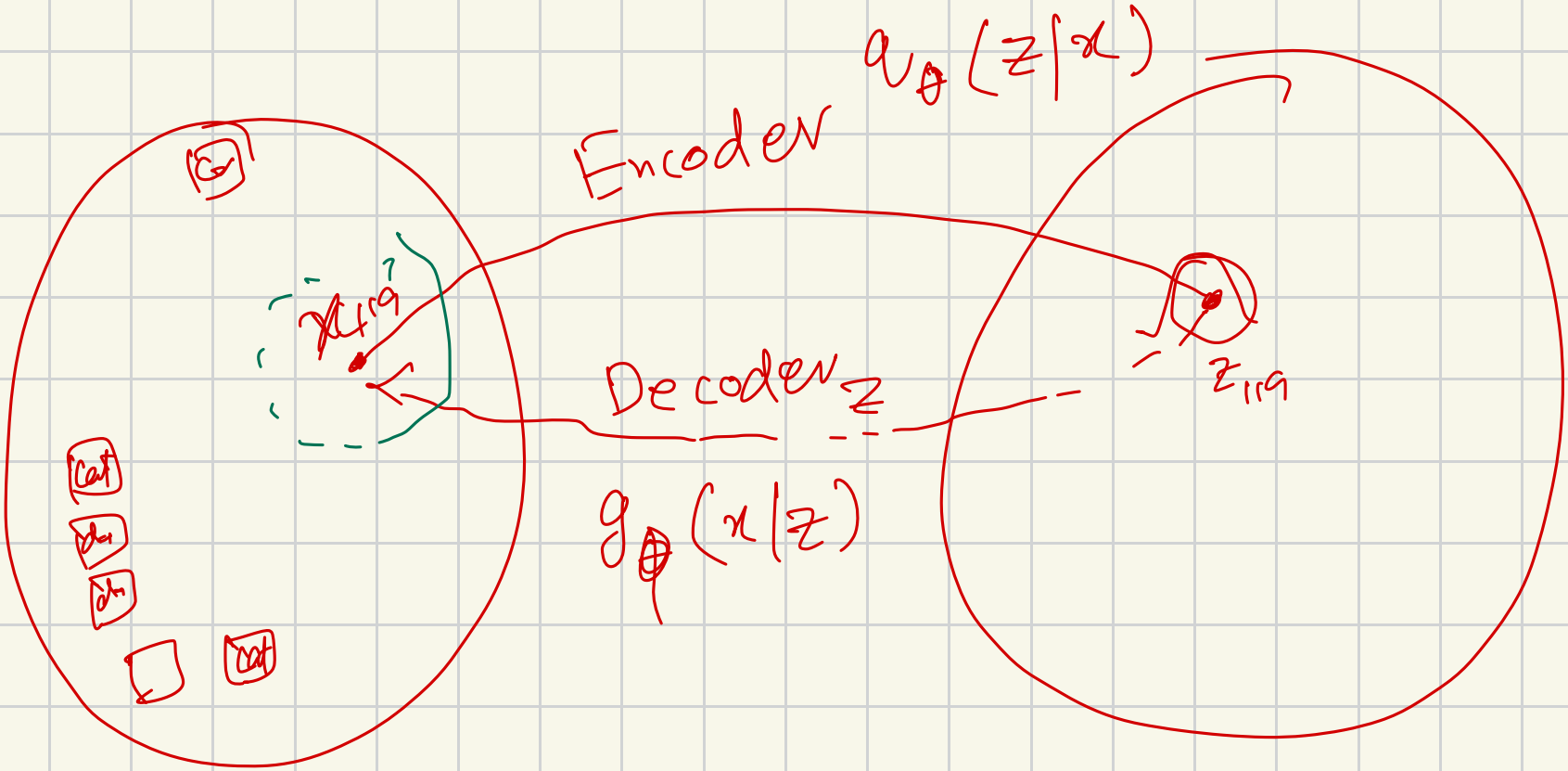
After this lecture, you will be able to:

- Explain the core principles behind diffusion-based generative models.
- Understand the forward and reverse processes in diffusion.
- Relate the training objective to variational inference and ELBO.
- Describe model architectures used in state-of-the-art diffusion models.
- Analyze and critique applications like GLIDE, DALL·E 2, Imagen, etc.

Diffusion Models: Introduction

Diffusion models are a class of probabilistic generative models that learn to reverse a gradual noising process applied to data. They have gained popularity due to their ability to generate samples with high fidelity and diversity.

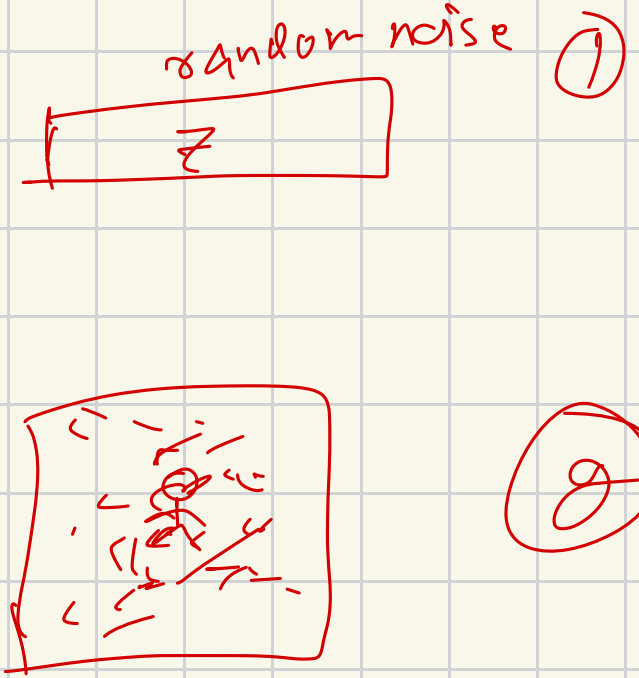
- **Inspiration:** Rooted in concepts from thermodynamics and stochastic processes.
- **Key Idea:**
  - *Forward process:* Progressively corrupt data by adding Gaussian noise.
  - *Reverse process:* Learn to recover the original data by reversing the noising process.
- **Popularity:** Known for producing high-quality and diverse generated samples.

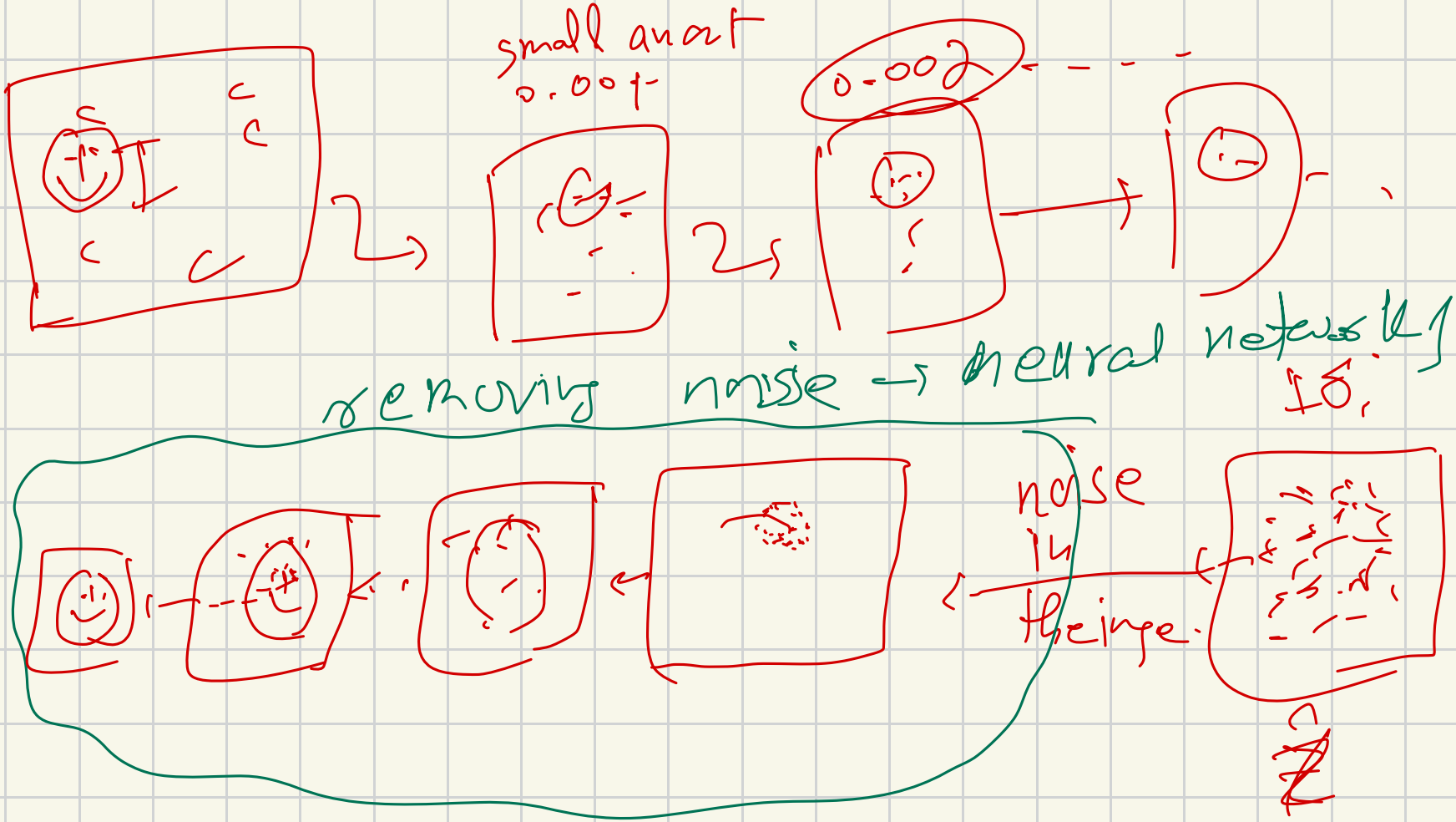


$X \rightarrow$ dataset

z

$p(z) \sim N(0, I)$.


random noise
z


small amount
0.001
0.002
removing noise → neural network is.
noise
in
the image.

Denoising Diffusion Probabilistic Models

Denoising diffusion models, also known as score-based generative models, have recently emerged as a powerful class of generative models. They achieve remarkable results in high-fidelity image generation, often outperforming GANs.

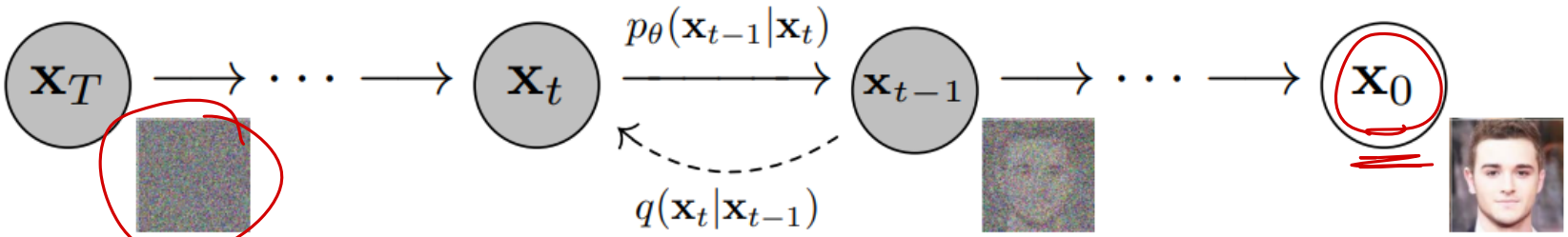
$\nabla \log p(x)$

Figure 2: Diffusion Models Beat GANs on Image Synthesis Dhariwal & Nichol, OpenAI, 2021

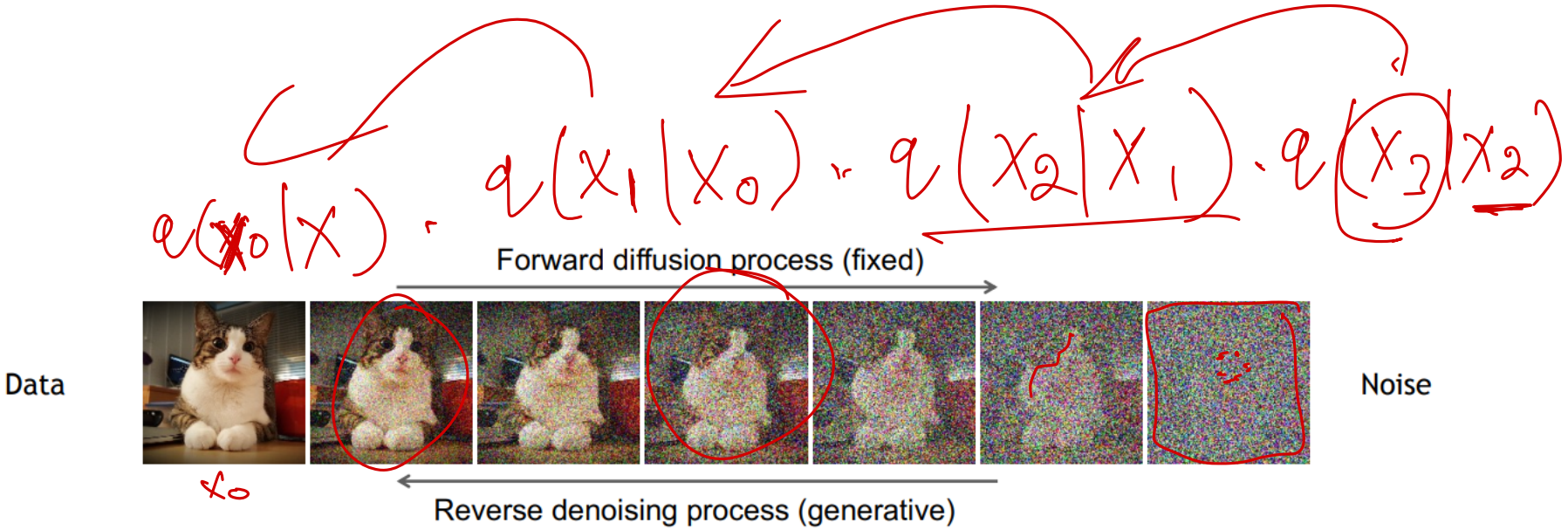
Denoising Diffusion Probabilistic Models (cont.)

Denoising diffusion models consist of two processes:

- A fixed (predefined) **forward diffusion process** q, which gradually adds Gaussian noise to an image until only pure noise remains.
- A learned **reverse denoising diffusion process** p_θ, where a neural network is trained to gradually denoise an image starting from pure noise, eventually recovering the original image.



Denoising Diffusion Probabilistic Models (cont.)



Forward Diffusion Process

- The forward process is a Markov chain that iteratively adds Gaussian noise to the image at each timestep.
- Given clean data $\mathbf{x}_0$, we generate $\mathbf{x}_t$ as:

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

- Over many steps (e.g., 1000), the data becomes indistinguishable from pure noise.
- This process is predefined and not learned.
- The full forward process:

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

Teacher take a cup of tea.

P(Teacher|$o s>)

↳ P(Take|$o s> Teache.)

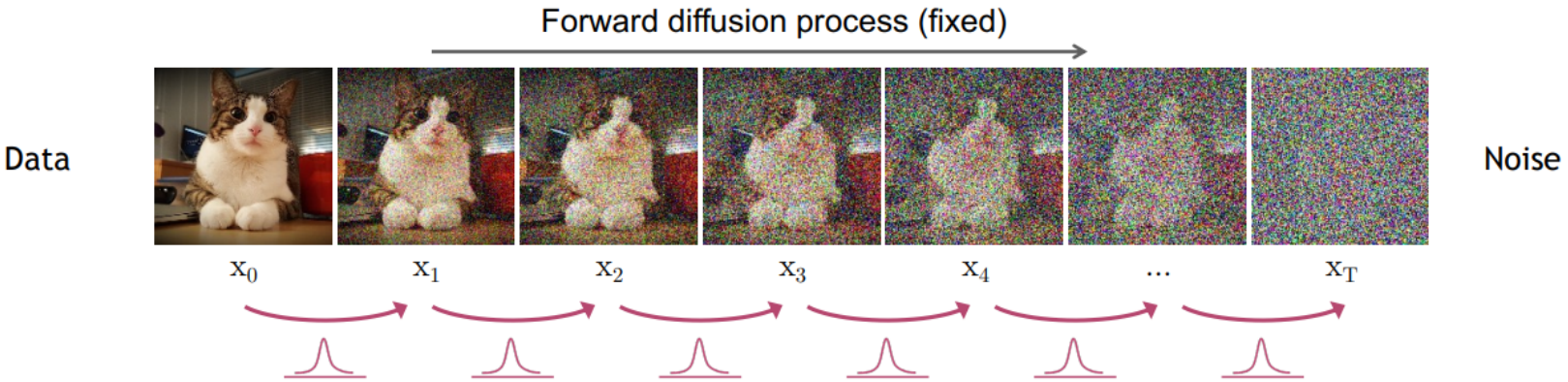
Forward Diffusion Process (cont.)

- Each new (slightly noisier) image at time step t is drawn from a conditional Gaussian distribution with $\mu_t = \sqrt{1-\beta_t}\mathbf{x}_{t-1}$ and $\sigma_t^2 = \beta_t$, which we can do by sampling $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ and then setting $\mathbf{x}_t = \sqrt{1-\beta_t}\mathbf{x}_{t-1} + \sqrt{\beta_t}\epsilon$.

previous image

adds more noise

Forward Diffusion Process (cont.)



- What if we want to go directly from q_0 to q_t?
- Let $\overline{\alpha}_t = \prod_{s=1}^{t}(1-\beta_s)$, then

$$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\overline{\alpha}_t}\mathbf{x}_0, (1-\overline{\alpha}_t)\mathbf{I})$$

- This allows us, during training, to optimize random terms of the loss function L (i.e., randomly sample t and optimize L_t).

Noise Schedules

- The noise schedule $\{\beta_t\}$ controls the amount of noise added at each timestep.
- Common schedules:
  - **Linear:** Simple and intuitive.
  - **Cosine:** Preserves perceptual signal longer; often yields better image generation results.
- The choice of schedule impacts training dynamics and the quality of generated samples.
- Visualizing different schedules helps understand how noise accumulates over time.

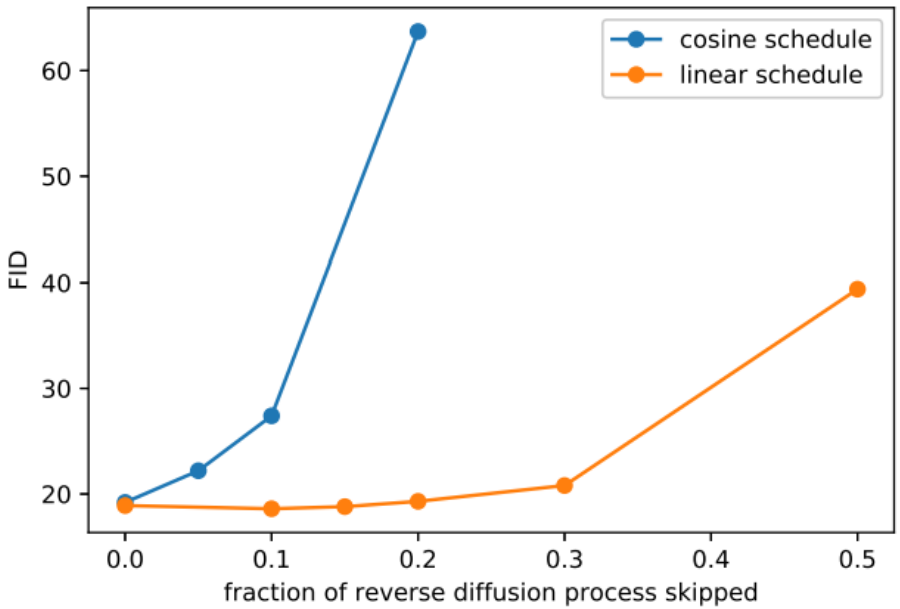


Figure 3: Comparison of linear and cosine noise schedules.

Reverse Denoising Process

In the reverse denoising process, we denoise Gaussian noise to generate an image.

- We start with a sample from the noise distribution $p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; 0, 1)$.
- The goal is to iteratively denoise this sample to recover the original image $\mathbf{x}_0$.
- At each time step t, we want to sample $\mathbf{x}_{t-1}$ given $\mathbf{x}_t$.
- The reverse process is defined as $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$, which we will learn using a neural network.

Reverse Denoising Process (cont.)

- The reverse process is a Markov chain that iteratively denoises the image.
- We want to sample $\mathbf{x}_{t-1}$ from $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$.
- However, $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ is unknown and needs to be learned.
- We approximate it with a neural network that predicts the mean and variance of the Gaussian distribution.
- If β_t is small enough at each time step, we can assume $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ is a Gaussian distribution:

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \mu_\theta(\mathbf{x}_t, t), \Sigma_\theta(\mathbf{x}_t, t))$$

where μ_θ and Σ_θ are neural networks conditioned on $\mathbf{x}_t$ and t.

Reverse Denoising Process (cont.)

- For simplicity, we can fix the variance Σ_θ to a constant value (e.g., $\beta_t \mathbf{I}$) and only learn the mean μ_θ.
- The reverse process can then be expressed as:

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \mu_\theta(\mathbf{x}_t, t), \beta_t \mathbf{I})$$

and the joint distribution over all time steps is:

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

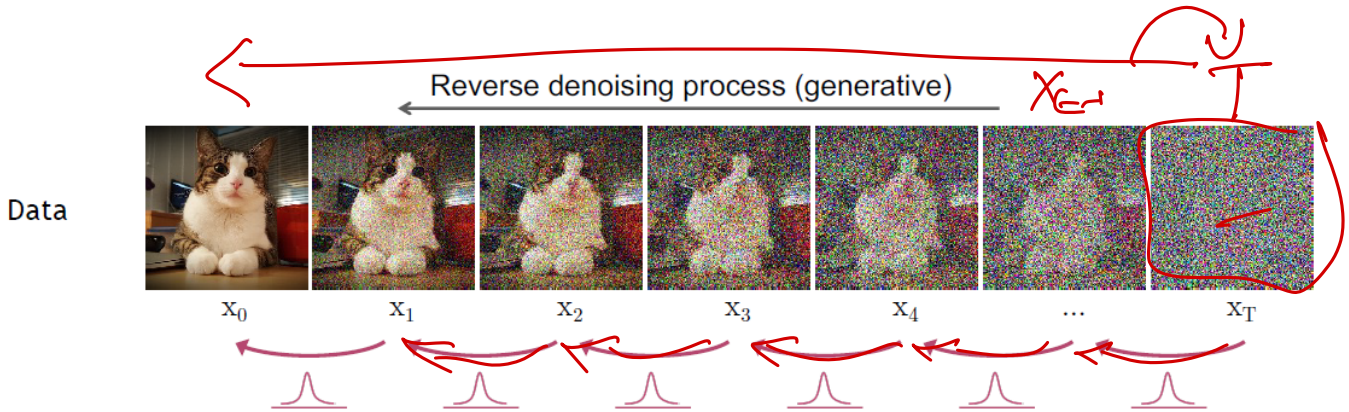


Figure 4: Reverse denoising process in diffusion models.

Direct maximization of the marginal likelihood $p(\mathbf{x})$ is often intractable.

Solution: Use the *Evidence Lower Bound* (ELBO) as a tractable proxy objective:

$$\log p(\mathbf{x}) \geq \mathbb{E}_{q(\mathbf{z}|\mathbf{x})}\left[\log \frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z}|\mathbf{x})}\right] = \text{ELBO}$$

ELBO Decomposition:

- **Reconstruction term:** Measures how well the model can reconstruct the data $\mathbf{x}$ from the latent variables $\mathbf{z}$.
- **KL divergence:** Penalizes the difference between the approximate posterior $q(\mathbf{z}|\mathbf{x})$ and the true/model prior $p(\mathbf{z})$.

Training: Maximize the ELBO to train the model, which encourages both accurate reconstruction and regularization of the latent space.

Learning Denoising Models

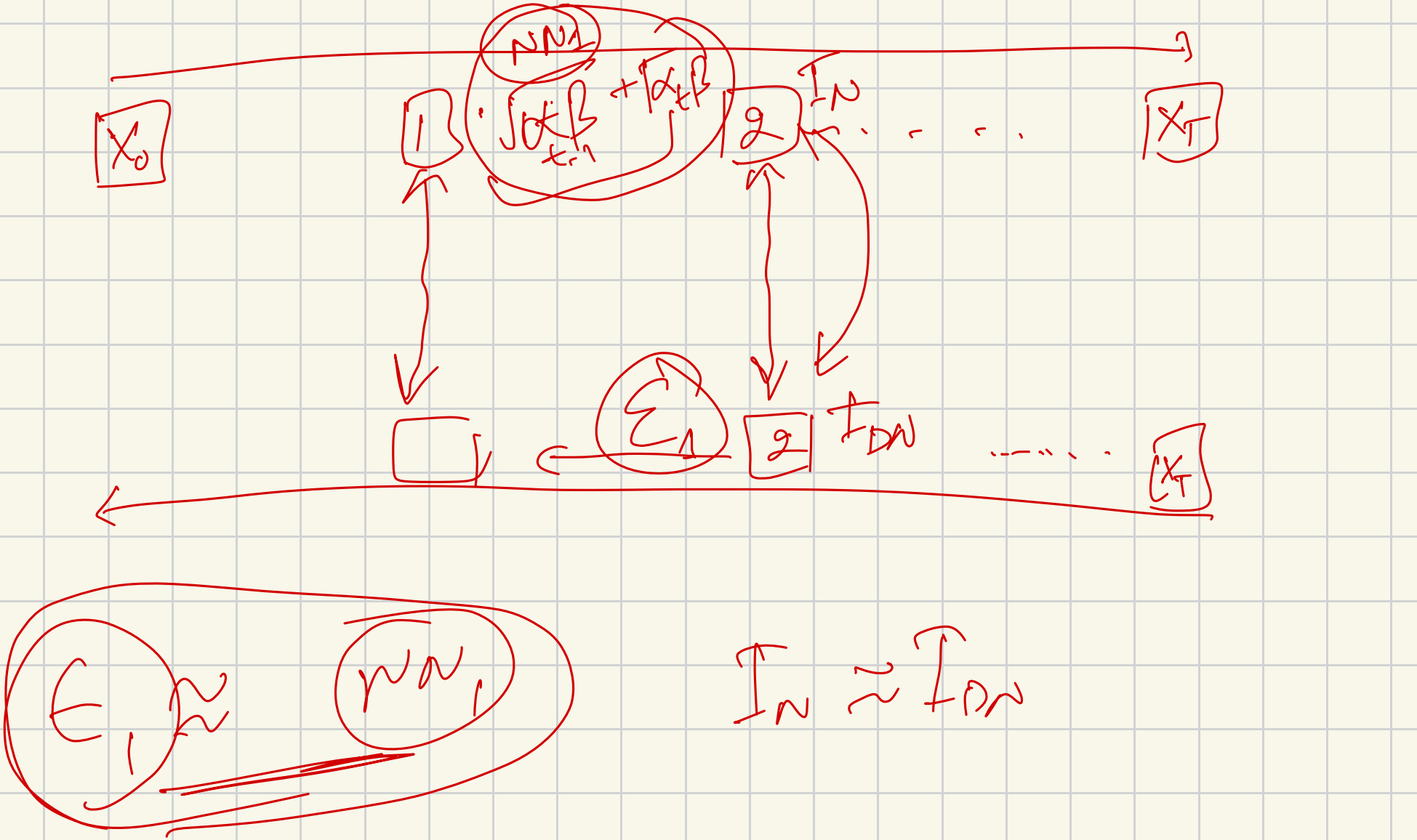
In diffusion models, we learn a denoising function that can reverse the noise addition process. The training objective is to minimize the difference between the predicted noise and the actual noise added at each step.

- For training, we can form a variational upper bound, commonly used for training variational autoencoders:

$$\mathbb{E}_{q(x_0)}\left[-\log p_\theta(\mathbf{x}_0)\right] \leq \mathbb{E}_{q(x_0)q(\mathbf{x}_{1:T}|x_0)}\left[-\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|x_0)}\right]$$

- The ELBO for this process can be expressed as a sum of losses at each time step t:

$$L = L_0 + L_1 + \cdots + L_T$$


NN1
x_0
1
$\alpha_{t-1}\beta$
$+\alpha_t\beta$
2
I_N
x_T
ε_1
2
I_{DN}
x_T
ε_1
NN1
$I_N \simeq I_{DN}$

Learning Denoising Models (cont.)

- We can reparametrize the mean so that the neural network learns to predict the added noise (using a network $\epsilon_\theta(\mathbf{x}_t, t)$ for noise level t in the KL terms that constitute the losses). This means our neural network becomes a noise predictor, rather than a direct mean predictor. The mean can be computed as:

$$\mu_\theta(\mathbf{x}_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(\mathbf{x}_t, t)\right)$$

- The final objective function L_t (for a random time step t and $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$) is:

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

- For a complete derivation, see here.

Algorithm

Algorithm 1 Training

1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $t \sim \text{Uniform}(\{1, \dots, T\})$
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

Training Algorithm

1. Sample x_0 from the data distribution.
2. Randomly select a timestep t.
3. Corrupt x_0 with noise to obtain x_t.
4. Model predicts noise $\epsilon_\theta(x_t, t)$.
5. Compute loss: mean squared error between predicted and true noise.
6. Optimize using SGD or Adam.

Algorithm (cont.)

Algorithm 2 Sampling

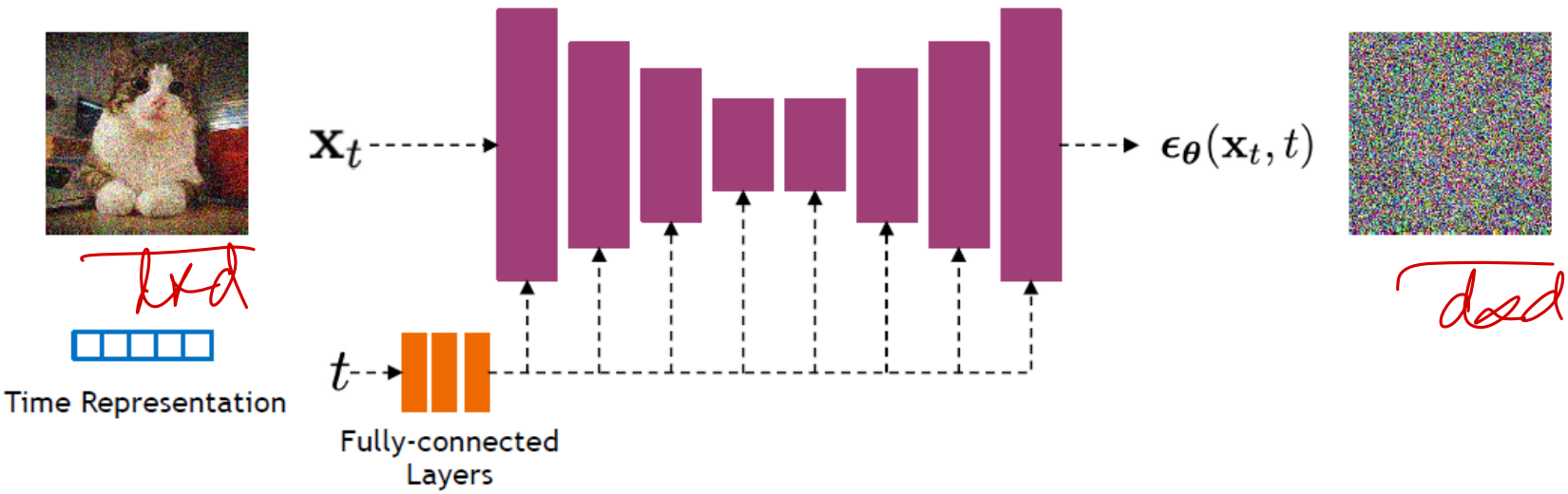
$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \ldots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

Sampling Algorithm

1. Start from Gaussian noise x_T.
2. For each timestep $t = T, \ldots, 1$:
   - 2.1 Predict noise $\epsilon_\theta(x_t, t)$.
   - 2.2 Compute posterior mean $\mu_\theta(x_t, t)$.
   - 2.3 Sample x_{t-1} from the Gaussian posterior.
   - 2.4 (Optional) Apply guidance (e.g., classifier-free) for improved results.

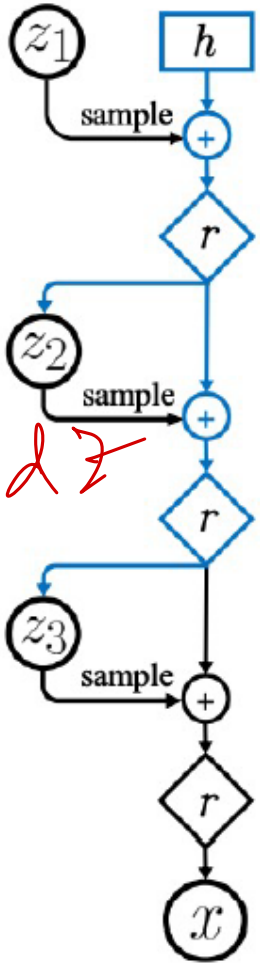
Network Architectures

- Diffusion models commonly use U-Net architectures with ResNet blocks and self-attention layers to represent $\epsilon_\theta(x_t, t)$.
- Time is encoded using sinusoidal positional embeddings or random Fourier features.



Connection to VAEs

- Diffusion models can be viewed as a special form of hierarchical VAEs (one VAE after another).
- In diffusion models:
  - The encoder is fixed.
  - The latent variables have the same dimension as the data.
  - The denoising model is shared across different timesteps.
  - The model is trained with a reweighted variational bound.



Problems with Diffusion Models

- **Slow Sampling:** Diffusion models require hundreds to thousands of iterative steps to generate a sample, making them computationally expensive and slow compared to other generative models.

Trilemma of Generative Learning

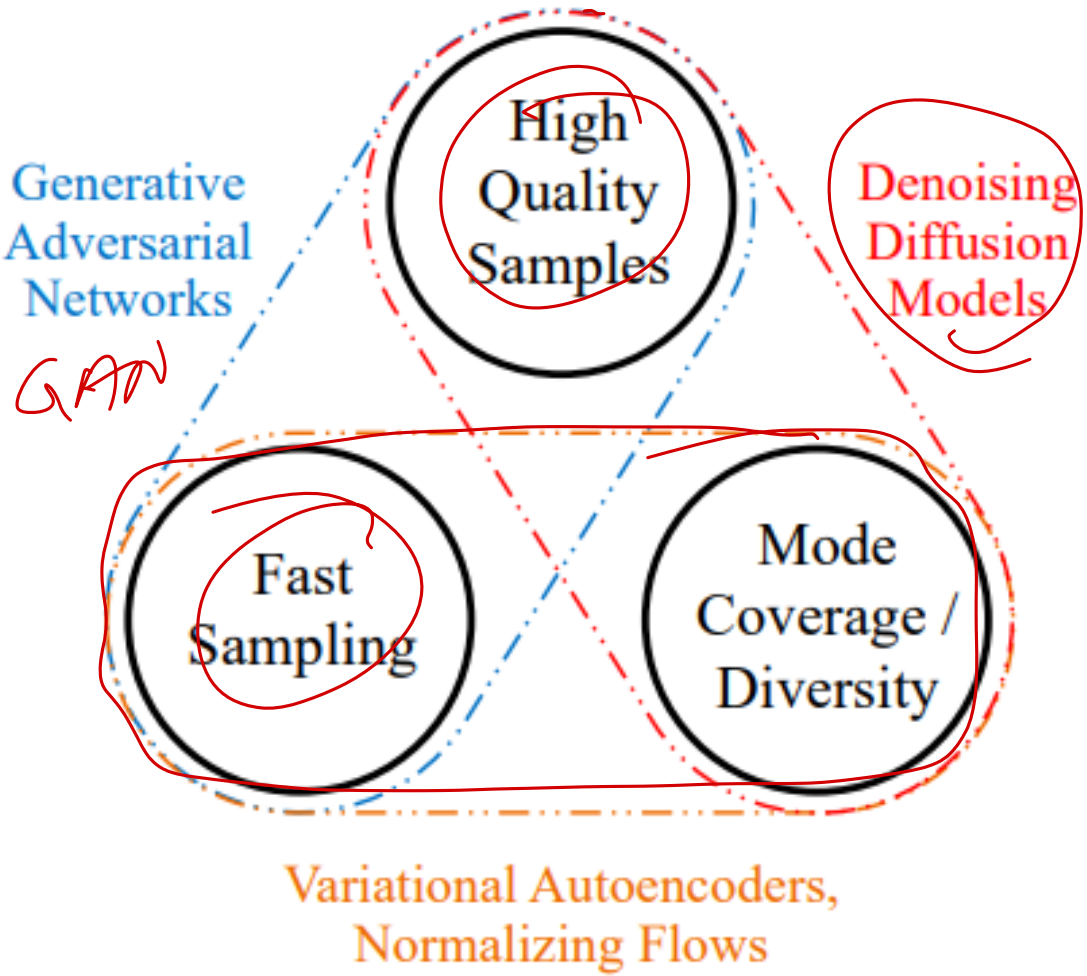


Figure 5: Generative Learning Trilemma: Balancing sample quality, diversity, and fast sampling.

[0] Tackling the Generative Learning Trilemma with Denoising Diffusion GANs

Diffusion Models: Current Research Directions

- **Faster Sampling:**
  - Denoising Diffusion Implicit Models (DDIM): Propose a non-Markovian process for faster and deterministic sampling by skipping steps and refining the sample.
- **Improved Training:**
  - Improved Denoising Diffusion Probabilistic Models: Learn the noise variance σ^2 during training, rather than fixing it, for better flexibility and performance.
- **Score-Based Modeling:**
  - Score-Based Generative Modeling through SDEs: Model the gradient of the log-density (score function) using stochastic differential equations for improved sample quality.
- **Combining GANs and Diffusion:**
  - Denoising Diffusion GANs: Use GANs to model each denoising step, addressing the trilemma by improving speed and sample quality.

Diffusion Models: Current Research Directions (cont.)

- **High-Fidelity Generation:**
  - Cascaded Diffusion Models: Employ a cascade of diffusion models at different resolutions to boost sample fidelity.

Application: GLIDE - OpenAI

Figure 6: Image Inpainting with GLIDE

[0] GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models

Application: DALL.E 2 - OpenAI

Figure 7: Text to image generation eith DAll.E 2

[0] Hierarchical Text-Conditional Image Generation with CLIP Latents

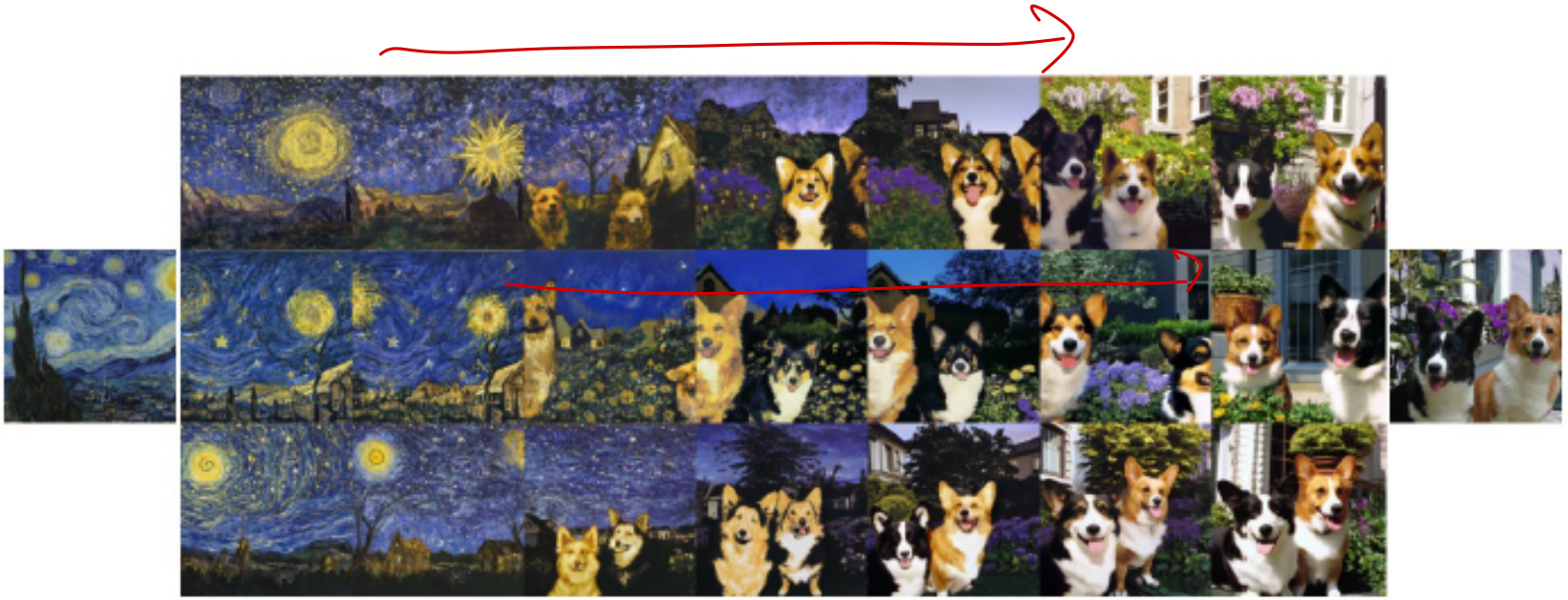
Fix the CLIP embedding $\mathbf{z}_i$

Decode using different decoder latents $\mathbf{x}_T$

Figure 8: Image Variations

[0] Hierarchical Text-Conditional Image Generation with CLIP Latents

DALL.E 2 - OpenAI



Interpolate image CLIP embeddings $\mathbf{z}_i$

Use different $\mathbf{x}_T$ to get different interpolation trajectories.

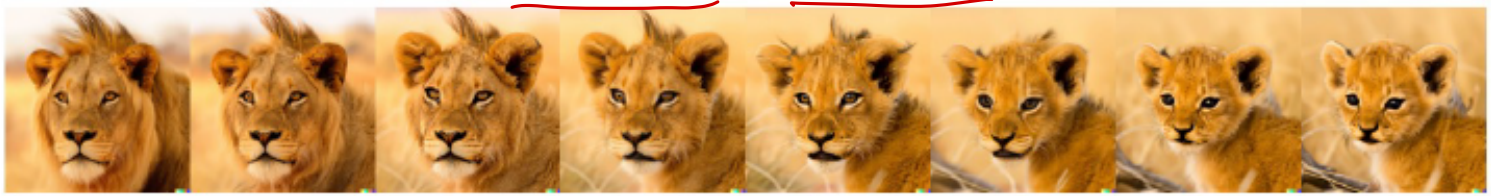
Figure 9: Image interpolation

[0] Hierarchical Text-Conditional Image Generation with CLIP Latents

DALL.E 2 - OpenAI

a photo of a cat → an anime drawing of a super saiyan cat, artstation

a photo of a victorian house → a photo of a modern house



a photo of an adult lion → a photo of lion cub

Change the image CLIP embedding towards the difference of the text CLIP embeddings of two prompts.

Decoder latent is kept as a constant.

Figure 10: Text Difference Image interpolation

[0] Hierarchical Text-Conditional Image Generation with CLIP Latents

Imagen - Google

A brain riding a rocketship heading towards the moon.

[0] Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding

Imagen - Google

A brain riding a rocketship heading towards the moon.

[0] Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding

Imagen - Google

A dragon fruit wearing karate belt in the snow.

[0] Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding

Imagen - Google

A relaxed garlic with a blindfold reading a newspaper while floating in a pool of tomato soup.

[0] Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding

Diffusion Autoencoders

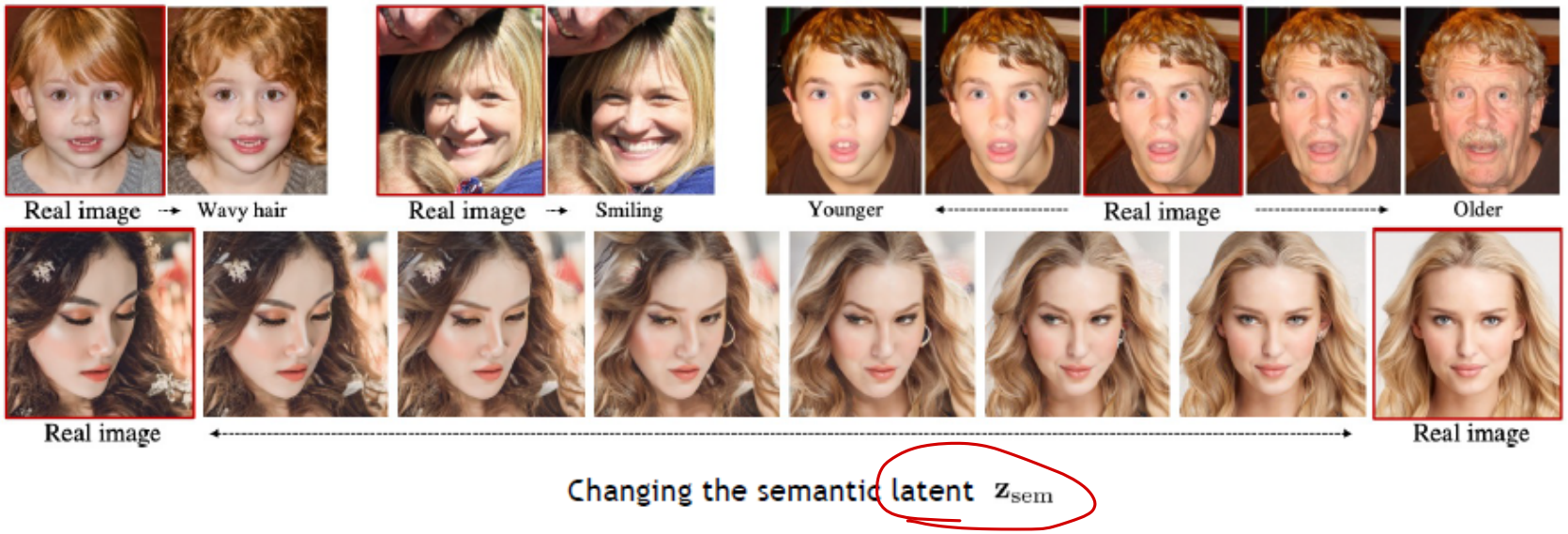


Figure 11: Learning semantic meaningful latent representations in diffusion models

[0] Diffusion Autoencoders: Toward a Meaningful and Decodable Representation

Super Resolution

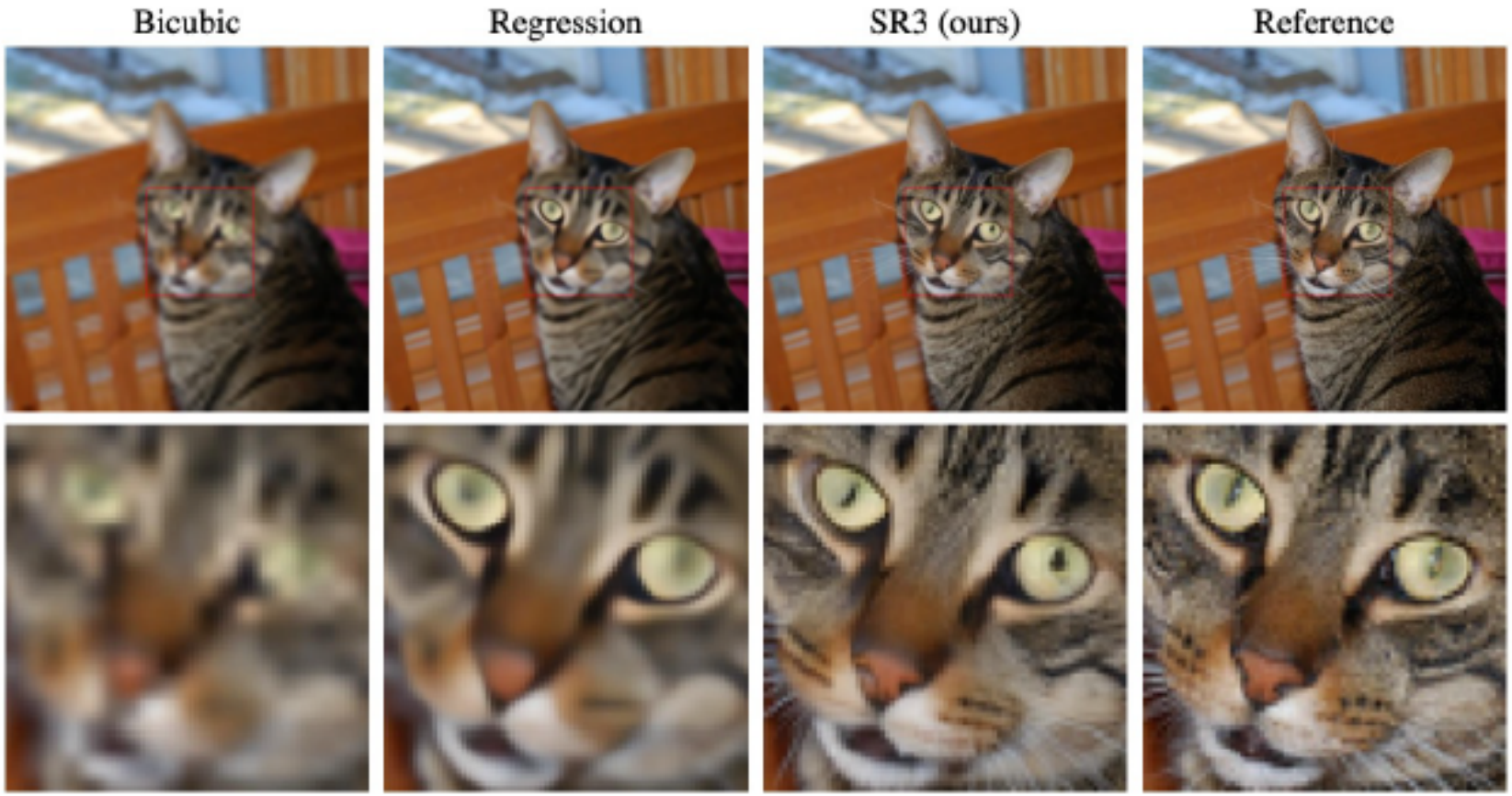
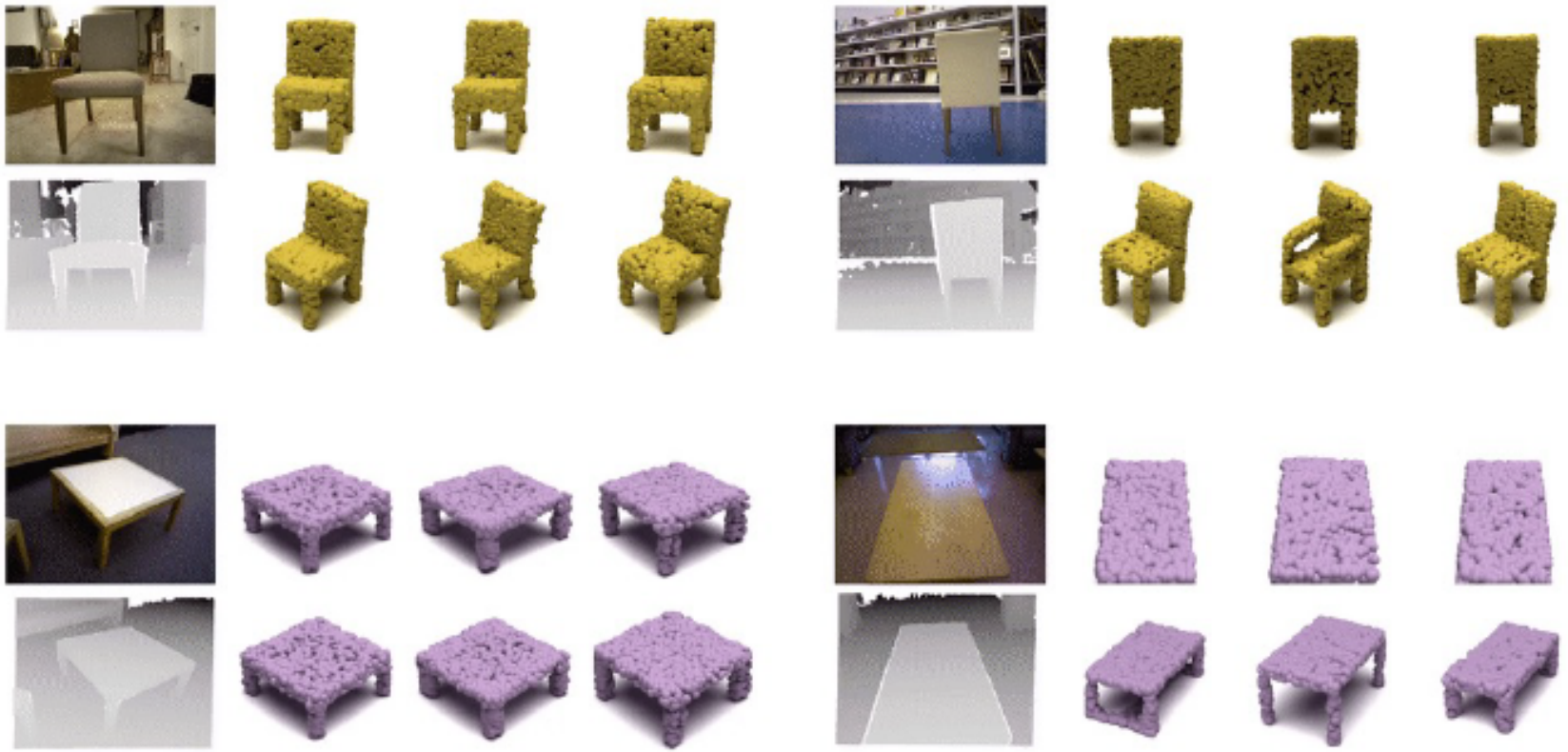


Figure 12: Natural Image Super Resolution $64 \times 64 \longrightarrow 256 \times 256$

[0] Image Super-Resolution via Iterative Refinement

3D Shape Generation



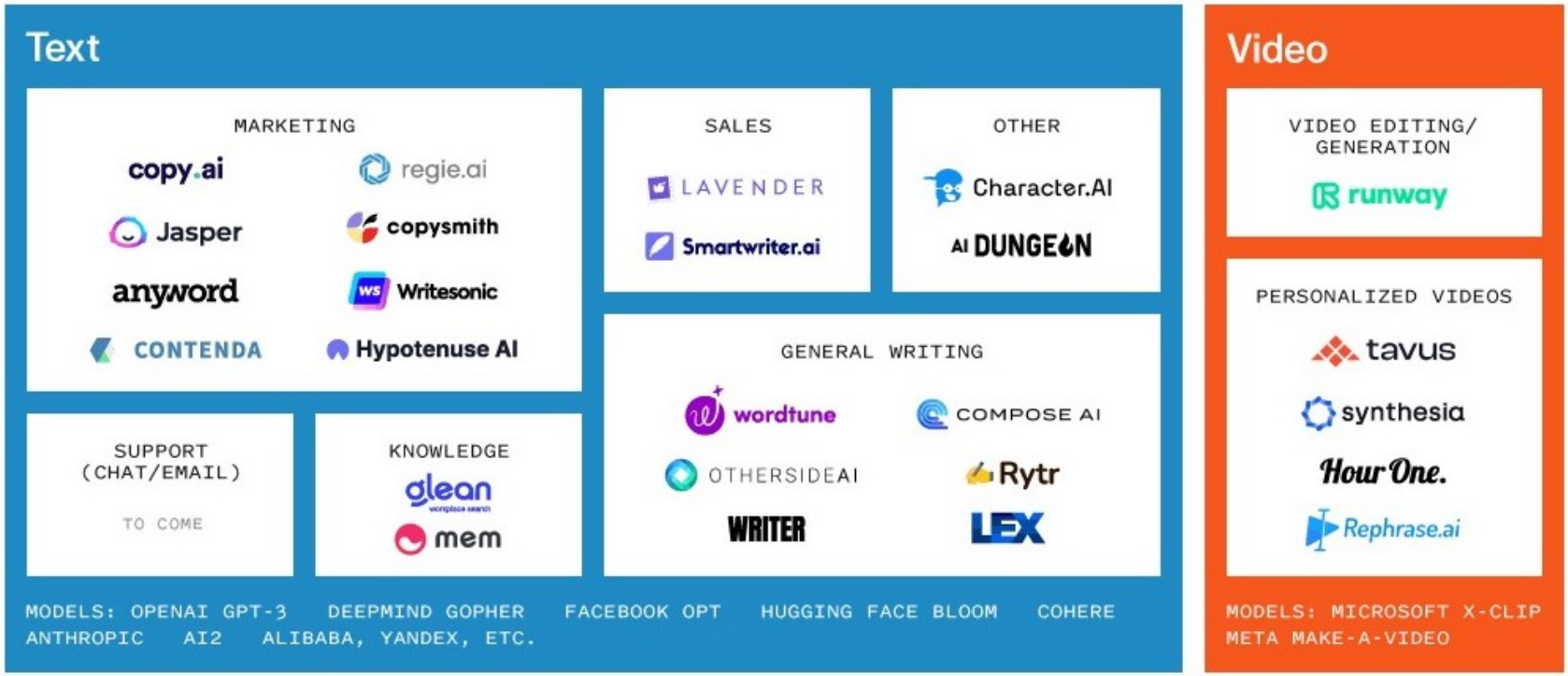
[0] 3D Shape Generation and Completion through Point-Voxel Diffusion

Try It Yourself!

Text to Image generation with stable diffusion.
https://huggingface.co/spaces/stabilityai/stable-diffusion

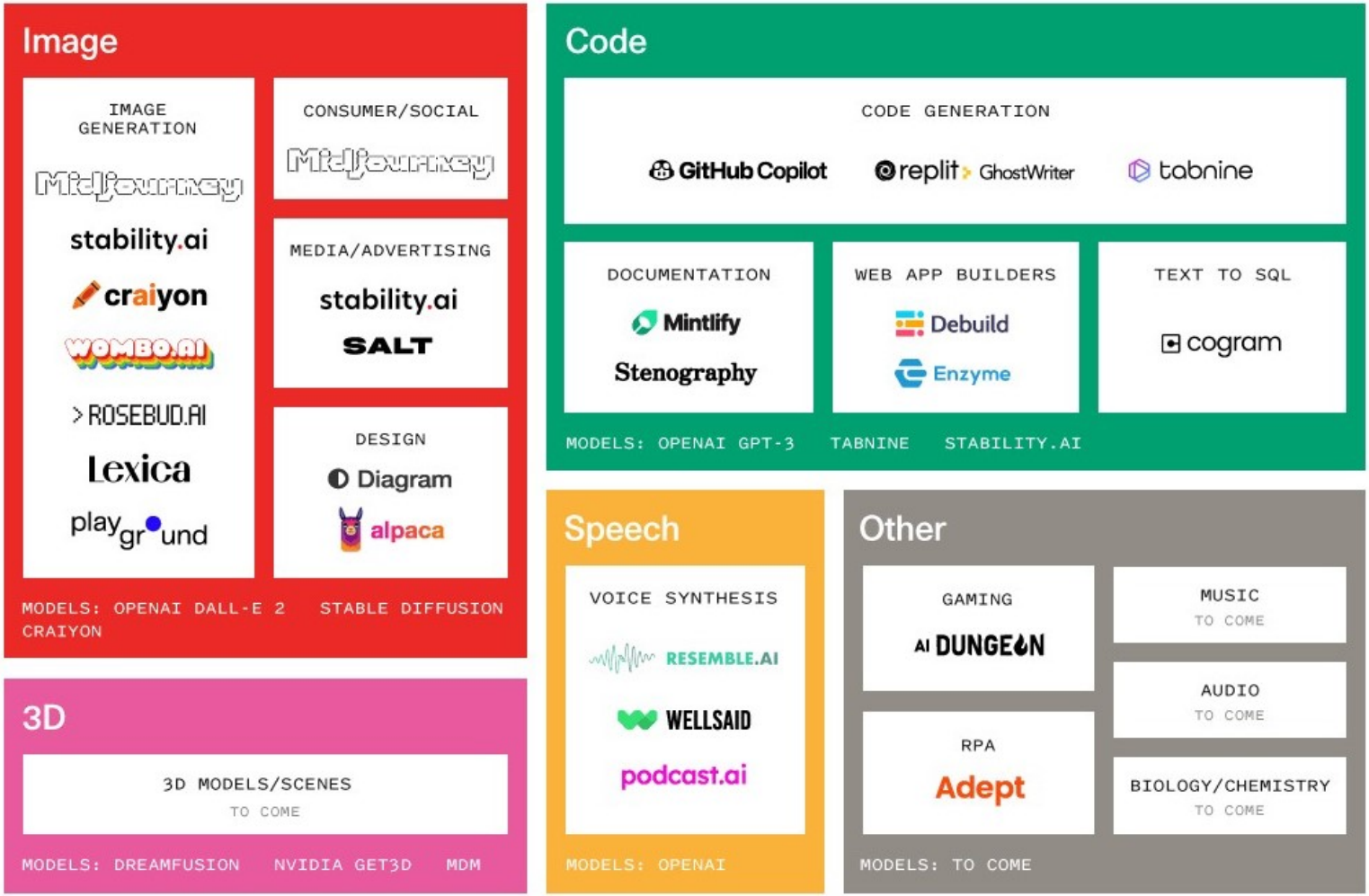
[0] High-Resolution Image Synthesis with Latent Diffusion Models

The Generative AI Landscape



[0] Sonya Huang (@sonyatweetybird)

The Generative AI Landscape



[0] Sonya Huang (@sonyatweetybird)

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Credits

Dr. Prashant Aparajeya

Computer Vision Scientist — Director(AISimply Ltd)

p.aparajeya@aisimply.uk

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