Diffusion Models

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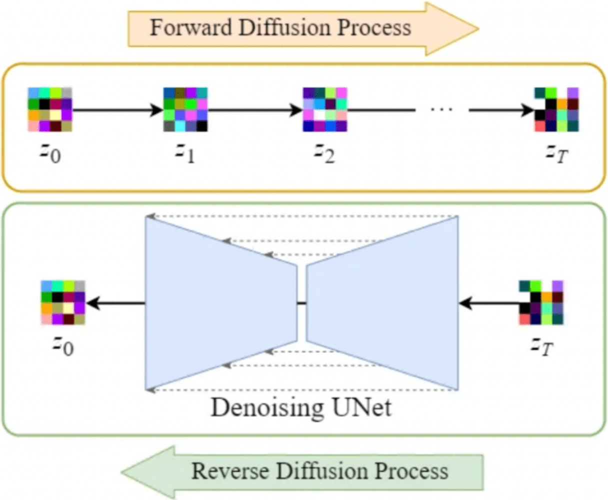
Table of Contents

Table of Contents (cont.)


Forward Diffusion Process
z_0
z_1
z_2
z_T
z_0
z_T
Denoising UNet
Reverse Diffusion Process

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:

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- 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.

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.

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

After this session, 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**

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  - *Forward process:* Progressively corrupt data by adding Gaussian noise.
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- **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.

Quick Overview

- **Forward:** Clean $\rightarrow$ Noise (additive Gaussian steps)
- **Reverse:** Learn **U-Net** to remove noise step by step
- **Training:** Model predicts the noise added
- **Sampling:** Roll back from pure noise to a data sample

Diffusion Models: **Denoising**

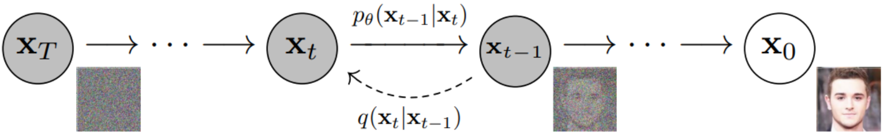
Denoising diffusion models, also known as score-based generative models, have recently emerged as a powerful class of generative models. They achieve remarkable results in high-fidelity image generation, often outperforming GANs.

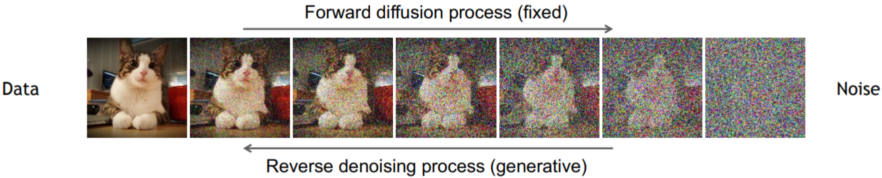
Diffusion Models Beat GANs on Image Synthesis Dhariwal & Nichol, OpenAI, 2021

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.





Forward diffusion process (fixed)
Data
Noise
Reverse denoising process (generative)

Diffusion Models: **Forward Process**

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.

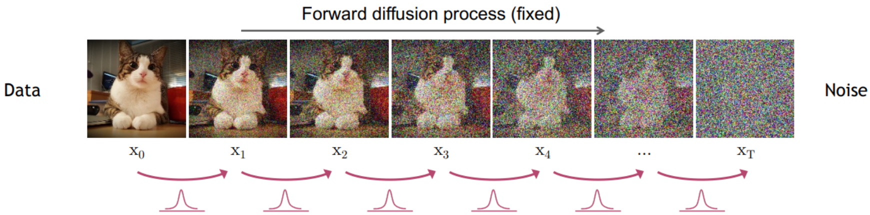
Forward Diffusion Process (cont.)

- This process is predefined and not learned.
- The full forward process:

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

- 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 $\mathbf{x}_t = \sqrt{1-\beta_t}\mathbf{x}_{t-1} + \sqrt{\beta_t}\epsilon$.

Forward Diffusion Process (cont.)



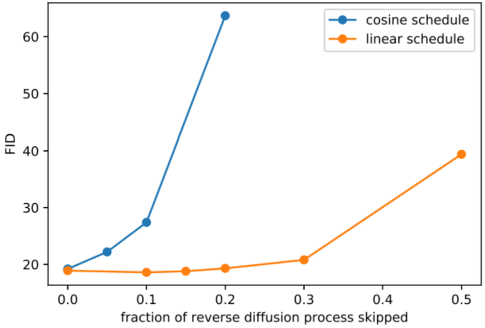
- What if we want to go directly from q_0 to q_t?
- Let $\overline{\alpha}_t = \prod_{s=1}^{t}(1-\beta_s)$, then

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

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

Diffusion Models: **Noise Schedules**

- The noise schedule $\{\beta_t\}$ controls the amount of noise added at each timestep.



Comparison of linear and cosine noise schedules.

Noise Schedules

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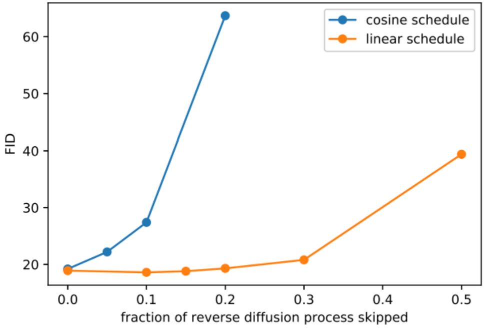
- Common schedules:
  - **Linear:** Simple and intuitive.
  - **Cosine:** Preserves perceptual signal longer; often yields better image generation results.



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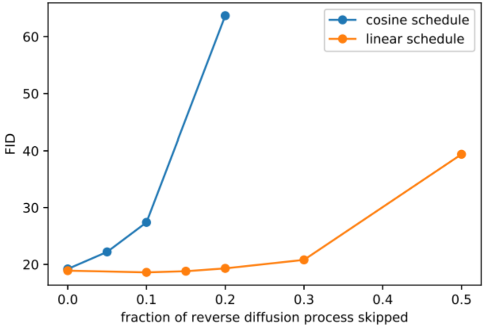

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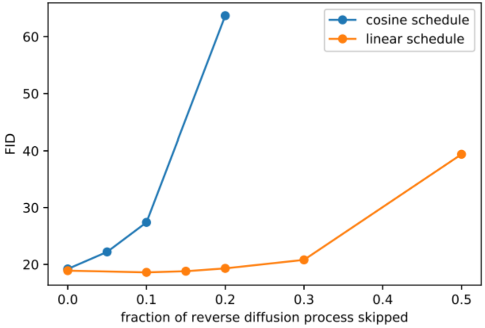
- Visualizing different schedules helps understand how noise accumulates over time.



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- 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

- 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.

Reverse Denoising Process (cont.)

- 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.

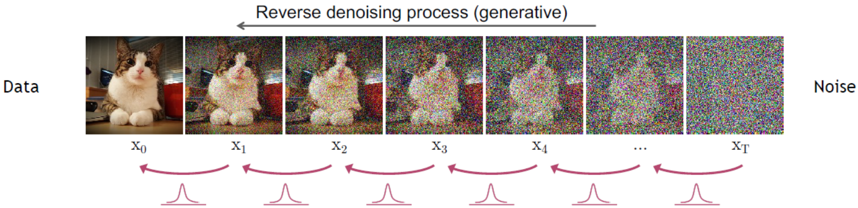
- For simplicity, we can fix the variance Σ_θ to a constant value (e.g., $\beta_t \mathbf{I}$) and only learn the mean μ_θ.

- 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:

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



Reverse denoising process in diffusion models.

Diffusion Models: **Evidence Lower Bound (ELBO) & Variational Inference**

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

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

ELBO & Variational Inference

أكاديمية كاوست
KAUST ACADEMY

LMH
Lady Margaret Hall

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- **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 $p(\mathbf{z})$.

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

Diffusion Models: **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:

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

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.

Diffusion Models: **Training & Sampling Algorithms**

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

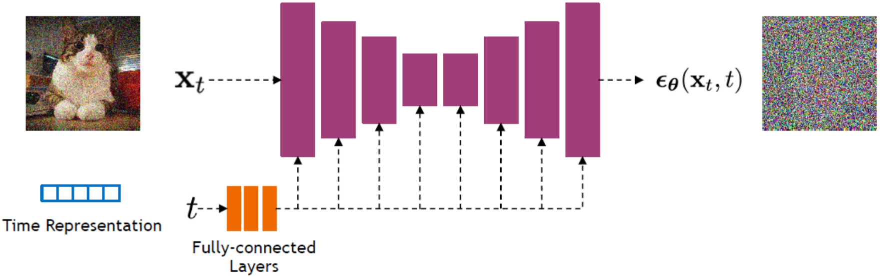
1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \ldots, 1$ **do**
3: $\quad \mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
4: $\quad \mathbf{x}_{t-1} = \boxed{\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t,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

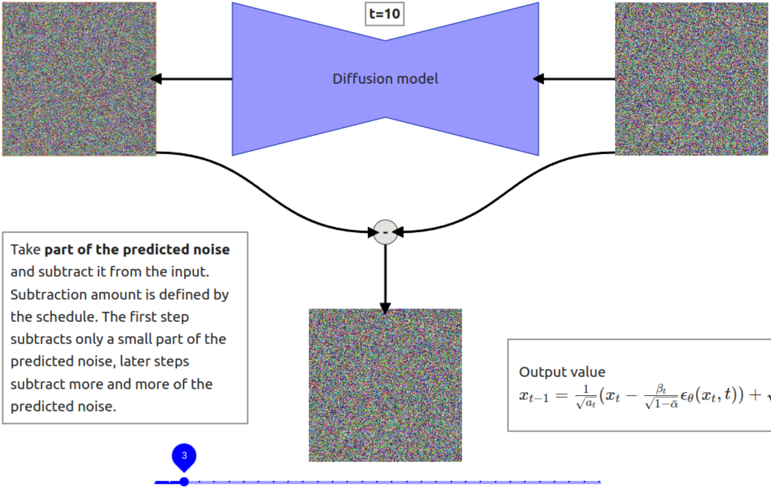
Sampling Algorithm

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.

Diffusion Models: **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.

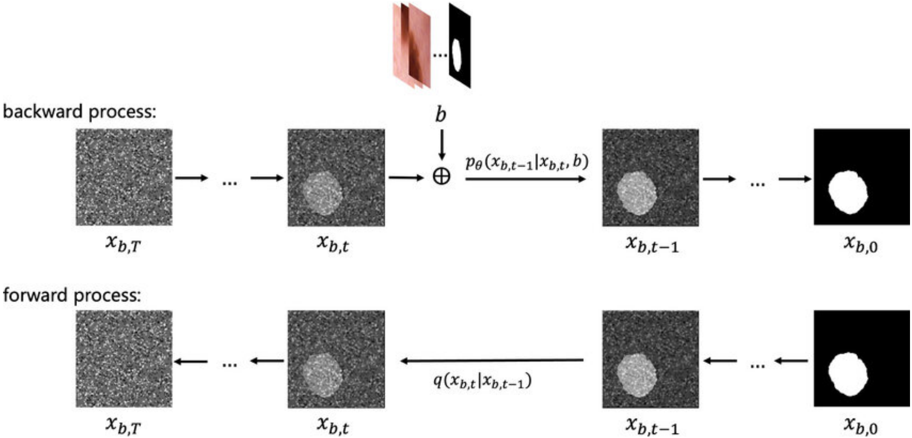




Take **part of the predicted noise** and subtract it from the input. Subtraction amount is defined by the schedule. The first step subtracts only a small part of the predicted noise, later steps subtract more and more of the predicted noise.

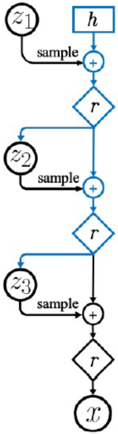
Output value

$$x_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}}}\epsilon_\theta(x_t, t)\right) + \sqrt{\beta_t}\epsilon$$


backward process:
b
$p_\theta(x_{b,t-1}|x_{b,t}, b)$
...
$x_{b,T}$
$x_{b,t}$
$x_{b,t-1}$
$x_{b,0}$
forward process:
$q(x_{b,t}|x_{b,t-1})$
$x_{b,T}$
$x_{b,t}$
$x_{b,t-1}$
$x_{b,0}$

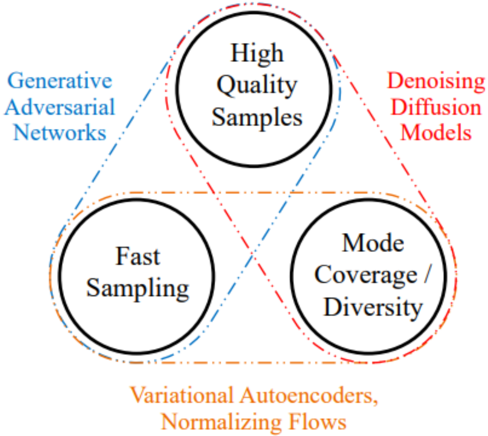
Connection to VAEs

- 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.



Diffusion Models: **Issues 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.



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

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

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

Diffusion Models: **Applications**

"a man wearing a white hat"

Image Inpainting with GLIDE

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

Application: DALL.E 2 - OpenAI

a shiba inu wearing a beret and black turtleneck

a close up of a handpalm with leaves growing from it

Text to image generation eith DAII.E 2

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

Image Variations

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

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

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

Image interpolation

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

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.

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.

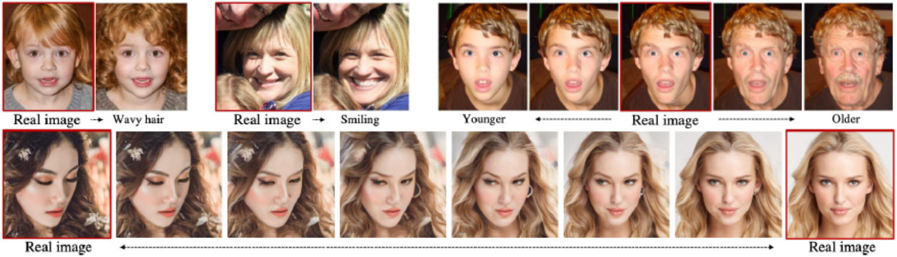
[0] Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding

A dragon fruit wearing karate belt in the snow.

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

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

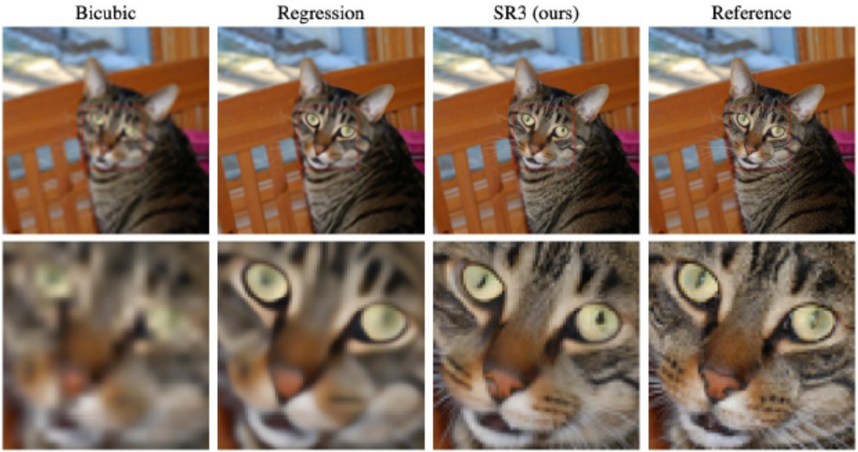


Changing the semantic latent $\mathbf{z}_{\text{sem}}$

Learning semantic meaningful latent representations in diffusion models

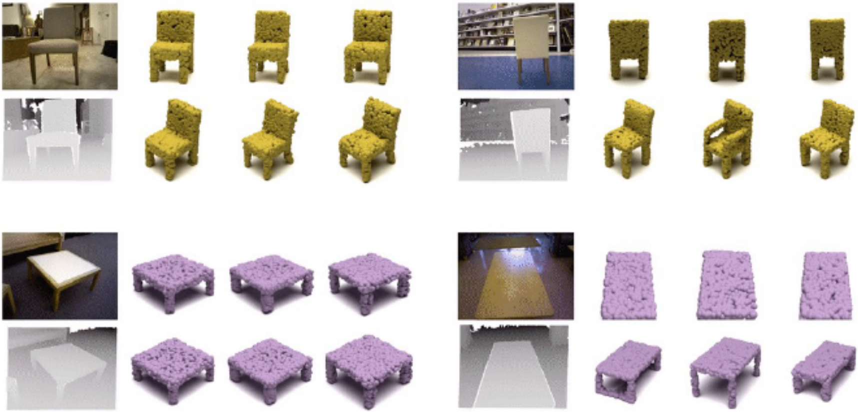
[0] Diffusion Autoencoders: Toward a Meaningful and Decodable Representation

Super Resolution



Natural Image Super Resolution $64 \times 64 \longrightarrow 256 \times 256$

0 Image Super-Resolution via Iterative Refinement



[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

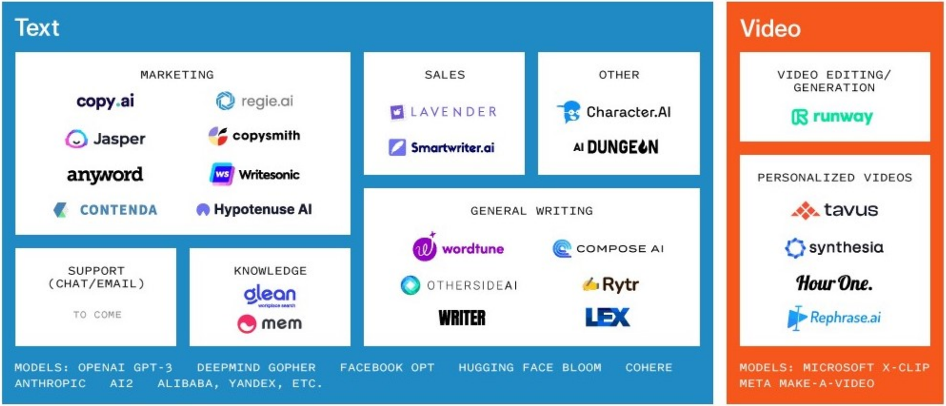
[0] High-Resolution Image Synthesis with Latent Diffusion Models

Diffusion Models: **Summary & Limitations**

Summary

- Diffusion models add noise to data and learn to reverse it
- Core task: Predict noise at different steps
- Training is efficient; Sampling is iterative and slow
- U-Nets with attention are the winning architecture

The Generative AI Landscape



[0] Sonya Huang (@sonyatweetybird)

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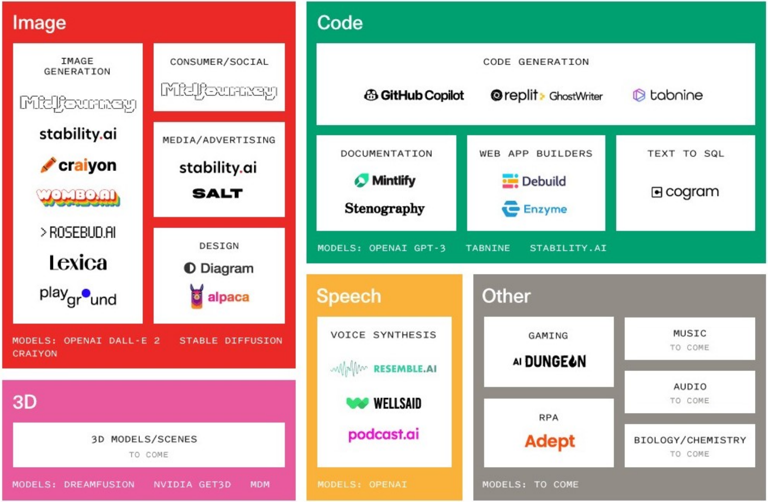

[0] Sonya Huang (@sonyatweetybird)

Limitations

- **Slow sampling** – iterative process
- **Data-heavy** – needs lots of varied data
- **Distribution miss** – struggles in tails of data
- **Compute needs** – high GPU/time investment
- **Misinformation concerns** – used in deepfake creation

Tutorials and Surveys

- Kreis, K., Gao, R., & Vahdat, A.: CVPR 2022 Tutorial: Diffusion Models
- Rogge, L., & Rasul, K.: The Annotated Diffusion Model
- Yang Song: Score-Based Generative Modeling: A Brief Overview
- Lilian Weng: What are Diffusion Models?

Foundational Papers

- Ho, J., Jain, A., & Abbeel, P. (2020). Denoising Diffusion Probabilistic Models
- Sohl-Dickstein, J., Weiss, E., Maheswaranathan, N., & Ganguli, S. (2015). Deep Unsupervised Learning using Nonequilibrium Thermodynamics
- Song, Y., & Ermon, S. (2019). Generative Modeling by Estimating Gradients of the Data Distribution
- Nichol, A., & Dhariwal, P. (2021). Improved Denoising Diffusion Probabilistic Models

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Applications and Notable Models

- Ramesh, A., et al. (2022). Hierarchical Text-Conditional Image Generation with CLIP Latents (DALL·E 2)
- Saharia, C., et al. (2022). Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding (Imagen)
- Nichol, A., Dhariwal, P., et al. (2021). GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models
- Preechakul, T., et al. (2022). Diffusion Autoencoders: Toward a Meaningful and Decodable Representation
- Saharia, C., et al. (2022). Image Super-Resolution via Iterative Refinement
- Poole, B., et al. (2022). DreamFusion: Text-to-3D using 2D Diffusion

GANs and Related Reading

- Goodfellow, I., et al. (2014). Generative Adversarial Nets
- Creswell, A., et al. (2018). Generative Adversarial Networks: An Overview

Credits

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