Lecture X: Denoising Diffusion Models



My Class 😕

Next few lectures: Generative models for direct image base rendering.



Current Image

Implicit: Use a Neural Network (Conditional Generative networks) Often, end-to-end.

- Viewpoint
- Lighting
- Reflectance
- Background
- Attributes
- Many others...

Slide Courtesy:

Denoising Diffusion-based Generative Modeling: Foundations and Applications, CVPR 2022 tutorial, Karsten Kreis, Ruiqi Gao, Arash Vahdat

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

@karsten_kreis



@RuiqiGao





@ArashVahdat

Deep Generative Learning

Learning to generate data









Neural Network



The Landscape of Deep Generative Learning

Variational Autoencoders

Generative Adversarial Networks

Energy-based Models Autoregressive Models Normalizing Flows

Denoising Diffusion Models

Denoising Diffusion Models Emerging as powerful generative models, outperforming GANs



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



"Cascaded Diffusion Models for High Fidelity Image Generation" Ho et al., Google, 2021

Image Super-resolution

Successful applications



Saharia et al., Image Super-Resolution via Iterative Refinement, ICCV 2021

SR3 Output : 1024x1024



Text-to-Image Generation

DALL·E 2

"a teddy bear on a skateboard in times square"



"Hierarchical Text-Conditional Image Generation with CLIP Latents" Ramesh et al., 2022





Imagen

A group of teddy bears in suit in a corporate office celebrating the birthday of their friend. There is a pizza cake on the desk.



<u>"Photorealistic Text-to-Image Diffusion Models with Deep</u> Language Understanding", Saharia et al., 2022

Text-to-Image Generation

Stable Diffusion



Stable Diffusion Applications: Twitter Mega Thread

"High-Resolution Image Synthesis with Latent Diffusion Models" Rombach et al., 2022

Q: What is a diffusion model?





Denoising Diffusion Models Learning to generate by denoising

Denoising diffusion models consist of two processes:

- Forward diffusion process that gradually adds noise to input
- Reverse denoising process that learns to generate data by denoising

Forward diffusion process (fixed)





Reverse denoising process (generative)

Sohl-Dickstein et al., Deep Unsupervised Learning using Nonequilibrium Thermodynamics, ICML 2015 Ho et al., Denoising Diffusion Probabilistic Models, NeurIPS 2020 Song et al., Score-Based Generative Modeling through Stochastic Differential Equations, ICLR 2021

Noise

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Forward Diffusion Process

The formal definition of the forward process in T steps:

Forward diffusion process (fixed)





Diffusion Kernel







What happens to a distribution in the forward diffusion?

So far, we discussed the diffusion kernel $q(\mathbf{x}_t|\mathbf{x}_0)$ but what about $q(\mathbf{x}_t)$?



We can sample $\mathbf{x}_t \sim q(\mathbf{x}_t)$ by first sampling $\mathbf{x}_0 \sim q(\mathbf{x}_0)$ and then sampling $\mathbf{x}_t \sim q(\mathbf{x}_t | \mathbf{x}_0)$ (i.e., ancestral sampling).

Generative Learning by Denoising

Recall, that the diffusion parameters are designed such that $q(\mathbf{x}_T) \approx \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$



Can we approximate $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$? Yes, we can use a Normal distribution if β_t is small in each forward diffusion step.

Diffused Data Distributions

Reverse Denoising Process

Formal definition of forward and reverse processes in T steps:



Data

Noise

How do we train? (summary version)

What is the loss function? (Ho et al. NeurIPS 2020)

$$L_{\text{simple}} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), t \sim \mathcal{U}(1, T)} \left[||\epsilon - \epsilon_{\theta} (\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{\bar{\alpha}_t}$$

 \mathbf{x}_t

Algorithm 1 Training

- 1: repeat
- 2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
- 3: $t \sim \text{Uniform}(\{1, \ldots, T\})$
- 4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
- 5: Take gradient descent step on

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

6: until converged

U-Net autoencoder takes x(t) as input and simply predict a noise. The goal of the training is to generate a noise pattern that is unit normal. Very similar to VAE, right?

 $(1 - \bar{\alpha}_t \epsilon, t) ||^2$

Summary

Training and Sample Generation

Algorithm 1 Training	Algorithm 2 S
1: repeat 2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$ 3: $t \sim \text{Uniform}(\{1, \dots, T\})$ 4: $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$ 5: Take gradient descent step on $\nabla_{\theta} \ \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta} (\sqrt{\overline{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \overline{\alpha}_t} \boldsymbol{\epsilon}, t) \ ^2$ 6: until converged	1: $\mathbf{x}_T \sim \mathcal{N}(0)$ 2: for $t = T$, . 3: $\mathbf{z} \sim \mathcal{N}(0)$ 4: $\mathbf{x}_{t-1} = \sqrt{2}$ 5: end for 6: return \mathbf{x}_0

Intuitively: During forward process we add noise to image. During reverse process we try to predict that noise with a U-Net and then subtract it from the image to denoise it.

Sampling $, \mathbf{I})$ $\ldots, 1$ do I) $\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t,t)\right) + \sigma_t \mathbf{z}$

Implementation Considerations

Network Architectures

Diffusion models often use U-Net architectures with ResNet blocks and self-attention layers to represent $\epsilon_{\theta}(\mathbf{x}_t,t)$



Time representation: sinusoidal positional embeddings or random Fourier features.

Time features are fed to the residual blocks using either simple spatial addition or using adaptive group normalization layers. (see <u>Dharivwal and Nichol NeurIPS 2021</u>)

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



Data

 $p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \mu_{\theta}(\mathbf{x}_t, t), \sigma_t^2 \mathbf{I})$

Above, β_t and σ_t^2 control the variance of the forward diffusion and reverse denoising processes respectively. Often a linear schedule is used for β_t , and σ_t^2 is set equal to β_t . Slowly increase the amount of added noise.

Kingma et al. NeurIPS 2022 introduce a new parameterization of diffusion models using signal-to-noise ratio (SNR), and show how to learn the noise schedule by minimizing the variance of the training objective.

We can also train σ_t^2 while training the diffusion model by minimizing the variational bound (Improved DPM by Nichol and Dhariwal ICML 2021) or after training the diffusion model (Analytic-DPM by Bao et al. ICLR 2022).

Noise



What happens to an image in the forward diffusion process?

Recall that sampling from $q(\mathbf{x}_t | \mathbf{x}_0)$ is done using $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{(1 - \bar{\alpha}_t)} \epsilon$ where $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$



In the forward diffusion, the high frequency content is perturbed faster.



Content-Detail Tradeoff

$$L_{\text{simple}} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), t \sim \mathcal{U}(1, T)} \left[|| \epsilon - \epsilon_{\theta} (\mathbf{y}_1) \right]$$



The weighting of the training objective for different timesteps is important!

Connection to VAEs

Diffusion models can be considered as a special form of hierarchical VAEs. However, in diffusion models:

- The encoder is fixed
- The latent variables have the same dimension as the data
- The denoising model is shared across different timestep
- The model is trained with some reweighting of the variational bound.



Summary

Denoising Diffusion Probabilistic Models

- Diffusion process can be reversed if the variance of the gaussian noise added at each step of the diffusion is small enough.
- To reverse the process we train a U-Net that takes input: current noisy image and timestamp, and predicts the noise map...
- Training goal is to make sure that the predicted noise map at each step is unit gaussian (Note that in VAE we also required the latent space to be unit gaussian).
- During sampling/generation, subtract the predicted noise from the noisy image at time t to generate the image at time t-1 (with some weighting).

The devil is in the details:

- Network architectures
- Objective weighting
- Diffusion parameters (i.e., noise schedule)

"Elucidating the Design Space of Diffusion-Based Generative Models" by Karras et al. for important design decisions. To be presented in the class!

Crash Course in Differential Equations

Ordinary Differential Equation (ODE):

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{f}(\mathbf{x}, t) \text{ or } \mathrm{d}\mathbf{x} = \mathbf{f}(\mathbf{x}, t)\mathrm{d}t$$



Iterative Numerical Solution:

$$\mathbf{x}(t + \Delta t) \approx \mathbf{x}(t) + \mathbf{f}(\mathbf{x}(t), t)\Delta t$$

Forward Diffusion Process as Stochastic Differential Equation

Consider the limit of many small steps: $q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I})$

Data

Forward diffusion process (fixed)



Song et al., "Score-Based Generative Modeling through Stochastic Differential Equations", ICLR, 2021

Noise

Forward Diffusion Process as Stochastic Differential Equation



Special case of more general SDEs used in generative diffusion models:

 $\mathrm{d}\mathbf{x}_t = f(t)\mathbf{x}_t\,\mathrm{d}t + g(t)\,\mathrm{d}\boldsymbol{\omega}_t$

$$\overline{)} \, \mathrm{d} \boldsymbol{\omega}_t$$

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The Generative Reverse Stochastic Differential Equation



Forward Diffusion SDE:

Reverse Generative

Diffusion SDE:

How do we obtain the "Score Function"?



Simulate reverse diffusion process: Data generation from random noise!

Song et al., ICLR, 2021 Anderson, in Stochastic Processes and their Applications, 1982

"Score Function"

Score Matching



Naïve idea, learn model for the score function by direct regression? 0

$$\min_{\boldsymbol{\theta}} \mathbb{E}_{t \sim \mathcal{U}(0,T)} \mathbb{E}_{\mathbf{x}_t \sim q_t(\mathbf{x}_t)} || \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}_t) || \mathbf{s}$$

But $\nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t)$ (score of the marginal diffused density $q_t(\mathbf{x}_t)$) is not tractable!



eural work

score of diffused data (marginal)

Denoising Score Matching



- Instead, diffuse individual data points \mathbf{x}_0 . Diffused $q_t(\mathbf{x}_t|\mathbf{x}_0)$ is tractable!
- **Denoising Score Matching:**

$$\begin{array}{c|c} \min \mathbb{E}_{t \sim \mathcal{U}(0,T)} \mathbb{E}_{\mathbf{x}_0 \sim q_0(\mathbf{x}_0)} \mathbb{E}_{\mathbf{x}_t \sim q_t(\mathbf{x}_t | \mathbf{x}_0)} || \mathbf{s}_{\mathbf{x}_t \sim q_t(\mathbf{x}_t$$

Vincent, in Neural Computation, 2011 Song and Ermon, NeurIPS, 2019 Song et al. ICLR, 2021





Denoising Score Matching Implementation Details



More sophisticated model parametrizations and loss weightings are possible!

Karras et al., "Elucidating the Design Space of Diffusion-Based Generative Models", arXiv, 2022

To be discussed in detail in paper presentation

Different loss weightings trade off between model with good perceptual quality vs. high log-likelihood



$$\sum_{t \sim \mathcal{U}(0,T)} \mathbb{E}_{\mathbf{x}_0 \sim q_0(\mathbf{x}_0)} \mathbb{E}_{\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0},\mathbf{I})} \frac{1}{\sigma_t^2} ||\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\boldsymbol{\theta}}(\mathbf{x}_t,t)||_2^2$$

$$\sum_{t \sim \mathcal{U}(0,T)} \mathbb{E}_{\mathbf{x}_0 \sim q_0(\mathbf{x}_0)} \mathbb{E}_{\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0},\mathbf{I})} \frac{\boldsymbol{\lambda}(t)}{\sigma_t^2} ||\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\boldsymbol{\theta}}(\mathbf{x}_t,t)||_2^2$$

Perceptual quality: $\lambda(t) = \sigma_t^2$ Maximum log-likelihood: $\lambda(t) = \beta(t)$ (negative ELBO)

Advanced Techniques Questions to address with advanced techniques

- Q1: How to accelerate the sampling process?
 - Advanced forward diffusion process
 - Advanced reverse process
 - Hybrid models & model distillation
- Q2: How to do high-resolution (conditional) generation?
 - Conditional diffusion models
 - Classifier(-free) guidance
 - Cascaded generation

Q: How to accelerate sampling process?





What makes a good generative model? The generative learning trilemma



Tackling the Generative Learning Trilemma with Denoising Diffusion GANs, ICLR 2022

Often requires 1000s of network evaluations!

What makes a good generative model? The generative learning trilemma

Tackle the trilemma by accelerating diffusion models



Tackling the Generative Learning Trilemma with Denoising Diffusion GANs, ICLR 2022

How to accelerate diffusion models?





- Naïve acceleration methods, such as reducing diffusion time steps in training or sampling every k time step in inference, lead to immediate worse performance.
- We need something cleverer.
- Given a limited number of functional calls, usually much less than 1000s, how to improve performance?

[Image credit: Ben Poole, Mohammad Norouzi]
Denoising diffusion implicit models (DDIM) Non-Markovian diffusion process



Main Idea

Design a family of non-Markovian diffusion processes and corresponding reverse processes.

The process is designed such that the model can be optimized by the same surrogate objective as the original diffusion model. \Box $L_{\text{simple}}(\theta) \coloneqq \mathbb{E}_{t,\mathbf{x}_0,\boldsymbol{\epsilon}} \Big[\Big\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta} (\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}, t) \Big\|^2 \Big]$

Therefore, can take a pretrained diffusion model but with more choices of sampling procedure.

Song et al., "Denoising Diffusion Implicit Models", ICLR 2021.

Denoising diffusion implicit models (DDIM) Non-Markovian diffusion process



Define a family of forward processes that meets the above requirement:

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0) = \mathcal{N}\left(\sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_{t-1}}\right)$$

The corresponding reverse process is

$$p(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}\left(\sqrt{\bar{\alpha}_{t-1}}\hat{\mathbf{x}}_0 + \sqrt{1 - \bar{\alpha}_{t-1}} - \tilde{\sigma}_t^2\right)$$
$$:= (\mathbf{x}_t - \sqrt{1 - \alpha_t} \cdot \epsilon_{\theta}^{(t)})$$

Intuitively, given noisy x_t we first predict the corresponding clean image x_0 and then use if to obtain a sample x_{t-1}

$$p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \mu_{\theta}(\mathbf{x}_t, t), \sigma_t^2 \mathbf{I})$$



Regular diffusion model

Denoising diffusion implicit models (DDIM) Non-Markovian diffusion process



The corresponding reverse process is

$$p(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}\left(\sqrt{\bar{\alpha}_{t-1}}\mathbf{\hat{x}}_0 + \sqrt{1 - \bar{\alpha}_{t-1}} - \tilde{\sigma}_t^2 \cdot \frac{\mathbf{x}_t - \sqrt{\bar{\alpha}_t}\mathbf{\hat{x}}_0}{\sqrt{1 - \bar{\alpha}_t}}, \tilde{\sigma}_t^2 \mathbf{I}\right)$$

Intuitively, given noisy x_t we first predict the corresponding clean image x_0 and then use if to obtain a sample x_{t-1}

$$\boldsymbol{x}_{t-1} = \sqrt{\alpha_{t-1}} \underbrace{\left(\frac{\boldsymbol{x}_t - \sqrt{1 - \alpha_t} \epsilon_{\theta}^{(t)}(\boldsymbol{x}_t)}{\sqrt{\alpha_t}} \right)}_{\text{"predicted } \boldsymbol{x}_0\text{"}} + \underbrace{\sqrt{1 - \alpha_{t-1} - \sigma_t^2} \cdot \epsilon_{\theta}^{(t)}(\boldsymbol{x}_t)}_{\text{"direction pointing to } \boldsymbol{x}_t\text{"}} + \underbrace{\sigma_t \epsilon_t}_{\text{random not}} \underbrace{\sigma_t \epsilon_t}_{\text{"random not}} \underbrace{\sigma_t \epsilon_t}_{\text{"random not}} + \underbrace{\sigma_t \epsilon_t}_{\text{"random not}} \underbrace{\sigma_t \epsilon_t}_{\text{"rand$$

Different choice of σ results in different generative process without re-training the model

- When $\sigma = 0$ for all t, we have a deterministic generative process, with randomness from only t=T (the last step).

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Advanced reverse process Approximate reverse process with more complicated distributions

Simple forward process slowly maps data to noise





Q: is normal approximation of the reverse process still accurate when there're less diffusion time steps?

Diffusion model



Advanced approximation of reverse process Normal assumption in denoising distribution holds only for small step

Denoising Process with Uni-modal Normal Distribution



Requires more complicated functional approximators!

Xiao et al., "Tackling the Generative Learning Trilemma with Denoising Diffusion GANs", ICLR 2022. Gao et al., "Learning energy-based models by diffusion recovery likelihood", ICLR 2021.



Denoising diffusion GANs Approximating reverse process by conditional GANs

$$\min_{\theta} \sum_{t \ge 1} \mathbb{E}_{q(\mathbf{x}_t)} \left[D_{\text{adv}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t) \| p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)) \right]$$



Xiao et al., "Tackling the Generative Learning Trilemma with Denoising Diffusion GANs", ICLR 2022.

- Compared to a one-shot GAN generator:
 - Both generator and discriminator are solving a much simpler problem.
 - Stronger mode coverage
 - Better training stability

Advanced modeling Latent space modeling & model distillation

Simple forward process slowly maps data to noise



- Can we do model distillation for fast sampling?
- Can we lift the diffusion model to a latent space that is faster to diffuse?

Progressive distillation

- Distill a deterministic DDIM sampler to the same model architecture. ullet
- At each stage, a "student" model is learned to distill two adjacent sampling steps of the "teacher" model to one sampling step.
- At next stage, the "student" model from previous stage will serve as the new "teacher" model.



Distillation stage

Salimans & Ho, "Progressive distillation for fast sampling of diffusion models", ICLR 2022.

Latent-space diffusion models

Variational autoencoder + score-based prior



Main Idea

Encoder maps the input data to an embedding space

Denoising diffusion models are applied in the latent space

Vahdat et al., "Score-based generative modeling in latent space", NeurIPS 2021. Rombach et al., "High-Resolution Image Synthesis with Latent Diffusion Models", CVPR 2022.

Latent Space Forward Diffusion $p(\mathbf{z_1})$

Latent Space Generative Denoising

Denoising Diffusion Prior



Latent-space diffusion models

Variational autoencoder + score-based prior



(1) The distribution of latent embeddings close to Normal distribution \rightarrow Simpler denoising, Faster Synthesis!

(2) Augmented latent space -> *More expressivity!*

(3) Tailored Autoencoders - More expressivity, Application to any data type (graphs, text, 3D data, etc.) !

Latent Space Forward Diffusion $p(\mathbf{z_1})$

Latent Space Generative Denoising

Denoising Diffusion Prior

Q: How to do high-resolution conditional generation?





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Impressive conditional diffusion models Text-to-image generation

DALL·E 2

"a propaganda poster depicting a cat dressed as french emperor napoleon holding a piece of cheese"



"A photo of a raccoon wearing an astronaut helmet, looking out of the window at night."



Ramesh et al., "Hierarchical Text-Conditional Image Generation with CLIP Latents", arXiv 2022. Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.

IMAGEN



Impressive conditional diffusion models Super-resolution & colorization





Super-resolution

Colorization

Colorization

Saharia et al., "Palette: Image-to-Image Diffusion Models", arXiv 2021.

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Impressive conditional diffusion models

Panorama generation← GeneratedInputGenerated



Generated \rightarrow

Conditional diffusion models Include condition as input to reverse process

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

Variational upper bound: $L_{\theta}(\mathbf{x}_{0}|\mathbf{c}) = \mathbb{E}_{q} \left[L_{T}(\mathbf{x}_{0}) + \sum_{t>1} D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \mathbf{x}_{0}) \parallel p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \mathbf{c})) - \log p_{\theta}(\mathbf{x}_{0}|\mathbf{x}_{1}, \mathbf{c}) \right].$

Incorporate conditions into U-Net

- Scalar conditioning: encode scalar as a vector embedding, simple spatial addition or adaptive group normalization layers.
- Image conditioning: channel-wise concatenation of the conditional image.
- Text conditioning: single vector embedding spatial addition or adaptive group norm / a seq of vector embeddings cross-attention.

Classifier guidance

Using the gradient of a trained classifier as guidance

Recap: What is a score function?

Forward Diffusion SDE:

$$d\mathbf{x}_{t} = -\frac{1}{2}\beta(t)\mathbf{x}_{t} dt + \sqrt{\beta(t)} d\omega_{t}$$

$$\underset{\text{Reverse Generative Diffusion SDE:}}{\text{d}\mathbf{x}_{t}} = \underbrace{\left[-\frac{1}{2}\beta(t)\mathbf{x}_{t} - \beta(t)\nabla_{\mathbf{x}_{t}}\log q_{t}(\mathbf{x}_{t})\right]}_{\text{"Score Function"}} dt + \sqrt{\beta(t)} d\bar{\omega}_{t}$$

$$\underset{\boldsymbol{\theta}}{\underset{\boldsymbol{\theta}}{\text{min } \mathbb{E}_{t \sim \mathcal{U}(0,T)} \mathbb{E}_{\mathbf{x}_{t} \sim q_{t}(\mathbf{x}_{t})}} ||\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}_{t},t) - \nabla_{\mathbf{x}_{t}}\log q_{t}(\mathbf{x}_{t})||_{2}^{2}}$$

$$\underset{\text{diffusion time } t \text{ diffused time } t \text{ network time } t \text{ diffused data } t \text{ diffused data } t \text{ network time } t \text{ diffused data } t \text{ network time } t \text{ diffused data } t \text{ network time } t \text{ diffused data } t \text{ network time } t \text{ diffused data } t \text{ diffused data } t \text{ network time } t \text{ diffused data } t \text{ diffused d$$



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Classifier guidance

Using the gradient of a trained classifier as guidance

Applying Bayes rule to obtain conditional score function

$$p(x \mid y) = rac{p(y \mid x) \cdot p(x)}{p(y)}$$

 $\implies \log p(x \mid y) = \log p(y \mid x) + \log p(x) - \log p(y)$

 $\implies \nabla_x \log p(x \mid y) = \nabla_x \log p(y \mid x) + \nabla_x \log p(x),$

$$abla_x \log p_\gamma(x \mid y) =
abla_x \log p(x) + \gamma
abla_x \log p(y \mid x).$$

Guidance scale: value >1 amplifies the influence of classifier signal.

$$p_\gamma(x \mid y) \propto p(x) \cdot p(y \mid x)^\gamma.$$

Slide Credits of guidance: https://benanne.github.io/2022/05/26/guidance.html

Classifier

Classifier guidance Using the gradient of a trained classifier as guidance

 $abla_x \log p_\gamma(x \mid y) =
abla_x \log p(x) + \gamma
abla_x \log p(y \mid x).$



Samples from an unconditional diffusion model with classifier guidance, for guidance scales 1.0 (left) and 10.0 (right), taken from Dhariwal & Nichol (2021).

Classifier guidance Using the gradient of a trained classifier as guidance

Algorithm 1 Classifier guided diffusion sampling, given a diffusion model $(\mu_{\theta}(x_t), \Sigma_{\theta}(x_t))$, classifier $p_{\phi}(y|x_t)$, and gradient scale s.

Input: class label y, gradient scale s Score model $x_T \leftarrow \text{sample from } \mathcal{N}(0, \mathbf{I})$ for all t from T to 1 do $\mu, \Sigma \leftarrow \mu_{\theta}(x_t), \Sigma_{\theta}(x_t)$ $x_{t-1} \leftarrow \text{sample from } \mathcal{N}(\mu + s\Sigma \nabla_{x_t} \log p_{\phi}(y|x_t), \Sigma)$ end for return x_0

- Train unconditional Diffusion model
- Take your favorite classifier, depending on the conditioning type

During inference / sampling mix the gradients of the classifier with the predicted score function of the unconditional diffusion model.

Classifier gradient

Classifier guidance

Problems of classifier guidance

$$abla_x \log p_\gamma(x \mid y) =
abla_x \log p(x) + \gamma
abla_x \log p(y \mid x).$$
Guidance scale: value >1 amplif the influence of classifier signal.

- At each step of denoising the input to the classifier is a noisy image x_t. Classifier is never trained on noisy image. So one needs to re-train classifier on noisy images! Can't use existing pre-trained classifiers.
- Most of the information in the input x is not relevant to predicting y, and as a result, taking the gradient of the classifier w.r.t. its input can yield arbitrary (and even adversarial) directions in input space.

- $g p(y \mid x)$. Classifier
- >1 amplifies

Classifier-free guidance

Get guidance by Bayes' rule on conditional diffusion models

$$p(y \mid x) = rac{p(x \mid y) \cdot p(y)}{p(x)}$$

$$\implies \log p(y \mid x) = \log p(x \mid y) + \log p(y)$$
 $\implies
abla_x \log p(y \mid x) =
abla_x \log p(x \mid y) -
abla_x \log p(x \mid y) =
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We proved this in classifier guidance.

$$abla_x \log p_\gamma(x \mid y) =
abla_x \log p(x) + \gamma
abla_x$$

$$abla_x \log p_\gamma(x \mid y) =
abla_x \log p(x) + \gamma \left(
abla$$

$$abla_x \log p_\gamma(x \mid y) = (1 - \gamma) \nabla_x \log p(x) + \gamma \nabla_x \log p(x \mid y).$$

 $\uparrow \qquad \uparrow$
Score function
for unconditional
diffusion model

 $diffusion model$

NCE diffusion models

$$-\log p(x)$$

 $\sum_{x} \log p(x).$

 $\log p(x \mid y) -
abla_x \log p(x)) \, ,$

Classifier-free guidance

Get guidance by Bayes' rule on conditional diffusion models

 $abla_x \log p_\gamma(x \mid y) =$

This is a barycentric combination of the conditional and the unconditional score function For $\gamma = 0$, we recover the unconditional model, and for $\gamma = 1$ we get the standard conditional model. But $\gamma > 1$ is where the magic happens. Below are some examples from OpenAl's GLIDE model⁸, obtained using classifier-free guidance.



Two sets of samples from OpenAI's GLIDE model, for the prompt 'A stained glass window of a panda eating bamboo.', taken from their paper. Guidance scale 1 (no guidance) on the left, guidance scale 3 on the right.

$$(1 - \gamma)
abla_x \log p(x) + \gamma
abla_x \log p(x \mid y).$$

unconditional diffusion model

tion for conditional diffusion model

Classifier-free guidance

Get guidance by Bayes' rule on conditional diffusion models

In practice:

- Train a conditional diffusion model p(x|y), with *conditioning dropout*: some percentage of the time, the conditioning information y is removed (10-20%) tends to work well).
- The conditioning is often replaced with a special input value representing the absence of conditioning information.
- The resulting model is now able to function both as a conditional model p(x|y), and as an unconditional model p(x), depending on whether the conditioning signal is provided.
- During inference / sampling simply mix the score function of conditional and unconditional diffusion model based on guidance scale.



Classifier-free guidance Trade-off for sample quality and sample diversity



Non-guidance

Guidance scale = 1

Large guidance weight (ω) usually leads to better individual sample quality but less sample diversity.

Ho & Salimans, "Classifier-Free Diffusion Guidance", 2021.

Guidance scale = 3

Classifier guidance





X Need to train a separate "noise-robust" classifier + + Train conditional & unconditional diffusion model jointly via drop-out.

X Gradient of the classifier w.r.t. input yields arbitrary + All pixels in input receive equally 'good' gradients. values.

Rather than constructing a generative model from classifier, we construct a classifier from a generative model!

Most recent papers use classifier-free guidance! Very simple yet very powerful idea!

Classifier-free guidance

 $\nabla_x \log p_\gamma(x \mid y) = (1 - \gamma) \nabla_x \log p(x) + \gamma \nabla_x \log p(x \mid y).$ \uparrow Score function for
Score function for

unconditional diffusion model Score function for conditional diffusion model

Cascaded generation Pipeline

Super-Resolution Diffusion Models 256×256



Similar cascaded / multi-resolution image generation also exist in GAN (Big-GAN & StyleGAN)

Cascaded Diffusion Models outperform Big-GAN in FID and IS and VQ-VAE2 in Classification Accuracy Score.

Ho et al., "Cascaded Diffusion Models for High Fidelity Image Generation", 2021.



Noise conditioning augmentation Reduce compounding error

Problem:

- During training super-resolution models are trained on original low-res images from the dataset.
- During inference, these low-res images are generated by class conditioned diffusion model, which has artifacts and poor quality than original low-res images used for training.

Solution: Noise conditioning augmentation.

- During training, add varying amounts of Gaussian noise (or blurring by Gaussian kernel) to the low-res images.
- During inference, sweep over the optimal amount of noise added to the low-res images.
- BSR-degradation process: applies JPEG compressions noise, camera sensor noise, different image interpolations for downsampling, Gaussian blur kernels and Gaussian noise in a random order to an image.

Ho et al., "Cascaded Diffusion Models for High Fidelity Image Generation", 2021. Nichol et al., "GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models", 2021.

Mismatch issue

Summary

Questions to address with advanced techniques

- Q1: How to accelerate the sampling process?
 - Advanced forward diffusion process
 - Advanced reverse process
 - Hybrid models & model distillation
- Q2: How to do high-resolution (conditional) generation?
 - Conditional diffusion models
 - Classifier(-free) guidance
 - Cascaded generation

Applications (1): Image Synthesis, Controllable Generation, Text-to-Image



GLIDE **OpenAl**

- A 64x64 base model + a 64x64 \rightarrow 256x256 super-resolution model.
- Tried classifier-free and CLIP guidance. Classifier-free guidance works better than CLIP guidance.







"robots meditating in a vipassana retreat"

"a hedgehog using a calculator"

"a corgi wearing a red bowtie and a purple party hat"

Samples generated with classifier-free guidance (256x256)

Nichol et al., "GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models", 2021.



"a fall landscape with a small cottage next to a lake"

CLIP guidance What is a CLIP model?

Trained by contrastive cross-entropy loss:

$$-\log \frac{\exp(f(\mathbf{x}_i) \cdot g(\mathbf{c}_j)/\tau)}{\sum_k \exp(f(\mathbf{x}_i) \cdot g(\mathbf{c}_k)/\tau)} - \log \frac{\exp(f(\mathbf{x}_i) \cdot g(\mathbf{c}_j)/\tau)}{\sum_k \exp(f(\mathbf{x}_k) \cdot g(\mathbf{c}_j)/\tau)}$$

The optimal value of $f(\mathbf{x}) \cdot g(\mathbf{c})$ is

$$\log \frac{p(\mathbf{x}, \mathbf{c})}{p(\mathbf{x})p(\mathbf{c})} = \log p(\mathbf{c}|\mathbf{x}) - \log p(\mathbf{c})$$



Radford et al., "Learning Transferable Visual Models From Natural Language Supervision", 2021. Nichol et al., "GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models", 2021.



CLIP guidance Replace the classifier in classifier guidance with a CLIP model

Sample with a modified score:

 $\nabla_{\mathbf{x}_t} [\log p(\mathbf{x}_t | \mathbf{c}) + \omega \log p(\mathbf{c} | \mathbf{x}_t)]$ $= \nabla_{\mathbf{x}_t} [\log p(\mathbf{x}_t | \mathbf{c}) + \omega (\log p(\mathbf{c} | \mathbf{x}_t) - \log p(\mathbf{c}))]$ CLIP model $= \nabla_{\mathbf{x}_t} [\log p(\mathbf{x}_t | \mathbf{c}) + \omega(f(\mathbf{x}_t) \cdot g(\mathbf{c}))]$



Pepper the

aussie pup

Radford et al., "Learning Transferable Visual Models From Natural Language Supervision", 2021. Nichol et al., "GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models", 2021.



GLIDE **OpenAl**

Fine-tune the model especially for inpainting: feed randomly occluded images with an additional mask channel as the input.



"an old car in a snowy forest"

Text-conditional image inpainting examples

Nichol et al., "GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models", 2021.

"a man wearing a white hat"

DALL·E 2 **OpenAl**



a shiba inu wearing a beret and black turtleneck

1kx1k Text-to-image generation. Outperform DALL-E (autoregressive transformer).

Ramesh et al., "Hierarchical Text-Conditional Image Generation with CLIP Latents", arXiv 2022.

a close up of a handpalm with leaves growing from it

DALL·E 2 Model components

Prior: produces CLIP image embeddings conditioned on the caption. Decoder: produces images conditioned on CLIP image embeddings and text.



Ramesh et al., "Hierarchical Text-Conditional Image Generation with CLIP Latents", arXiv 2022.

DALL·E 2 Model components



Why conditional on CLIP image embeddings?

CLIP image embeddings capture high-level semantic meaning.

Latents in the decoder model take care of the rest.

The bipartite latent representation enables several text-guided image manipulation tasks.




DALL·E 2 Model components (1/2): prior model



Prior: produces CLIP image embeddings conditioned on the caption.

- Option 1. autoregressive prior: quantize image embedding to a seq. of discrete codes and predict them autoregressively.
- Option 2. diffusion prior: model the continuous image embedding by diffusion models conditioned on caption.

DALL·E 2

Model components (2/2): decoder model



Decoder: produces images conditioned on CLIP image embeddings (and text).

- Cascaded diffusion models: 1 base model (64x64), 2 super-resolution models (64x64 \rightarrow 256x256, 256x256 \rightarrow 1024x1024).
- Largest super-resolution model is trained on patches and takes full-res inputs at inference time.
- Classifier-free guidance & noise conditioning augmentation are important.

DALL·E 2 Bipartite latent representations



Bipartite latent representations $(\mathbf{z}, \mathbf{x}_T)$

z: CLIP image embeddings

 \mathbf{x}_T : inversion of DDIM sampler (latents in the decoder model)





Near exact reconstruction



Fix the CLIP embedding \mathbf{Z}_{\cdot} Decode using different decoder latents \mathbf{x}_{T}







DALL·E 2 Image interpolation





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

DALL·E 2 Text Diffs



a photo of a cat \rightarrow an anime drawing of a super saiyan cat, artstation



a photo of a victorian house \rightarrow a photo of a modern house



a photo of an adult lion \rightarrow 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.



Output: 1kx1k images Input: text;

- An unprecedented degree of photorealism •
 - SOTA automatic scores & human ratings
- A deep level of language understanding •
- Extremely simple ٠
 - no latent space, no quantization



Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.

A brain riding a rocketship heading towards the moon.



A photo of a Shiba Inu dog with a backpack riding a bike. It is wearing sunglasses and a beach hat.

Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.



A dragon fruit wearing karate belt in the snow.

Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.



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

Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.

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A cute hand-knitted koala wearing a sweater with 'CVPR' written on it.

Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.



Key modeling components:

- Cascaded diffusion models
- Classifier-free guidance and dynamic thresholding.
- Frozen large pretrained language models as text encoders. (T5-XXL)



"A Golden Retriever dog wearing a blue checkered beret and red dotted turtleneck."

Text Embedding

 256×256 Image







Key observations:

- Beneficial to use text conditioning for all super-res models.
 - Noise conditioning augmentation weakens information from low-res models, thus needs text conditioning as extra information input.
- Scaling text encoder is extremely efficient.
 - More important than scaling diffusion model size.
- Human raters prefer T5-XXL as the text encoder over CLIP encoder on DrawBench.



Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.

"A Golden Retriever dog wearing a blue checkered beret and red dotted turtleneck."

Text Embedding

 256×256 Image







Imagen Dynamic thresholding

Large classifier-free guidance weights \rightarrow better text alignment, worse image quality



Better text alignment





Imagen Dynamic thresholding

- Large classifier-free guidance weights \rightarrow better text alignment, worse image quality
- Hypothesis : at large guidance weight, the generated images are saturated due to the very large gradient updates during sampling
- Solution dynamic thresholding: adjusts the pixel values of samples at each sampling step to be within a dynamic range computed over the statistics of the current samples.

Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.



Dynamic thresholding



Static thresholding

Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.

dates during

|ynamic

Dynamic thresholding



DrawBench: new benchmark for text-to-image evaluations

- A set of 200 prompts to evaluate text-to-image models across multiple dimensions.
 - E.g., the ability to faithfully render different colors, numbers of objects, spatial relations, text in the scene, unusual interactions between objects.
 - Contains complex prompts, e.g, long and intricate descriptions, rare words, misspelled prompts.

Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.



DrawBench: new benchmark for text-to-image evaluations

- A set of 200 proi
 - E.g., the interactio
 - Contains (



A brown bird and a blue bear.



One cat and two dogs sitting on the grass.



A small blue book sitting on a large red book.



A blue coloured pizza.



A pear cut into seven pieces arranged in a ring.



A photo of a confused grizzly bear in calculus class.

Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.

cene, unusual

A sign that says 'NeurIPS'.



A wine glass on top of a dog.



A small vessel propelled on water by oars, sails, or an engine.



Imagen **Evaluations**

Imagen got SOTA automatic evaluation scores on COCO dataset

Model	FID-30K	Zero-shot FID-30K
AttnGAN [76]	35.49	
DM-GAN [83]	32.64	
DF-GAN [69]	21.42	
DM-GAN + CL [78]	20.79	
XMC-GAN [81]	9.33	
LAFITE [82]	8.12	
Make-A-Scene [22]	7.55	
DALL-E [53]		17.89
LAFITE [82]		26.94
GLIDE [41]		12.24
DALL-E 2 [54]		10.39
Imagen (Our Work)		7.27



Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.

Imagen is preferred over recent work by human raters in sample quality & image-text alignment on DrawBench.



Stable Diffusion

Latest & Publicly available text-to-image generation To be discussed in detail in paper presentation

High-Resolution Image Synthesis with Latent Diffusion Models Robin Rombach*, Andreas Blattmann*, Dominik Lorenz, Patrick Esser, Björn Ommer CVPR '22 Oral | GitHub | arXiv | Project page



Stable Diffusion is a latent text-to-image diffusion model. Thanks to a generous compute donation from Stability AI and support from LAION, we were able to train a Latent Diffusion Model on 512x512 images from a subset of the LAION-5B database. Similar to Google's Imagen, this model uses a frozen CLIP ViT-L/14 text encoder to condition the model on text prompts. With its 860M UNet and 123M text encoder, the model is relatively lightweight and runs on a GPU with at least 10GB VRAM. See this section below and the model card.

Stable Diffusion

Latest & Publicly available text-to-image generation

Input



HW assignment: Use stable diffusion API to generate 'interesting' image from text prompt. All submissions will be rated for top 3!

Outputs



Applications (2): Image Editing, Image-to-Image, Super-resolution, Segmentation



Diffusion Autoencoders Learning semantic meaningful latent representations in diffusion models



To be discussed in detail in paper presentation

Preechakul et al., "Diffusion Autoencoders: Toward a Meaningful and Decodable Representation", CVPR 2022.

Diffusion Autoencoders Learning semantic meaningful latent representations in diffusion models



Real image

Changing the semantic latent $z_{\rm sem}$

Very similar to StyleGAN based editing. Zsem is the latent representation similar to the W/W+ space of StyleGAN

Preechakul et al., "Diffusion Autoencoders: Toward a Meaningful and Decodable Representation", CVPR 2022.

Real image

Diffusion Autoencoders Learning semantic meaningful latent representations in diffusion models



Preechakul et al., "Diffusion Autoencoders: Toward a Meaningful and Decodable Representation", CVPR 2022.

Varying stochastic subcode $(\mathbf{z}_{sem}, \mathbf{x}_T^i)$

Super-Resolution

Super-Resolution via Repeated Refinement (SR3)

Image super-resolution can be considered as training $p(\mathbf{x}|\mathbf{y})$ where y is a low-resolution image and x is the corresponding high-resolution image

Train a score model for x conditioned on y using:

$$\mathbb{E}_{\mathbf{x},\mathbf{y}} \mathbb{E}_{\epsilon \sim \mathcal{N}(\mathbf{0},\mathbf{I})} \mathbb{E}_{t} || \epsilon_{\theta}(\mathbf{x}_{t},t;\mathbf{y}) - \epsilon$$

The conditional score is simply a U-Net with x_t and y (resolution image) concatenated.



Saharia et al., Image Super-Resolution via Iterative Refinement, 2021

 $||_p^p$

Super-Resolution

Super-Resolution via Repeated Refinement (SR3)

Natural Image Super-Resolution $64 \times 64 \rightarrow 256 \times 256$

Bicubic

Regression

SR3 (ours)



Reference



Image-to-Image Translation Palette: Image-to-Image Diffusion Models

Many image-to-image translation applications can be considered as training $p(\mathbf{x}|\mathbf{y})$ where y is the input image. For example, for colorization, \mathbf{x} is a colored image and \mathbf{y} is a gray-level image. Train a score model for x conditioned on y using:

$$\mathbb{E}_{\mathbf{x},\mathbf{y}} \mathbb{E}_{\epsilon \sim \mathcal{N}(\mathbf{0},\mathbf{I})} \mathbb{E}_{t} || \epsilon_{\theta}(\mathbf{x}_{t},t;\mathbf{y}) - \epsilon$$

The conditional score is simply a U-Net with x_t and y concatenated.



Saharia et al., Palette: Image-to-Image Diffusion Models, 2022

 $||_p^p$



Image-to-Image Translation Palette: Image-to-Image Diffusion Models



Conditional Generation

Iterative Latent Variable Refinement (ILVR)

To be discussed in detail in paper presentation

A simple technique to guide the generation process of an unconditional diffusion model using a reference image.

Given the conditioning (reference) image y the generation process is modified to pull the samples towards the reference image.



Conditional Generation Iterative Latent Variable Refinement (ILVR)

(a) Generation from various downsampling factors Reference N = 4N = 8N = 16

(b) Image Translation



Portrait



Realistic Image



Oil Painting



Realistic Image

Choi et al., ILVR: Conditioning Method for Denoising Diffusion Probabilistic Models, ICCV 2021

N = 32

N = 64



(d) Editing with Scribbles



Scribbled



New Watermark

Semantic Segmentation

Label-efficient semantic segmentation with diffusion models

Can we use representation learned from diffusion models for downstream applications such as semantic segmentation?



Baranchuk et al., Label-Efficient Semantic Segmentation with Diffusion Models, ICLR 2022

ion diffusion models

Semantic Segmentation Label-efficient semantic segmentation with diffusion models

The experimental results show that the proposed method outperforms Masked Autoencoders, GAN and VAE-based models.



Baranchuk et al., Label-Efficient Semantic Segmentation with Diffusion Models, ICLR 2022

Image Editing **SDEdit**

Goal: Given a stroke painting with color, generate a photorealistic image Key Idea:

- Latent Distribution of stroke and real images do not overlap. -
- But once we apply forward diffusion on them, their distribution start overlapping as finally it becomes gaussian noise.



Meng et al., SDEdit: Guided Image Synthesis and Editing with Stochastic Differential Equations, ICLR 2022





Input

Output

Image Editing SDEdit



LSUN bedroom

LSUN church

CelebA

Video Synthesis, Medical Imaging, 3D Generation, Discrete State Models




Samples from a text-conditioned video diffusion model, conditioned on the string *fireworks*.

Ho et al., "Video Diffusion Models", arXiv, 2022 Harvey et al., "Flexible Diffusion Modeling of Long Videos", arXiv, 2022 Yang et al., "Diffusion Probabilistic Modeling for Video Generation", arXiv, 2022 Höppe et al., "Diffusion Models for Video Prediction and Infilling", arXiv, 2022 Voleti et al., "MCVD: Masked Conditional Video Diffusion for Prediction, Generation, and Interpolation", arXiv, 2022

Video Generation Tasks:

- Unconditional Generation (Generate all frames) ullet
- Future Prediction (Generate future from past fames) \bullet
- Past Prediction (Generate past from future fames) \bullet
- Interpolation (Generate intermediate frames) •

Learn a model of the form: $p_{\boldsymbol{\theta}}(\mathbf{x}^{t_1},\cdots,\mathbf{x}^{t_K}|\mathbf{x}^{\tau_1},\cdots,\mathbf{x}^{\tau_M})$

Given frames:

 $\mathbf{x}^{ au_1},\cdots,\mathbf{x}^{ au_M}$

Frames to be predicted: $\mathbf{x}^{t_1}, \cdots, \mathbf{x}^{t_K}$

Ho et al., "Video Diffusion Models", arXiv, 2022 Harvey et al., "Flexible Diffusion Modeling of Long Videos", arXiv, 2022 Yang et al., "Diffusion Probabilistic Modeling for Video Generation", arXiv, 2022 Höppe et al., "Diffusion Models for Video Prediction and Infilling", arXiv, 2022 Voleti et al., "MCVD: Masked Conditional Video Diffusion for Prediction, Generation, and Interpolation", arXiv, 2022

Learn one model for everything:

- Architecture as one diffusion model over all frames concatenated.
- Mask frames to be predicted; provide conditioning frames; vary applied masking/conditioning for different tasks during training.
- Use time position encodings to encode times.



(image from: Harvey et al., "Flexible Diffusion Modeling of Long Videos", arXiv, 2022)

Architecture Details:

Data is 4D (image height, image width, #frames, channels) •

- Option (1): 3D Convolutions. Can be computationally expensive.
- Option (2): Spatial 2D Convolutions + Attention Layers along frame axis.



(image from: Harvey et al., "Flexible Diffusion Modeling of Long Videos", arXiv, 2022)

Video Generation Results

Long term video generation in hierarchical manner:

- 1. Generate future frames in sparse manner, conditioning on frames far back
- 2. Interpolate in-between frames



Test Data:

Generated:

(video from: Harvey et al., "Flexible Diffusion Modeling of Long Videos", *arXiv*, 2022, https://plai.cs.ubc.ca/2022/05/20/flexible-diffusion-modeling-of-long-videos/)



1+ hour coherent video generation possible!

Solving Inverse Problems in Medical Imaging

Forward CT or MRI imaging process (simplified):



(image from: Song et al., "Solving Inverse Problems in Medical Imaging with Score-Based Generative Models", ICLR, 2022)



Inverse Problem: Reconstruct original image from sparse measurements.

Solving Inverse Problems in Medical Imaging

High-level idea: Learn Generative Diffusion Model as "prior"; then guide synthesis conditioned on sparse observations:



(a) FISTA-TV (b) cGAN (d) SIN-4c-PRN (c) Neumann (image from: Song et al., "Solving Inverse Problems in Medical Imaging with Score-Based Generative Models", ICLR, 2022)

Outperforms even fully-supervised methods.

Song et al., "Solving Inverse Problems in Medical Imaging with Score-Based Generative Models", ICLR, 2022

PSNR: 15.32, SSIM: 0.796 PSNR: 17.79, SSIM: 0.454 PSNR: 17.60, SSIM: 0.471 PSNR: 27.88, SSIM: 0.908 PSNR: 35.57, SSIM: 0.929

(e) Ours (f) Ground truth

Solving Inverse Problems in Medical Imaging Lots of Literature

- Song et al., "Solving Inverse Problems in Medical Imaging with Score-Based Generative Models", <u>ICLR</u>, 2022
- Chung and Ye, "Score-based diffusion models for accelerated MRI", Medical Image Analysis, 2022
- Chung et al., "Come-Closer-Diffuse-Faster: Accelerating Conditional Diffusion Models for Inverse Problems through Stochastic Contraction", <u>CVPR</u>, 2022
- Peng et al., "Towards performant and reliable undersampled MR reconstruction via diffusion model sampling", <u>arXiv</u>, 2022
- Xie and Li, "Measurement-conditioned Denoising Diffusion Probabilistic Model for Under-sampled Medical Image Reconstruction", arXiv, 2022 •
- Luo et al, "MRI Reconstruction via Data Driven Markov Chain with Joint Uncertainty Estimation", arXiv, 2022
- . . .



orring inverse Frediente in medical imaging with coole-based constants model

3D Shape Generation

- Point clouds as 3D shape representation can be diffused easily and intuitively
- Denoiser implemented based on modern point cloud-processing networks (PointNets & Point-VoxelCNNs)



(image from: Zhou et al., "3D Shape Generation and Completion through Point-Voxel Diffusion", ICCV, 2021)

Zhou et al., "3D Shape Generation and Completion through Point-Voxel Diffusion", ICCV, 2021 Luo and Hu, "Diffusion Probabilistic Models for 3D Point Cloud Generation", CVPR, 2021



3D Shape Generation

- Point clouds as 3D shape representation can be diffused easily and intuitively
- Denoiser implemented based on modern point cloud-processing networks (PointNets & Point-VoxelCNNs)



(video from: Zhou et al., "3D Shape Generation and Completion through Point-Voxel Diffusion", *ICCV*, 2021, https://alexzhou907.github.io/pvd)

Zhou et al., "3D Shape Generation and Completion through Point-Voxel Diffusion", ICCV, 2021

/ ointNets & Point-VoxelCNNs)

3D Shape Generation Shape Completion

Can train conditional shape completion diffusion model (subset of points fixed to given conditioning points):



(video from: Zhou et al., "3D Shape Generation and Completion through Point-Voxel Diffusion", ICCV, 2021, https://alexzhou907.github.io/pvd)

Zhou et al., "3D Shape Generation and Completion through Point-Voxel Diffusion", ICCV, 2021

3D Shape Generation

Shape Completion - Multimodality



(video from: Zhou et al., "3D Shape Generation and Completion through Point-Voxel Diffusion", *ICCV*, 2021, https://alexzhou907.github.io/pvd)

Zhou et al., "3D Shape Generation and Completion through Point-Voxel Diffusion", ICCV, 2021

DN lity

3D Shape Generation Shape Completion - Multimodality - On Real Data



(video from: Zhou et al., "3D Shape Generation and Completion through Point-Voxel Diffusion", ICCV, 2021, https://alexzhou907.github.io/pvd)

Zhou et al., "3D Shape Generation and Completion through Point-Voxel Diffusion", ICCV, 2021





Towards Discrete State Diffusion Models

So far:

Continuous diffusion and denoising processes.





But what if data is discrete? Categorical? Continuous perturbations are not possible!

> (Text, Pixel-wise Segmentation Labels, Discrete Image Encodings, etc.)

Categorical diffusion: $q(\mathbf{x}_t | \mathbf{x}_{t-1}) = Cat(\mathbf{x}_t; \mathbf{p} = \mathbf{x}_{t-1}\mathbf{Q}_t)$ **X**_t : one-hot state vector \mathbf{Q}_t : transition matrix $[\mathbf{Q}_t]_{ij} = q(\mathbf{x}_t = j | \mathbf{x}_{t-1} = i)$



(image from: Hoogeboom et al., "Argmax Flows and Multinomial Diffusion: Learning Categorical Distributions", NeurIPS, 2022)

Austin et al., "Structured Denoising Diffusion Models in Discrete State-Spaces", NeurIPS, 2021 Hoogeboom et al., "Argmax Flows and Multinomial Diffusion: Learning Categorical Distributions", NeurIPS, 2022

Reverse process can be parametrized categorical distribution.





(image from: Austin et al., "Structured Denoising Diffusion Models in Discrete State-Spaces", NeurIPS, 2021)

Austin et al., "Structured Denoising Diffusion Models in Discrete State-Spaces", NeurIPS, 2021



(image from: Austin et al., "Structured Denoising Diffusion Models in Discrete State-Spaces", NeurIPS, 2021)

Austin et al., "Structured Denoising Diffusion Models in Discrete State-Spaces", NeurIPS, 2021

Modeling Categorical Image Pixel Values

Progressive denoising starting from allmasked state.

Progressive denoising starting from random uniform state.

(with discretized Gaussian denoising model)



(image from: Austin et al., "Structured Denoising Diffusion Models in Discrete State-Spaces", NeurIPS, 2021)

Modeling Discrete Image Encodings



Encoding images into latent space with discrete tokens, and modeling discrete token distribution



(images from: Chang et al., "MaskGIT: Masked Generative Image Transformer", CVPR, 2022)

Chang et al., "MaskGIT: Masked Generative Image Transformer", CVPR, 2022 Esser et al., "ImageBART: Bidirectional Context with Multinomial Diffusion for Autoregressive Image Synthesis", NeurIPS, 2021



Class-conditional model samples



Modeling Pixel-wise Segmentations



(image from: Hoogeboom et al., "Argmax Flows and Multinomial Diffusion: Learning Categorical Distributions", NeurIPS, 2022)

Hoogeboom et al., "Argmax Flows and Multinomial Diffusion: Learning Categorical Distributions", NeurIPS, 2022

Conclusions, Open Problems and Final Remarks



Summary: Denoising Diffusion Probabilistic Models "Discrete-time" Diffusion Models

We started with denoising diffusion probabilistic models:

Forward diffusion process (fixed)

Data

Reverse denoising process (generative)

We showed how the denoising model can be trained by predicting noise injected in each diffused image:

$$L_{\text{simple}} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), t \sim \mathcal{U}(1, T)} \left[||\epsilon - \epsilon_\theta (\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t)||^2 \right]$$



Noise

Summary: Advanced Techniques Acceleration, Guidance and beyond

In the third part, we discussed several advanced topics in diffusion models.

How can we accelerate the sample generation?



How to scale up diffusion models to high-resolution (conditional) generation?

- Cascaded models
- Guided diffusion models

[Image credit: Ben Poole, Mohammad Norouzi]

Summary: Applications

We covered many successful applications of diffusion models:

- Image generation, text-to-image generation, controllable generation
- Image editing, image-to-image translation, super-resolution, segmentation, adversarial robustness
- Discrete models, 3D generation, medical imaging, video synthesis

Open Problems (1)

- Diffusion models are a special form of VAEs and continuous normalizing flows
 - Why do diffusion models perform so much better than these models?
 - How can we improve VAEs and normalizing flows with lessons learned from diffusion models?

- Sampling from diffusion models is still slow especially for interactive applications
 - The best we could reach is 4-10 steps. How can we have one step samplers?
 - Do we need new diffusion processes?

- Diffusion models can be considered as latent variable models, but their latent space lacks semantics
 - How can we do latent-space semantic manipulations in diffusion models

Open Problems (2)

- How can diffusion models help with discriminative applications?
 - Representation learning (high-level vs low-level)
 - Uncertainty estimation
 - Joint discriminator-generator training

- What are the best network architectures for diffusion models?
 - Can we go beyond existing U-Nets?
 - How can we feed the time input and other conditioning?
 - How can we improve the sampling efficiency using better network designs?

Open Problems (3)

- How can we apply diffusion models to other data types?
 - 3D data (e.g., distance functions, meshes, voxels, volumetric representations), video, text, graphs, etc.
 - How should we change diffusion models for these modalities?

- Compositional and controllable generation
 - How can we go beyond images and generate scenes?
 - How can we have more fine-grained control in generation?

- Diffusion models for X
 - Can we better solve applications that were previously addressed by GANs and other generative models?
 - Which applications will benefit most from diffusion models?

Thanks!



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



@RuiqiGao

@karsten_kreis







@ArashVahdat

