

Advanced Topics in Deep Learning

Summer Semester 2024 6. Generative Models II 10.07.2024

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Course Topics

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- 1. Interpretability.
- 2. Attention and Transformers.
- Self-supervised Learning I.
- 4. Self-supervised Learning II.
- 5. Similarity Learning.
- Generative Models.
- 7. Model Compression.
- 8. Transfer learning, domain adaptation, few-shot learning.
- 9. Uncertainty Estimation.
- 10. Geometric Deep Learning.
- 11. Recap and Q&A.
- The exam will be written.
- We will have an exam preparation test.

<u>Acknowledgements</u>

Special thanks Arij Bouazizi, Julia Hornauer, Julian Wiederer, Adrian Holzbock and Youssef Dawoud for contributing to the lecture preparation.



Recap

- ***Not for sharing (LMS, Friedrich-Alexander-Universität Erlangen-Nürnberg)***
- Generative models with Deep Neural Networks.
- Generative Adversarial Networks.
- Auto-Encoders.
- Variational Auto-Encoders.



Today's Agenda and Objectives

- Generative Models.
- Diffusion Models.
- Forward Process.
- Reverse Process.
- Sampling.
- Conditional Diffusion Models.



Generative Models

- We focus on generative models where no labels are provided, similar to unsupervised learning and self-learning.
 - Consider the training set $D = \{\{x_1\}, ..., \{x_n\}\}$. Each sample can be, for instance, an image.
 - The generative model $p_{\theta}(x)$ will learn to form images based on the training set D, which expresses the data distribution $p_{data}(x)$.
- By learning the data distribution based on the training set, the generative model can used for sampling, e.g., sample new images.



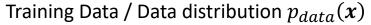


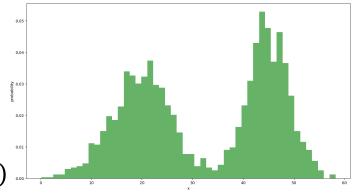
Generated with DiffusionBee.

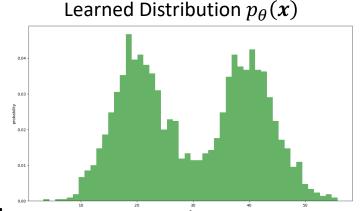


Generative Model Training

- We have seen two approaches to training the generative model $p_{\theta}(x)$ to match the data distribution $p_{data}(x)$.
 - Maximize the expected log-likelihood
 - **Minimize** the divergence between $p_{\theta}(\mathbf{x})$ and $p_{data}(\mathbf{x})$.
- Generative Adversarial Networks (GANs)
 - Minimize the Jensen-Shannon divergence.
- Variational Autoencoders (VAEs)
 - Maximize the log-likelihood of the ELBO.









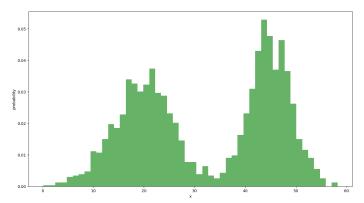


Generative Model Training

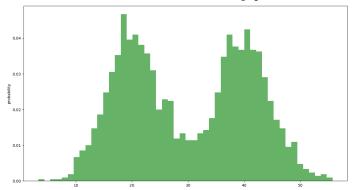
Not for sharing (LMS, Friedrich-Alexander-Universität Erlangen-Nürnberg)

- Generative Adversarial Networks (GANs)
 - Minimize the Jensen-Shannon divergence.
 - $\min_{G} \max_{D} \mathbb{E}_{x \sim p_{data}(x)[Log(D(x))]} + \mathbb{E}_{z \sim p_{z}(z)[Log(1-D(G(z)))]}$
- Variational Autoencoders (VAEs)
 - Maximize the log-likelihood of the ELBO.
 - $\mathcal{L}(\theta, \varphi; x^{i}) =$ $D_{KL}(q_{\phi}(z|x^{i})||p_{\theta}(z)) +$ $\mathbb{E}_{q_{\phi}(z|x^{i})}[log p_{\theta}(x^{i}|z)].$

Training Data / Data distribution $p_{data}(x)$



Learned Distribution $p_{\theta}(x)$

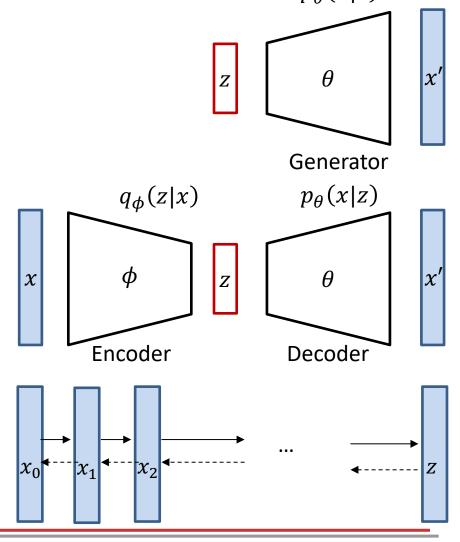






Generative Model Sampling

- How do we generate a new sample?
- Both GANs and VAEs sample
 noise z (based on a prior
 distribution) in the latent space to
 create a new sample in a single
 step.
- Diffusion models start with a fully noisy sample and gradually (in multiple steps) denoise it to an image.
 - We deal with noisy on the sample space, e.g., image space. It's possible to have noise in the latent space as well (latent diffusion).





Diffusion Models

- The motivation is to start from a based distribution, like a Gaussian distribution and gradually (in multiple steps) convert it to the target data distribution, like an image.
 - This process is like a Markov chain. Each step in the transition from noise to image is a step in the chain.
 - Moreover, it is assumed that the current step depends only on the previous one (Markov property).
 - By making the Markov chain assumption, we can define the diffusion process as a sequence of Gaussian transitions. In the end, it is assumed to have an isotropic Gaussian distribution given a large number of steps.
- Diffusion models contain the step-wise* functionality not only during sampling but also during training.
- A diffusion model consists of:
 - Forward process (image to noise transition).
 - Reverse process (noise to image transition).
 - Sampling (noise to image transition).
- The forward and reverse processed are required to perform training.

^{*}Ho, Jonathan, Ajay Jain, and Pieter Abbeel. "Denoising diffusion probabilistic models." Advances in neural information processing systems 33 (2020): 6840-6851.



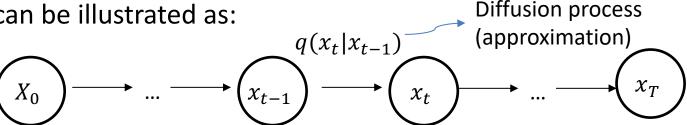


Forward Process

- Consider the sample X_0 that is noise free, e.g. an image.
- In the **forward** process, we gradually add small amounts of **Gaussian** noise to the image. Each steps makes the image x_t noisier until we end with noise x_T .
- The process of adding noise is repeated for T steps.
- Ideally, we will end up with pure noise (isotropic Gaussian distribution) after a large number of iterations.











Forward Process Derivation

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For each time step, the image noising is given by:

$$- x_t = \sqrt{1 - \beta_t} x_{t-1} + \sqrt{\beta_t} \epsilon.$$

- With $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ and β_t the noise variance.
- The noise variance $\beta_1 \dots \beta_T$ is from 0 to 1. It tells us the amount of noise to add at the current step.
- Based on the update step x_t , we can now write the sampling as a **Gaussian** distribution:

$$- q(x_t|x_{t-1}) = \mathcal{N}(\sqrt{1-\beta_t}x_{t-1}, \beta_t \mathbf{I}).$$

- $-\beta_t$ corresponds to the current variance schedule.
- $-\sqrt{1-\beta_t}x_{t-1}$ is the mean value.
- To derive the above, consider that:

•
$$\mathcal{N}(\sqrt{1-\beta_t}x_{t-1}, \beta_t \mathbf{I}) = \sqrt{1-\beta_t}x_{t-1} + \beta_t \mathcal{N}(\mathbf{0}, \mathbf{I}).$$





Forward Process Derivation (Cont.)

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For each time step, the image noising is given by:

$$- x_t = \sqrt{1 - \beta_t} x_{t-1} + \sqrt{\beta_t} \epsilon.$$

- With $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ and β_t the noise variance.
- We can rewrite x_t as:

$$- x_t = \sqrt{a_t} x_{t-1} + \sqrt{1 - a_t} \epsilon.$$

- We define $a_t = 1 \beta_t$ with $a_t \in (0,1)$.
- Also define $\bar{a}_t = \prod_{i=1}^t \alpha_i$.
- The forward process is a recurrence. It can be written as:

$$- x_t = \sqrt{1 - \beta_t} x_{t-1} + \sqrt{\beta_t} \epsilon = \sqrt{a_t} x_{t-1} + \sqrt{1 - a_t} \epsilon = \sqrt{a_t} \left(\sqrt{a_{t-1}} x_{t-2} + \sqrt{1 - a_{t-1}} \epsilon \right) + \sqrt{1 - a_t} \epsilon = \dots = \sqrt{a_t \dots a_1} x_0 + \sqrt{1 - a_t \dots a_1} \epsilon = \sqrt{\bar{a}_t} x_0 + \sqrt{1 - \bar{a}_t} \epsilon.$$

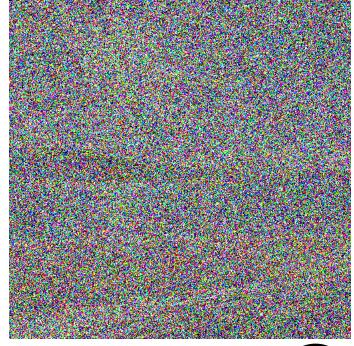
- We can thus **always** express x_t w.r.t. x_0 as $q(x_t|x_0) = \mathcal{N}(\sqrt{\overline{a_t}}x_0, (1 - \overline{a_t})\mathbf{I})$. Also, we have $q(x_t|x_{t-1}) = \mathcal{N}(\sqrt{a_t}x_{t-1}, 1 - a_t\mathbf{I})$.

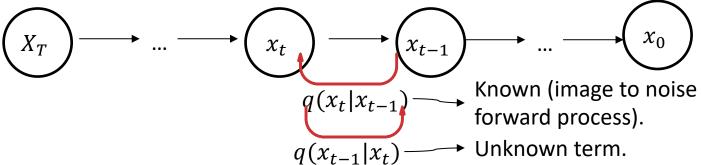




Reverse Process

- The noising steps cannot help us to create an image. However, the opposite approach (denoising) can lead to the formation of an image from Gaussian noise in several steps.
 - This is called the reverse process.
- Our goal is to learn with the diffusion model to go from the noise to the each using a multiple step process $q(x_{t-1}|x_t)$.
- We generate data from random noise.
- The process can be illustrated as:









Reverse Process

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• The reverse prices $q(x_{t-1}|x_t)$ is clear unknown. For that reason, we consider first the Bayer rule:

$$- f(a|b) = \frac{f(a,b)}{f(b)} = \frac{f(a)f(b|a)}{f(b)}.$$

•
$$q(x_{t-1}|x_t) = \frac{q(x_{t-1},x_t)}{q(x_t)} = \frac{q(x_{t-1})q(x_t|x_{t-1})}{q(x_t)} = q(x_t|x_{t-1})\frac{q(x_{t-1})}{q(x_t)}$$

- $q(x_t)$ is computationally intractable because we must compute $q(x_t) = \int q(x_t|x_{t-1}) \, q(x_{t-1}) dx$.
- $q(x_t|x_{t-1})$ is a Gaussian distribution that we know (image to noise).

• We have to reply on some **approximation** to compute $q(x_{t-1}|x_t)$... x_t ...



Reverse Process

- We can assume forward process steps with very **small** noise schedule β_t .
 - Based on this assumption, we further assume that the reverse process can be a Gaussian distribution similar to the forward process.
- The reverse process approximation is a Gaussian with unknown mean and variance.
 - We rely on a neural network to learn the Gaussian parameters for the reverse process.
 - Our neural network model is defined as $p_{\theta} = (x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t); \Sigma_{\theta}(x_t, t)).$
- Our goal in training the neural network is to maximize the log-likelihood of the generated data using the reverse process.
 - Our objective is similar to VAEs training.
 - Recall that for VAEs, we have:

•
$$\mathcal{L}(\theta, \varphi; x^i) = -D_{KL}(q_{\phi}(z|x^i)||p_{\theta}(z)) + \mathbb{E}_{q_{\phi}(z|x^i)}[log p_{\theta}(x^i|z)] \rightarrow$$

- $\mathbb{E}_{q_{\phi}(z|x^i)}[log p_{\theta}(x^i|z)] D_{KL}(q_{\phi}(z|x^i)||p_{\theta}(z)) \leq log p_{\theta}(x)$
- We can use the same objective for the diffusion process as well.





Learning the Reverse Process

- ***Not for sharing (LMS, Friedrich-Alexander-Universität Erlangen-Nürnberg)***
- We want to learn the reverse process $p_{\theta}(x_{t-1}|x_t)$ from the available forward process $q(x_t|x_{t-1})$.
- We will use the KL divergence as objective function where we will consider all time steps *T*. We have thus:
 - $D_{KL}(q(x_{1:T}|x_0)||p_{\theta}(x_{1:T}|x_0)).$
- Similar to VAEs, we apply variational inference and optimize an evidence lower bound on the likelihood $p_{\theta}(x_0)$ of the sample x_0 .

$$- \log p_{\theta}(x_{0}) \geq \log p_{\theta}(x_{0}) - D_{KL}(q(x_{1:T}|x_{0})||p_{\theta}(x_{1:T}|x_{0})) = \log p_{\theta}(x_{0}) - \mathbb{E}_{x_{1}:T \sim q(x_{1:T}|x_{0})} \left[\log \frac{q(x_{1:T}|x_{0})}{\frac{p_{\theta}(x_{1:T}|x_{0})}{p_{\theta}(x_{0})}} \right] = \log p_{\theta}(x_{0}) - \mathbb{E}_{q} \left[\log \frac{q(x_{1:T}|x_{0})}{p_{\theta}(x_{0:T})} + \log p_{\theta}(x_{0}) \right] = -\mathbb{E}_{q} \left[\log \frac{q(x_{1:T}|x_{0})}{p_{\theta}(x_{0:T})} \right].$$





Learning the Reverse Process (Cont.)

- Now we have $log p_{\theta}(x_0) \ge -\mathbb{E}_q \left[log \frac{q(x_{1:T}|x_0)}{p_{\theta}(x_{0:T})}\right]$.
 - Note that q is fixed and we optimise only for p_{θ} .

$$- -\mathbb{E}_q \left[log \frac{q(x_{1:T}|x_0)}{p_{\theta}(x_{0:T})} \right]$$

- Next, we would like to transform the above bound (ELBO) into a sum of simpler terms.
 - $\text{ Consider the variational lower bound loss } L_{VLB} = \mathbb{E}_{q} \left[log \frac{q(x_{1:T}|x_{0})}{p_{\theta}(x_{0:T})} \right] = \\ \mathbb{E}_{q} \left[log \frac{\prod_{t=1}^{T} q(x_{t}|x_{t-1})}{p_{\theta}(x_{T}) \prod_{t=1}^{T} p_{\theta}(x_{t-1}|x_{t})} \right] = \cdots = \mathbb{E}_{q} \left[D_{KL} \left(q(x_{T}|x_{0}) || p_{\theta}(x_{T}) \right) \right] + \\ \sum_{t=2}^{T} D_{KL} \left(q(x_{t-1}|x_{t},x_{0}) || p_{\theta}(x_{t-1}|x_{t}) \right) log \; p_{\theta}(x_{0}|x_{1}).$
 - We have three terms in L_{VLB} .
 - We can write it as $L_{VLB} = L_T + L_{T-1} + \cdots + L_0$





Learning the Reverse Process (Cont.)

- $L_T = D_{KL}(q(x_T|x_0)||p_{\theta}(x_T))$ corresponds to the prior loss and compares the final x_T with x_0 .
- The reconstruction term $L_0 = -log p_{\theta}(x_0|x_1)$ is the probability of the true x_0 given the current prediction x_1 .
- The diffusion loss is $L_t = D_{KL}(q(x_{t-1}|x_t,x_0)||p_{\theta}(x_{t-1}|x_t)) = D_{KL}(q(x_t|x_{t+1},x_0)||p_{\theta}(x_t|x_{t+1}))$ for $1 \le t \le T-1$.
 - It measures the similarity of the learned reverse process $p_{\theta}(x_t|x_{t+1})$ with the real reverse process $q(x_t|x_{t+1},x_0)$.
 - This part of the the variational lower bound loss L_{VLB} is important.





Diffusion Loss

- ***Not for sharing (LMS, Friedrich-Alexander-Universität Erlangen-Nürnberg)***
- The diffusion loss is:

$$- L_t = D_{KL}(q(x_t|x_{t+1},x_0)||p_{\theta}(x_t|x_{t+1})) \text{ for } 1 \le t \le T-1.$$

- We know that:
 - $q(x_t|x_0) = \mathcal{N}(\sqrt{\overline{a}_t}x_0, (1-\overline{a}_t)I) \text{ with } \overline{a}_t = \prod_{i=1}^t \alpha_i.$
 - $q(x_t|x_{t-1}) = \mathcal{N}(\sqrt{a_t}x_{t-1}, 1 a_t I) \text{ with } a_t = 1 \beta_t.$
- Using the Bayes' rule, it can be shown that:
 - $q(x_t|x_t,x_0) = \mathcal{N}(\tilde{\mu}(x_t,x_0),\tilde{\beta}_t \mathbf{I}) \text{ for some } \tilde{\mu} \text{ and } \tilde{\beta}.$
- We also assume that:
 - $p(x_{t-1}|x_t) = \mathcal{N}(\mu_{\theta}(x_t), \widetilde{\beta}_t \mathbf{I}).$
 - $-\mu_{\theta}\left(\cdot\right)$ corresponds to a neural network.
- Based on μ_{θ} (x_t) and $\tilde{\mu}(x_t, x_0)$, the **diffusion** loss becomes to **minimize** their different while assuming the same variance $\tilde{\beta}_t$.





Diffusion Loss (Cont.)

- ***Not for sharing (LMS, Friedrich-Alexander-Universität Erlangen-Nürnberg)***
- The term $q(x_t|x_t,x_0) = \mathcal{N}(\tilde{\mu}(x_t,x_0),\tilde{\beta}_t I)$ can be further worked by considering $\tilde{\mu}(x_t,x_0)$ to that:

$$- \tilde{\mu}_t = \frac{1}{\sqrt{a_t}} \left(x_t - \frac{1 - a_t}{\sqrt{1 - \bar{a}_t}} \epsilon_t \right).$$

- $-\epsilon_t$ now corresponds to the noise added to x_0 and resulted in x_t .
- We can now our model as:

$$- \mu_{\theta}(x_t, t) = \frac{1}{\sqrt{a_t}} \left(x_t - \frac{1 - a_t}{\sqrt{1 - \bar{a}_t}} \epsilon_{\theta}(x_t, \tau) \right).$$

- $-\epsilon_{\theta}(x_t,t)$ corresponds to the neural network model of the noise ϵ_t .
- With this model and parametrization, minimizing the **diffusion** loss L_t refers to predicting the noise ϵ_t using the neural network model $\epsilon_{\theta}(\cdot)$ and then removing it from x_t .





Diffusion Loss (Cont.)

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• Finally, we can write the **diffusion** loss L_t as:

$$-L_t = \mathbb{E}_{x_0,\epsilon}[C_1 \cdot \|\tilde{\mu}(x_t, x_0) - \mu_{\theta}(x_t, t)\|^2] = \mathbb{E}_{x_0,\epsilon}[C_2 \cdot \|\epsilon_t - \epsilon_{\theta}(x_t, t)\|^2] = \mathbb{E}_{x_0,\epsilon}[C_2 \cdot \|\epsilon_t - \epsilon_{\theta}(\sqrt{\bar{a}_t x_0} + \sqrt{1 - \bar{a}_t}\epsilon_t, t)\|^2].$$

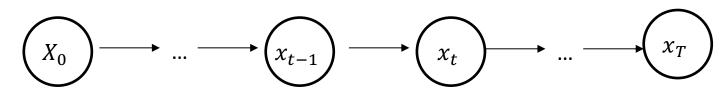
- With $x_t = \sqrt{\overline{a}_t x_0} + \sqrt{1 \overline{a}_t} \epsilon_t$.
- C_1 , C_2 are positive constants that we can ignore.
- So, optimizing the diffusion loss is given as:
 - Sample x_0 .
 - Sample a time step t, \dots, T .
 - Sample noise $\epsilon_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$.
 - Generate noisy $x_t = \sqrt{\overline{a}_t x_0} + \sqrt{1 \overline{a}_t} \epsilon_t$.
 - Compute loss $L_t = \|\epsilon_t \epsilon_\theta(x_t, t)\|^2$.
 - Perform gradient descent on L_t .
- Training takes place until convergence.

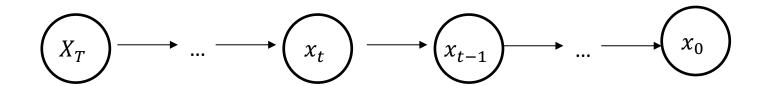




Diffusion Loss Interpretation

- During the forward process, we can randomly pick up a time step and add noise ϵ_t to our noisy sample (image).
- In the reverse process, we take a noisy sample x_t and denoise it using the neural network $\epsilon_{\theta}(\cdot)$. However, the neural network does not directly remove the noise from the sample. Instead, it produces the noise that we need to remove from the sample.









Sample Generation

***Not for sharing (LMS, Friedrich-Alexander-l

- Diffusion models are commonly used to generate images, videos and graphs, among other things.
- The most common architecture for images is to rely on a U-Net* style architecture.



Generated with DiffusionBee.

^{*}Ronneberger, O., Fischer, P., & Brox, T. (2015). U-net: Convolutional networks for biomedical image segmentation. In Medical image computing and computer-assisted intervention–MICCAI 2015: 18th international conference, Munich, Germany, October 5-9, 2015, proceedings, part III 18 (pp. 234-241). Springer International Publishing.





Sample Generation (Cont.)

***Not for sharing (LMS, Friedrich-Alexander-Li

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Comparison to other Generative Models

- ***Not for sharing (LMS, Friedrich-Alexander-Universität Erlangen-Nürnberg)***
- 2 main metrics are used in the literature to evaluate the performance of generative models
- SOTA comparison regarding the Inception Score(IS) & Frechet Inception Distance(FID)
 - FID: Calculates the statistical difference between real and generated images' feature representations extracted from a pre-trained Inception-v3 model. A lower FID score suggests better quality and diversity of the generated images compared to the real ones.
 - -> lower FID is better.
 - IS: Measures the quality by classification confidence and measure the diversity. Additionally measures image diversity by the spread of predicted classes across generated images.
 - -> higher IS is better.

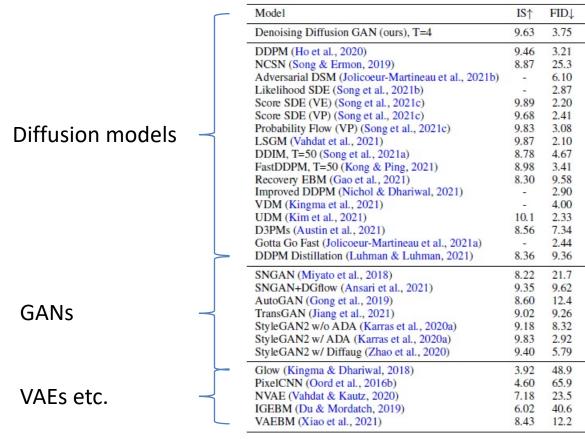




Comparison to other Generative Models (Cont.)

Not for sharing (LMS, Friedrich-Alexander-Universität Erlangen-Nürnberg)

Results on standard benchmarks for image generation.



Source: Xiao, Z., Kreis, K., & Vahdat, A. (2021). Tackling the generative learning trilemma with denoising diffusion gans. arXiv preprint arXiv:2112.07804





Latent Diffusion Models

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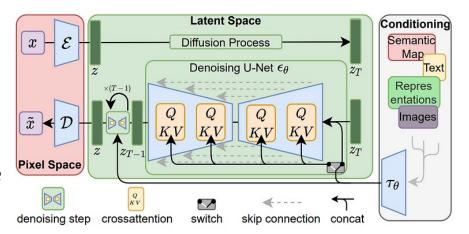
- Latent diffusion modes (LDMs):
 - Pixel space diffusion models have huge drawbacks:
 - Sampling speed is very slow
 - Training on high-resolution images is resource intensive
 - LDMs* fix these issues with a simple idea:

1. Encode everything into a latent space with the help of a pretrained

VQGAN encoder ϵ .

2. perform diffusion in the latent space of the VQGAN.

- → diffusion is applied in lower dimension
- 3. decode back to pixel space with the VQGAN decoder *D*



^{*} Rombach, R., Blattmann, A., Lorenz, D., Esser, P., & Ommer, B. (2022). High-resolution image synthesis with latent diffusion models. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition* (pp. 10684-10695).





Denoising Diffusion Implicit Models

Not for sharing (LMS, Friedrich-Alexander-Universität Erlangen-Nürnberg)

- Latent diffusion modes (LDMs):
 - Pixel space diffusion models have huge drawbacks
 - LDMs fix the computation issue with encoding to a latent space
 Sampling speed is still problematic!
 - Change sampling strategy, e.g., deterministic sampling (DDIM)*
 - Trade sampling speed for quality with Denoising Diffusion Implicit Models (DDIM):

DDIM

DDPM

•	Using	only	T =	100	steps.
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DDIM reaches only slightly.

Higher FID score than DDPM.

• When using T = 1000.

CIFAR10 (32×32)								
10	20	50	100	1000				
13.36	6.84	4.67	4.16	4.04				
14.04	7.11	4.77	4.25	4.09				
16.66	8.35	5.25	4.46	4.29				
41.07	18.36	8.01	5.78	4.73				
367.43	133.37	32.72	9.99	3.17				

FID scores for both DDPMs and DDIMs on CIFAR10 data.

^{*} Song, J., Meng, C., & Ermon, S. (2020). Denoising diffusion implicit models. arXiv preprint arXiv:2010.02502.



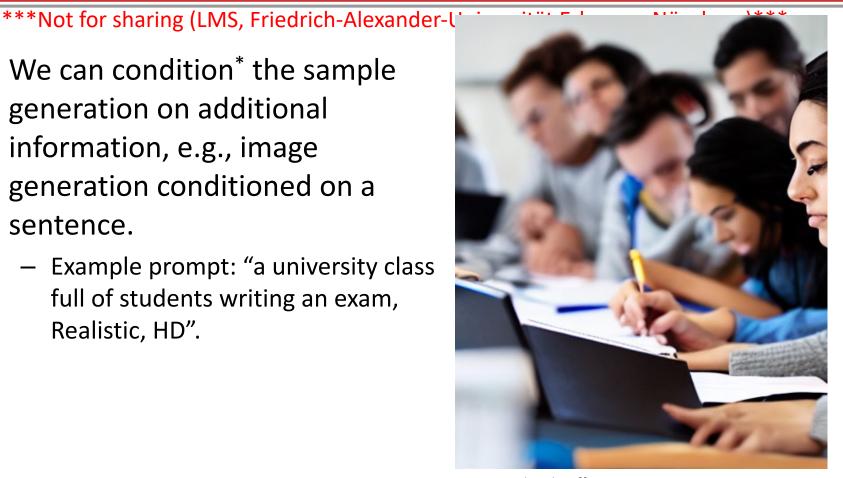


Conditional Sampling & Guidance

We can condition* the sample generation on additional information, e.g., image generation conditioned on a

sentence.

 Example prompt: "a university class" full of students writing an exam, Realistic, HD".



Generated with DiffusionBee.

^{*} Dhariwal, Prafulla, and Alexander Nichol. "Diffusion models beat gans on image synthesis." Advances in neural information processing systems 34 (2021): 8780-8794.





Study Material

- ***Not for sharing (LMS, Friedrich-Alexander-Universität Erlangen-Nürnberg)***
- Ho, Jonathan, Ajay Jain, and Pieter Abbeel. "Denoising diffusion probabilistic models." Advances in neural information processing systems 33 (2020): 6840-6851.
- Song, Yang, et al. "Score-based generative modeling through stochastic differential equations." arXiv preprint arXiv:2011.13456 (2020).
- Sohl-Dickstein, J., Weiss, E., Maheswaranathan, N., & Ganguli, S. (2015, June). Deep unsupervised learning using nonequilibrium thermodynamics. In International conference on machine learning (pp. 2256-2265). PMLR.
- Song, J., Meng, C., & Ermon, S. (2020). Denoising diffusion implicit models. arXiv preprint arXiv:2010.02502.





Next Lecture

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Model Compression



