

# The Emergence of Reproducibility and Consistency in Diffusion Models

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# Outline

- 1 Introduction
- 2 Reproducibility for Unconditional Diffusion Models
- 3 Correlation between Reproducibility, Memorizability & Generalizability
- 4 Reproducibility beyond Unconditional Diffusion Models
- 5 Future Directions

# Model reproducibility in deep learning

- **Definition:** You can repeatedly run your algorithm on certain datasets and obtain the same (or similar) results on a particular project <sup>1</sup>.

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- **Very general in diffusion model**

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# Introduction of diffusion model

- **A powerfule generative model:**
  - **Stable Diffusion [14]:** Large text-to-image diffusion model

*'An oil painting of a latent space.'*

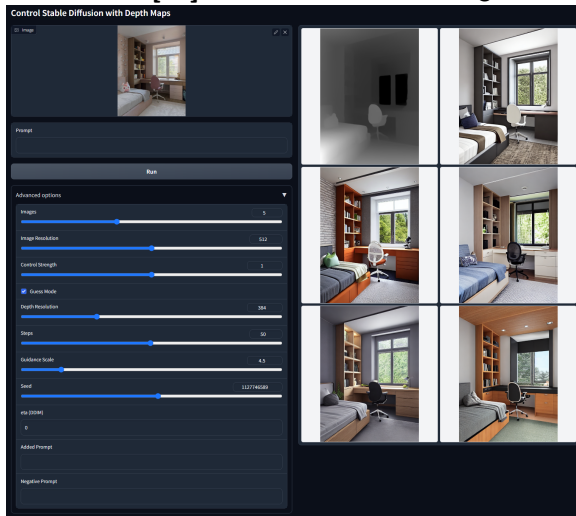


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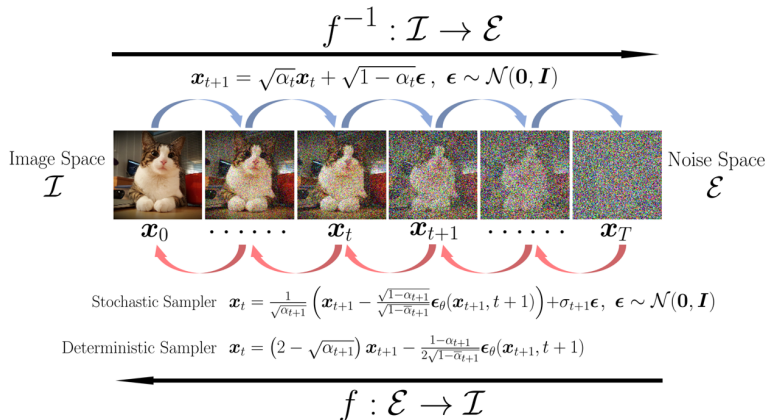
# Introduction of diffusion model

- **A powerfule generative model:**
  - **ControlNet [22]:** Diffusion model with high flexiable guidance



# Introduction of diffusion model

- Definition:** A generative model  $f : \mathcal{E} \mapsto \mathcal{I}$  mapping from the gaussian noise space  $\mathcal{E}$  to the image manifold  $\mathcal{I}$



# Introduction of diffusion model

- **Training:** Only the denoiser function  $\epsilon_\theta$  requires training, following an easy pipeline:

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## Algorithm 1 Training

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

$$\nabla_\theta \left\| \epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t) \right\|^2$$
  - 6: **until** converged
-

# Outline

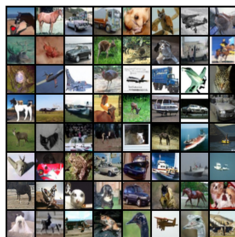
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# Samples Visualization

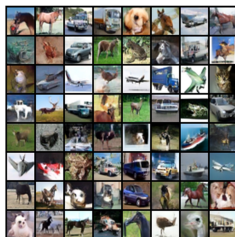
**Q1:** *Starting from the **same noise input**, how are the generated data samples from various diffusion models related to each other?*

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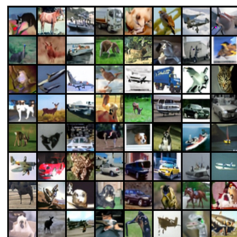
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(a) DDPMv4



(b) CT

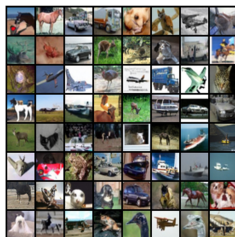


(c) U-ViT

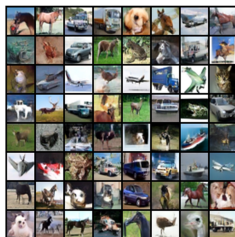


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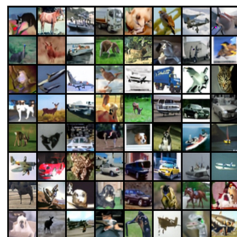
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Training on the same dataset, sampling by a deterministic sampler.

## Quantitative analysis

- **Metric:** We define *reproducibility (RP) score* to measure the this phenomenon:

$$\text{RP Score} := \mathbb{P}(\mathcal{M}_{\text{SSCD}}(\mathbf{x}_1, \mathbf{x}_2) > 0.6),$$

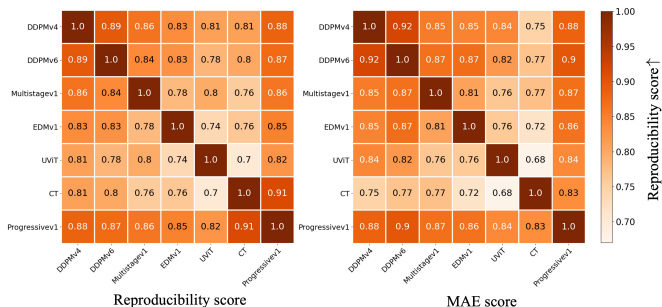
represents the *probability* of a generated sample pair  $(\mathbf{x}_1, \mathbf{x}_2)$  from two different diffusion models to have *self-supervised copy detection* (SSCD) similarity  $\mathcal{M}_{\text{SSCD}}$  larger than 0.6. We sampled 10K noise to estimate the probability. The SSCD similarity is first introduced in [12] to measure the replication between image pair  $(\mathbf{x}_1, \mathbf{x}_2)$ , which is defined as the following:

$$\mathcal{M}_{\text{SSCD}}(\mathbf{x}_1, \mathbf{x}_2) = \frac{\text{SSCD}(\mathbf{x}_1) \cdot \text{SSCD}(\mathbf{x}_2)}{\|\text{SSCD}(\mathbf{x}_1)\|_2 \cdot \|\text{SSCD}(\mathbf{x}_2)\|_2}$$

where  $\text{SSCD}(\cdot)$  represents a neural descriptor for copy detection.

# Quantitative analysis

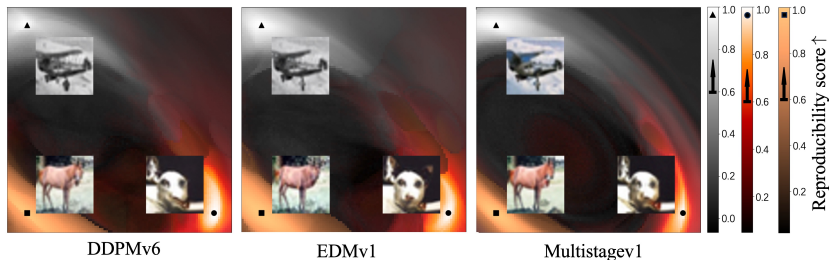
## Results:



**C2:** *Diffusion models consistently generate **nearly identical contents**, irrespective of network architectures, training and sampling procedures, and perturbation kernels.*

# Mapping from Noise Hyperplane to Image Manifold

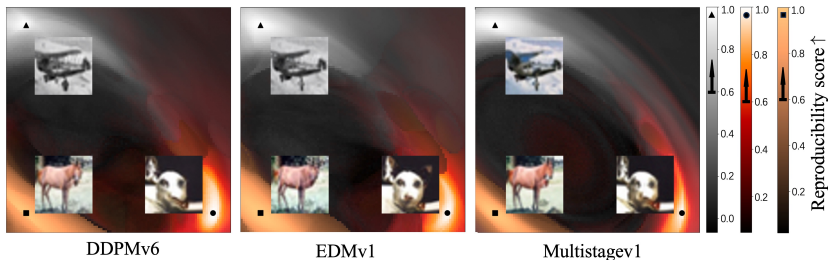
- Results:**



Pick three initial noises  $(\epsilon_1, \epsilon_2, \epsilon_3)$  to generate clear images  $(x_1, x_2, x_3)$  in the image manifold  $\mathcal{I}$ . Second, we create a 2D noise hyperplane with  $\epsilon(\alpha, \beta) = \alpha \cdot (\epsilon_2 - \epsilon_1) + \beta \cdot (\epsilon_3 - \epsilon_1) + \epsilon_1$ . And utilize them to generate images  $x(\alpha, \beta)$ , and RP Score  $:= \max_{k \in \{1, 2, 3\}} [\mathcal{M}_{\text{SSCD}}(x_k, x(\alpha, \beta))]$

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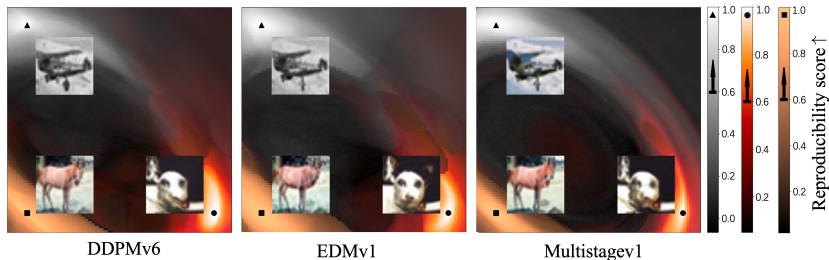
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## Conclusions:

- Similar unique encoding maps across different network architectures.

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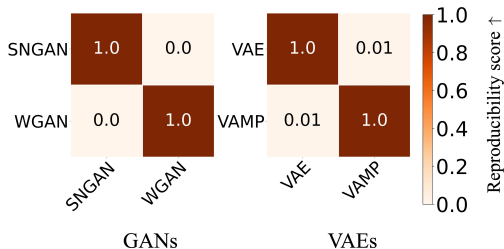
- Similar unique encoding maps across different network architectures.
- Local Lipschitzness of the unique encoding from noise to image space.

# Reproducibility for other generative models

- **Question:** Does model reproducibility appear to other generative models?

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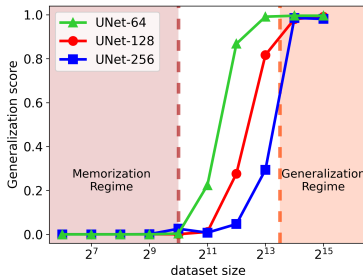
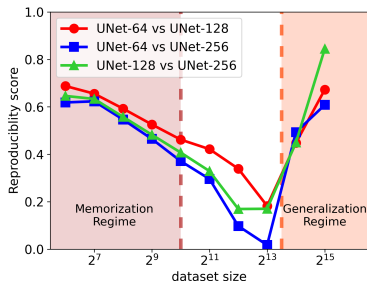
- Conclusion:** Reproducibility doesn't appear for GAN and general VAE;



# Outline

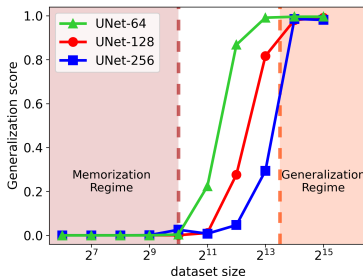
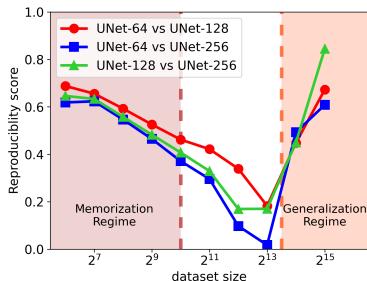
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# “Memorization” and “Generalization” regimes



generalization (GL) score  $:= 1 - \mathbb{P}(\max_{i \in [N]} [\mathcal{M}_{\text{SSCD}}(\mathbf{x}, \mathbf{y}_i)] > 0.6)$  between the generated sample  $\mathbf{x}$  and all samples from training dataset  $\{\mathbf{y}_i\}_{i=1}^N$ .

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**C3:** The reproducibility of diffusion models manifests in two distinct training regimes, both **strongly correlated** with the model's generalizability.

# Theory for reproducibility in Memorization Regime

## Theorem (1)

Suppose we train a diffusion model denoiser function  $\epsilon_{\theta}(\mathbf{x}, t)$  with parameter  $\theta$  on a training dataset  $\{\mathbf{y}_i\}_{i=1}^N$  of  $N$ -samples, by minimizing the training loss

$$\min_{\theta} \mathcal{L}(\epsilon_{\theta}; t) = \mathbb{E}_{\mathbf{x}_0 \sim p_{\text{data}}(\mathbf{x})} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{x}_0)} [\|\epsilon - \epsilon_{\theta}(\mathbf{x}, t)\|^2], \quad (1)$$

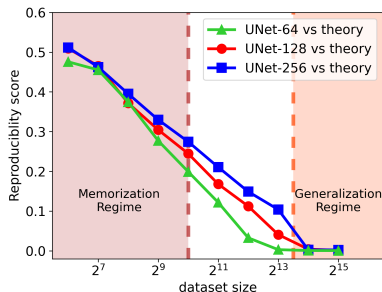
assuming data  $\mathbf{x}_0$  follows a multi-delta distribution  $p_{\text{data}}(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{y}_i)$ , and the perturbation kernel  $p_t(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; s_t \mathbf{x}_0, s_t^2 \sigma_t^2 \mathbf{I})$  with parameters  $s_t, \sigma_t$ . Then we show the optimal denoiser  $\epsilon_{\theta}^*(\mathbf{x}; t) = \arg \min_{\epsilon_{\theta}} \mathcal{L}(\epsilon_{\theta}; t)$  is:

$$\epsilon_{\theta}^*(\mathbf{x}; t) = \frac{1}{s_t \sigma_t} \left[ \mathbf{x} - s_t \frac{\sum_{i=1}^N \mathcal{N}(\mathbf{x}; s_t \mathbf{y}_i, s_t^2 \sigma_t^2 \mathbf{I}) \mathbf{y}_i}{\sum_{i=1}^N \mathcal{N}(\mathbf{x}; s_t \mathbf{y}_i, s_t^2 \sigma_t^2 \mathbf{I})} \right]. \quad (2)$$

Moreover, suppose a trained diffusion model could converge to the optimal denoiser  $\epsilon_{\theta}^*(\mathbf{x}; t)$  and we use a deterministic ODE sampler to generate images using  $\epsilon_{\theta}^*(\mathbf{x}; t)$ , then  $f: \mathcal{E} \mapsto \mathcal{I}$ , which is determined by the  $\epsilon_{\theta}^*(\mathbf{x}; t)$  and the ODE sampler, is an invertible mapping and the inverse mapping  $f^{-1}$  is a unique identifiable encoding.

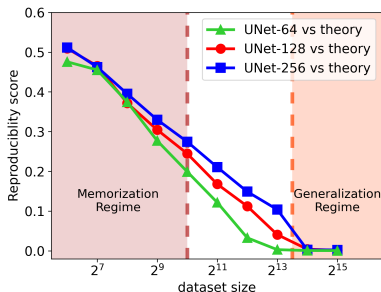
# Experimental verification of Theorem (1)

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- Conclusion:** Diffusion model could converge to the theoretical solution when model capacity is enough.

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# More than unconditional diffusion model

**C4:** *Model reproducibility holds **more generally** across conditional diffusion models, diffusion models for inverse problems, the fine-tuning of diffusion models.*



# Intro to conditional diffusion model

- Enable conditional generation, e.g. class condition, text-to-image, image-to-image translation.[14].

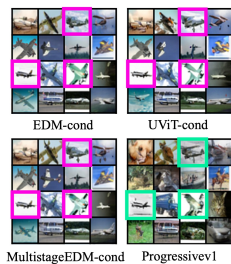
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- Enable conditional generation, e.g. class condition, text-to-image, image-to-image translation.[14].
- Change the denoiser from  $\epsilon_{\theta}(\mathbf{x}_t, t)$  to  $\epsilon_{\theta}(\mathbf{x}_t, t, c)$  for  $c \in \mathcal{C}$ . Total class  $\mathcal{C}$  could be the class label, text, image, and so on.

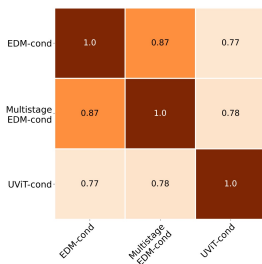
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- Utilize  $\epsilon_{\theta}(\mathbf{x}_t, t, c)$  for both training and sampling.

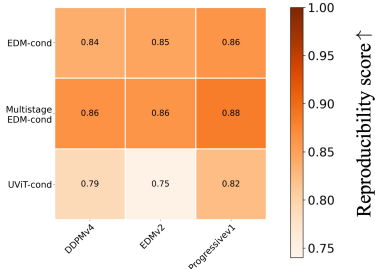
# Reproducibility of conditional diffusion model



(a) Visualization

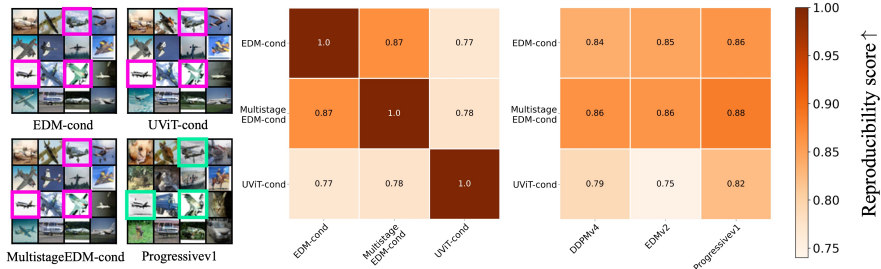


(b) Conditional diffusion models



(c) Conditional and unconditional diffusion models

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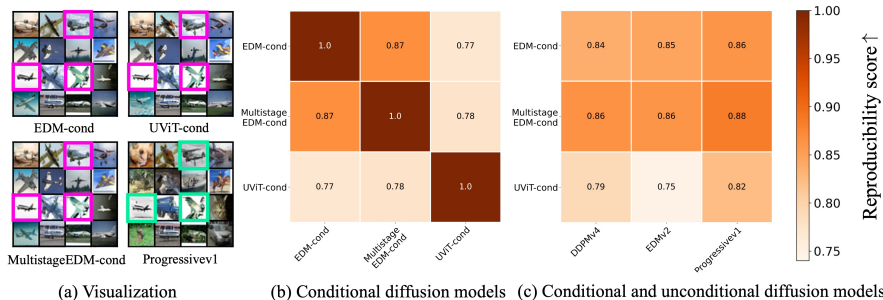
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$RP_{cond} \text{ Score} := \mathbb{P}(\mathcal{M}_{SSCD}(\mathbf{x}_1^c, \mathbf{x}_2^c) > 0.6 \mid c \in \mathcal{C})$ ,  $(\mathbf{x}_1^c, \mathbf{x}_2^c)$  are generated by two conditional models from the same initial noise and conditioned on the class  $c \in \mathcal{C}$

$RP_{between} \text{ Score} := \mathbb{P}(\max_{c \in \mathcal{C}} [\mathcal{M}_{SSCD}(\mathbf{x}_1, \mathbf{x}_2^c)] > 0.6)$ , for an unconditional generation  $\mathbf{x}_1$  and conditional generation  $\mathbf{x}_2^c$  starting from the same noise.

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Model reproducibility of conditional models is evident and linked with unconditional counterparts.

# Intro to diffusion model for inverse problem

- Inverse problem: reconstruct an unknown signal  $\mathbf{u}$  from the measurements  $\mathbf{z}$  of the form  $\mathbf{z} = \mathcal{A}(\mathbf{u}) + \boldsymbol{\eta}$ , where  $\mathcal{A}$  denotes some (given) sensing operator and  $\boldsymbol{\eta}$  is the noise.
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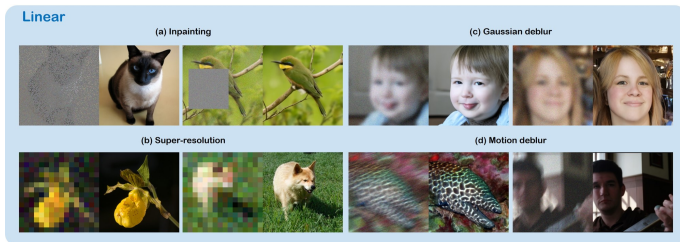
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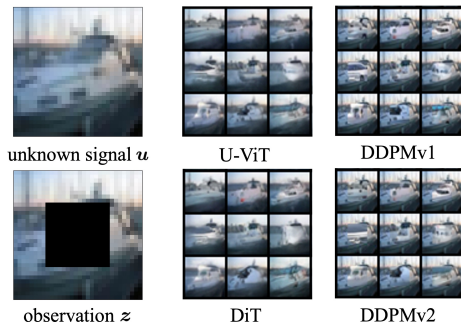
$$\mathbf{x}_t \leftarrow \mathbf{x}_t - \xi_t \nabla_{\mathbf{x}_t} \|\mathbf{u} - \mathcal{A}(\hat{\mathbf{x}}_0)\|_2^2$$

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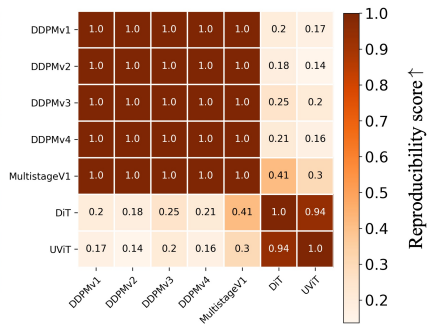
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- Diffusion Posterior Sampling (DPS) [1]



# Reproducibility of diffusion model for inverse problem

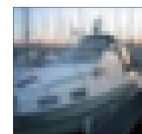
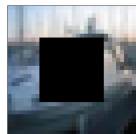


(a) Visualization



(b) Reproducibility Score

# Reproducibility of diffusion model for inverse problem

unknown signal  $u$ observation  $z$ 

U-ViT



DiT

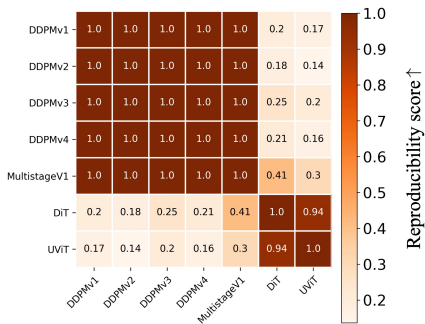


DDPMv1



DDPMv2

(a) Visualization



(b) Reproducibility Score

Model reproducibility largely holds only within the same type of network architectures.

# Intro to diffusion model fine-tuning

- Pre-trained large diffusion model (e.g. stable diffusion), fine-tuning only part of the diffusion model (e.g. attention layer, txt embedding.) and on few-shot images.

# Intro to diffusion model fine-tuning

- Pre-trained large diffusion model (e.g. stable diffusion), fine-tuning only part of the diffusion model (e.g. attention layer, txt embedding.) and on few-shot images.
- Obtain incredible generalizability, e.g. DreamBooth [15].



Input images



in the Acropolis



swimming



sleeping



in a doghouse

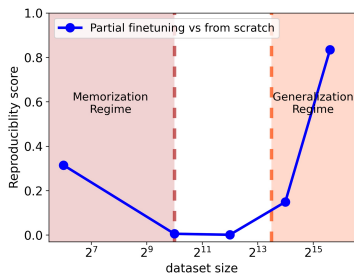


in a bucket

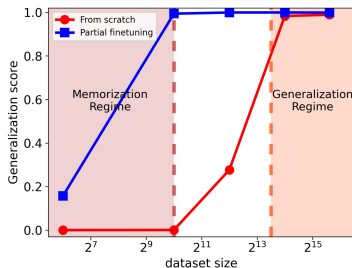


getting a haircut

# Reproducibility of diffusion model fine-tuning



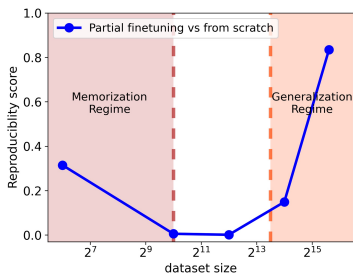
(a) Reproducibility



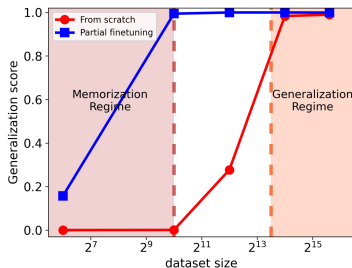
(b) Generalizability

Pretrained on CIFAR-100, fine-tuning on CIFAR-10. Only fine-tuning the attention layer.

# Reproducibility of diffusion model fine-tuning



(a) Reproducibility



(b) Generalizability

Pretrained on CIFAR-100, fine-tuning on CIFAR-10. Only fine-tuning the attention layer.

Partial fine-tuning reduces reproducibility but improves generalizability in “memorization regime”.



# Outline

- 1 Introduction
- 2 Reproducibility for Unconditional Diffusion Models
- 3 Correlation between Reproducibility, Memorizability & Generalizability
- 4 Reproducibility beyond Unconditional Diffusion Models
- 5 Future Directions**

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  - Connection between diffusion models and the Schrödinger bridge [16, 3, 11, 4, 9, 8] (an optimal transport problem).

# Q & A





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