



ICML 2026 Tutorial

Diffusion and Flow Matching

From Memorization to Generalization & Beyond

Quentin Bertrand & Mathurin Massias

<https://memorization-generalization.github.io>

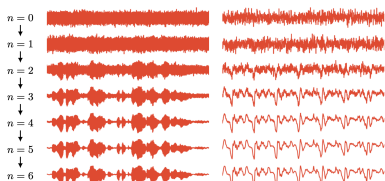
Inria | ENS Lyon | Laboratoire Hubert Curien | Mila Affiliated Member | CIFAR Global Scholar

Diffusion and Flow matching are everywhere

- Diffusion introduced in 2015¹, took off in 2020^{2,3}
- Flow matching introduced in 2023^{4,5,6}
- Current SOTA techniques for generation of images, audio, videos, proteins...



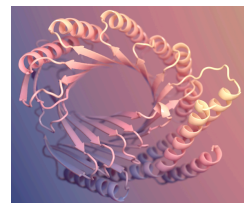
Stable Diffusion



WaveGrad



Sora



RF Diffusion

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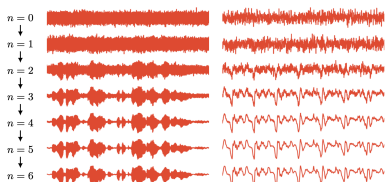
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- And even for text now



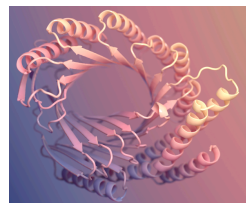
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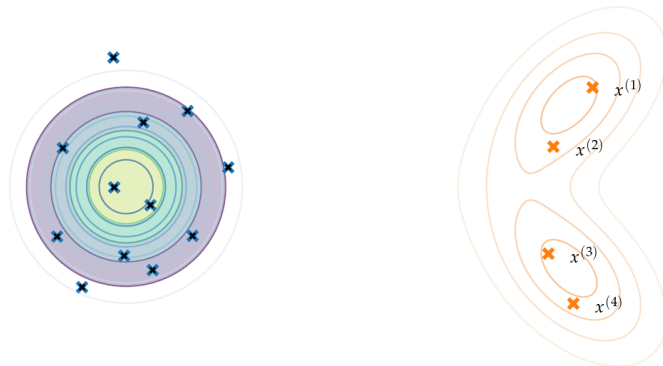
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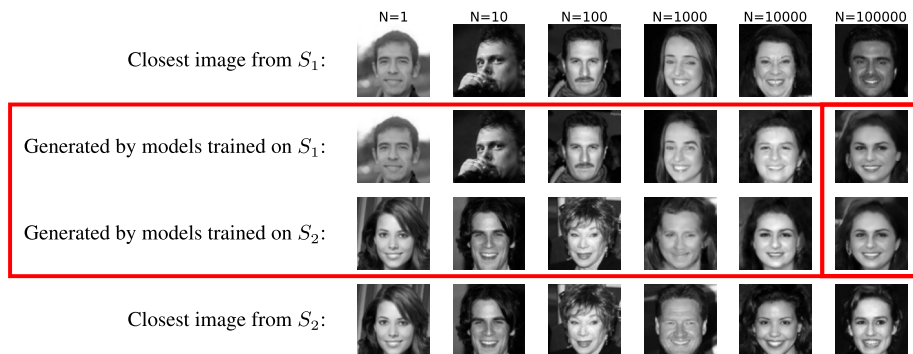
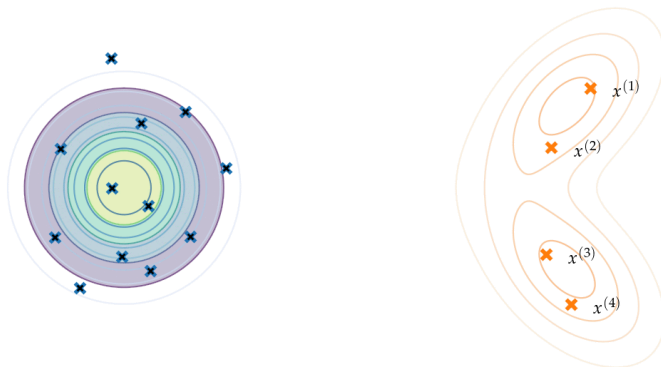
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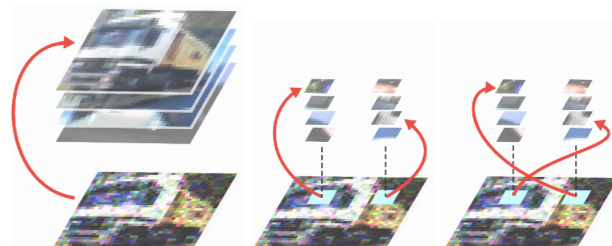
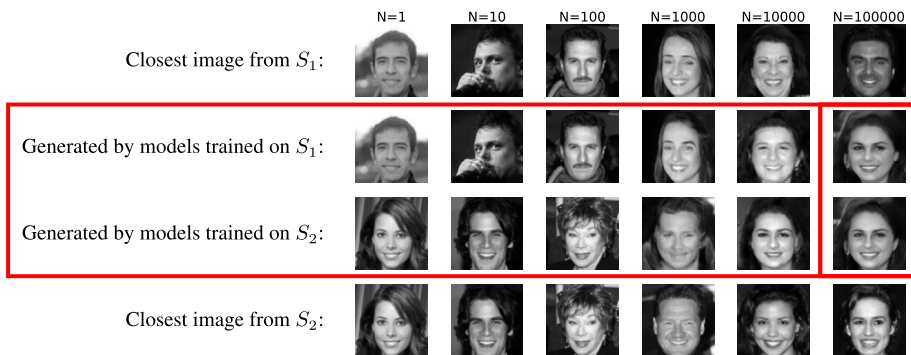
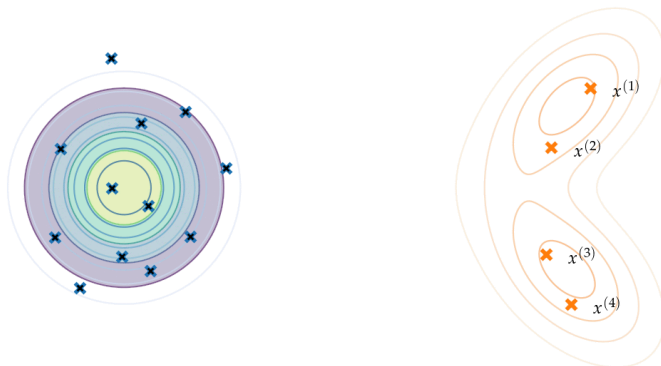
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- Optimal models should only generate training data?⁷
- Models trained on different datasets generate the same images?⁸
- Generated images are patchworks of training images?⁹



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Tutorial goal

When, how, and why do Diffusion & Flow matching create new data?

Plan

- Introduction to Flow matching and Diffusion: why should they memorize? (40 min)
- Discussion #1 (10 min)

Training Set



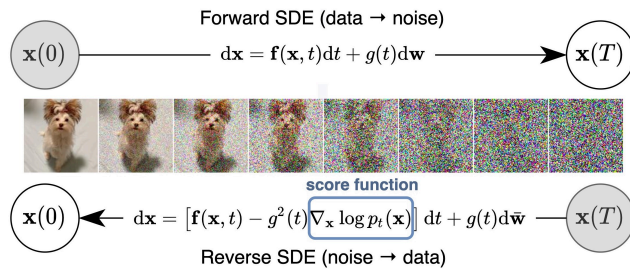
Caption: Living in the light with Ann Graham Lotz

Generated Image

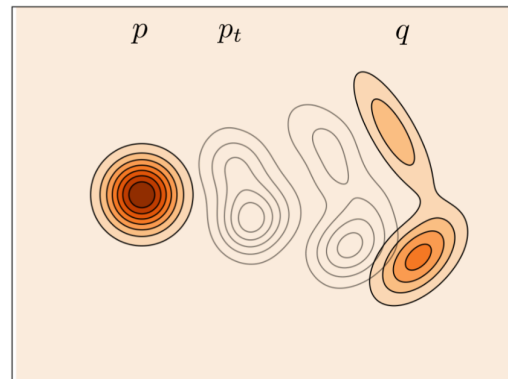


Prompt: Ann Graham Lotz

Extracting Training Data from Diffusion Models Carlini et al. (2023)



<https://yang-song.net/blog/2021/score/>



Flow Matching Guide and Code, Lipman et al. (2025)

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- Discussion #2 (10 min)

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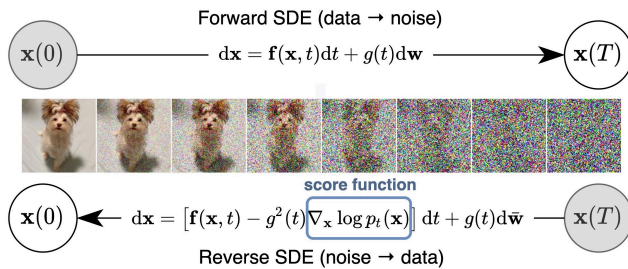
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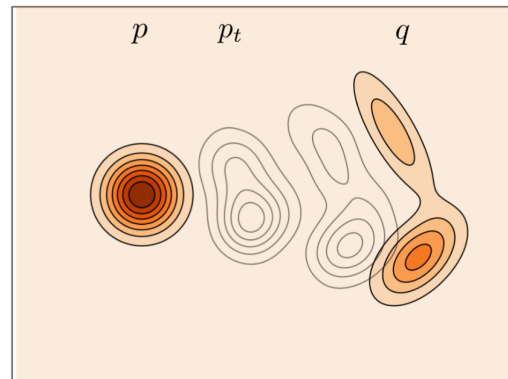


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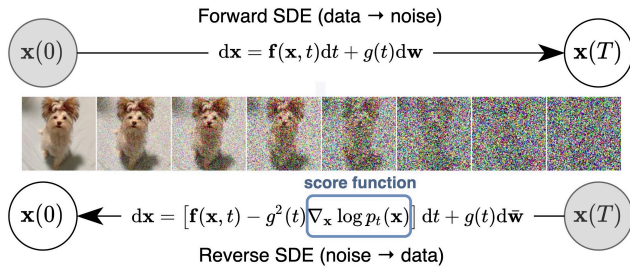
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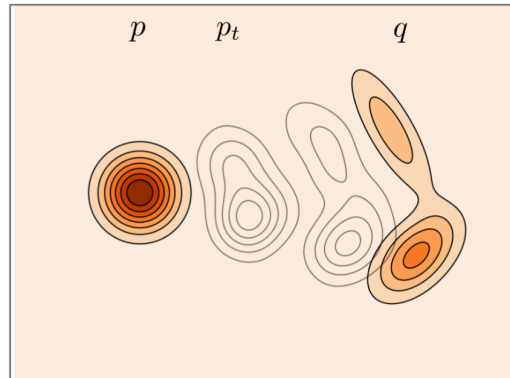
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- Discussion #2 (10 min)
- Beyond generalization (30 min)
- Current open problems (15 min)
- Discussion #3 (15 min)



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Training Set



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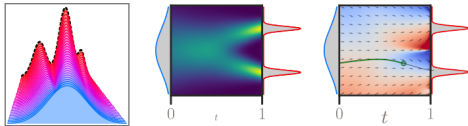
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Who we are

- Researchers at Inria (France)
- Blog post¹⁰ and contributions in memorization^{11,12}

A Visual Dive into Conditional Flow Matching



On the Closed-Form of Flow Matching: Generalization Does Not Arise from Target Stochasticity

Quentin Bertrand¹⁵; Anne Gagneux²; Mathurin Massias³; Rémi Emonet^{14*}

TRAINING FLOW MATCHING: THE ROLE OF WEIGHTING AND PARAMETERIZATION

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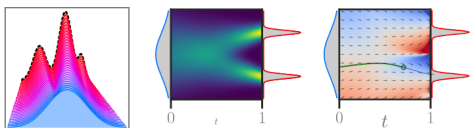
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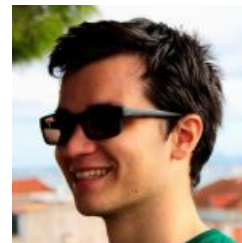
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- Many thanks to Rémi Emonet, Ségolène Martin, Anne Gagneux, Georges Le Bellier and Eloi Tanguy who contributed to the material



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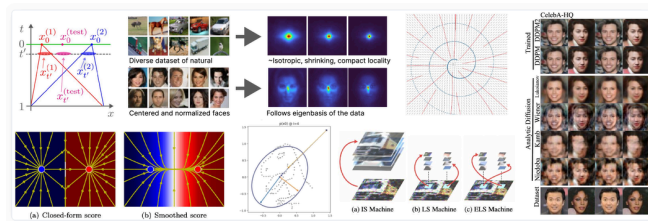
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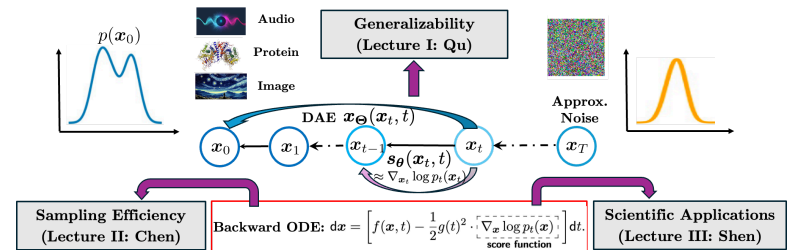
Analytic Understanding of Diffusion Models

A deep dive into the mathematical foundations and analytic perspectives behind modern diffusion-based generative models.



<https://analytic-diffusion.github.io/> CVPR 2026

Harnessing Low Dimensionality in Diffusion Models: From Theory to Practice



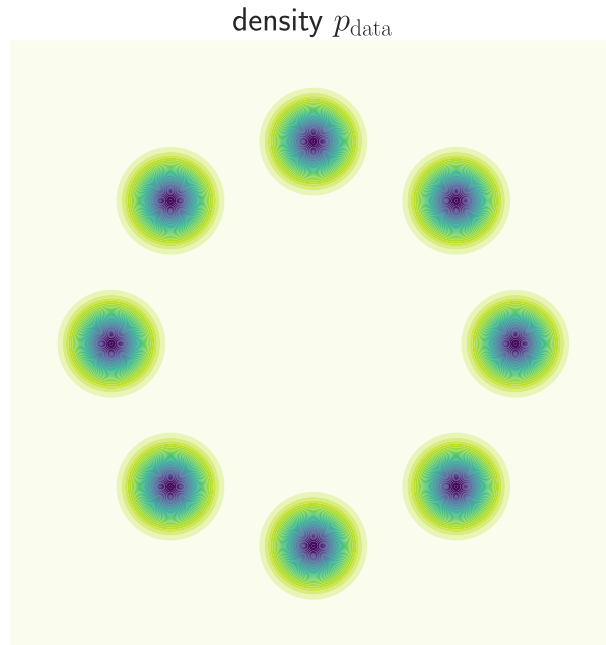
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Introduction to Flow matching and Diffusion

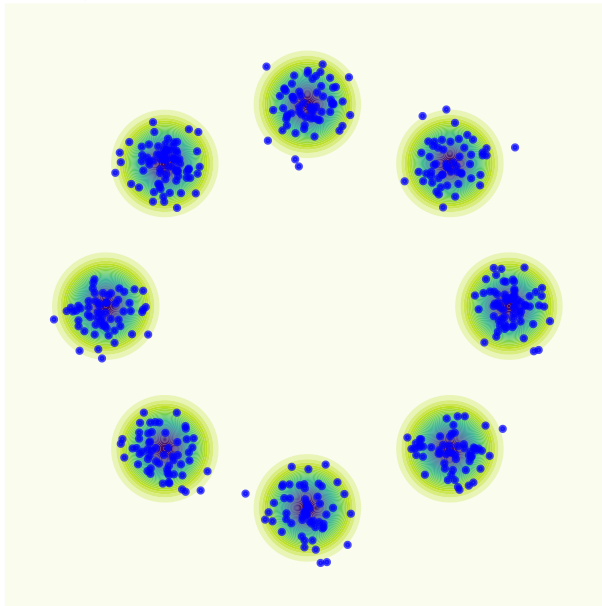
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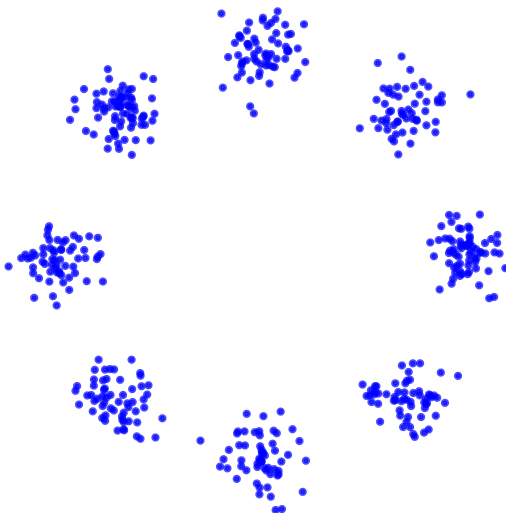
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density p_{data} + samples $x^{(1)}, \dots, x^{(n)} \sim p_{\text{data}}$



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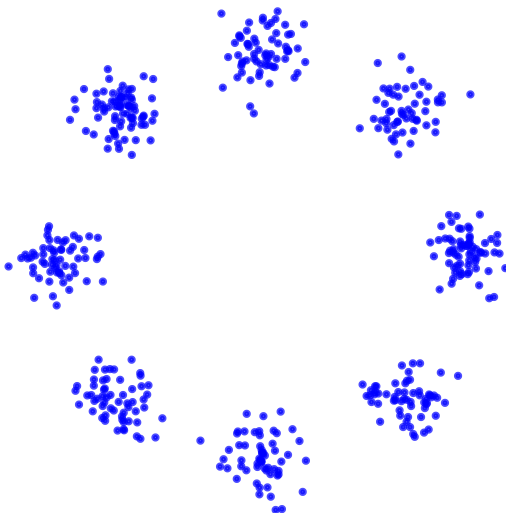


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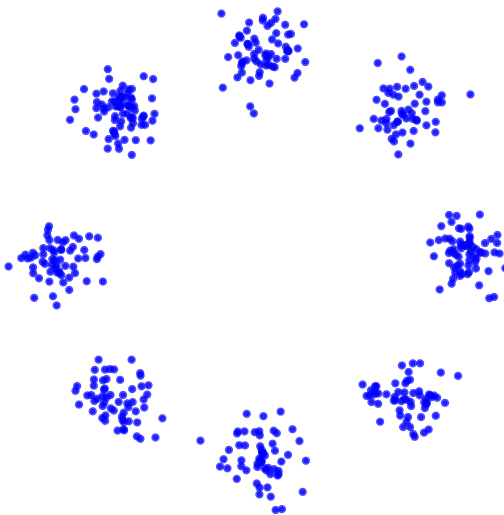


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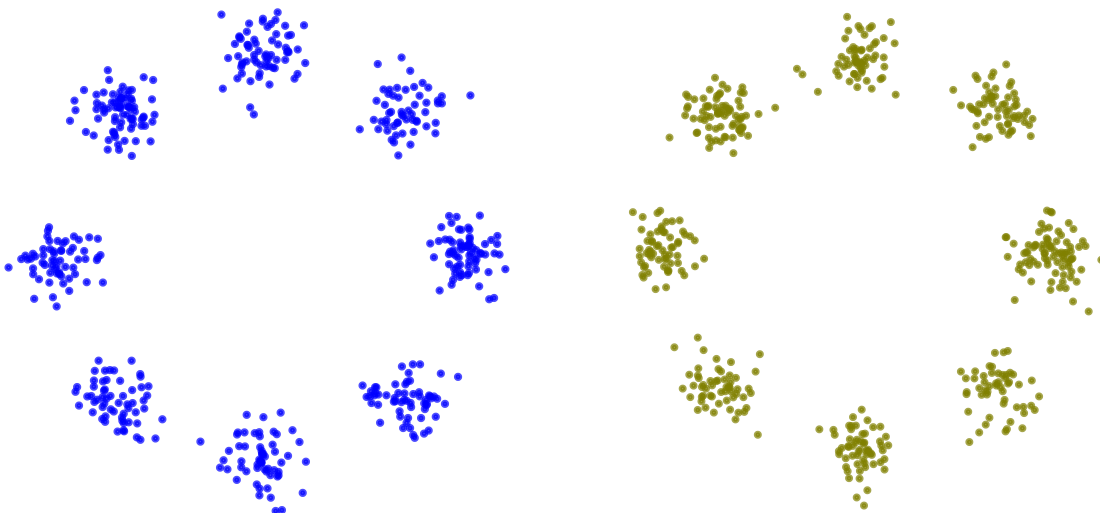
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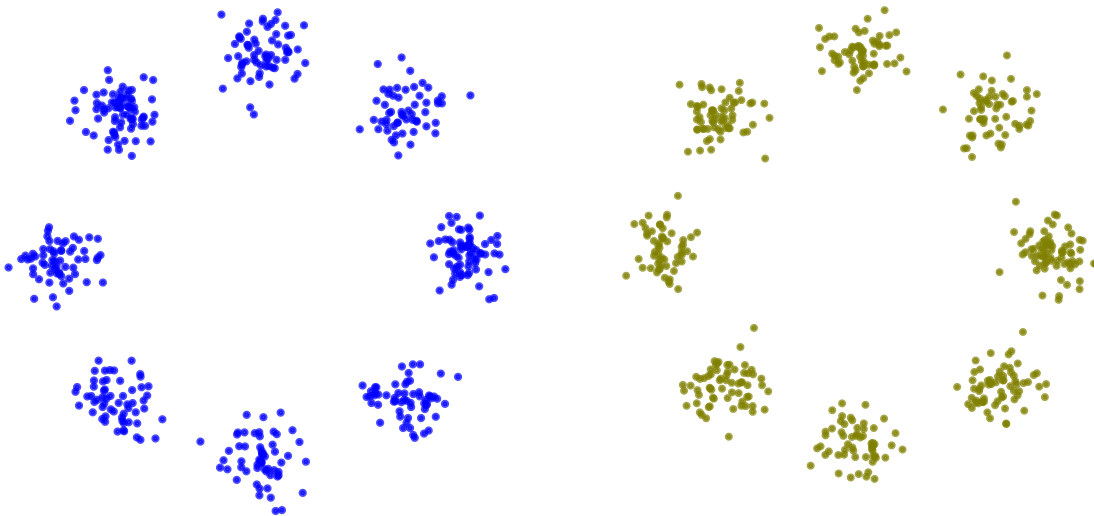
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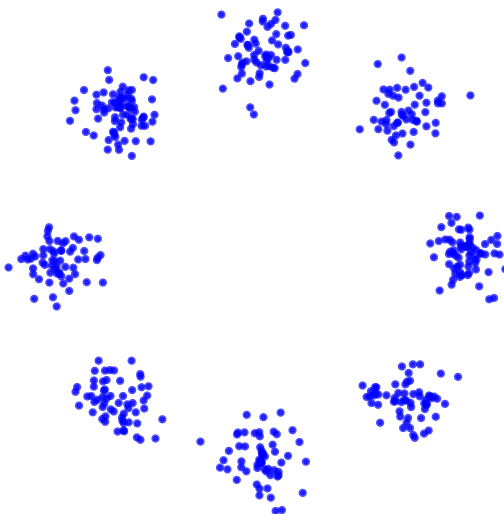
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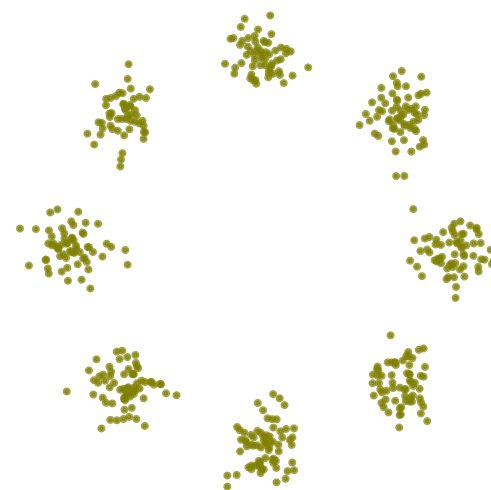
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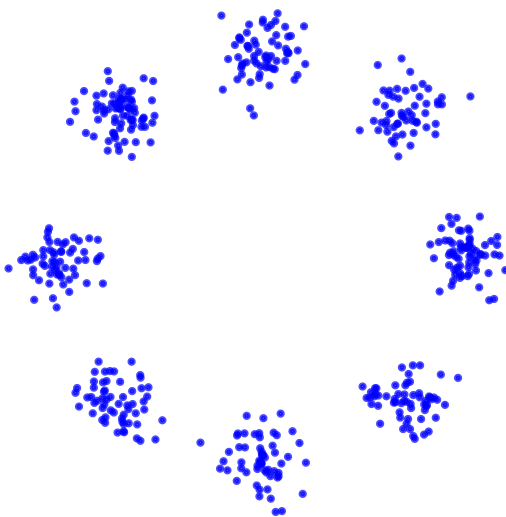
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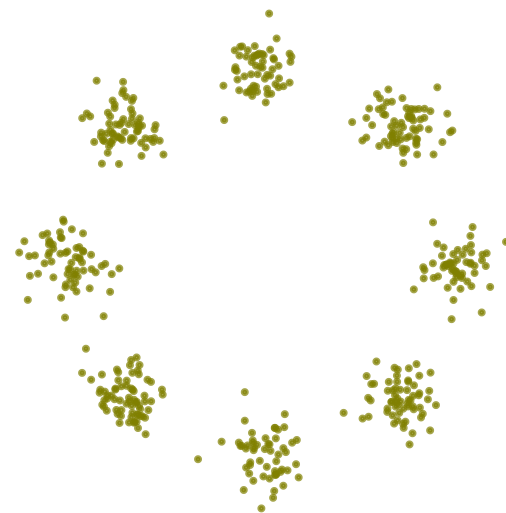
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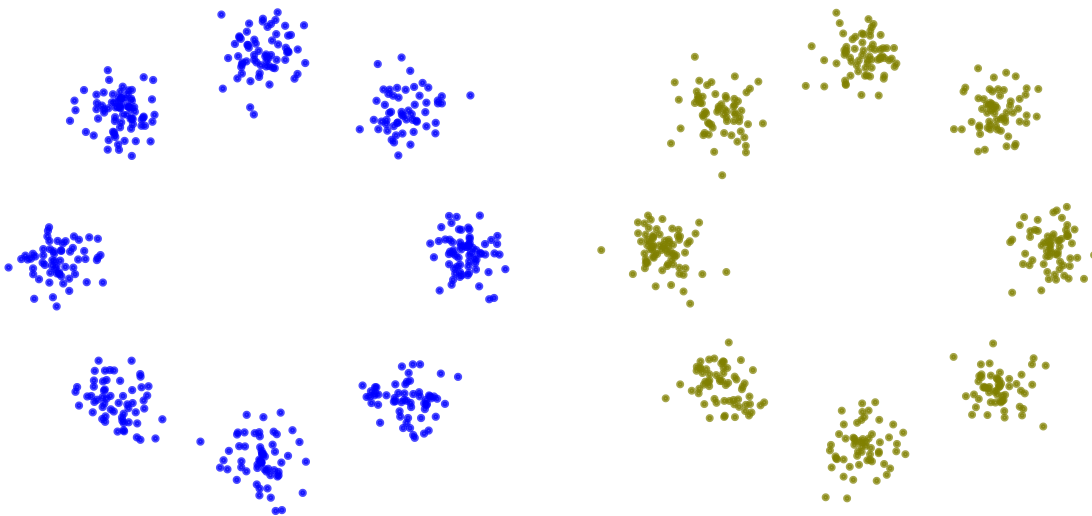
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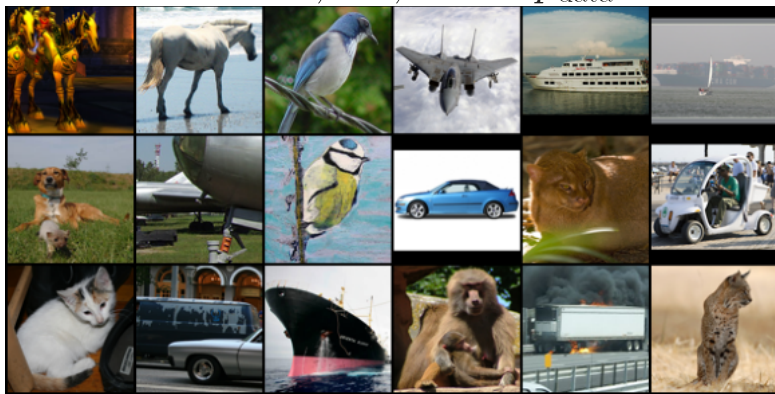
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Generative modeling: an image example

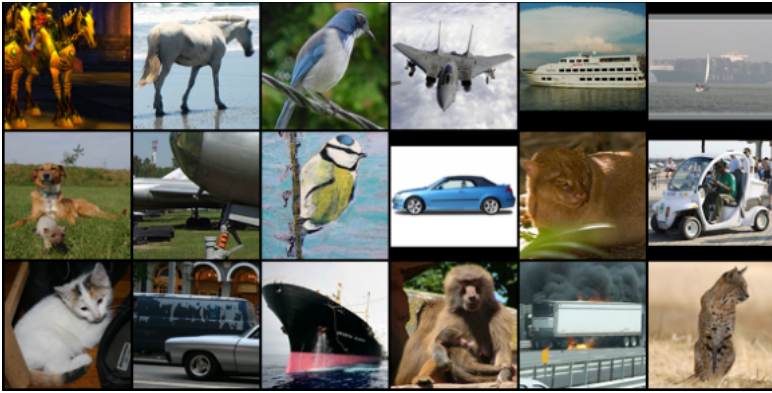
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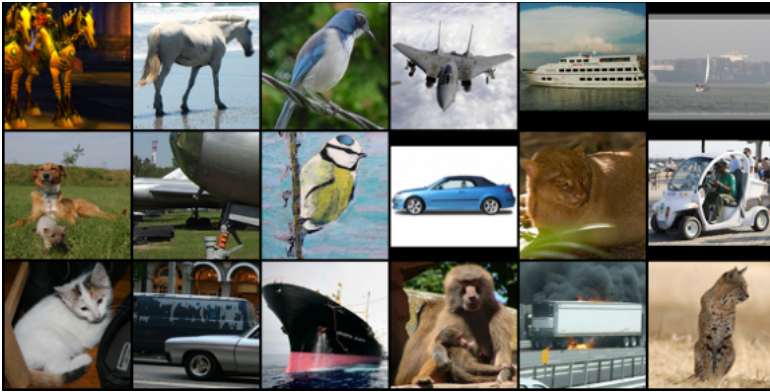


Data:

- Access to samples $x^{(1)}, \dots, x^{(n)} \in \mathbb{R}^d$
- Drawn from $p_{\text{data}} : \underbrace{x^{(1)}, \dots, x^{(n)}}_{\text{known}} \sim \underbrace{p_{\text{data}}}_{\text{unknown}}$
- Could also be audio, texts, proteins, etc

Generative modeling: an image example

data $x^{(1)}, \dots, x^{(n)} \sim p_{\text{data}}$



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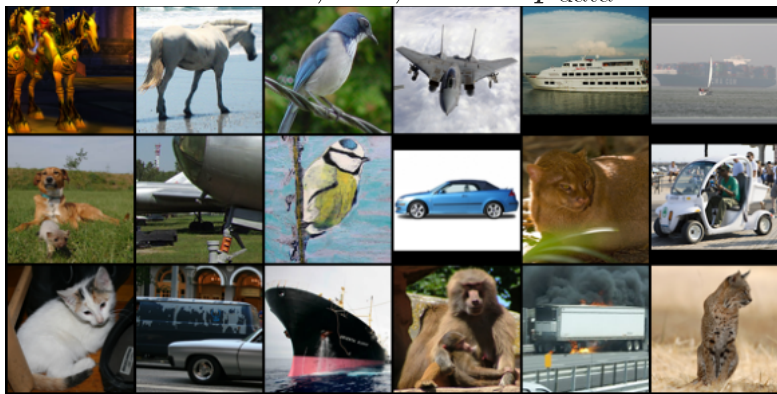
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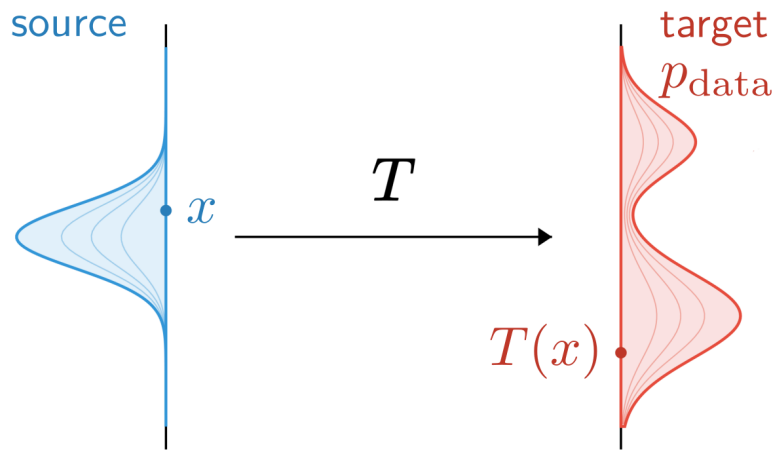
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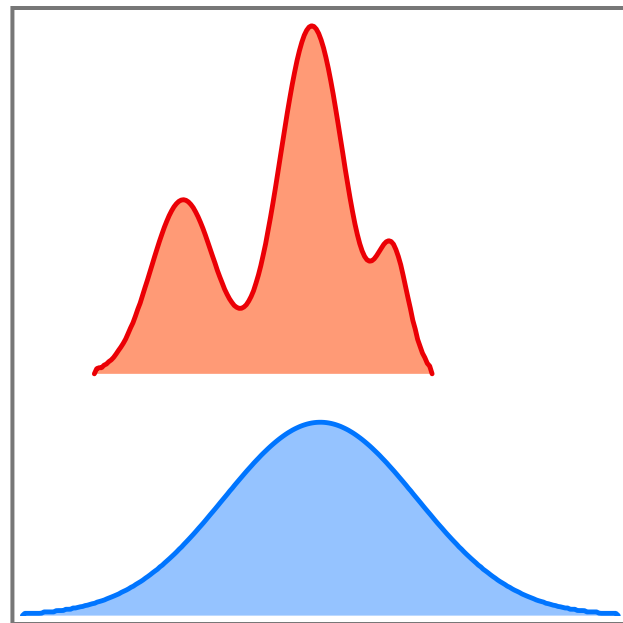
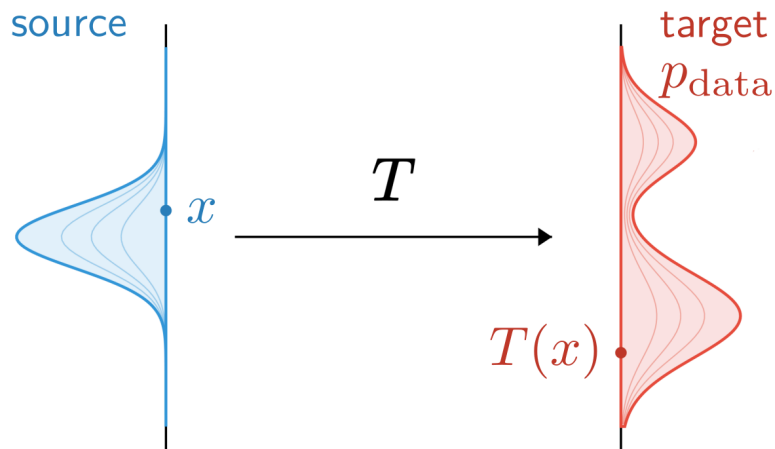
- Learn mapping T sending samples from **source distribution** to samples from **target distribution** p_{data}



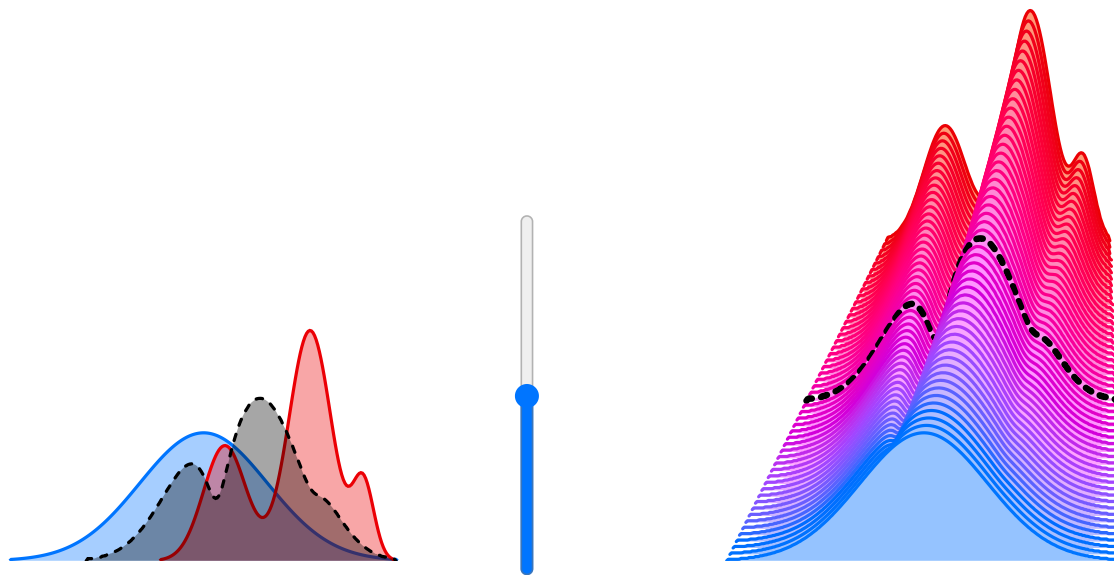
Diffusion and Flow matching: the big picture

Common idea:

- Learn mapping T sending samples from **source distribution** to samples from **target distribution** p_{data}
- Rely on a continuous interpolation between the source and target distributions



Play with paths from to source and target distributions!



NB: Diffusion only supports Gaussian **source distribution**

Flow matching

Flow matching

- Convention: go from time $t = 0$ (source) to time $t = 1$ (target)

Flow matching

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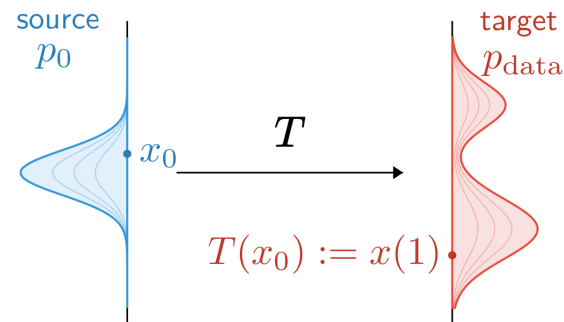
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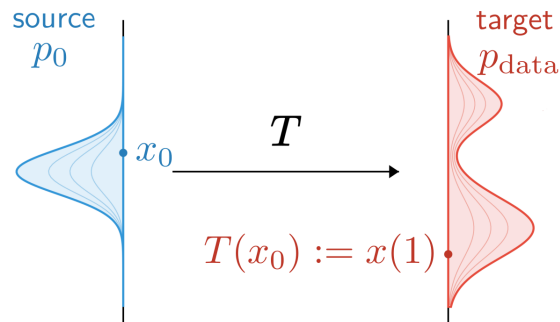


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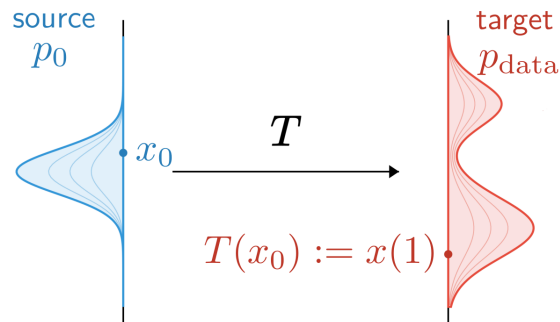
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$x(1)$ is random because x_0 is



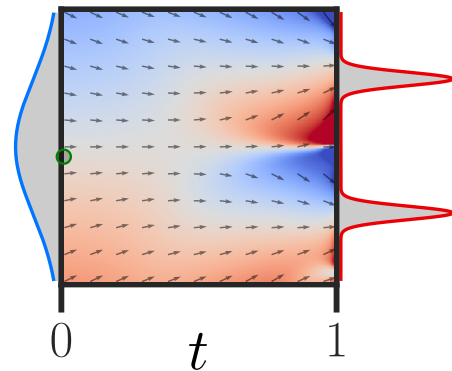
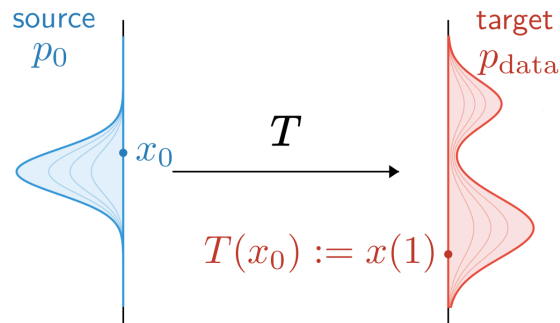
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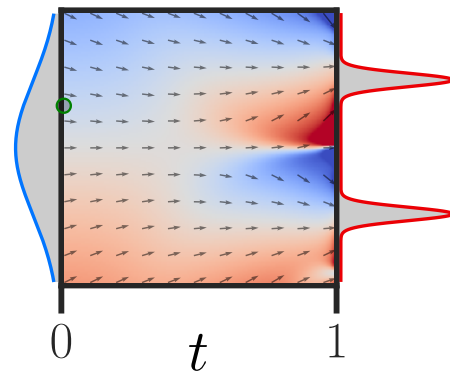
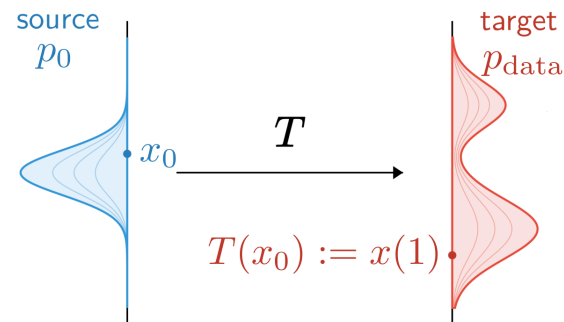
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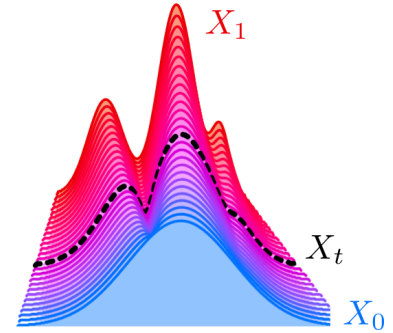


But how to find a *good* velocity $u(x, t)$?

How to find a good velocity?

Setup: define three random variables

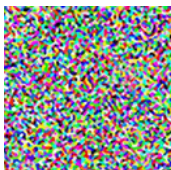
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- $X_t := (1 - t)X_0 + tX_1$ interpolation: noised image



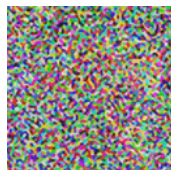
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$X_{t=0}$



$X_{t=0.25}$



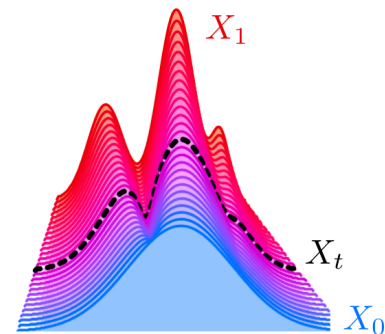
$X_{t=0.5}$



$X_{t=0.75}$



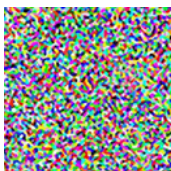
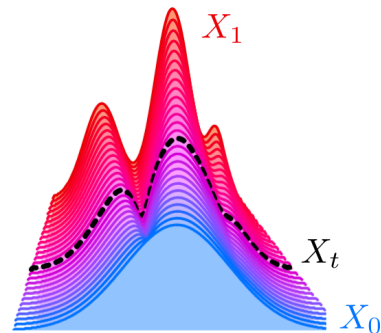
$X_{t=1}$



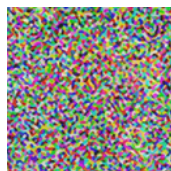
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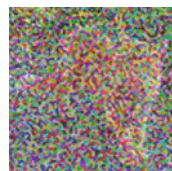
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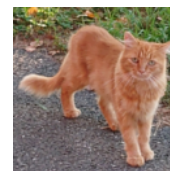
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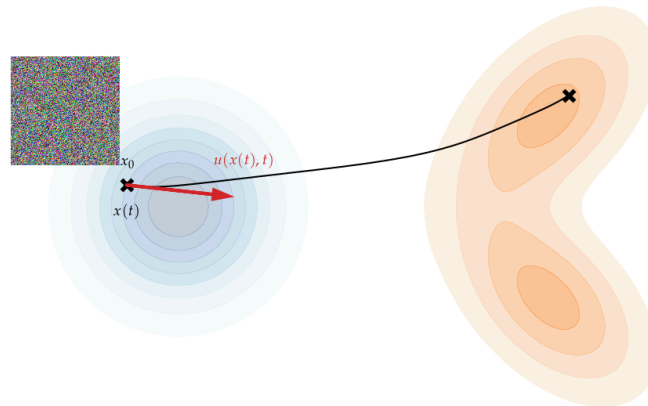
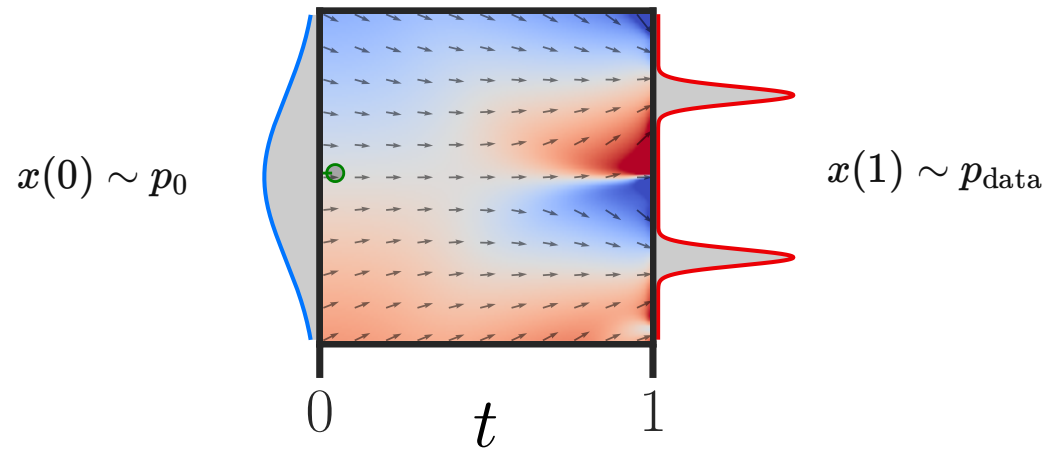
The FM magic^{5,13,14}: $u(x, t) := \mathbb{E}[X_1 - X_0 | X_t = x]$ is a *good* velocity:

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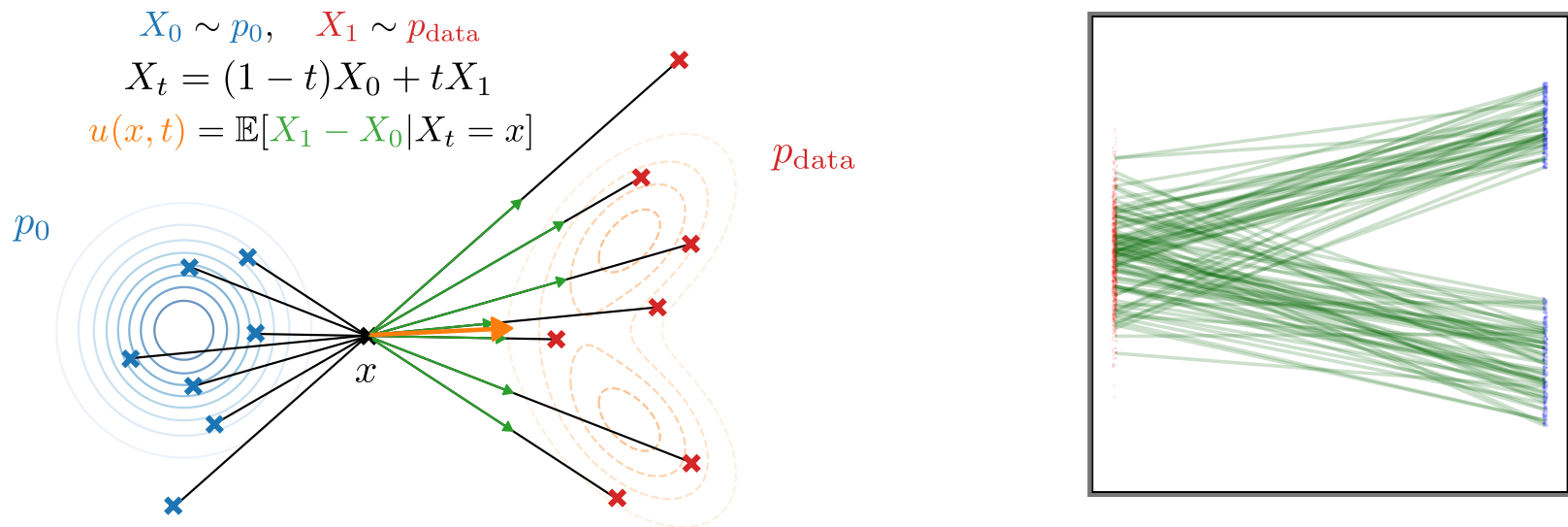
⁵ M. Albergo et al., *Building Normalizing Flows with Stochastic Interpolants*, In: ICLR, 2023.

¹³ Y. Lipman et al., *Flow Matching for Generative Modeling*, In: ICLR, 2023.

¹⁴ X. Liu et al., *Flow Straight and Fast: Learning to Generate and Transfer Data with Rectified Flow*, In: ICLR, 2023.



Why the conditional expectation is "good"



More in our blog post: **A Visual dive into conditional flow matching**¹⁰: <https://dl.heeere.com/cfm/>

¹⁰ A. Gagneux et al., A Visual Dive into Conditional Flow Matching, In: ICLR Blogposts, 2025.

How to train a Flow matching model?

$$\min_{u_\theta} \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim p_{\text{data}} \\ t \sim \text{unif}([0,1])}} \left\| u_\theta(\underbrace{(1-t)x_0 + tx_1}_{=x_t}, t) - (x_1 - x_0) \right\|^2$$

Train practically with:

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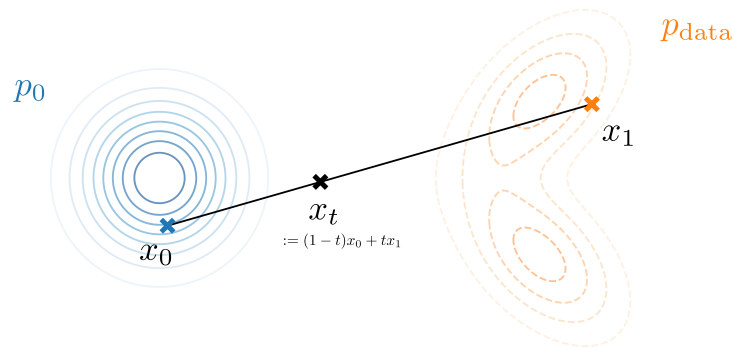
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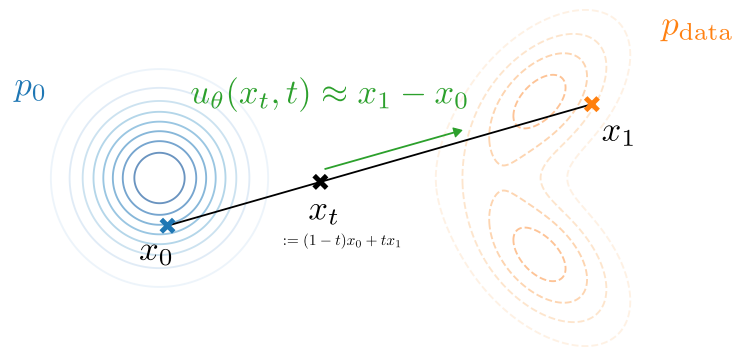
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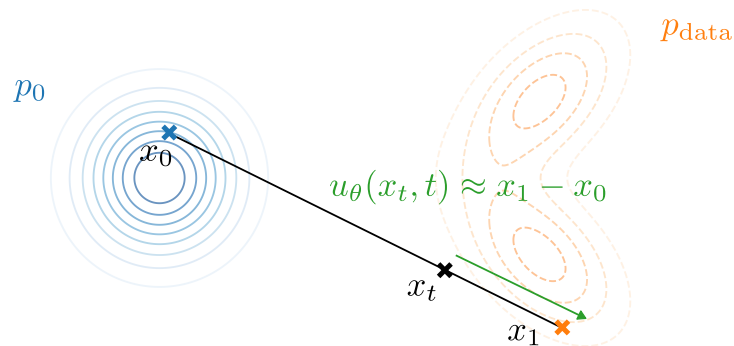
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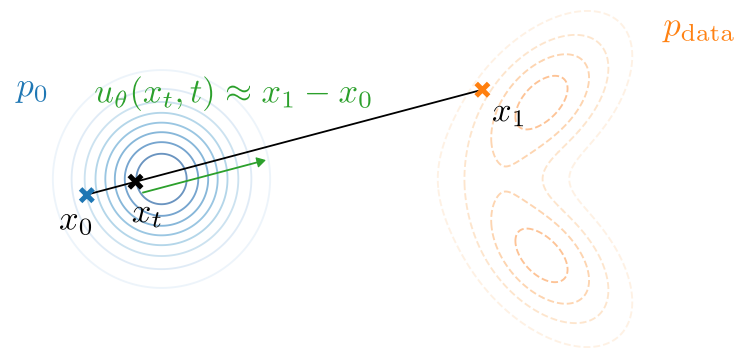
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$$\text{the minimizer is } u(x, t) = \mathbb{E}[X_1 - X_0 | X_t = x]$$

Bonus: much more to FM^{15,16}

- Source distribution p_0 can be arbitrary
- Time sampling need not be uniform
- In training, x_0 and x_1 need not be sampled independently^{17,18}
- X_t need not equal $(1 - t)X_0 + tX_1$
- In practice guidance/conditioning is used a lot

¹⁵ E. Pierret et al., **Flow Matching for Applied Mathematicians**, In: , 2026.

¹⁶ Y. Lipman et al., **Flow matching guide and code**, In: arXiv preprint arXiv:2412.06264, 2024.

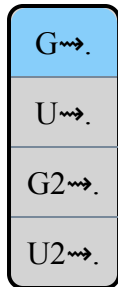
¹⁷ A. Pooladian et al., **Multisample flow matching: Straightening flows with minibatch couplings**, In: ICML, 2023.

¹⁸ A. Tong et al., **Improving and generalizing flow-based generative models with minibatch optimal transport**, In: TMLR, 2023.

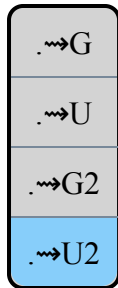
Much more to FM: playground!



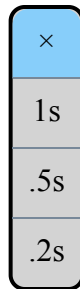
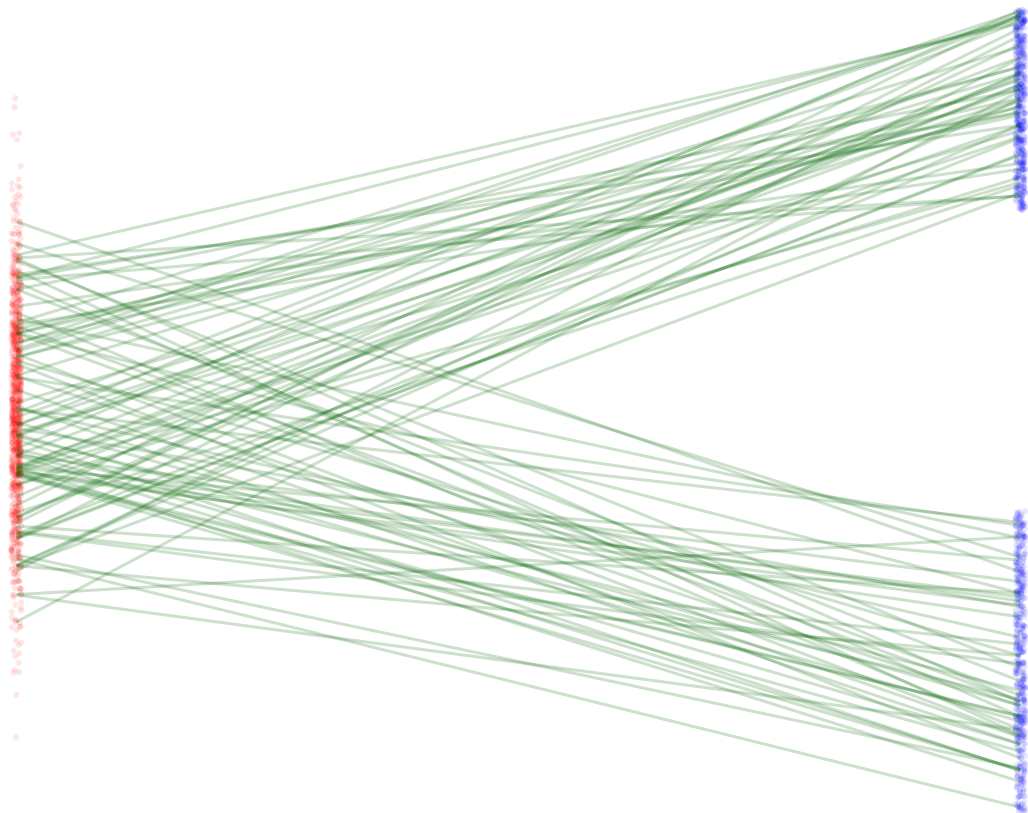
p_0



p_1



z



Diffusion

Only thing to know: it's equivalent to Flow matching¹⁹!

Diffusion Meets Flow Matching: Two Sides of the Same Coin



<https://diffusionflow.github.io/>

¹⁹ R. Gao et al., *Diffusion Meets Flow Matching: Two Sides of the Same Coin*, In: ICLR Blogposts, 2025.

Diffusion

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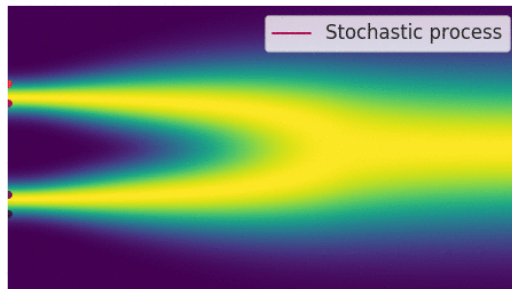
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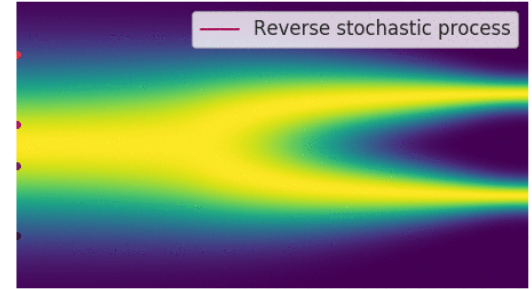
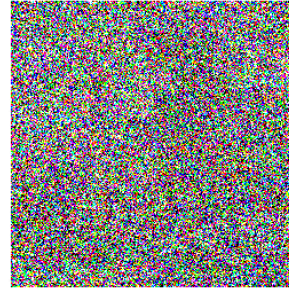
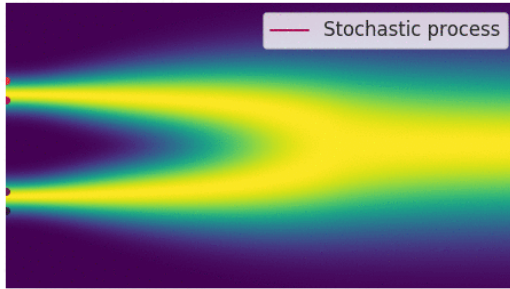
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<https://yang-song.net/blog/2021/score/>

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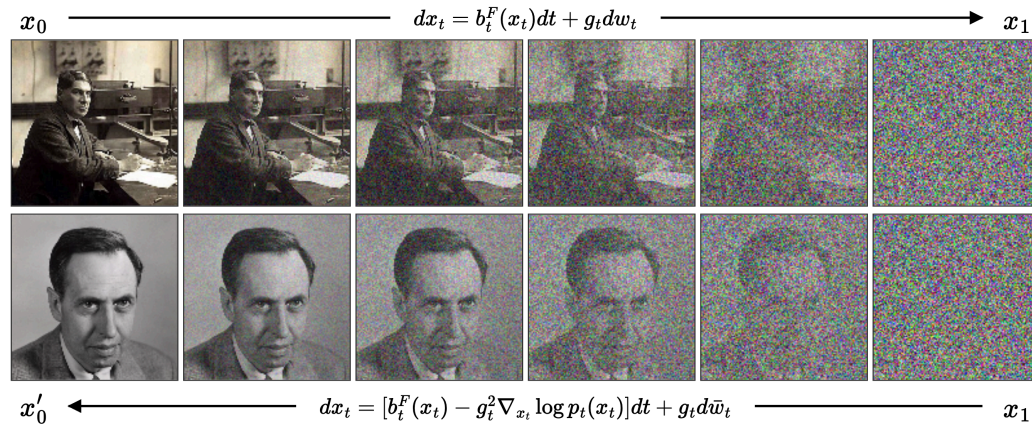
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- One learns to reverse the noising process



<https://yang-song.net/blog/2021/score/>

Learning Diffusion

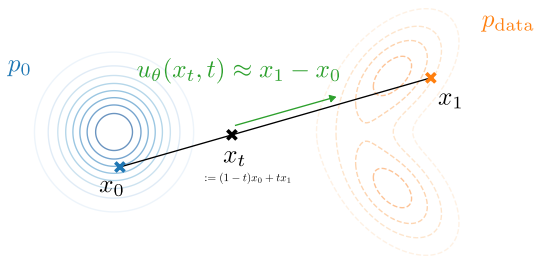
- Instead of learning the velocity u , diffusion learns to reverse the corruption process
- It is driven by a Stochastic Differential Equation (SDE)



- A key quantity to learn is the *score* $\nabla \log p_t(x_t) \in \mathbb{R}^d$ (p_t is the density of X_t)
It is theoretically equivalent to learn to predict the score, the added noise or the original image from the corrupted image x_t
- Training procedure is similar to Flow matching: sample clean image, noise it, learn to denoise it

Memorization in Diffusion & Flow Matching

A small caveat in training



Flow matching training:

$$x_0 \sim p_0 = \mathcal{N}(0, \text{Id}_d)$$

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Flow matching code

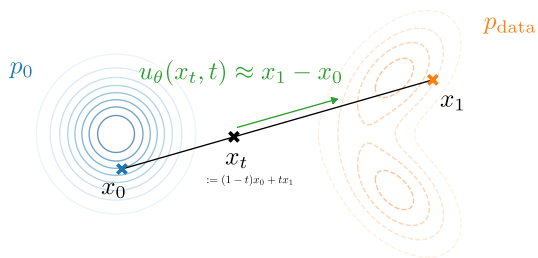
Flow Matching

Yaron Lipman¹, Marton Havas
Ricky T. Q. Chen¹, David Lopez
¹FAIR at Meta, ²MIT CSAIL

```
24 # training
25 flow = Flow()
26 optimizer = torch.optim.Adam(flow.parameters(), 1e-2)
27 loss_fn = nn.MSELoss()
28
29 for _ in range(10000):
30     x_1 = Tensor(make_moons(256, noise=0.05)[0])
31     x_0 = torch.randn_like(x_1)
32     t = torch.rand(len(x_1), 1)
33     x_t = (1 - t) * x_0 + t * x_1
34     dx_t = x_1 - x_0
35     optimizer.zero_grad()
36     loss_fn(flow(x_t, t), dx_t).backward()
37     optimizer.step()
38
```

No si
ODE

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SGD step on θ with loss $\|u_\theta(x_t, t) - (x_1 - x_0)\|^2$

Flow matching code

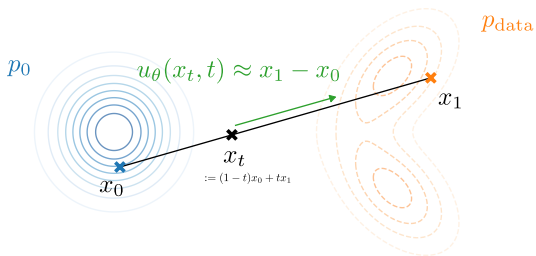
Flow Matching

Yaron Lipman¹, Marton Havas
Ricky T. Q. Chen¹, David Lopez
¹FAIR at Meta, ²MIT CSAIL

```
24 # training
25 flow = Flow()
26 optimizer = torch.optim.Adam(flow.parameters(), 1e-2)
27 loss_fn = nn.MSELoss()
28
29 for _ in range(10000):
30     x_1 = Tensor(make_moons(256, noise=0.05)[0])
31     x_0 = torch.randn_like(x_1)
32     t = torch.rand(len(x_1), 1)
33     x_t = (1 - t) * x_0 + t * x_1
34     dx_t = x_1 - x_0
35     optimizer.zero_grad()
36     loss_fn(flow(x_t, t), dx_t).backward()
37     optimizer.step()
38
```

No si
ODE

A small caveat in training



Flow matching training:

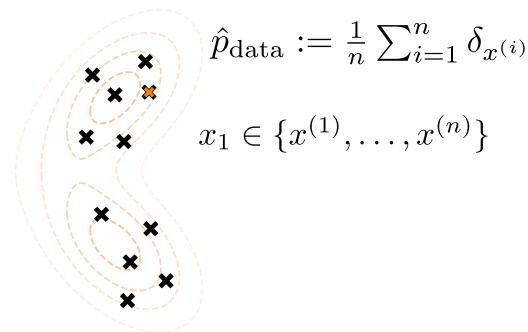
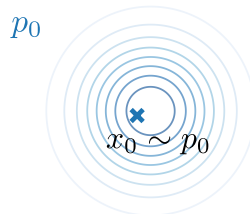
$$x_0 \sim p_0 = \mathcal{N}(0, \text{Id}_d)$$

$$x_1 \sim p_{\text{data}}$$

$$t \sim \text{Uniform}([0, 1])$$

$$x_t = (1 - t)x_0 + tx_1$$

SGD step on θ with loss $\|u_\theta(x_t, t) - (x_1 - x_0)\|^2$



only usable loss: $\mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \text{unif}([0,1])}} \|u_\theta((1 - t)x_0 + tx_1, t) - (x_1 - x_0)\|^2$

Expectation vs reality

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Proposition: when p_{data} is replaced by $\hat{p}_{\text{data}} := \frac{1}{n} \sum_{i=1}^n \delta_{x^{(i)}}$, the FM loss minimizer has a closed-form:

$$\hat{u}^*(x, t) := \sum_{i=1}^n \lambda_i(x, t) \frac{x^{(i)} - x}{1-t}$$

with $\lambda_i(x, t) = \frac{\exp(-\frac{1}{2(1-t)^2} \|x - tx^{(i)}\|^2)}{\sum_{i'=1}^n \exp(-\frac{1}{2(1-t)^2} \|x - tx^{(i')}\|^2)}$

$\lambda(x, t) = \text{softmax}((- \frac{1}{2(1-t)^2} \|x - tx^{(i')}\|^2)_{i'=1, \dots, n}) \in \mathbb{R}^n$

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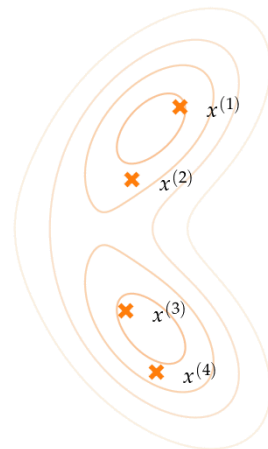
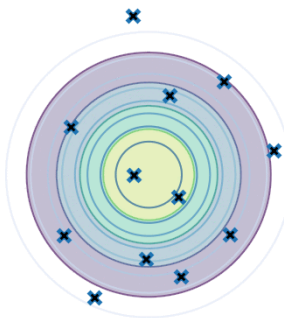
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it only generates training points!



What about diffusion?

- Training diffusion is a particular instance of Flow matching parametrization
- The ideal diffusion score $s^*(x, t) = \nabla \log p_t(x)$ is related to the ideal velocity by $s(x, t) = \frac{tu^*(x, t) - x}{1-t}$
- Closed-form minimizer for velocity \implies closed-form minimizer for score! (which also blows up)

Diffusion suffers from the same curse!

Wrap-up of Part I

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- Flow matching & Diffusion: powerful generative models
- Simple training algorithms
- Closed-form for the ideal score/velocity
- Closed-form can only generate training samples
- Properly trained Flow matching and diffusion should only generate training data (like all unregularized generative models)
- So why do they generate new samples?



ICML 2026 Tutorial

Diffusion and Flow Matching

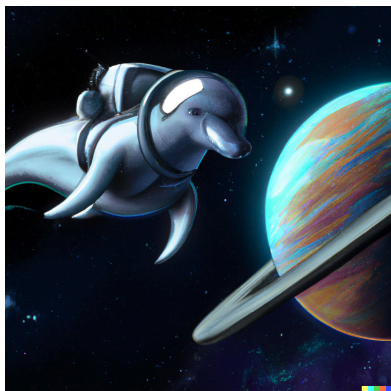
Part II: From Memorization to Generalization

Quentin Bertrand & Mathurin Massias

<https://memorization-generalization.github.io>

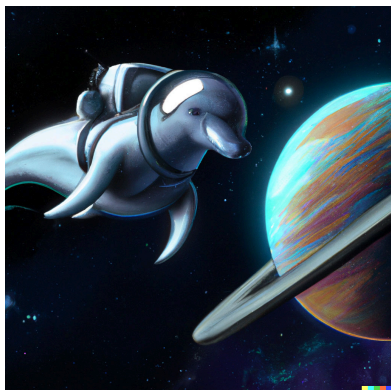
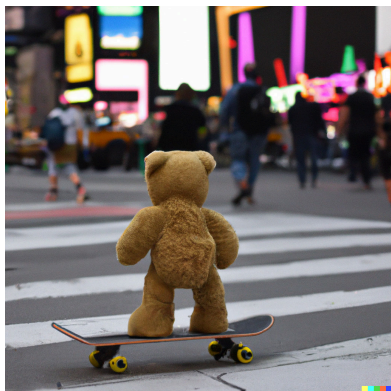
Inria | ENS Lyon | Laboratoire Hubert Curien | Mila Affiliated Member | CIFAR Global Scholar

Generative models: high dimensional density estimation



DALL-E, Ramesh et al.

Generative models: high dimensional density estimation



Diffusion & Flow matching models sample from **high dimensional densities**

DALL-E, Ramesh et al.

An unavoidable curse?

- Data in dimension d
 - e.g. moderate size images $d = 256 \times 256 \times 3$
- Estimation of the joint density $p(x_1, \dots, x_d)$
- Number of samples needed to estimate a density for data in dimension d ?
 - Standard machine learning theory: exponential in d

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- Number of samples needed to estimate a density for data in dimension d ?
 - Standard machine learning theory: exponential in d

In theory: density estimation in such high dimension should fail!

From memorization to generalization

Memorization and closed-form minimizers
observed since 2023^{2,3}

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$n = 1$
closest training
image in S_n^1

A small square image showing a close-up of a man's face, which is the closest training image in the set S_n^1 for n=1.


generated by
model trained on S_n^1

A small square image showing a close-up of a man's face, generated by a model trained on the set S_n^1.

generated by
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A small square image showing a close-up of a man's face, generated by a model trained on the set S_n^2.

closest training
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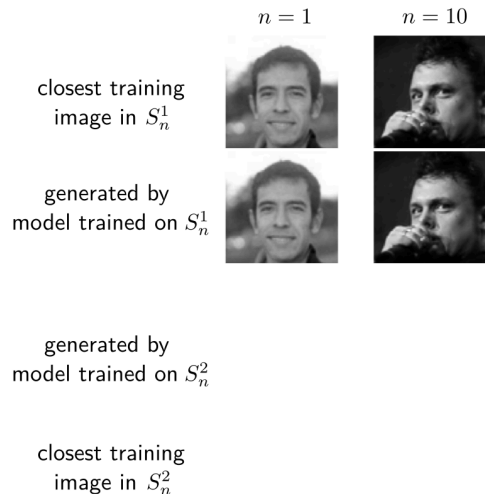
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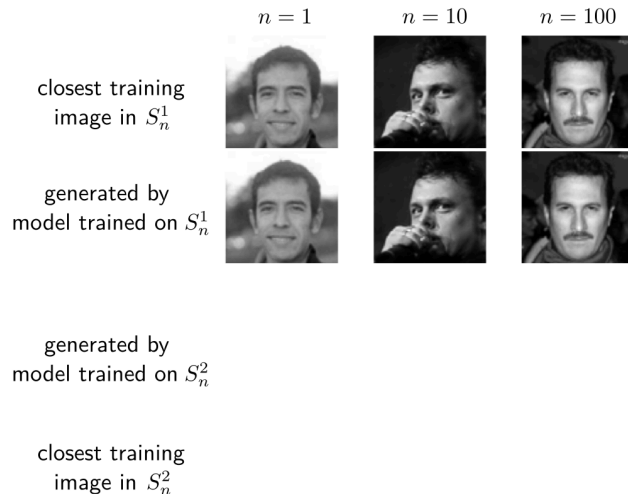
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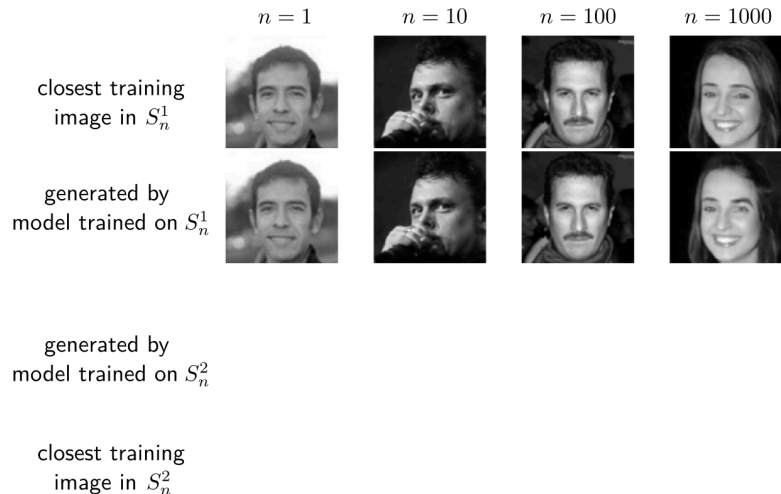
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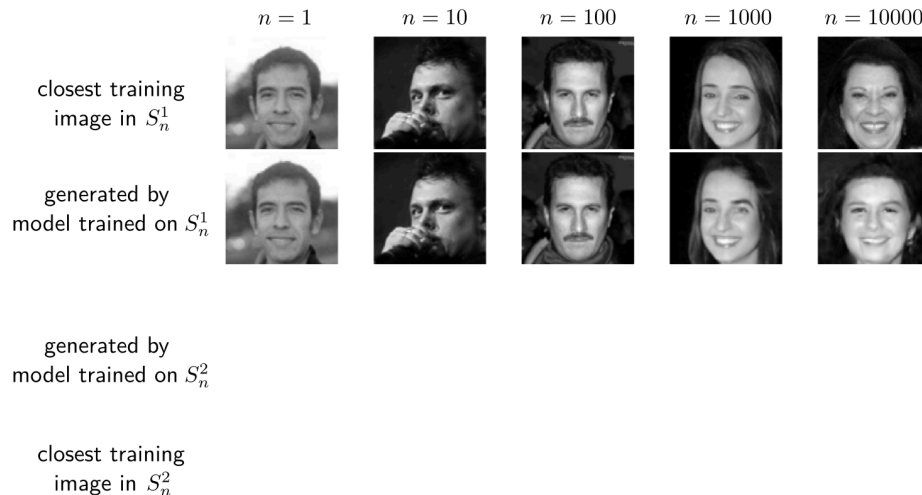
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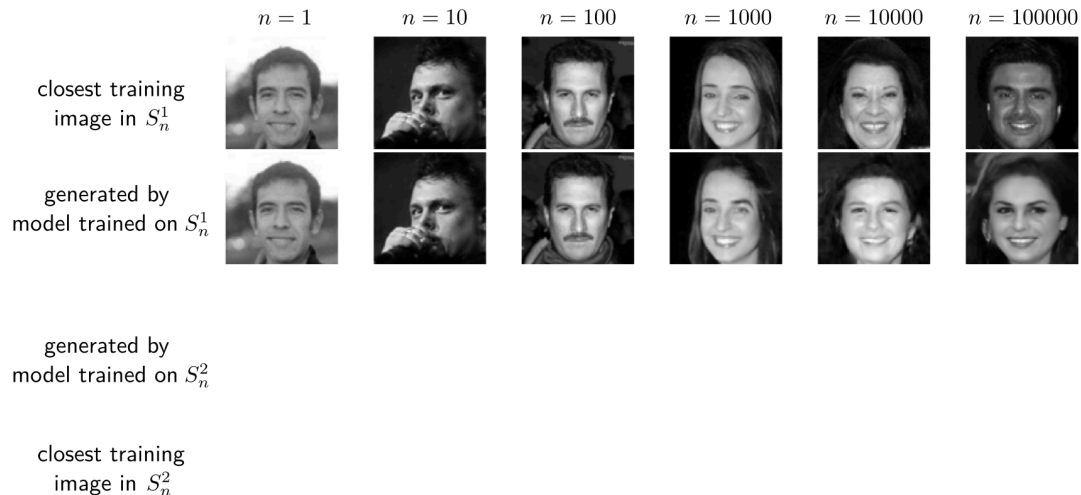
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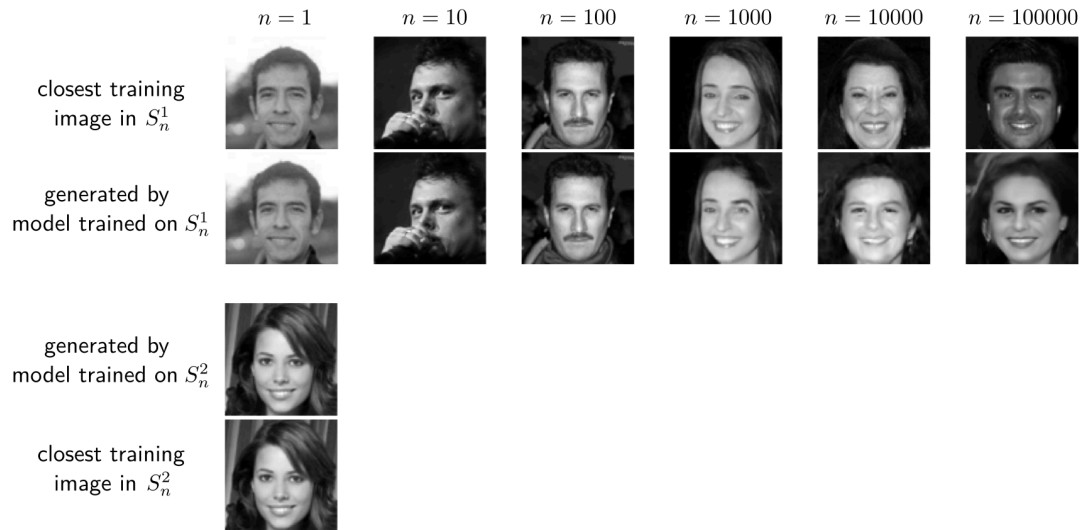
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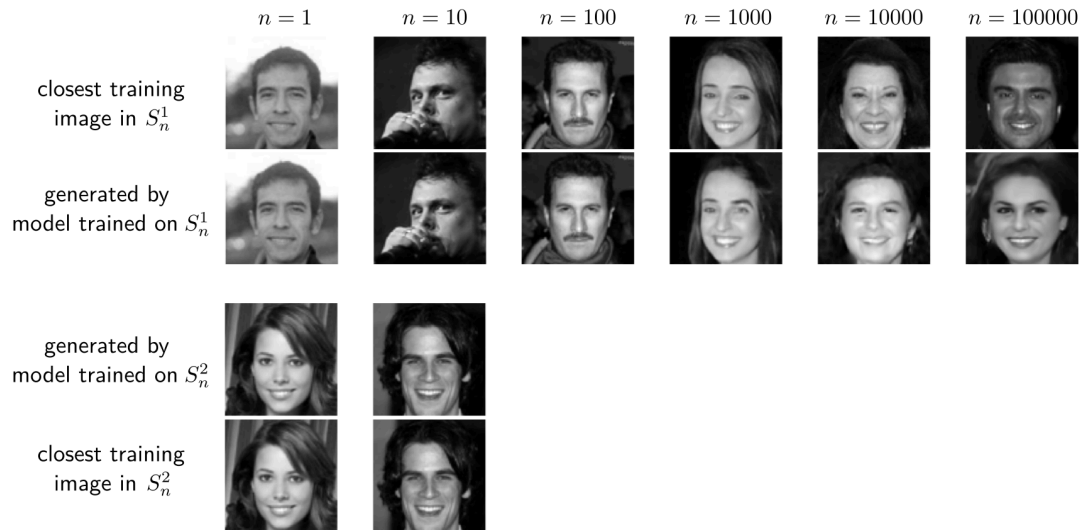
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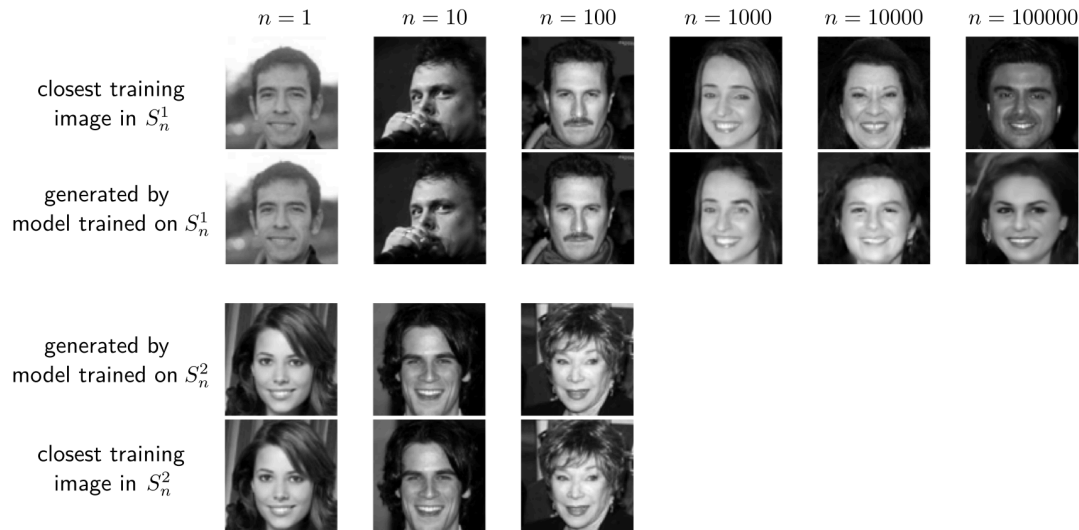
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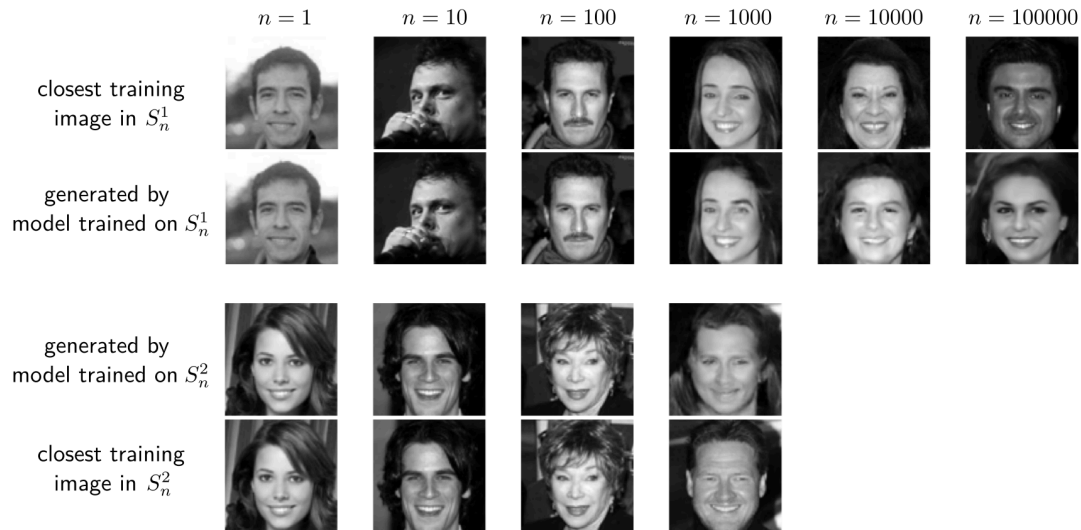
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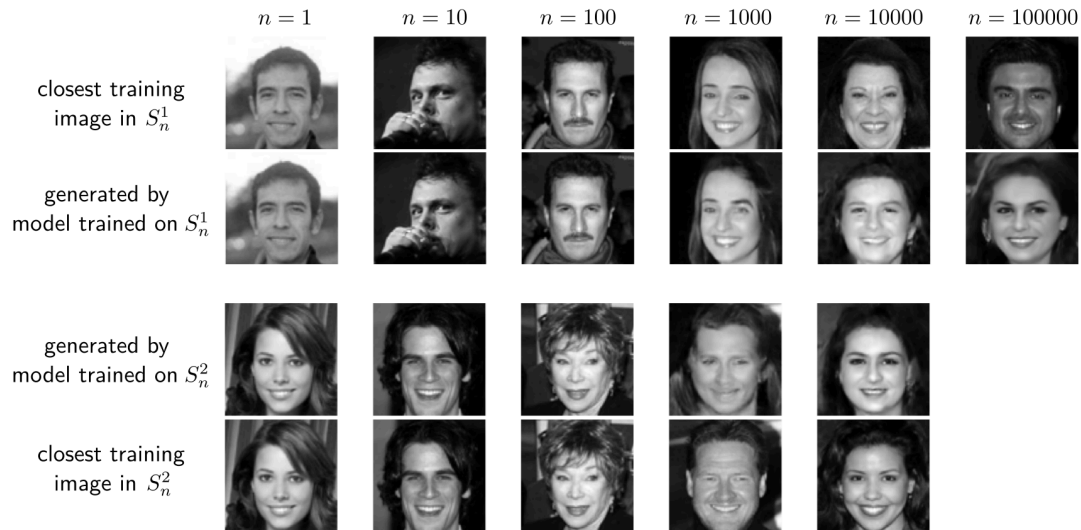
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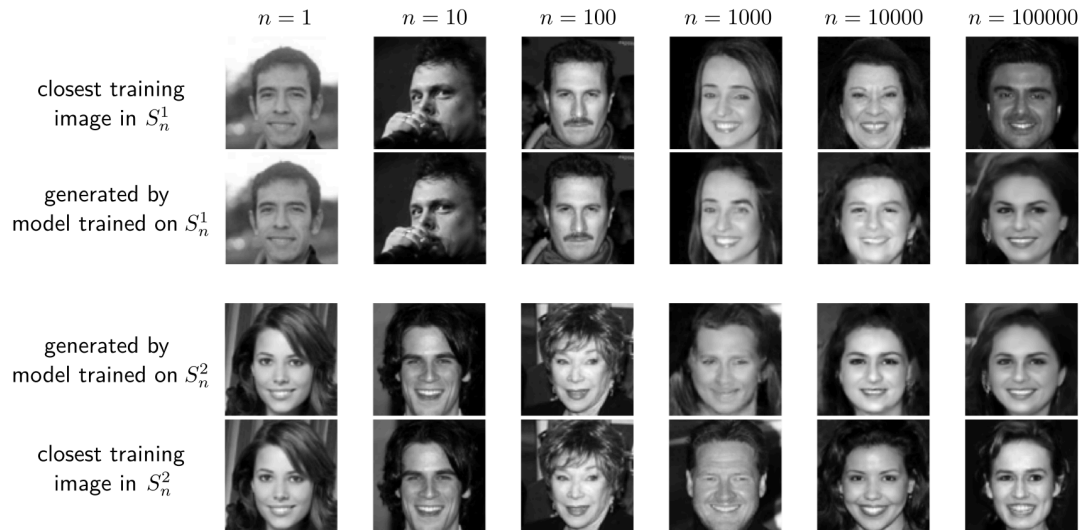
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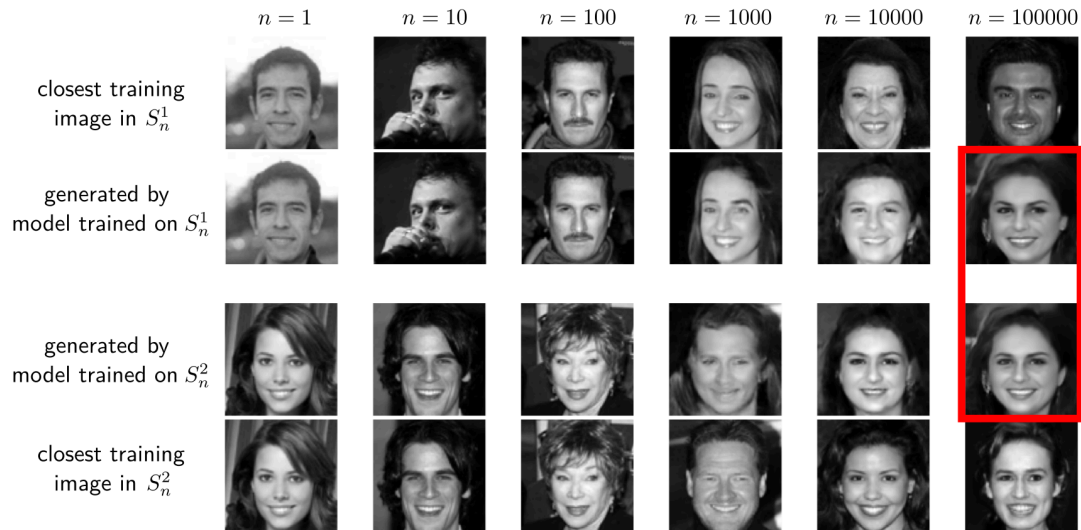
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From memorization to generalization

Memorization and closed-form minimizers
observed since 2023^{2,3}

Seminal experiment in 2024⁴:

- Split the training set
 - 2 **disjoints** sets S_n^1 and S_n^2
 - of size n
- For training set sample size n
 - Train a model on set S_n^1
 - Train a model on set S_n^2
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- In theory:
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How to resolve this incompatibility?

Additional mystery: models generate the same data!



Memorization and generalization in Flow matching and Diffusion

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- Commonly accepted definition: generating samples too similar to training data

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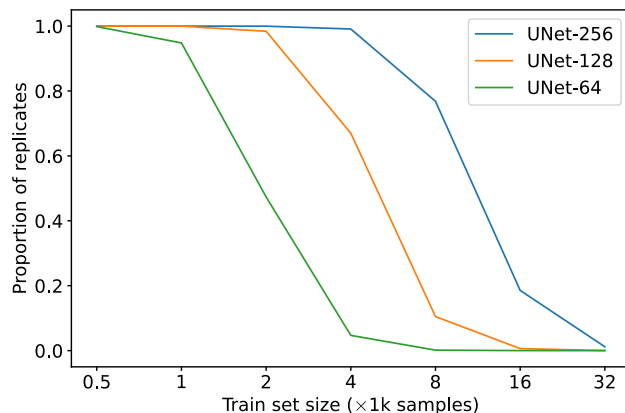
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- Relatively easy to quantify: a generated sample is *memorized* if "its distance to the nearest training sample is smaller than $1/3$ of that to the second nearest training sample"⁵

the distance used and factor $1/3$ can vary

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the distance used and factor $1/3$ can vary
- Memorization ratio: generate many samples and measure proportions of memorized generated samples



Yoon et al. (2023)

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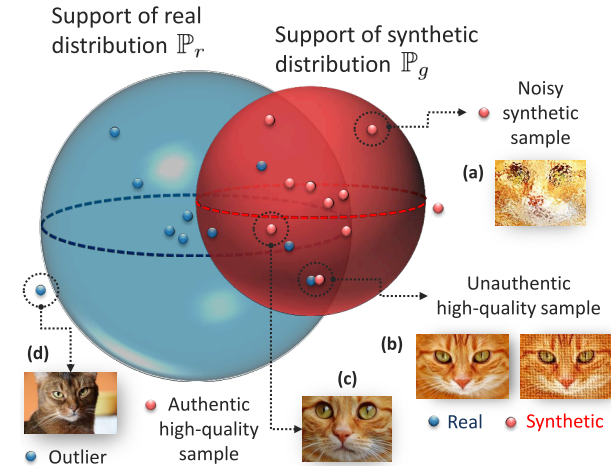
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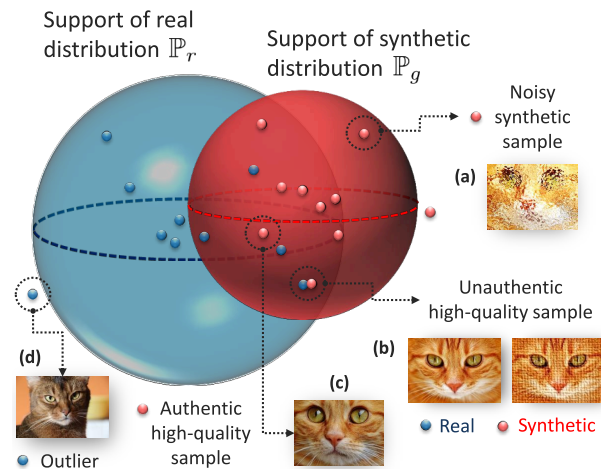


Alaa et al. (2022)

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many complements/alternatives^{9,10,11} to FID that we cannot cover...



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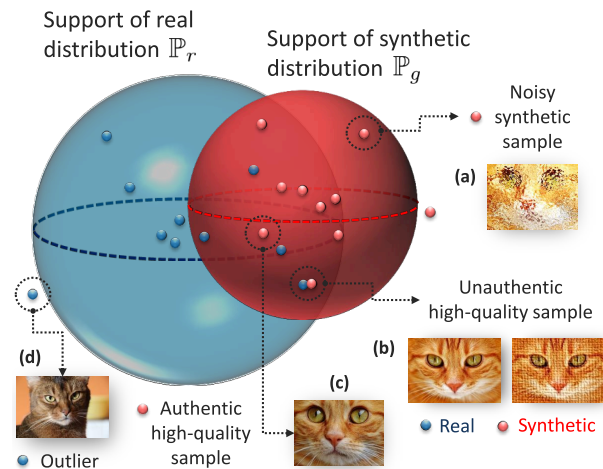
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- Memorization and generalization are often treated as a dichotomy^{5,8}

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Abstract

In this work, we study the training of diffusion probabilistic models through a series of hypotheses and carefully designed experiments. We call our key finding the memorization-generalization dichotomy, and it asserts that generalization and memorization are mutually exclusive phenomena.

Diffusion Probabilistic Models Generalize when They Fail to Memorize

TaeHo Yoon¹ Joo Young Choi¹ Shyun Kwon² Ernest K. Ryu^{1,2}

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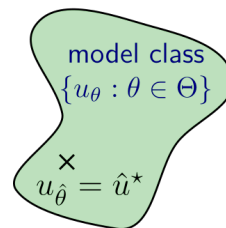
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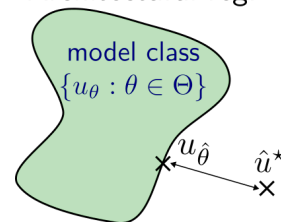
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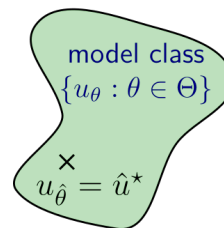
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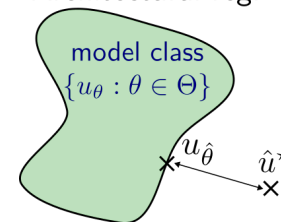
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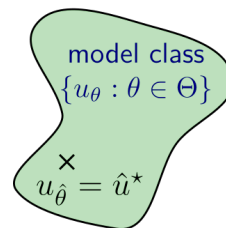
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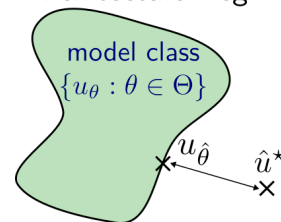
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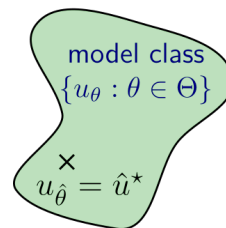
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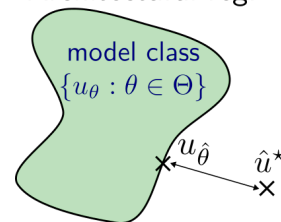
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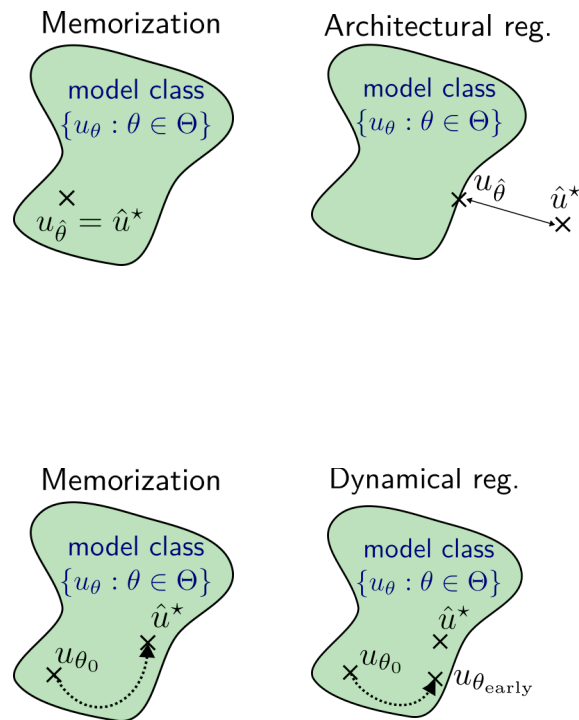
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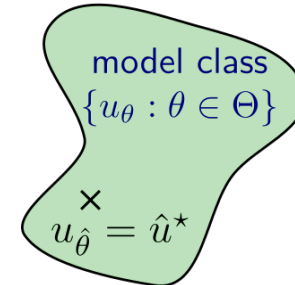
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Dynamical and architectural regularization

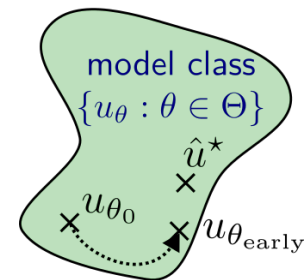
Inductive bias and optimization

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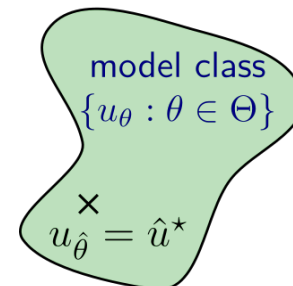


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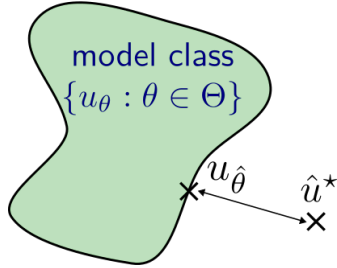


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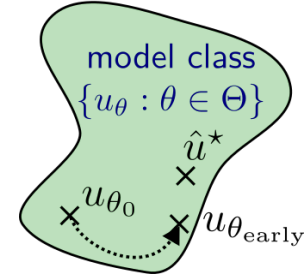


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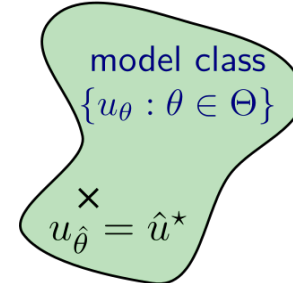
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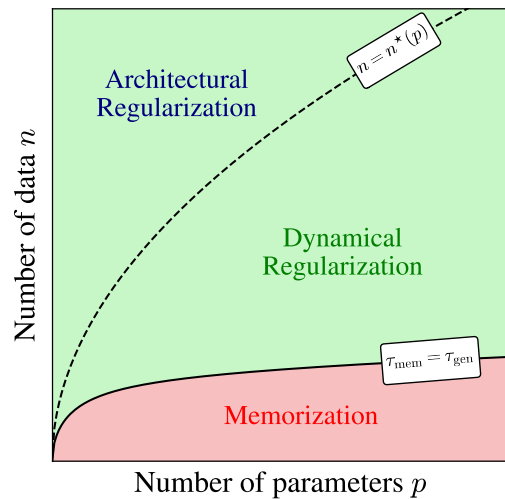
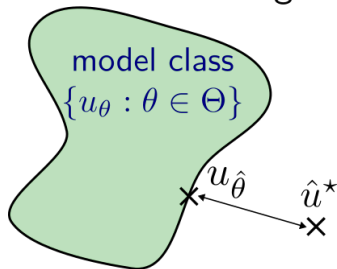


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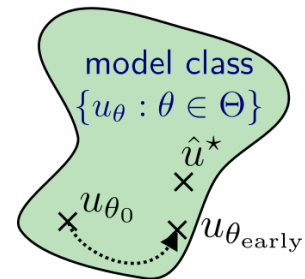
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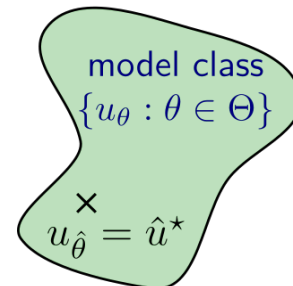


Bonnaire et al. (2026)

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Dynamical^{14,15} then Architectural^{4,12,13}?

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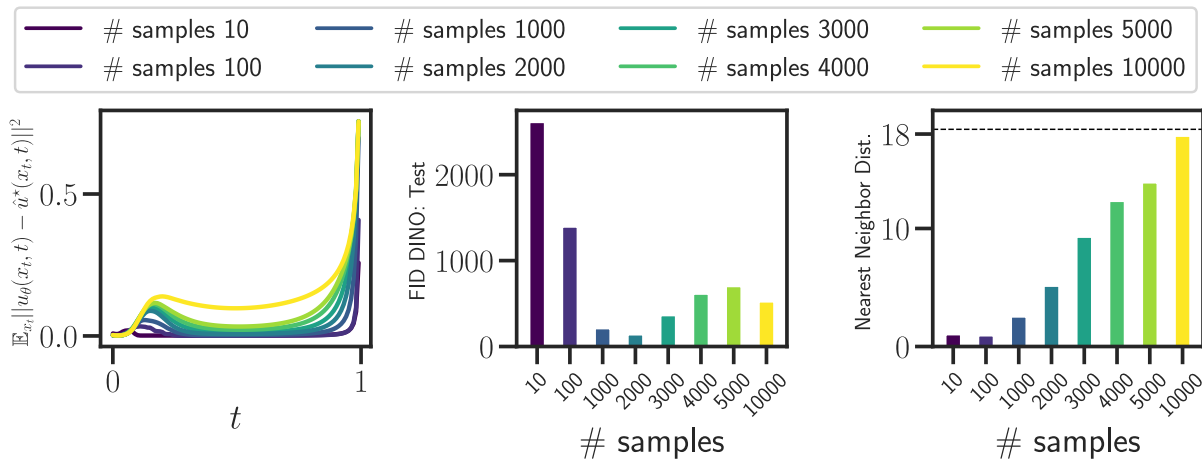
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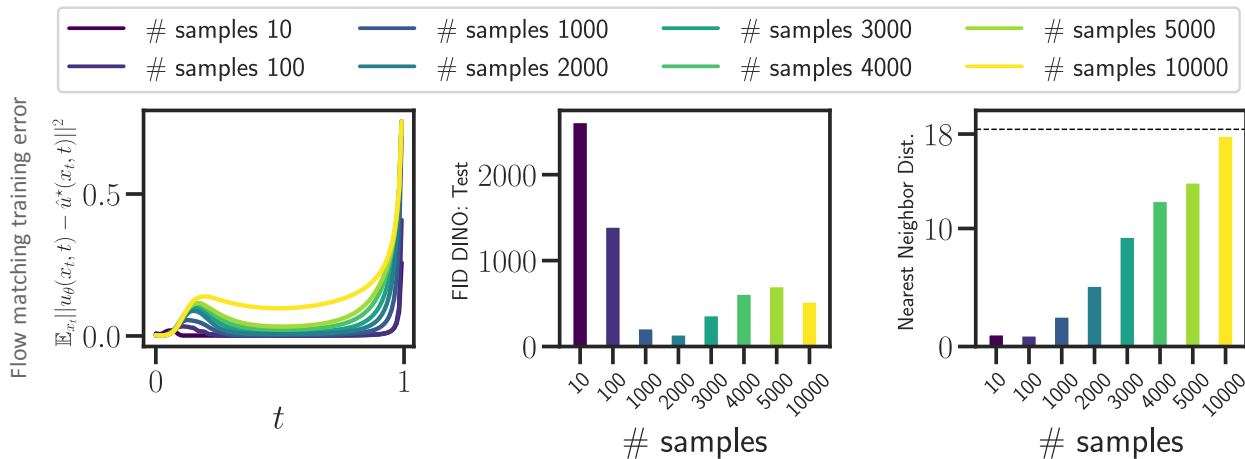
- Fixed architecture size, increase number of training samples n (CIFAR-10)



¹⁶Q. Bertrand et al., On the Closed-Form of Flow Matching: Generalization Does Not Arise from Target Stochasticity, In: NeurIPS, 2025.

Architectural regularization¹⁶

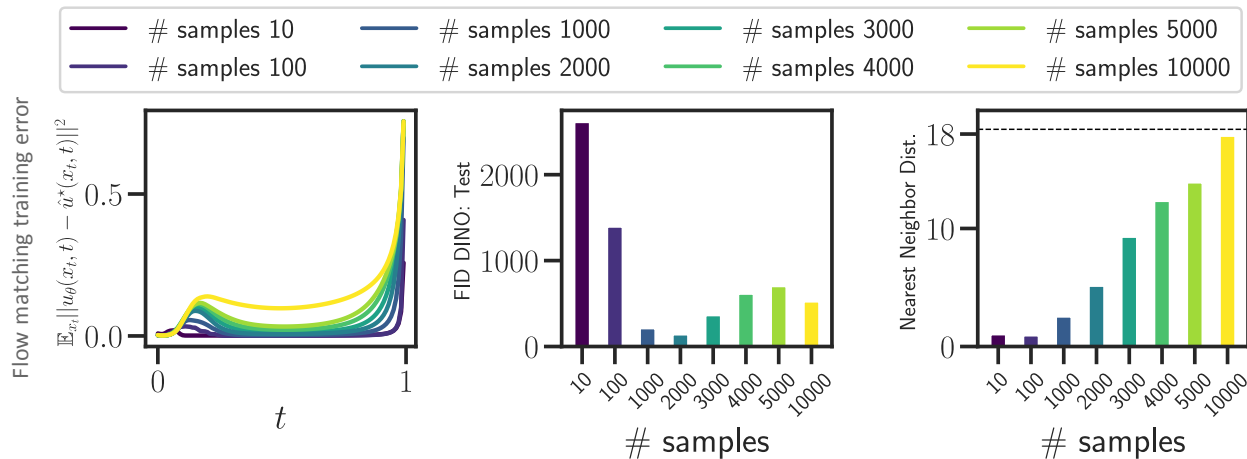
- Fixed architecture size, increase number of training samples n (CIFAR-10)



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Architectural regularization¹⁶

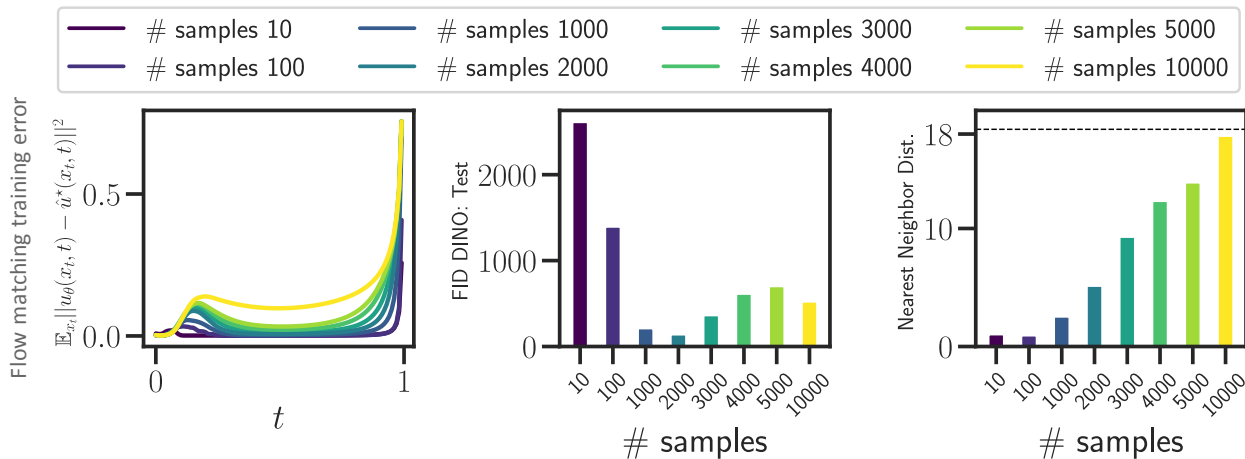
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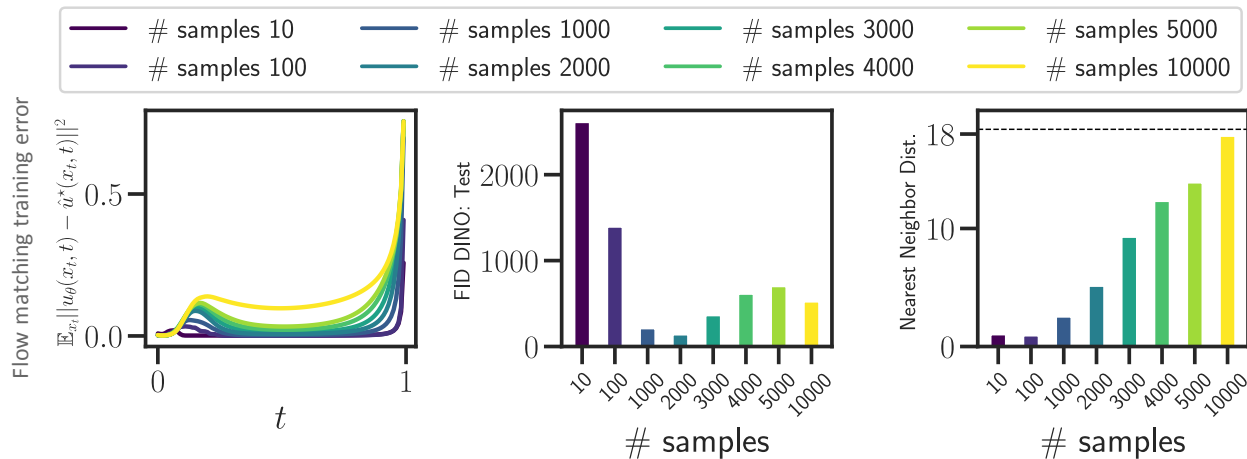
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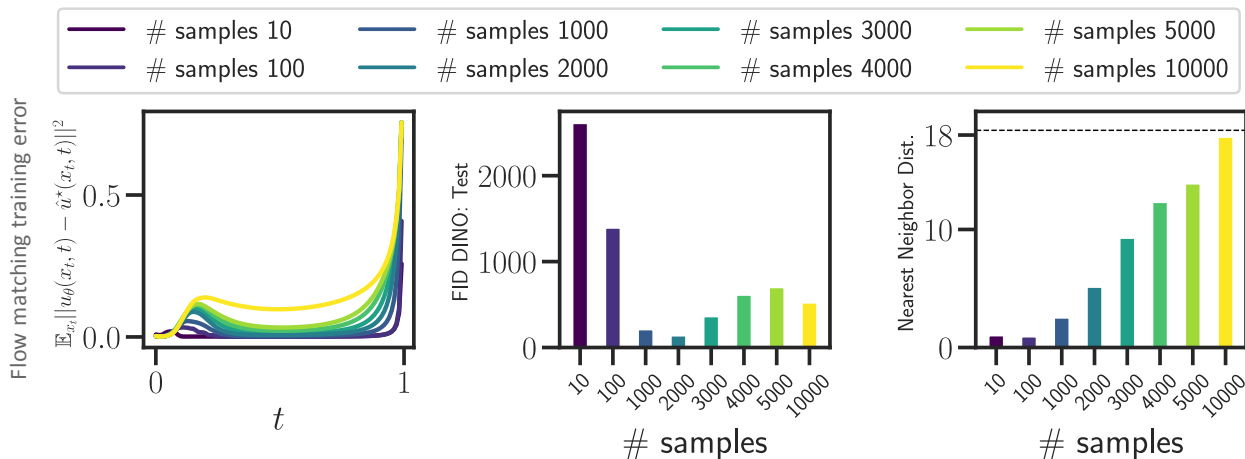
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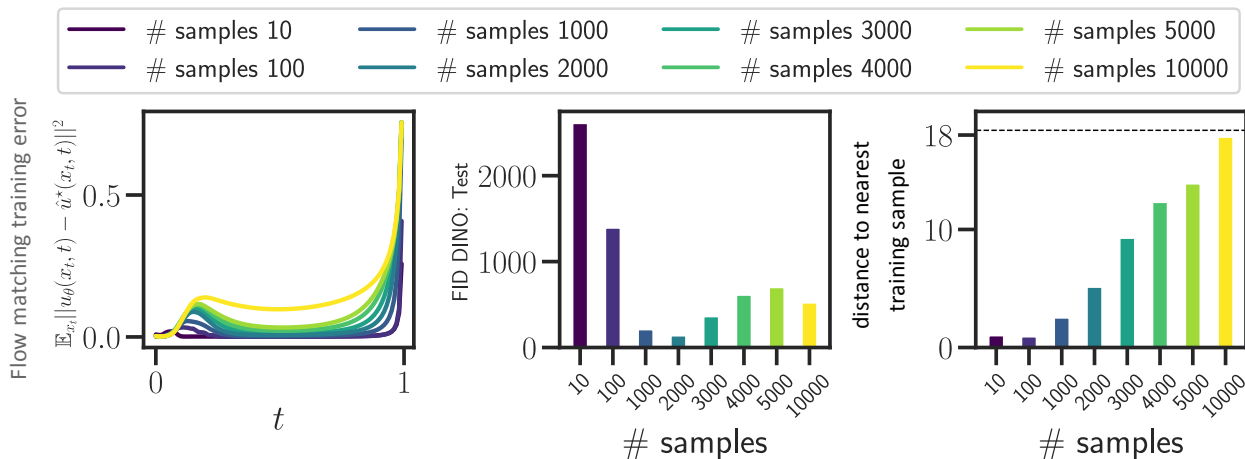


(FID going down at $n = 1000$ is a problem of FID)

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Architectural regularization¹⁶

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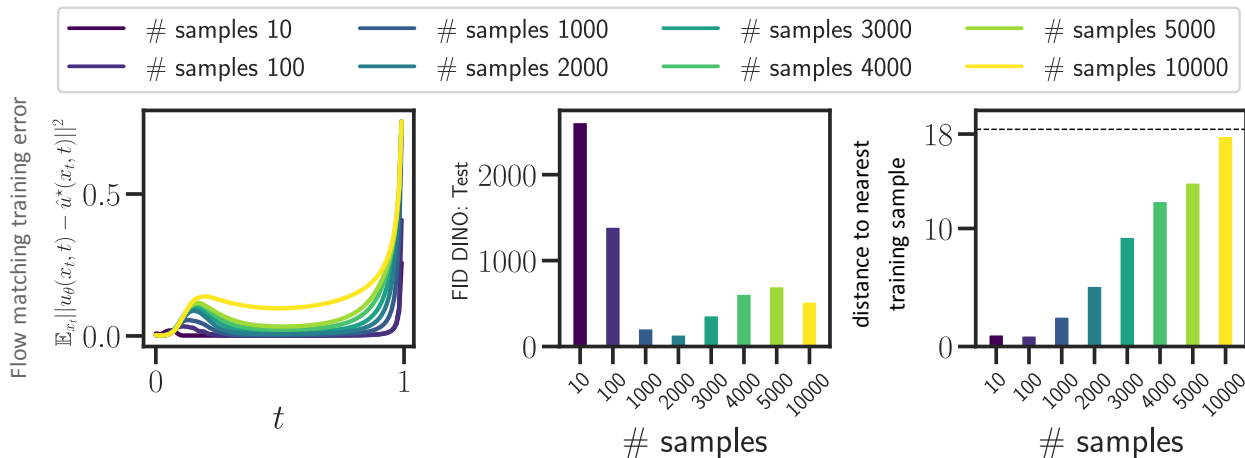


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- Fixed architecture size, increase number of training samples n (CIFAR-10)



(FID going down at $n = 1000$ is a problem of FID)

Models stop memorizing when they can no longer fit \hat{u}^*

Importance of small times¹⁶

From a good trained u_θ , we build a **hybrid model** (fixed $\tau \in [0, 1]$):

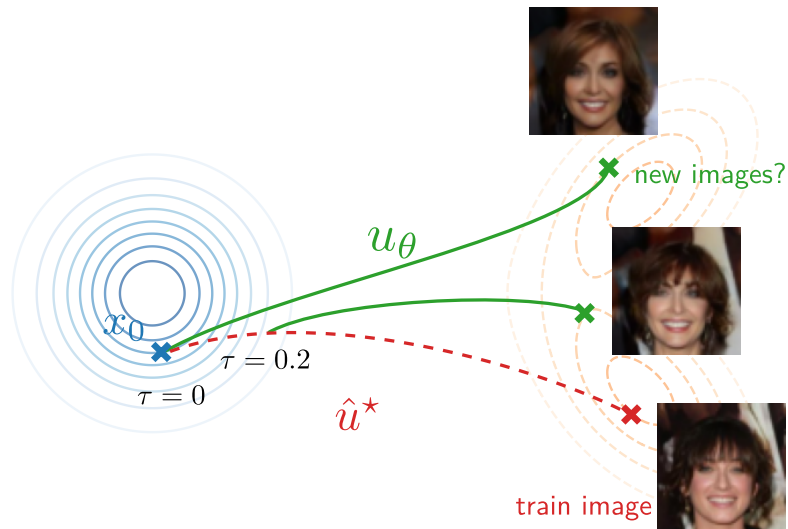
- on $[0, \tau]$: follow \hat{u}^*
- on $[\tau, 1]$: follow u_θ
- $\tau = 1$ means completely following \hat{u}^* (full memorization)
- $\tau = 0$ means completely following u_θ (good generalization)

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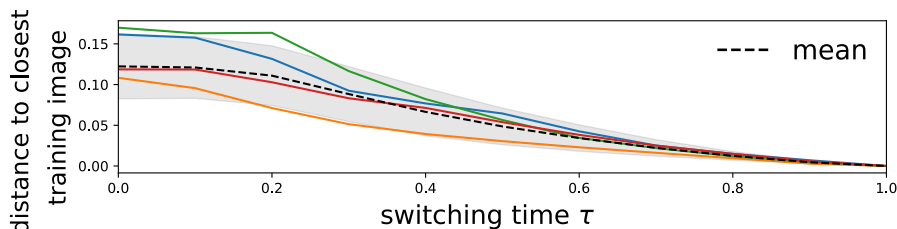
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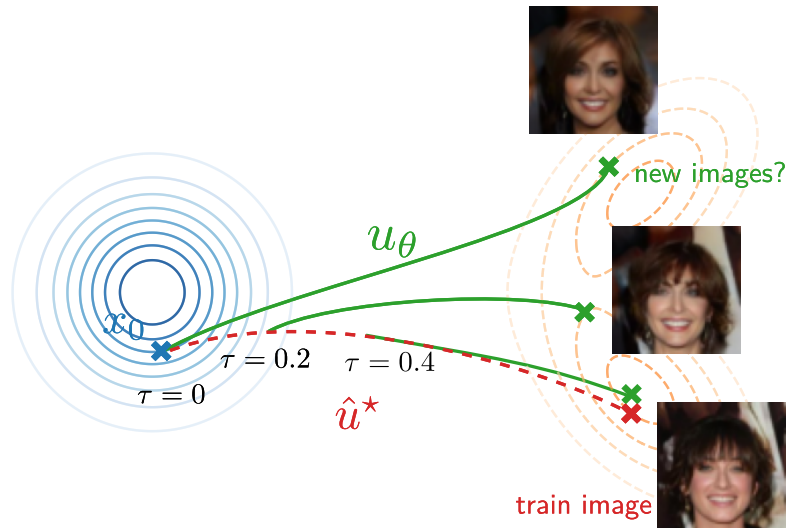
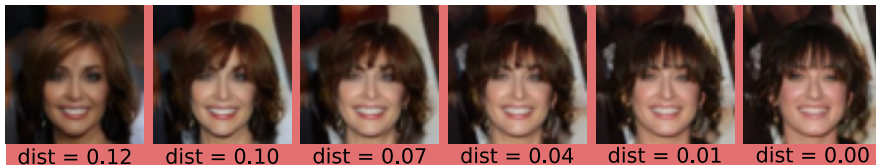
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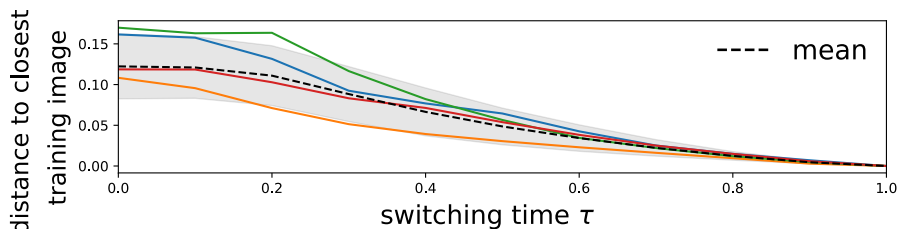
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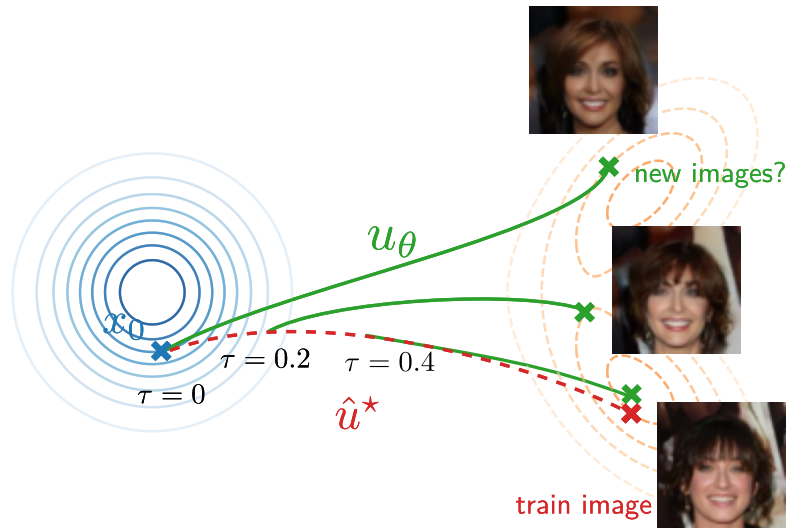
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Not fitting small times is critical

Dynamical regularization^{14,15}

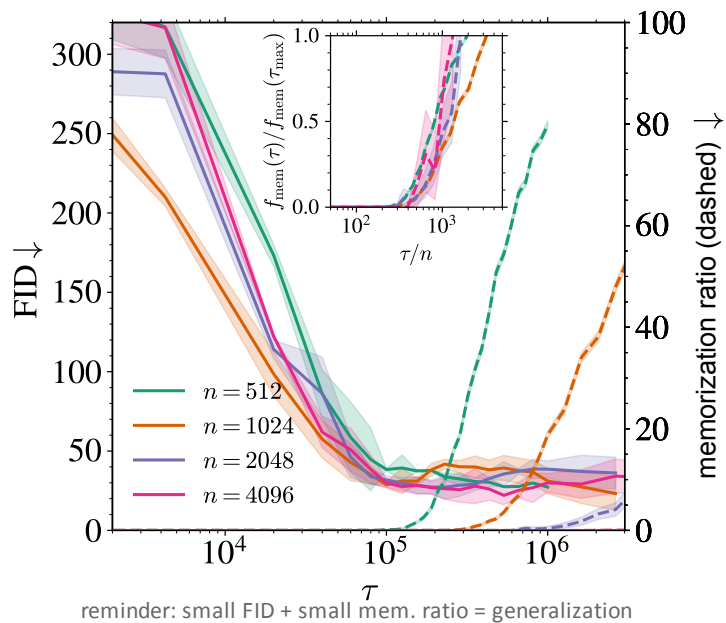
- Fixed architecture size, increase number of training samples n (CelebA 32×32)

¹⁴ T. Bonnaire et al., **Why Diffusion Models Don't Memorize: The Role of Implicit Dynamical Regularization in Training**, In: NeurIPS, 2025.

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Dynamical regularization^{14,15}

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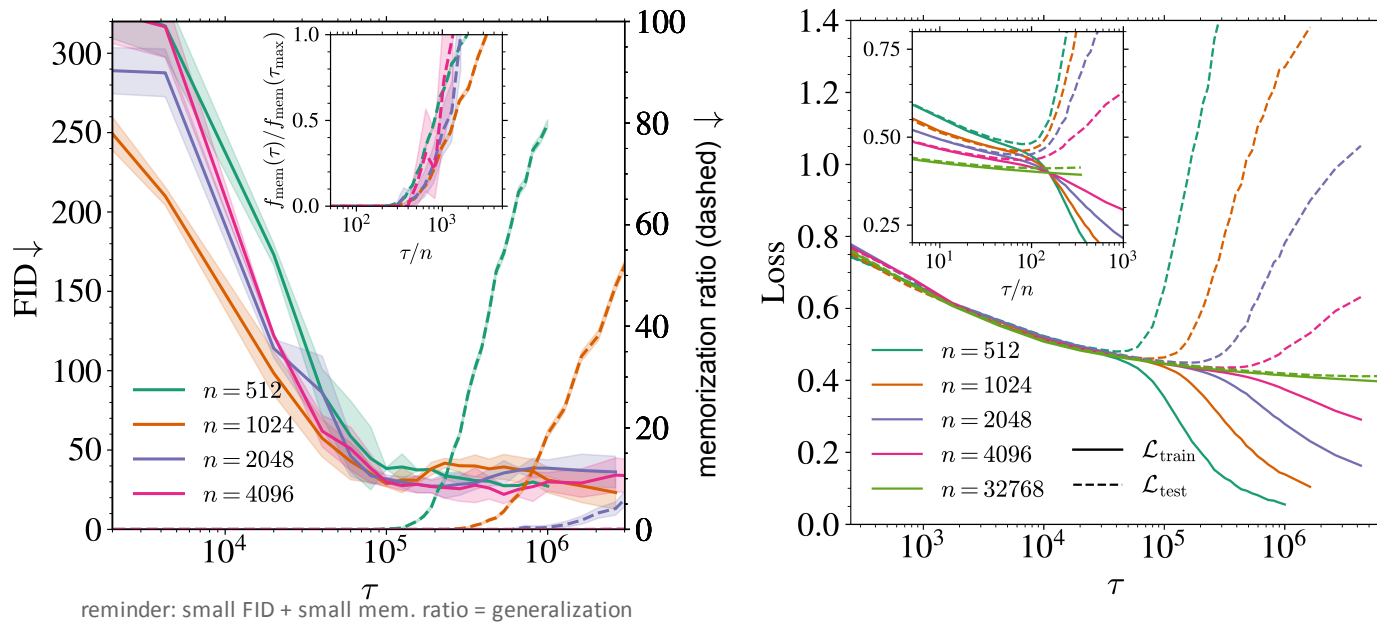


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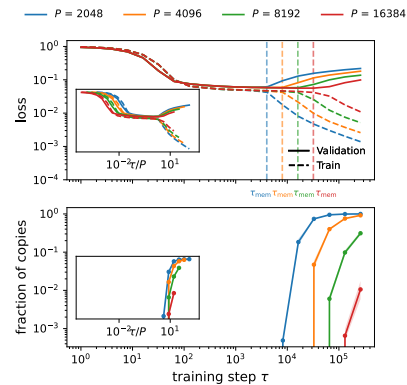
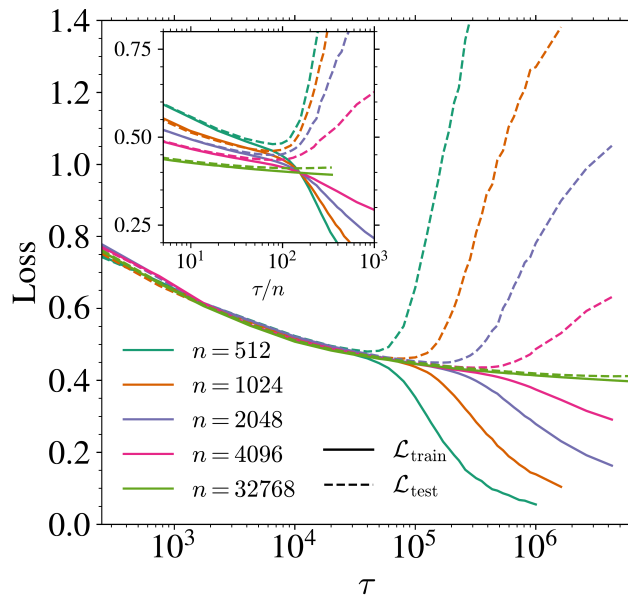
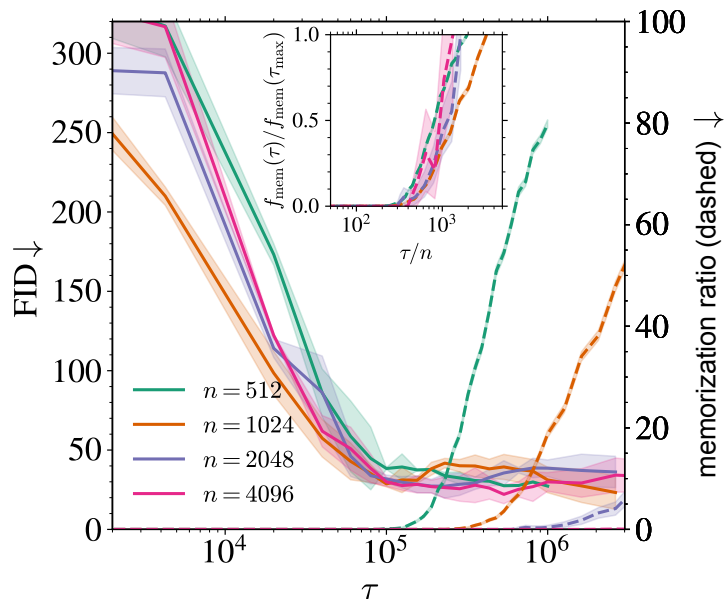


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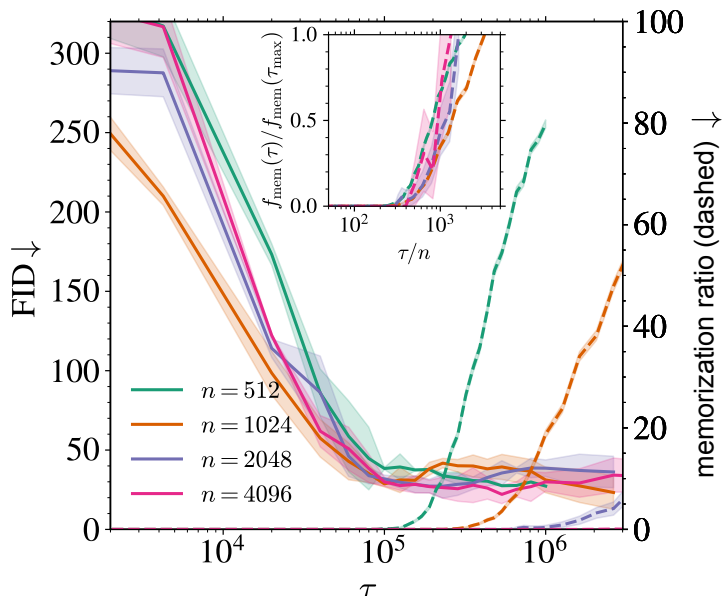
same result by Favero et al (2026)

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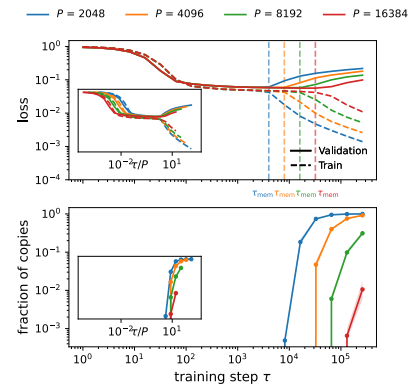
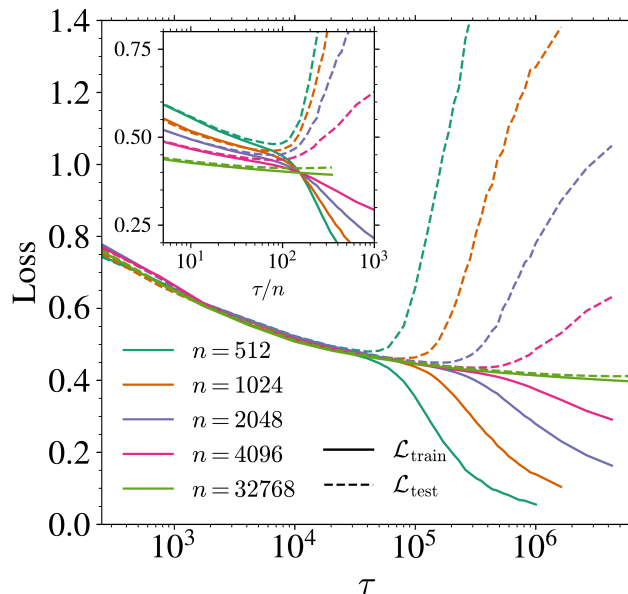
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Dynamical regularization^{14,15}

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reminder: small FID + small mem. ratio = generalization



same result by Favero et al (2026)

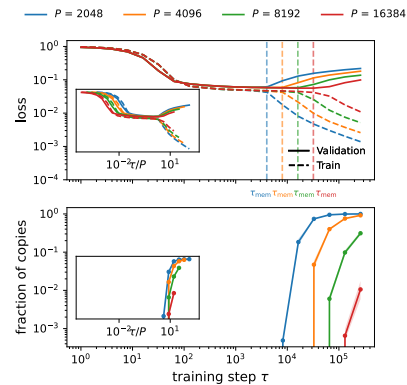
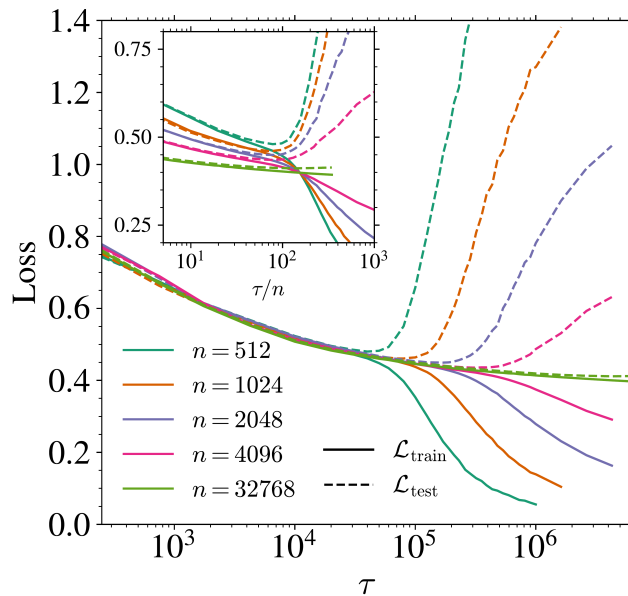
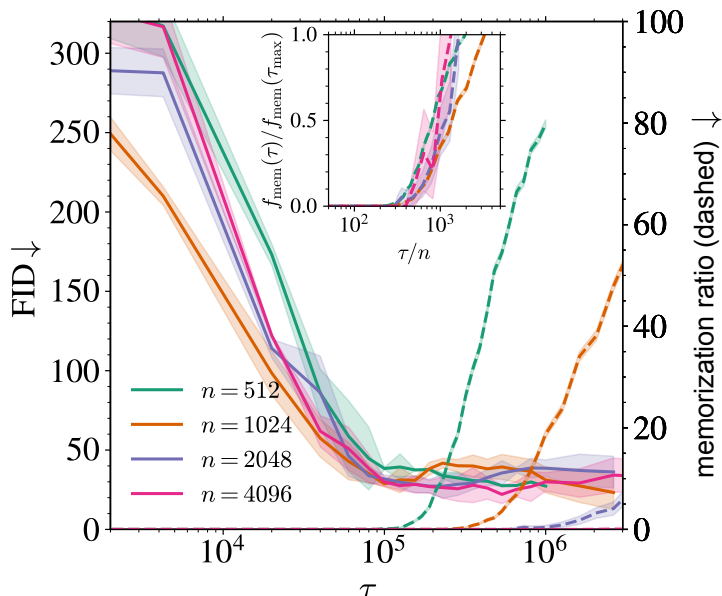
Overparametrized models can still generalize if early stopped

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Dynamical regularization^{14,15}

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same result by Favero et al (2026)

Memorization starts at $\tau_{\text{mem}} = \mathcal{O}(\#\text{samples})$

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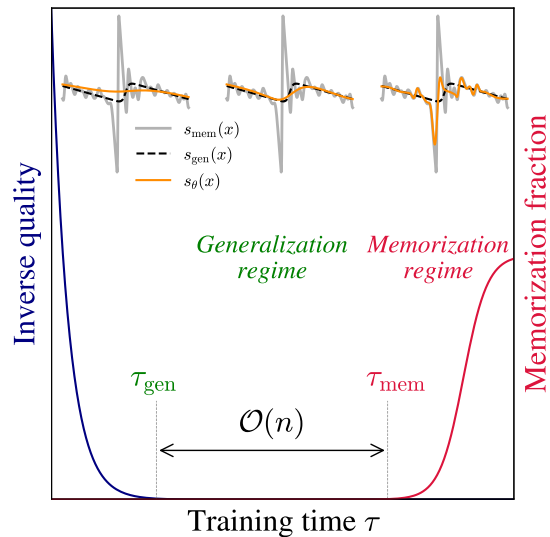
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Generalization and memorization times^{14,15}

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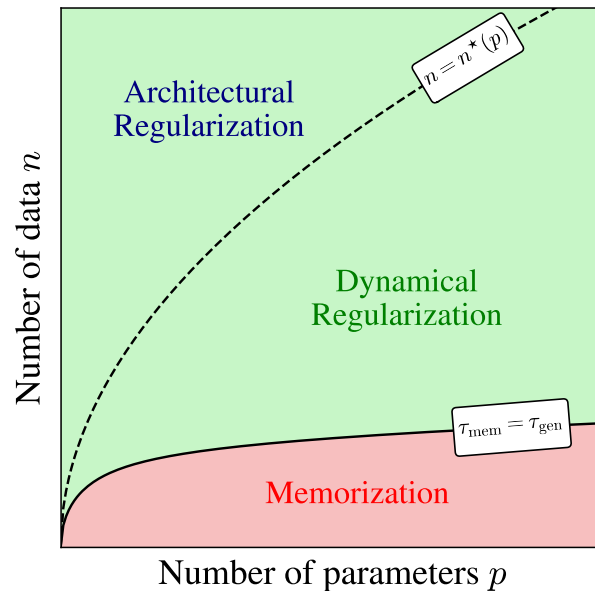
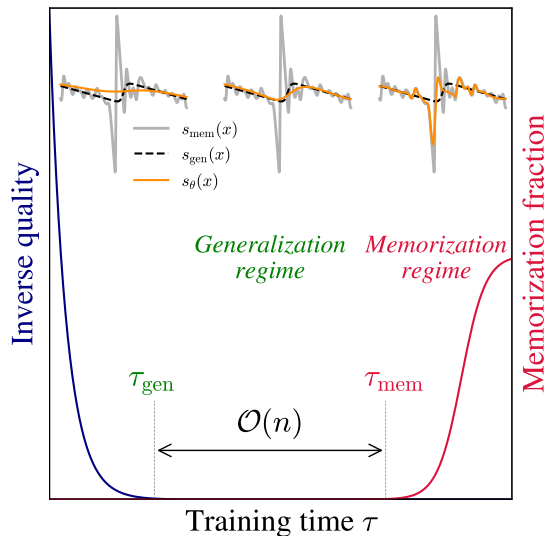
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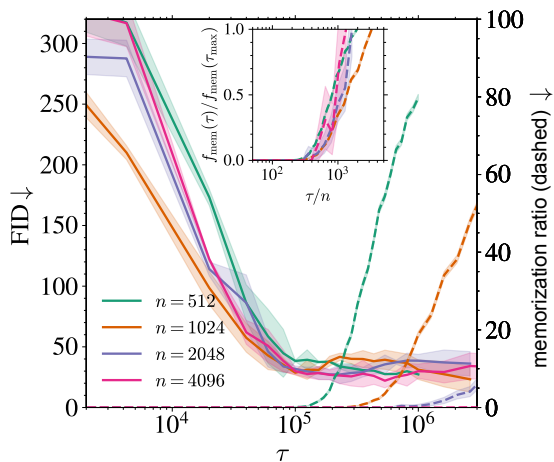
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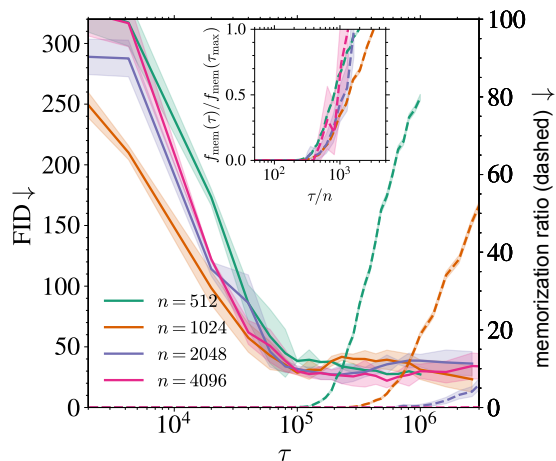
Caveats in overparametrization and early stopping¹⁴



Data & architecture. We conduct our experiments on the CelebA face dataset [26], which we convert to **grayscale downsampled** images of size $d = 32 \times 32$, and vary the training set size n from 128 up to 32768. Our score model has a U-Net architecture [35] with three resolution levels, and a base channel

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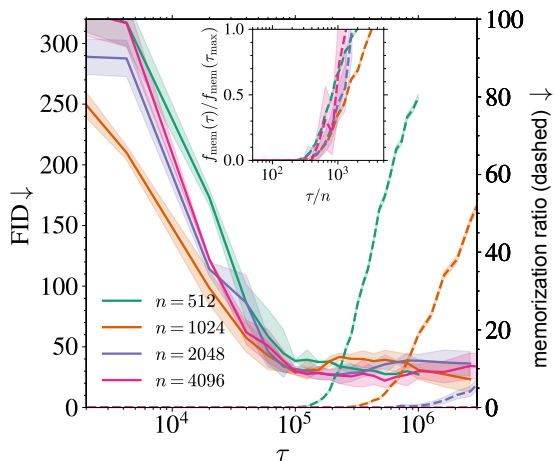


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- In this experiment the dataset size is very reduced (both through n and d)

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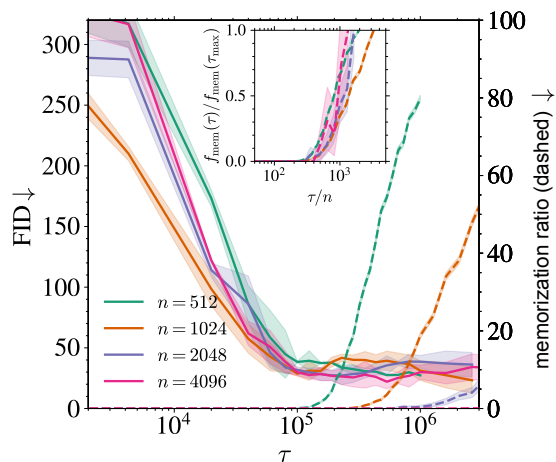


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- In this experiment the dataset size is very reduced (both through n and d)
- Real CelebA has $178 \times 218 \times 3 \times 200000 \approx 2.3 \times 10^{10}$ pixels

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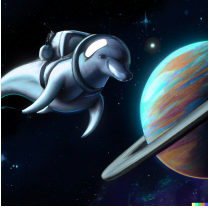


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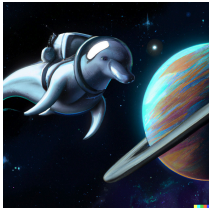
- In this experiment the dataset size is very reduced (both through n and d)
- Real CelebA has $178 \times 218 \times 3 \times 200000 \approx 2.3 \times 10^{10}$ pixels
- Open question: do models have enough capacity to memorize their datasets?

¹⁴ T. Bonnaire et al., **Why Diffusion Models Don't Memorize: The Role of Implicit Dynamical Regularization in Training**, In: NeurIPS, 2025.

Conclusion

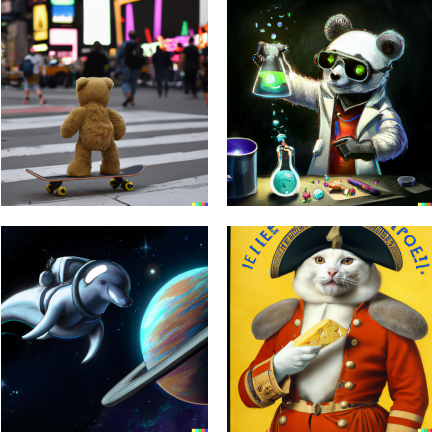


Conclusion



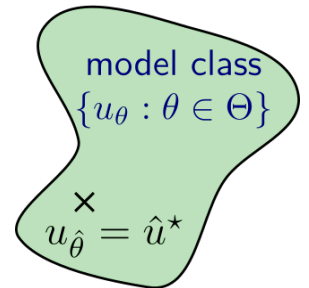
The generalization properties of flow matching/diffusion are poorly understood

Conclusion

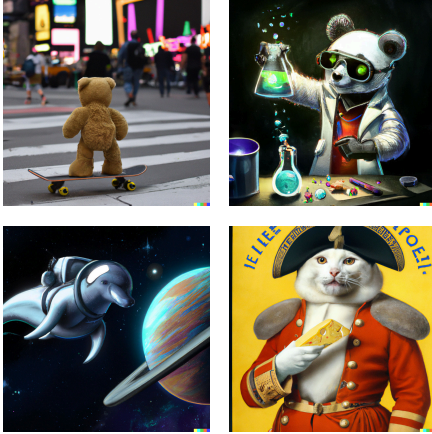


The generalization properties of flow matching/diffusion are poorly understood

Memorization

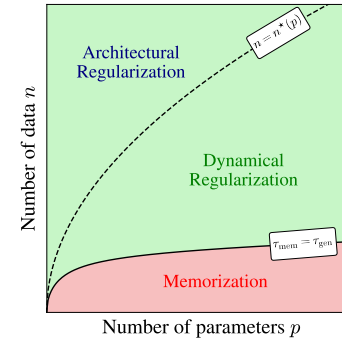


Conclusion



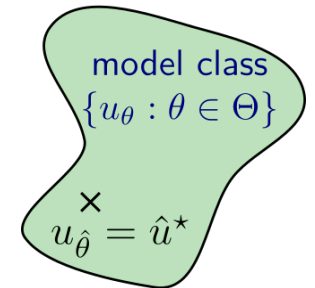
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- Mainly two hypotheses:

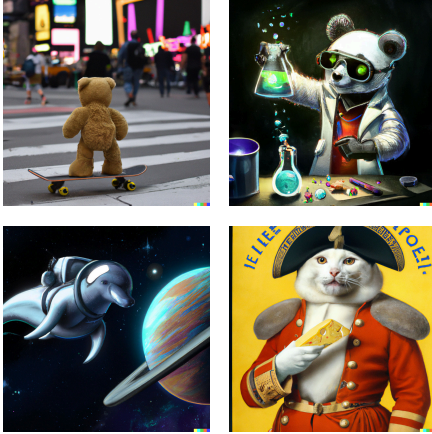


Bonnaire et al. (2026)

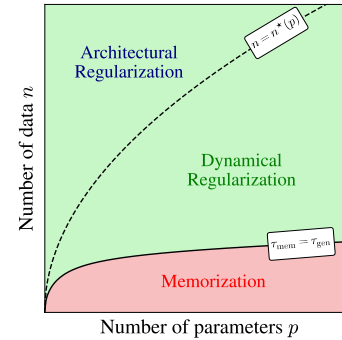
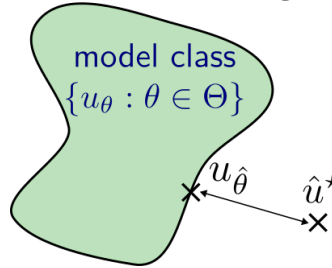
Memorization



Conclusion

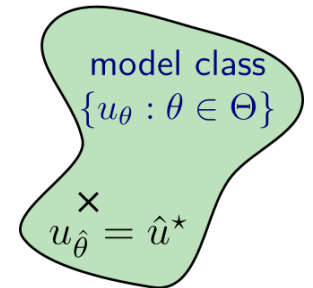


Architectural reg.



Bonnaire et al. (2026)

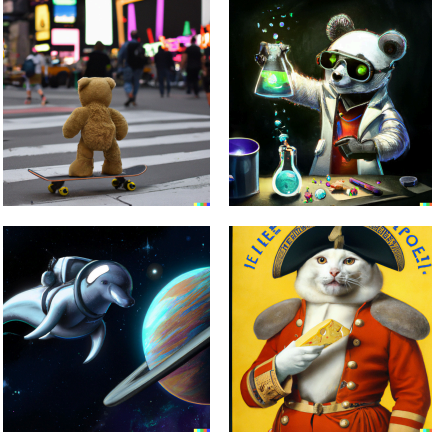
Memorization



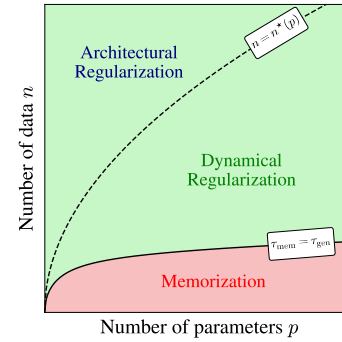
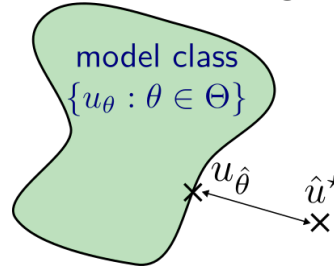
The generalization properties of flow matching/diffusion are poorly understood

- Mainly two hypotheses:
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Conclusion

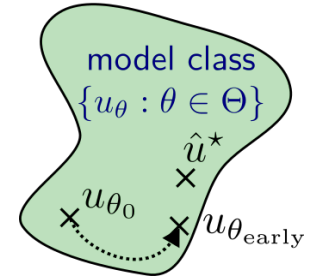


Architectural reg.

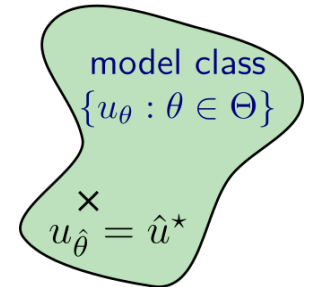


Bonnaire et al. (2026)

Dynamical reg.



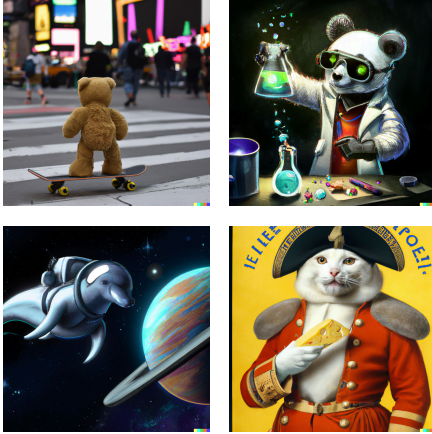
Memorization



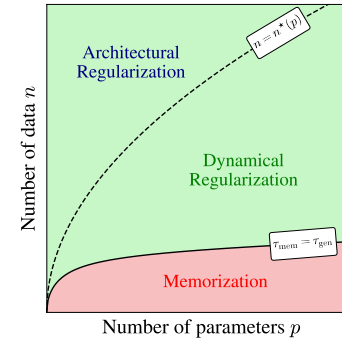
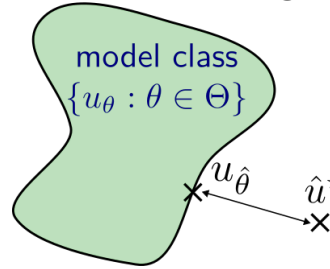
The generalization properties of flow matching/diffusion are poorly understood

- Mainly two hypotheses:
 - Architecture regularization
 - Dynamical regularization through optimization

Conclusion

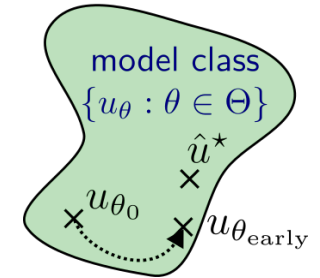


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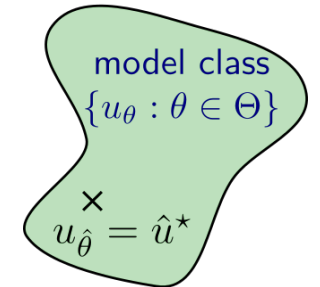


Bonnaire et al. (2026)

Dynamical reg.



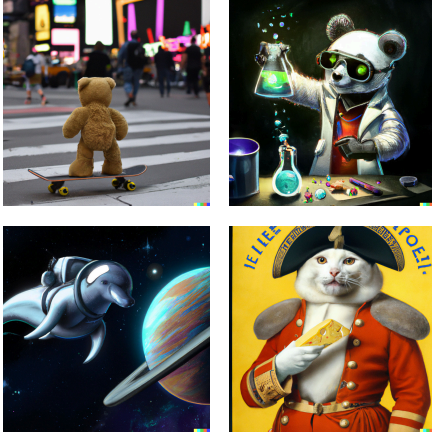
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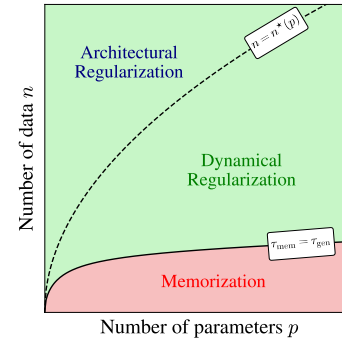
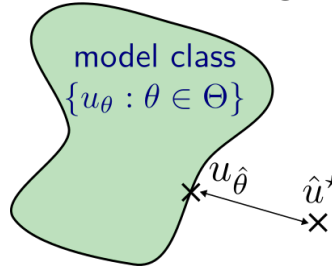
The generalization properties of flow matching/diffusion are poorly understood

- Mainly two hypotheses:
 - Architecture regularization
 - Dynamical regularization through optimization
- Other source for the generalization

Conclusion

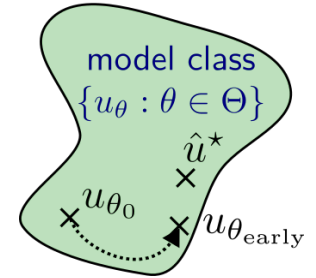


Architectural reg.

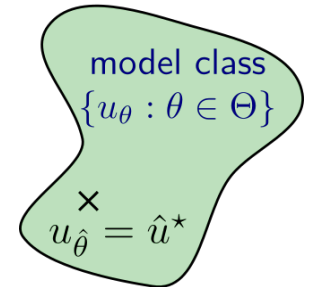


Bonnaire et al. (2026)

Dynamical reg.



Memorization



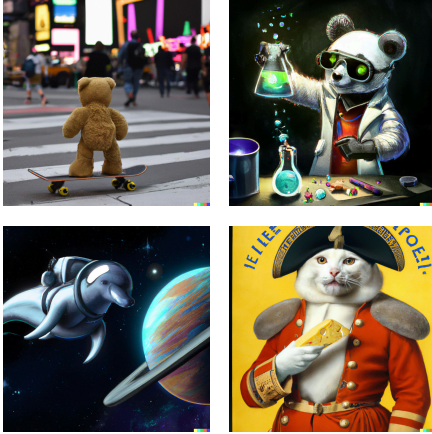
The generalization properties of flow matching/diffusion are poorly understood

- Mainly two hypotheses:
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 - Dynamical regularization through optimization
- Other source for the generalization
 - Stochasticity at inference/Errors in numerical ODE/SDE resolution^{17,18}

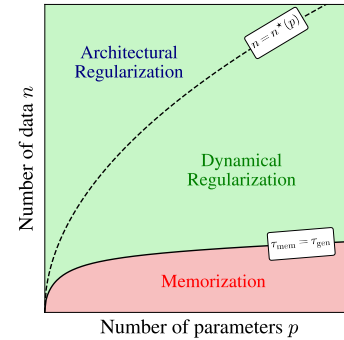
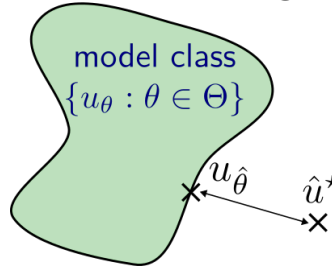
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Conclusion



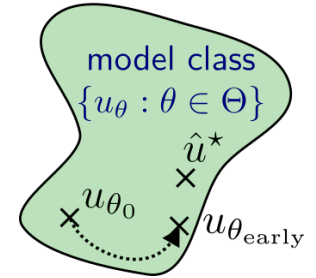
Architectural reg.



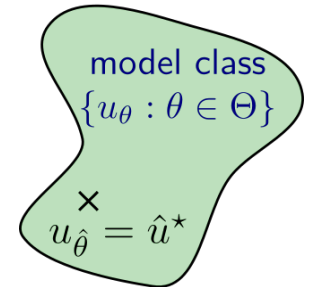
Bonnaire et al. (2026)

Thank you for your attention!

Dynamical reg.



Memorization



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ICML 2026 tutorial

Diffusion and Flow Matching

Part III: Beyond Generalization: Creativity

Quentin Bertrand & Mathurin Massias

<https://memorization-generalization.github.io>

Inria | ENS Lyon | Laboratoire Hubert Curien | Mila Affiliated Member | CIFAR Global Scholar

Why do Diffusion & Flow matching work so well?

Reminders:

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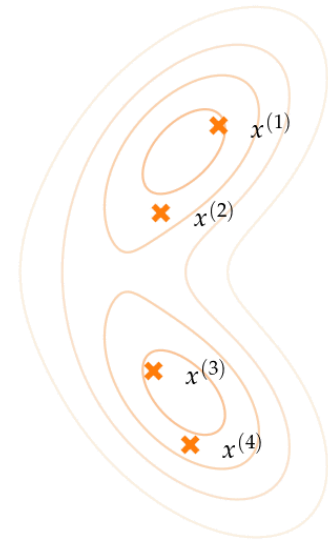
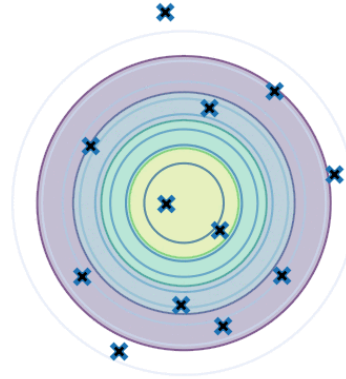
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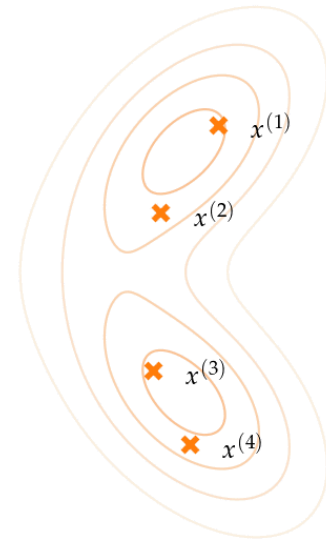
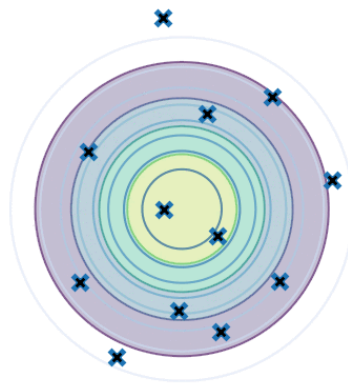


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Diffusion/flow matching models



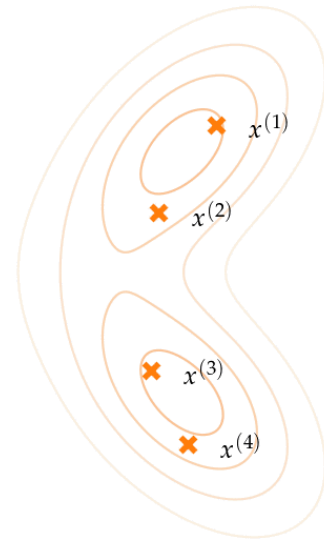
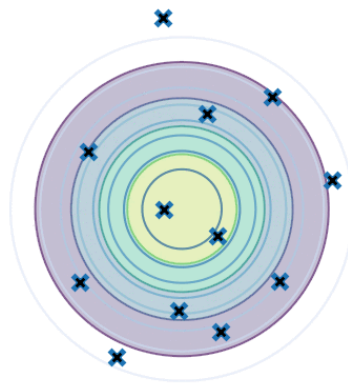
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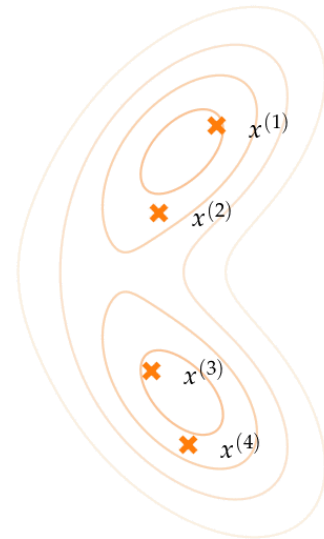
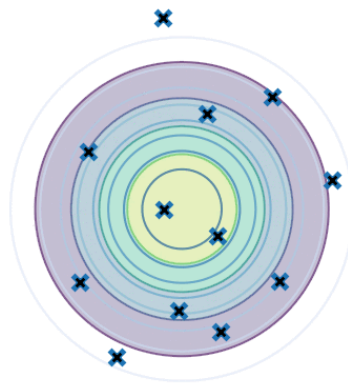
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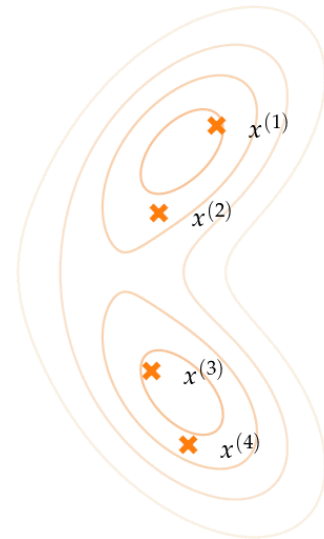
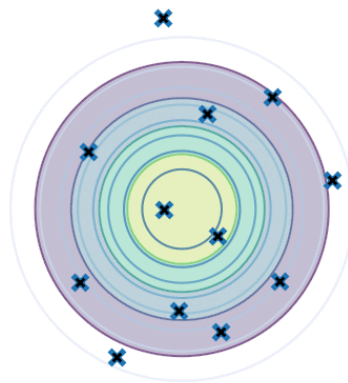
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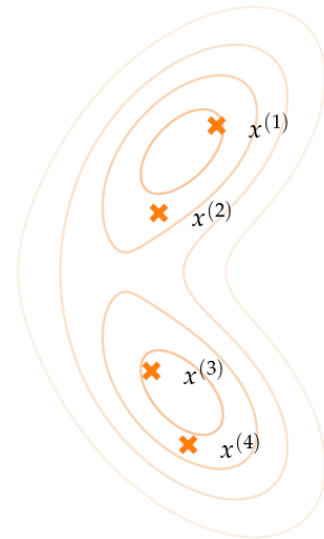
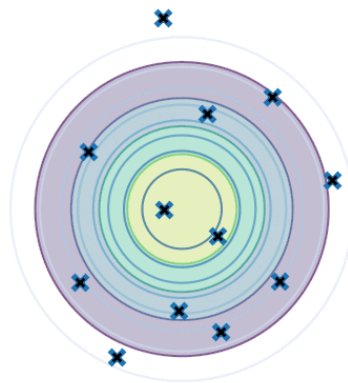
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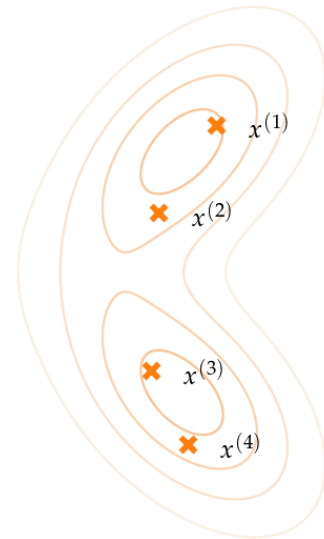
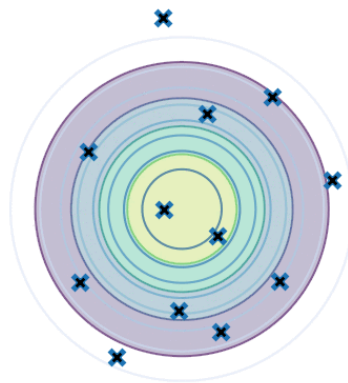
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- And easily mix and match images/concepts
- How can diffusion/flow matching combine concepts?



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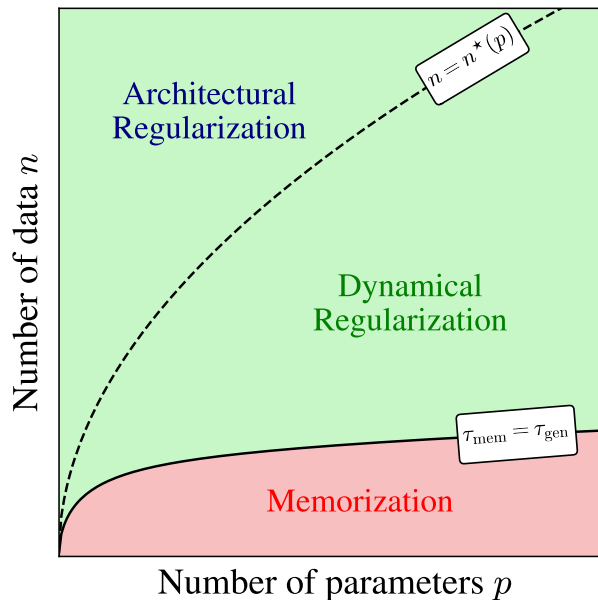
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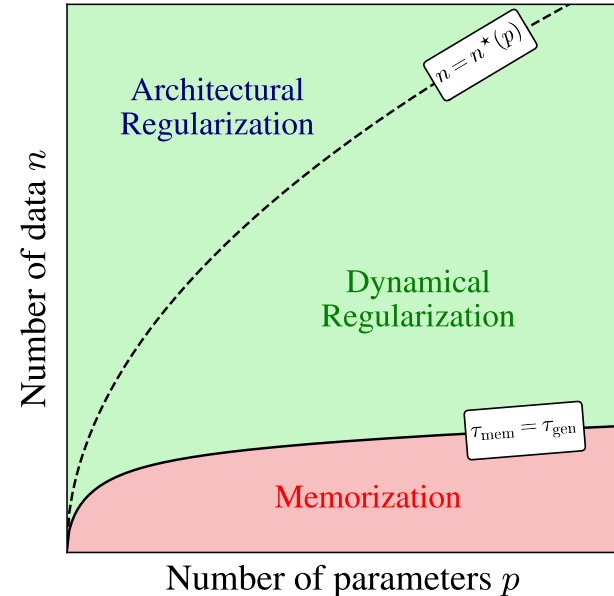
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Rest of this part: architectural regularization



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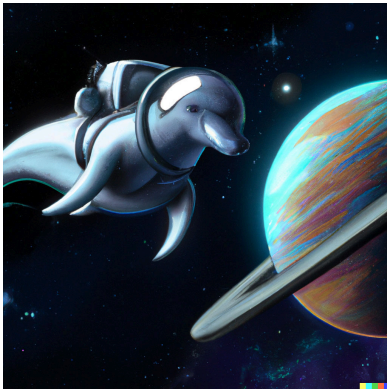
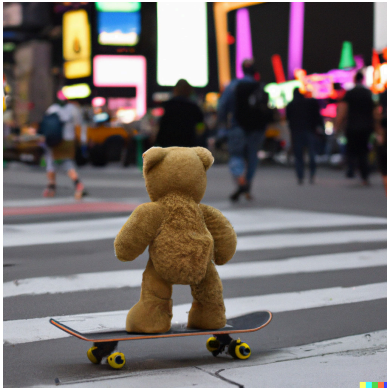
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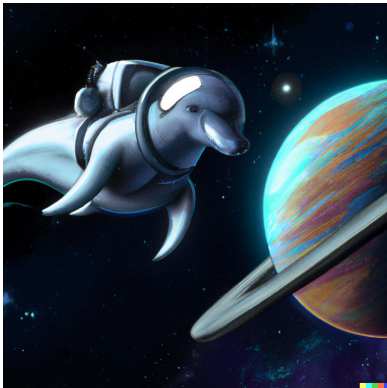
Beyond memorization: Mix and Match capabilities⁴



DALL-E, Ramesh et al.

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How to understand diffusion mix and match capabilities in a minimalistic framework?

DALL-E, Ramesh et al.

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- Goal: Understand diffusion/flow matching "generalization" capabilities

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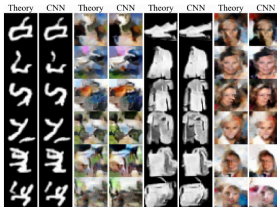
- An analytic theory of creativity in convolutional diffusion models⁴

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Mason Kamb¹ Surya Ganguli¹

Abstract

We obtain an analytic, interpretable and predictive theory of creativity in convolutional diffusion models. Indeed, score-matching diffusion models can generate highly original images that lie far from their training data. However, optimal score-matching theory suggests that these models should only be able to produce memorized training examples. To reconcile this theory-experiment gap, we identify two simple inductive biases, locality and equivariance, that: (1) induce a form of combinatorial creativity by preventing optimal score-matching; (2) result in fully analytic, completely mechanistically interpretable, local score



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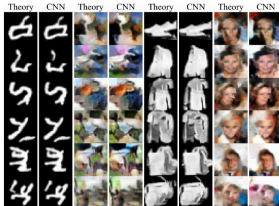
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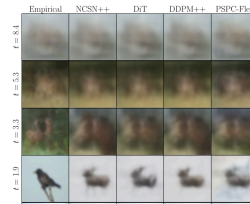


Towards a Mechanistic Explanation of Diffusion Model Generalization

Matthew Niedoba^{1,2} Berend Zwartsberg² Kevin Murphy¹ Frank Wood^{1,2,3}

Abstract

We propose a simple, training-free mechanism which explains the generalization behaviour of diffusion models. By comparing pre-trained diffusion models to their theoretically optimal empirical counterparts, we identify a shared local inductive bias across a variety of network architectures. From this observation, we hypothesize that network denoisers generalize through localized denoising operations, as these operations approximate the training objective well over much of the training distribution. To validate our hypothesis, we introduce novel denoising algorithms which aggregate local empirical denoisers to replicate



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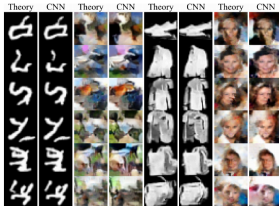


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Mason Kamb¹ Surya Ganguli¹

Abstract

We obtain an analytic, interpretable and predictive theory of creativity in convolutional diffusion models. Indeed, score-matching diffusion models can generate highly original images that lie far from their training data. However, optimal score-matching theory suggests that these models should only be able to produce memorized training examples. To reconcile this theory-experiment gap, we identify two simple inductive biases, locality and equivariance, that: (1) induce a form of combinatorial creativity by preventing optimal score-matching; (2) result in fully analytic, completely mechanistically interpretable, local score

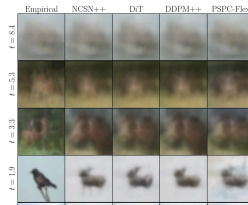


Towards a Mechanistic Explanation of Diffusion Model Generalization

Matthew Niedoba^{1,2} Berend Zwartenberg² Kevin Murphy¹ Frank Wood^{1,2,3}

Abstract

We propose a simple, training-free mechanism which explains the generalization behaviour of diffusion models. By comparing pre-trained diffusion models to their theoretically optimal empirical counterparts, we identify a shared local inductive bias across a variety of network architectures. From this observation, we hypothesize that network denoisers generalize through localized denoising operations, as these operations approximate the training objective well over much of the training distribution. To validate our hypothesis, we introduce novel denoising algorithms which aggregate local empirical denoisers to replicate



Locality in Image Diffusion Models Emerges from Data Statistics

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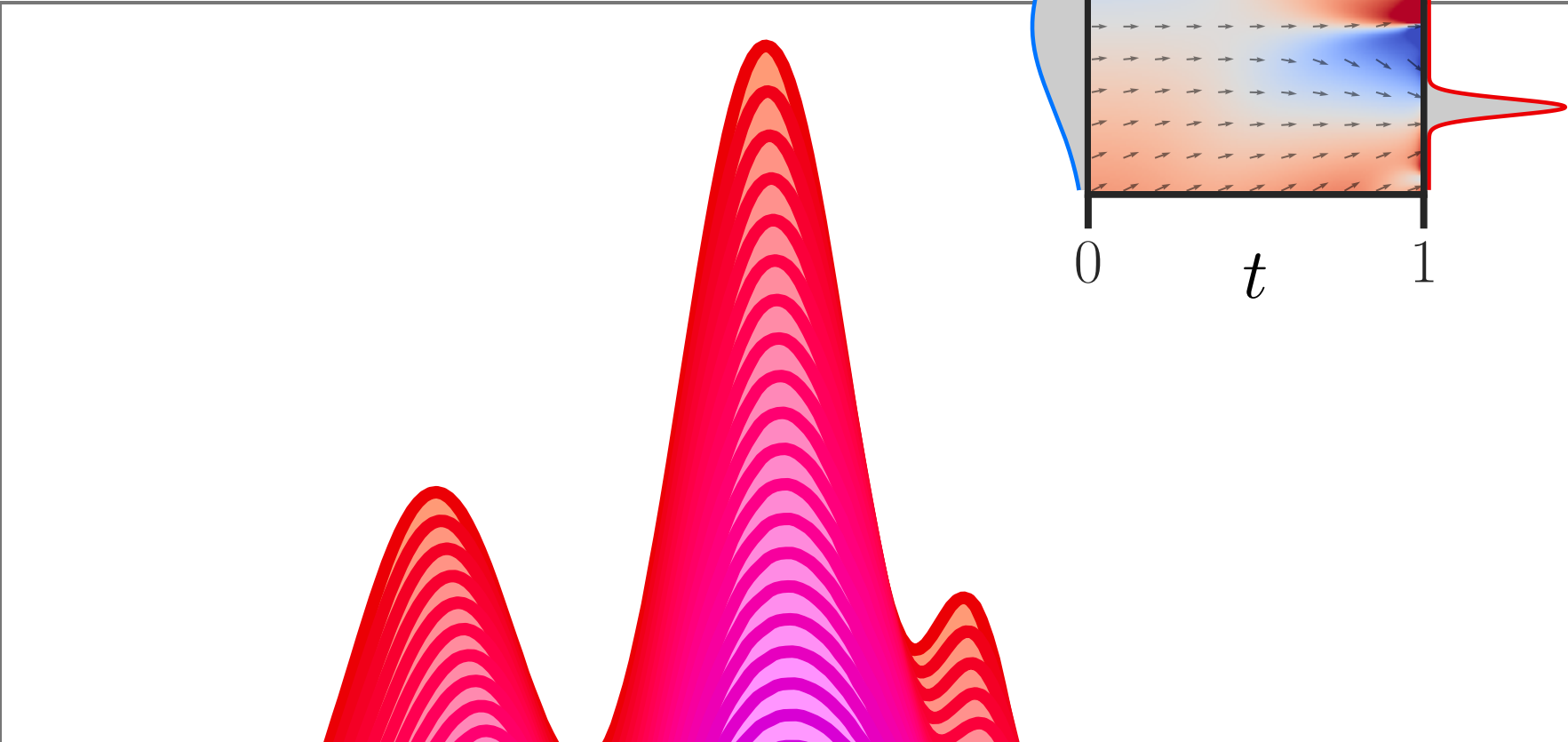
<https://locality.lukoianov.com>

⁴ M. Kamb et al., **An Analytic Theory of Creativity in Convolutional Diffusion Models**, In: ICML, 2025.

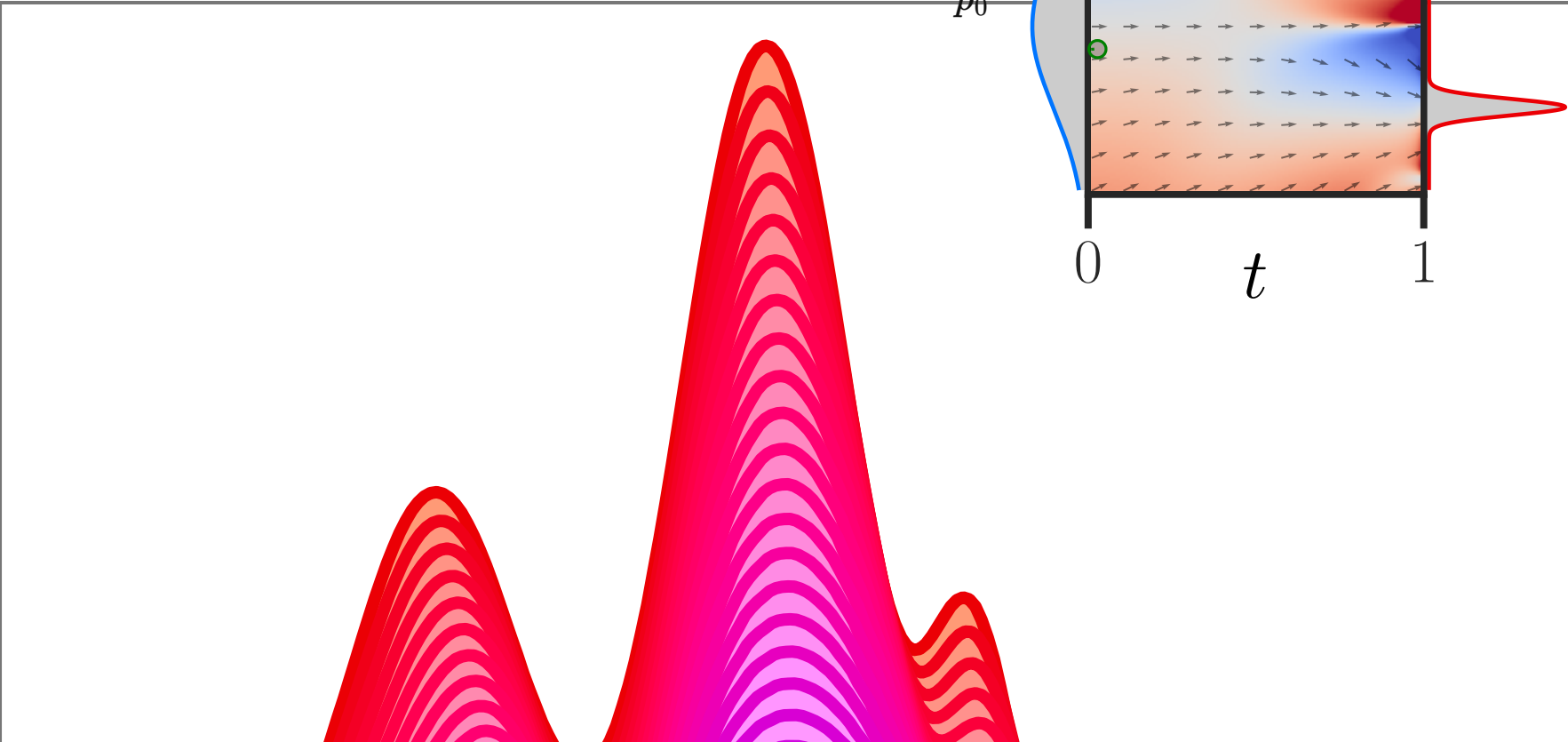
⁵ M. Niedoba et al., **Towards a mechanistic explanation of diffusion model generalization**, In: ICML, 2025.

⁶ A. Lukoianov et al., **Locality in Image Diffusion Models Emerges From Data Statistics**, In: NeurIPS, 2025.

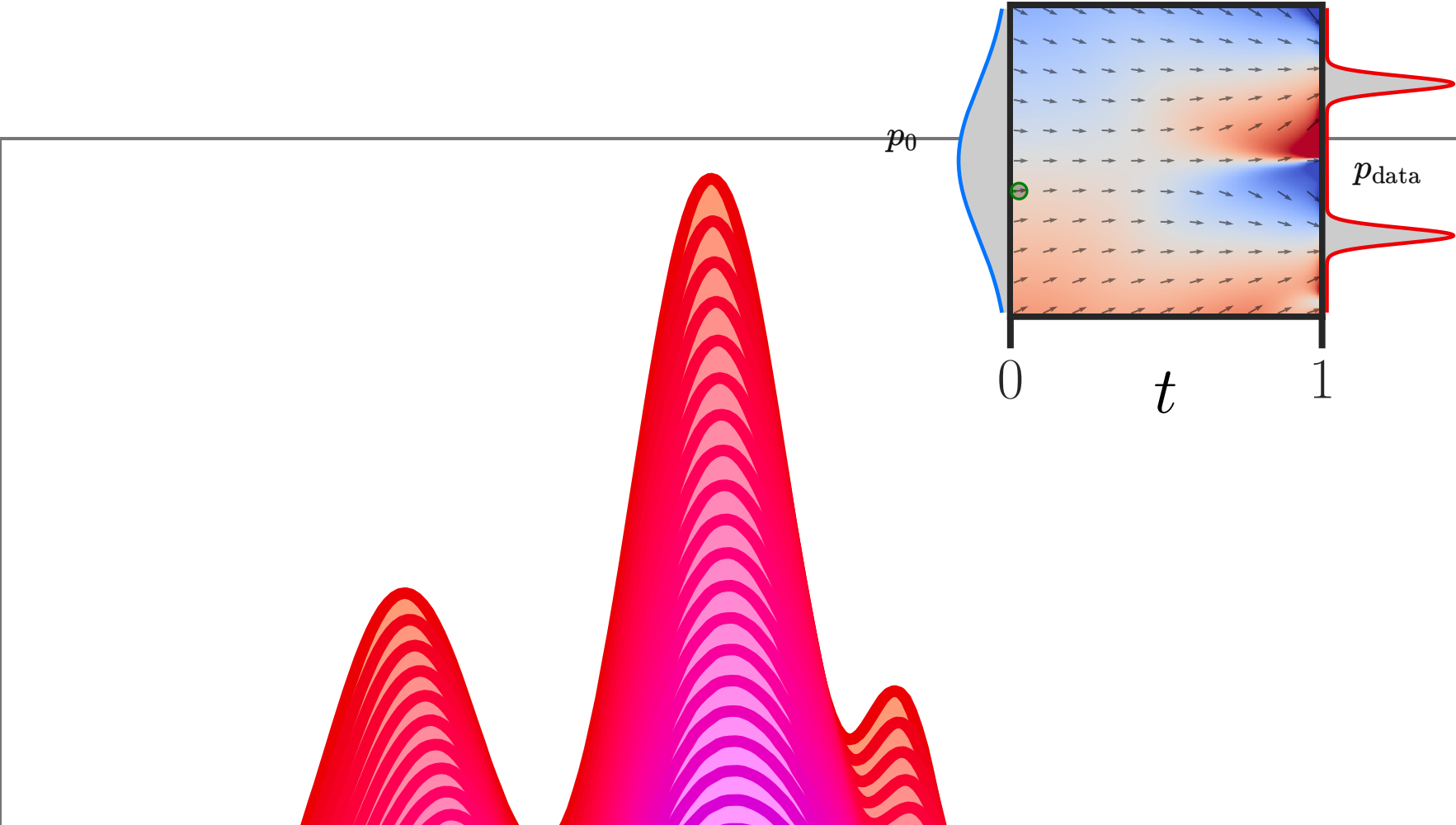
Reminder



Reminder



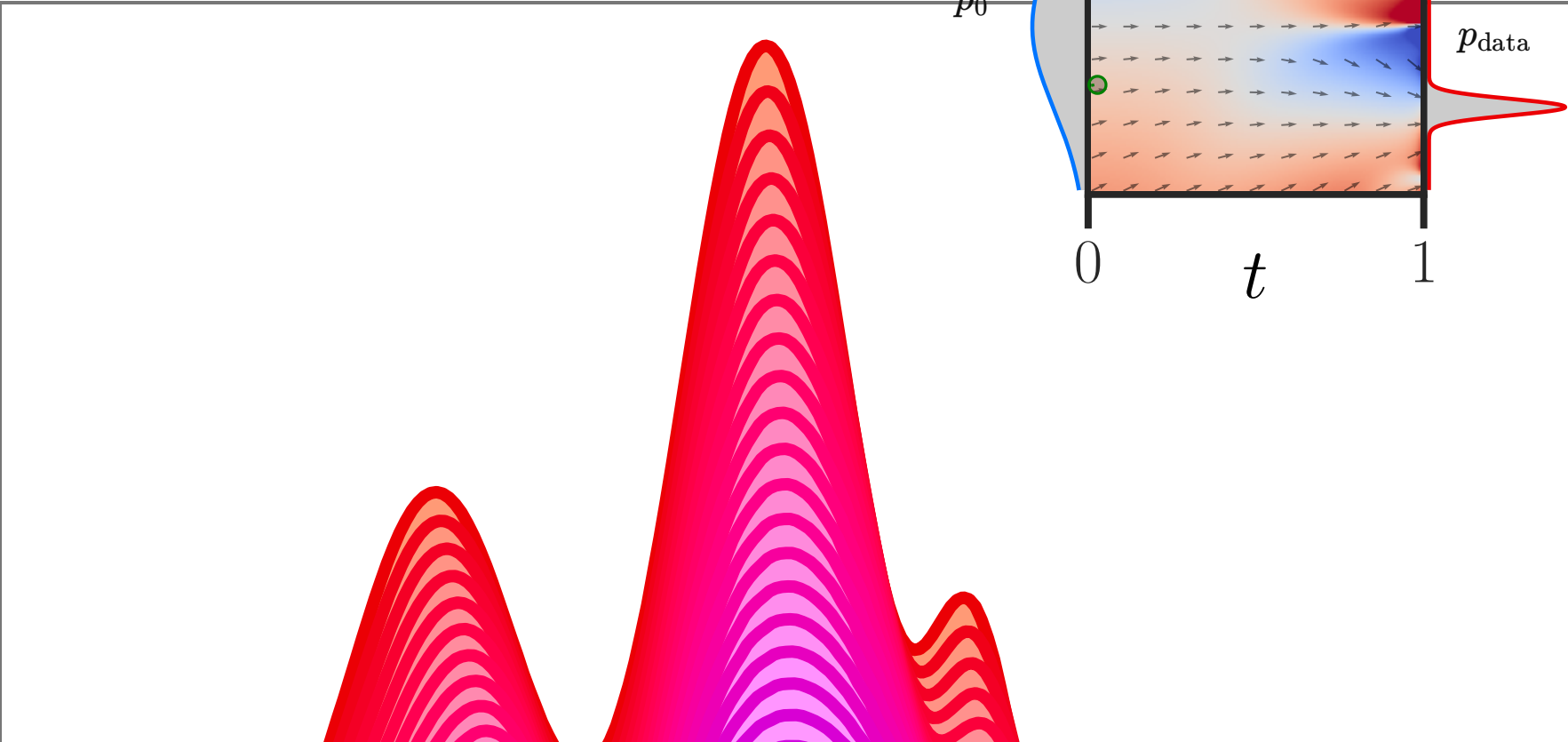
Reminder



Problem Setting:

- Access to n samples $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)} \in \mathbb{R}^d$
- $\underbrace{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}}_{\text{known}} \sim \underbrace{p_{\text{data}}}_{\text{unknown}}$

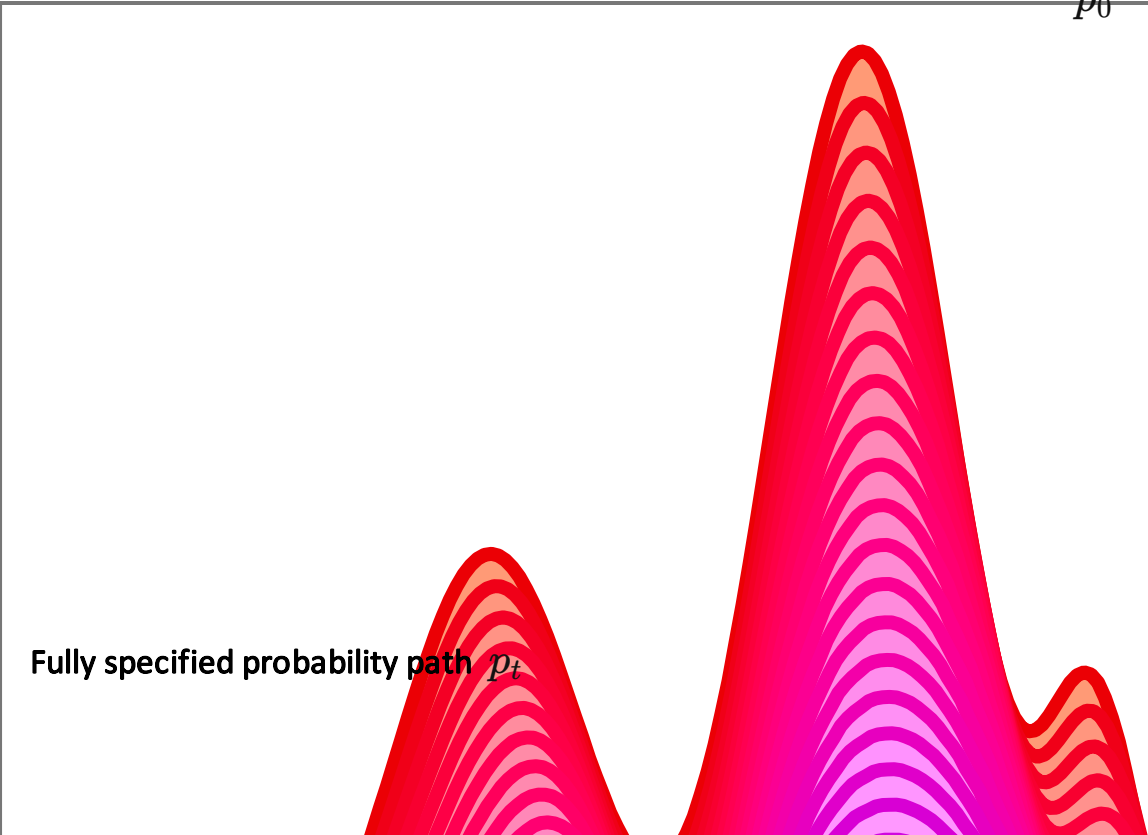
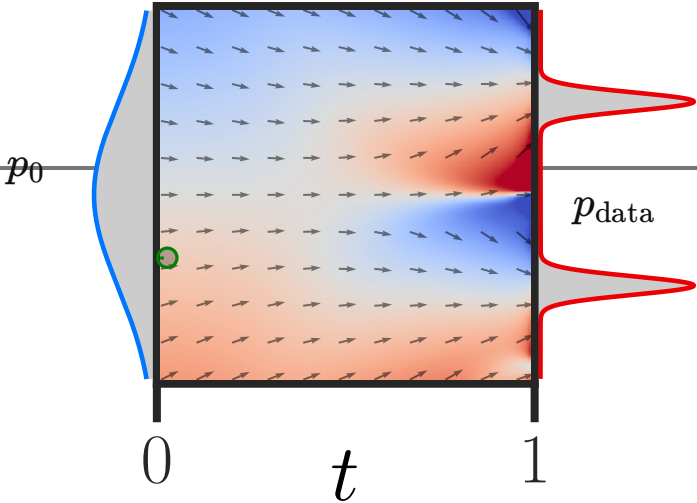
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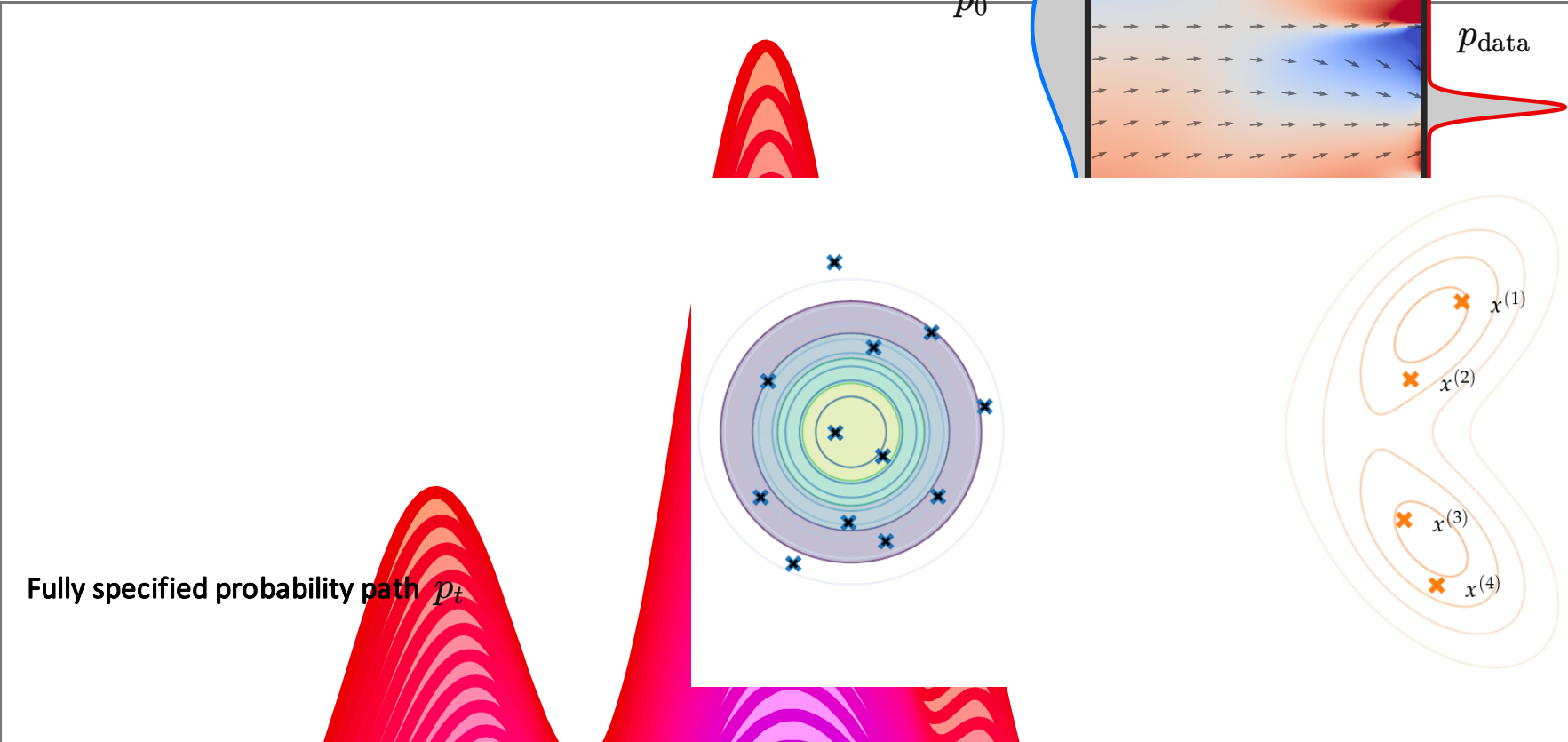
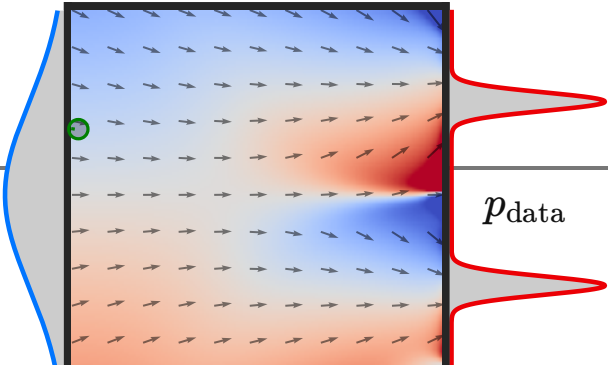
Reminder



Problem Setting:

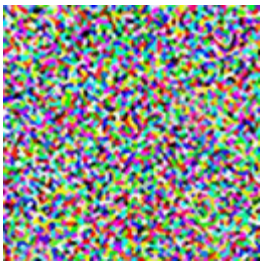
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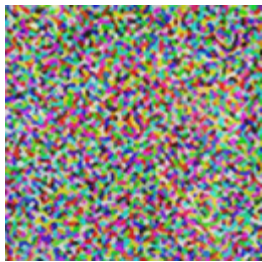


Flow matching reminder

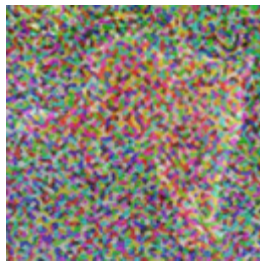
Goal: learn a velocity field $u : \mathbb{R}^d \times [0, 1] \rightarrow \mathbb{R}^d$



$X_{t=0}$



$X_{t=0.25}$



$X_{t=0.5}$



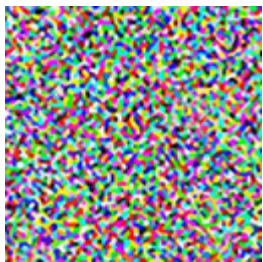
$X_{t=0.75}$



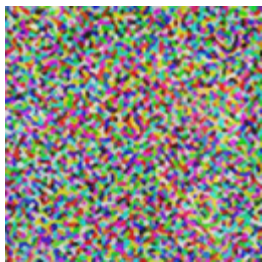
$X_{t=1}$

Flow matching reminder

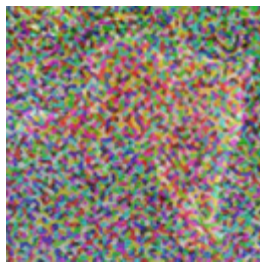
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$X_{t=1}$

Practical loss^{9,10,11}:

$$\min_{u_\theta} \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u_\theta((1-t)x_0 + tx_1, t) - (x_1 - x_0)\|^2$$

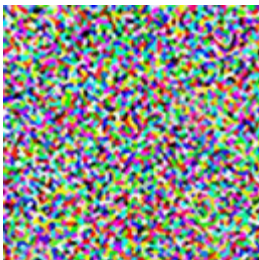
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Flow matching reminder

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$X_{t=0}$

Closed-form solution for the minimizer \hat{u}^*

$$\hat{u}^*(x, t) = \sum_{i=1}^n \lambda_i(x, t) \frac{x^{(i)} - x}{1 - t}$$

(if infinite capacity/no constraints on u_θ)



$X_{t=1}$

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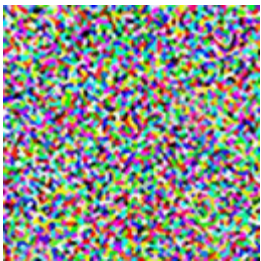
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$X_{t=1}$

Can only generate samples $x^{(1)}, \dots, x^{(n)}$ from the training set

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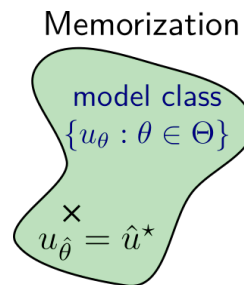
Explicit architectural regularization: idea

$$\min_{u_\theta} \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u_\theta((1-t)x_0 + tx_1, t) - (x_1 - x_0)\|^2$$

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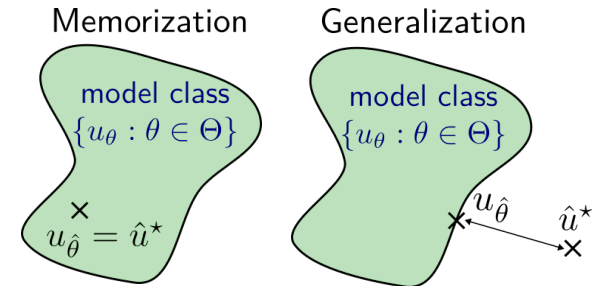
- If no constraints on u_θ /infinite capacity: **memorization**



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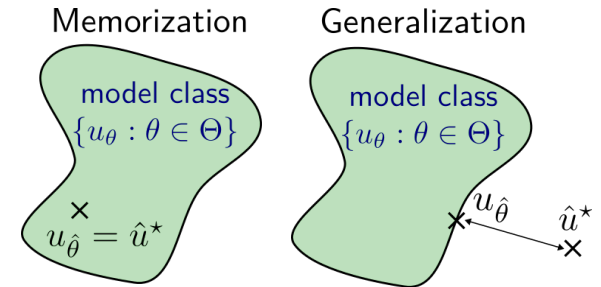
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- **In practice:** architecture regularization $u_\theta, \theta \in \Theta$
- **Minimalist model:** what about explicit constraints on the velocity field u ?^{4,5}



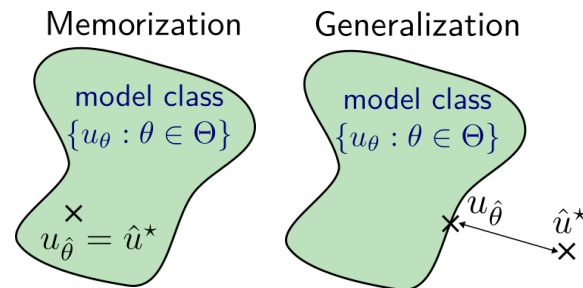
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Main idea: add explicit regularization on the score/velocity u

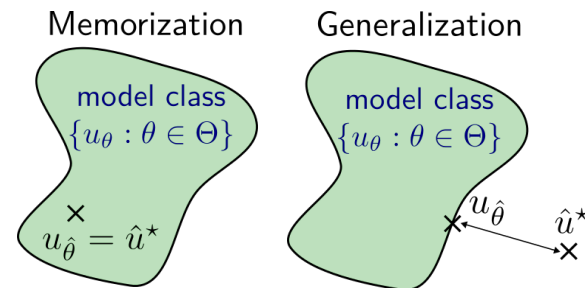
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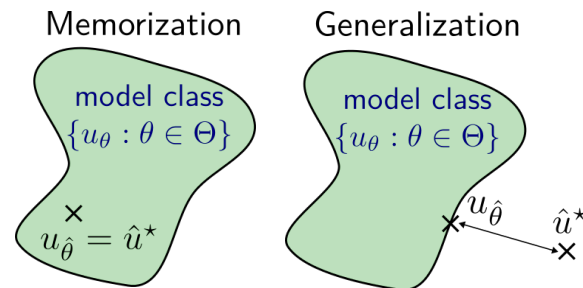
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s.t. u satisfies equivariance constraints (E)

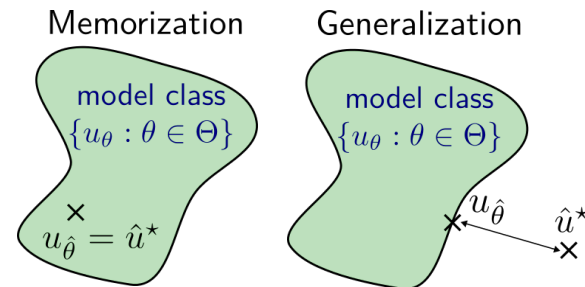
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Main idea: add explicit regularization on the score/velocity u

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u((1-t)x_0 + tx_1, t) - (x_1 - x_0)\|^2$$

s.t. u satisfies equivariance constraints (E)

u satisfies locality constraints (L)

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⁵ M. Niedoba et al., **Towards a mechanistic explanation of diffusion model generalization**, In: ICML, 2025.

Explicit architectural regularization: idea

Main results:

- Derive a closed-form formula for this constrained optimization problem
- Show that it matches images generated by a U-Net in practice

Main idea: add explicit regularization on the score/velocity u

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u((1-t)x_0 + tx_1, t) - (x_1 - x_0)\|^2$$

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Explicit architectural regularization #1: Equivariance⁴

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s.t. u satisfies equivariance constraints (Eq.)

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$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u((1-t)x_0 + tx_1, t) - (x_1 - x_0)\|^2$$

s.t. $T(u(x, t)) = u(T(x), t)$, for all 2D translations T (Eq.)

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Explicit architectural regularization #1: Equivariance⁴

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u((1-t)x_0 + tx_1, t) - (x_1 - x_0)\|^2$$

$$\text{s.t. } T(u(x, t)) = u(T(x), t), \text{ for all 2D translations } T \text{ (Eq.)}$$

Closed-form solution for the minimizer $\hat{u}_{\text{Eq.}}^*$ with equivariance constraints

$$\hat{u}_{\text{Eq.}}^*(x, t) := \sum_{i=1}^n \sum_{T \in \mathcal{T}^{2D}} \lambda_{i,T}(x, t) \left(\frac{T(x^{(i)}) - x}{1-t} \right)$$

$$\lambda_{i,T}(x, t) := \text{softmax} \left(-\frac{\|tT(x^{(j)}) - x\|^2}{2(1-t)^2} \right)_{i,T}$$

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Explicit architectural regularization #1: Equivariance⁴

Reminder: closed-form formula without equivariance

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Equivalent to data augmentation

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Explicit architectural regularization #2: Locality⁴

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Explicit architectural regularization #2: Locality⁴

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u((1-t)x_0 + tx_1, t) - (x_1 - x_0)\|^2$$

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Explicit architectural regularization #2: Locality⁴

$$\begin{aligned} \min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} & \quad \left\| u((1-t)x_0 + tx_1, t) - (x_1 - x_0) \right\|^2 \\ \text{s.t. } u & \text{ satisfies locality constraints (Loc.)} \end{aligned}$$

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Explicit architectural regularization #2: Locality⁴

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u((1-t)x_0 + tx_1, t) - (x_1 - x_0)\|^2$$

$$\text{s.t. } u^q(x, t) = u^q(M_t^q \odot x, t) \text{ (Loc.)}$$

M_t^q : binary mask centered on pixel q

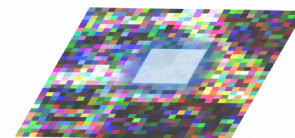
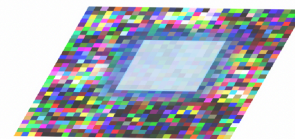
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$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u((1-t)x_0 + tx_1, t) - (x_1 - x_0)\|^2$$

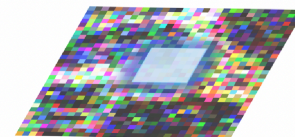
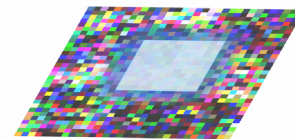
$$\text{s.t. } u^q(x, t) = u^q(M_t^q \odot x, t) \text{ (Loc.)}$$

M_t^q : binary mask centered on pixel q

Closed-form solution for the minimizer $\hat{u}_{\text{Loc.}}^*$ with locality constraints

$$\hat{u}_{\text{Loc.}}^*(x, t) = \sum_{i=1}^n \lambda_i(x, t) \odot \left(\frac{x^{(i)} - x}{1-t} \right)$$

$$\lambda_i(x, t)^q = \text{softmax} \left(-\frac{\|M_t^q \odot (tx^{(j)} - x)\|^2}{2(1-t)^2} \right)_i$$



⁴ M. Kamb et al., An Analytic Theory of Creativity in Convolutional Diffusion Models, In: ICML, 2025.

Explicit architectural regularization #2: Locality⁴

Constraint is on the denoiser. Not on the velocity field.

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u((1-t)x_0 + tx_1, t) - (x_1 - x_0)\|^2$$

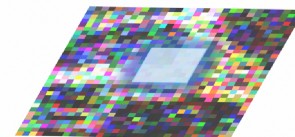
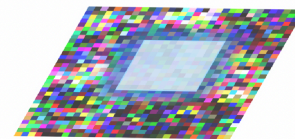
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$$\lambda_i(x, t)^q = \text{softmax} \left(-\frac{\|M_t^q \odot (tx^{(j)} - x)\|^2}{2(1-t)^2} \right)_i$$



⁴ M. Kamb et al., An Analytic Theory of Creativity in Convolutional Diffusion Models, In: ICML, 2025.

Equivariance AND Locality⁴

⁴ M. Kamb et al., **An Analytic Theory of Creativity in Convolutional Diffusion Models**, In: ICML, 2025.

Equivariance AND Locality⁴

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u((1-t)x_0 + tx_1, t) - (x_1 - x_0)\|^2$$

⁴ M. Kamb et al., *An Analytic Theory of Creativity in Convolutional Diffusion Models*, In: ICML, 2025.

Equivariance AND Locality⁴

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u((1-t)x_0 + tx_1, t) - (x_1 - x_0)\|^2$$

s.t. u satisfies equivariance constraints (Eq.)

s.t. u satisfies locality constraints (Loc.)

⁴ M. Kamb et al., *An Analytic Theory of Creativity in Convolutional Diffusion Models*, In: ICML, 2025.

Equivariance AND Locality⁴

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u((1-t)x_0 + tx_1, t) - (x_1 - x_0)\|^2$$

s.t. $T(u(x, t)) = u(T(x), t)$, for all 2D translations T (Eq.)

s.t. $u^q(x, t) = u^q(M_t^q \odot x, t)$ (Loc.)

M_t^q : Binary mask centered on pixel q

⁴ M. Kamb et al., An Analytic Theory of Creativity in Convolutional Diffusion Models, In: ICML, 2025.

Equivariance AND Locality⁴

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u((1-t)x_0 + tx_1, t) - (x_1 - x_0)\|^2$$

s.t. $T(u(x, t)) = u(T(x), t)$, for all 2D translations T (Eq.)

s.t. $u^q(x, t) = u^q(M_t^q \odot x, t)$ (Loc.)

M_t^q : Binary mask centered on pixel q

Closed-form solution for the minimizer $\hat{u}_{\text{E+L}}^*$ with locality constraints

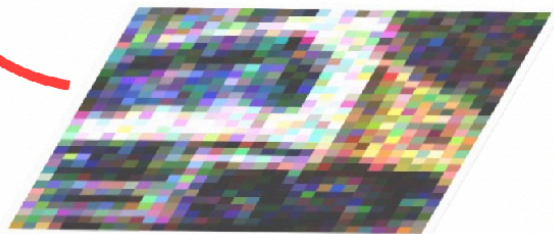
$$\hat{u}_{\text{Eq.}+\text{Loc.}}^*(x, t) = \sum_{i=1}^n \sum_{T \in \mathcal{T}^{2D}} \lambda_{i,T}(x, t) \odot \left(\frac{T(x^{(i)}) - x}{1-t} \right)$$

$$\lambda_{i,T}(x, t)^q = \text{softmax} \left(-\frac{\|M_t^q \odot (tT(x^{(j)}) - x)\|^2}{2(1-t)^2} \right)_{i,T}$$

⁴ M. Kamb et al., An Analytic Theory of Creativity in Convolutional Diffusion Models, In: ICML, 2025.

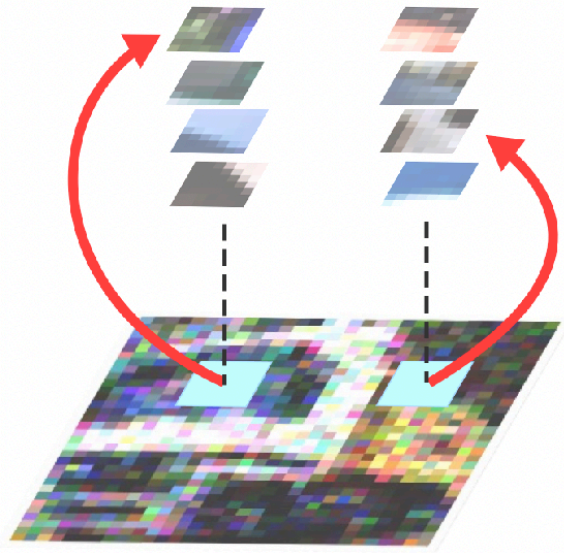
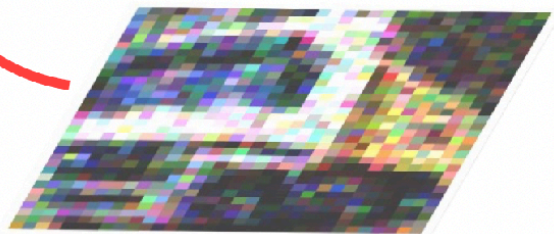
Illustration of the impact of locality & equiv. constraints

Illustration of the impact of locality & equiv. constraints



Vanilla closed-form

Illustration of the impact of locality & equiv. constraints



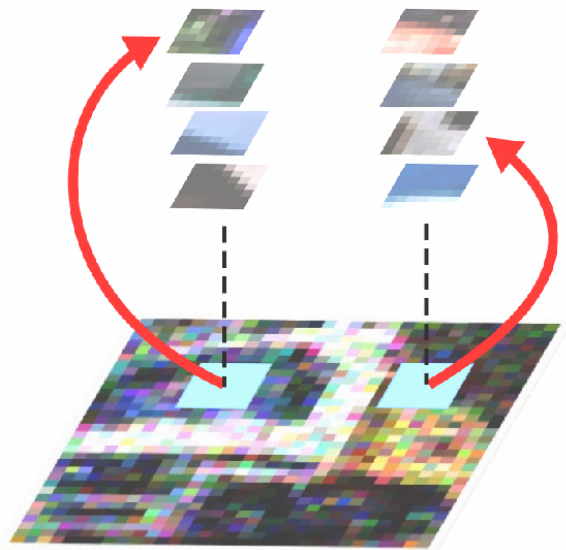
Vanilla closed-form

Closed-form for
locality constraints

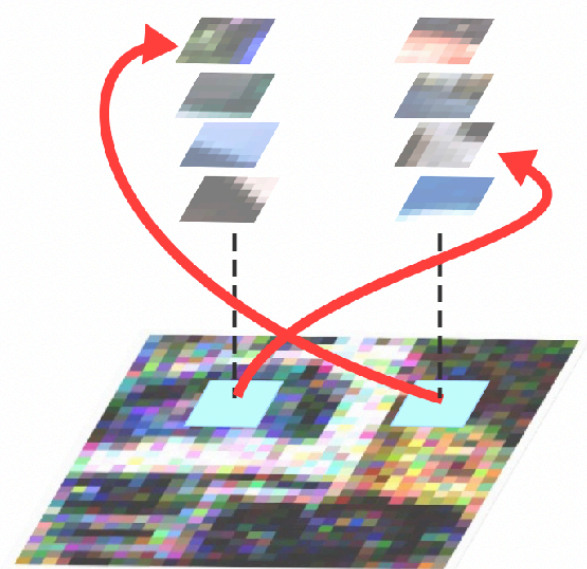
Illustration of the impact of locality & equiv. constraints



Vanilla closed-form



Closed-form for
locality constraints



Closed-form for locality +
equivariance constraints₁₂

Empirical validation: closed-form vs U-Net

Empirical validation: closed-form vs U-Net

Left: Closed-Form with Locality and Equivariance Constraints

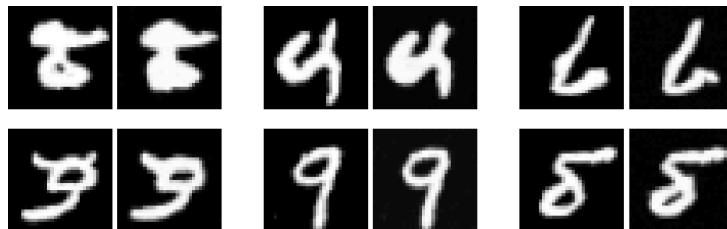
Right: Learned (small) U-Net

Empirical validation: closed-form vs U-Net

Left: Closed-Form with Locality and Equivariance Constraints

Right: Learned (small) U-Net

MNIST

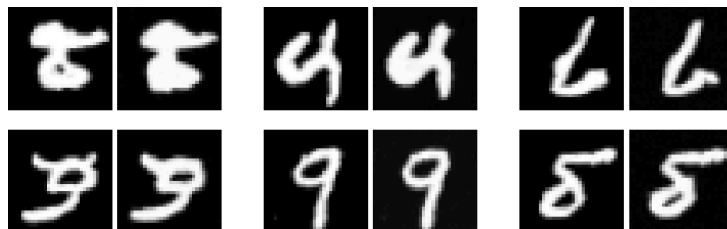


Empirical validation: closed-form vs U-Net

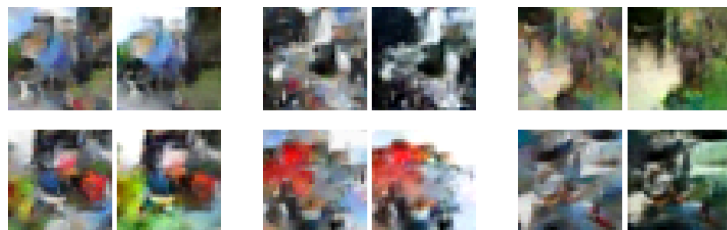
Left: Closed-Form with Locality and Equivariance Constraints

Right: Learned (small) U-Net

MNIST



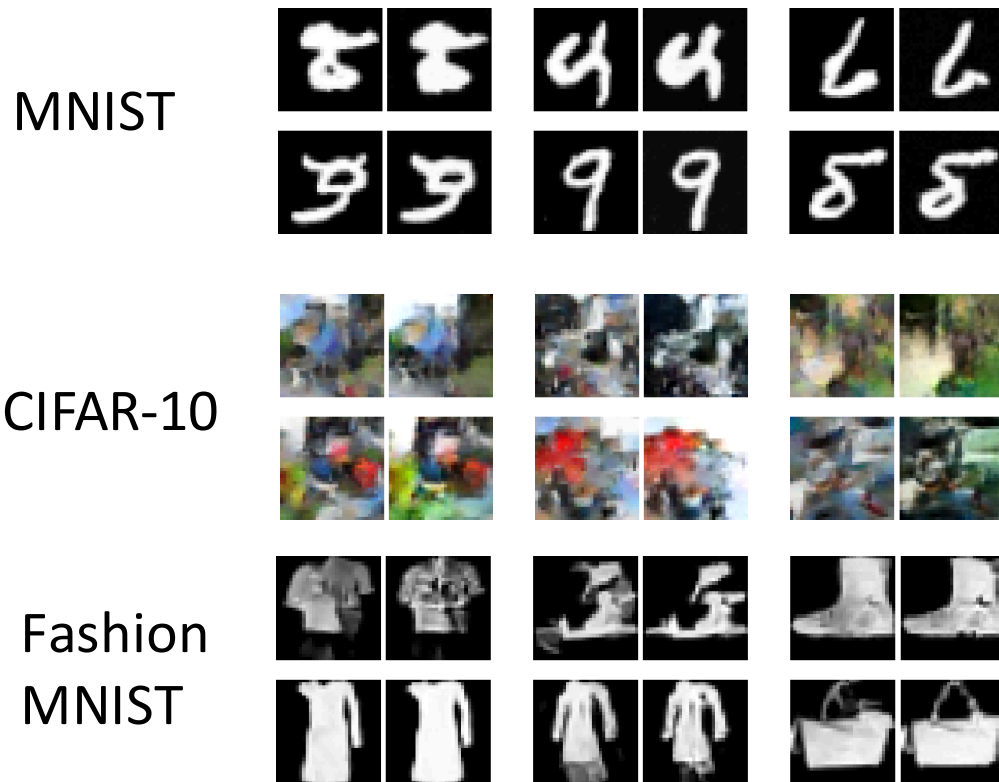
CIFAR-10



Empirical validation: closed-form vs U-Net

Left: Closed-Form with Locality and Equivariance Constraints

Right: Learned (small) U-Net

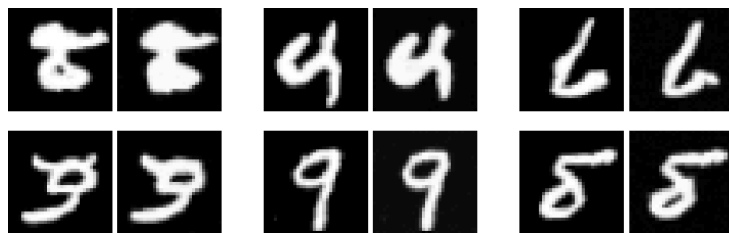


Empirical validation: closed-form vs U-Net

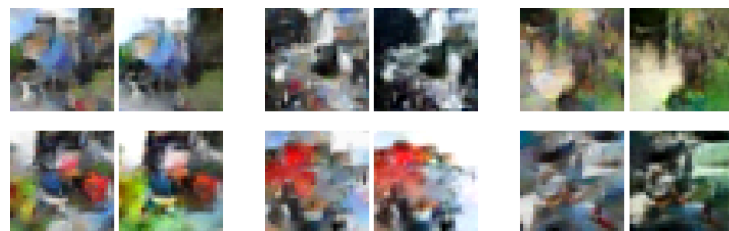
Left: Closed-Form with Locality and Equivariance Constraints

Right: Learned (small) U-Net

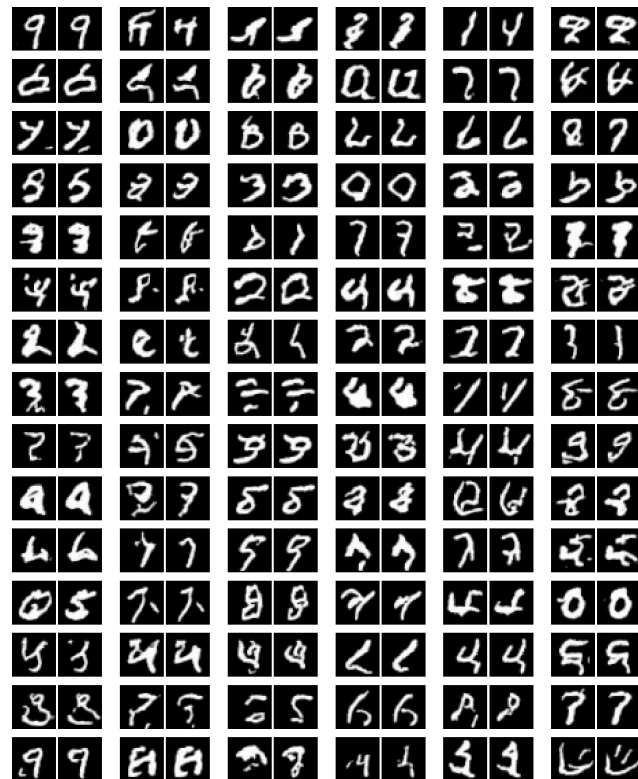
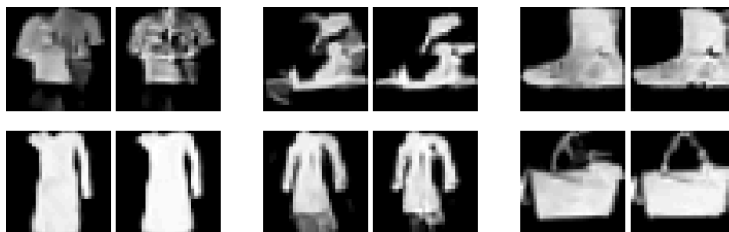
MNIST



CIFAR-10



Fashion
MNIST



Empirical validation: receptive field comparison 1/2

Empirical validation: receptive field comparison 1/2

What is a receptive field?

Empirical validation: receptive field comparison 1/2

- Learned velocity field $u_\theta(x, t)$

What is a receptive field?

Empirical validation: receptive field comparison 1/2

- Learned velocity field $u_\theta(x, t)$
image
- Learned velocity field $u_\theta(\underbrace{x}_{\text{image}}, t)$

What is a receptive field?

Empirical validation: receptive field comparison 1/2

- Learned velocity field $u_\theta(x, t)$
- Learned velocity field $u_\theta(\underbrace{x}_{\text{image}}, t)$
- Value of the velocity field at pixel q : $u_\theta^q(\underbrace{x}_{\text{image}}, t)$
 $\in \mathbb{R}$, real valued

What is a receptive field?

Empirical validation: receptive field comparison 1/2

- Learned velocity field $u_\theta(x, t)$
- Learned velocity field $u_\theta(\underbrace{x}_{\text{image}}, t)$ What is a receptive field?
- Value of the velocity field at pixel q : $u_\theta^q(\underbrace{x}_{\text{image}}, t)$ Question
 $\in \mathbb{R}$, real valued

Empirical validation: receptive field comparison 1/2

- Learned velocity field $u_\theta(x, t)$

- Learned velocity field $u_\theta(\overbrace{x}^{\text{image}}, t)$

What is a receptive field?

- Value of the velocity field at pixel q : $u_\theta^q(\overbrace{x}^{\text{image}}, t)$
 $\in \mathbb{R}$, real valued

Question

What is the size of $\nabla_x u_\theta^q(\overbrace{x}^{\text{image}}, t)$?

Empirical validation: receptive field comparison 1/2

- Learned velocity field $u_\theta(x, t)$

- Learned velocity field $u_\theta(\underbrace{x}_{\text{image}}, t)$

What is a receptive field?

- Value of the velocity field at pixel q : $u_\theta^q(\underbrace{x}_{\text{image}}, t)$
 $\in \mathbb{R}$, real valued

Question

- $\underbrace{\nabla_x u_\theta^q(\underbrace{x}_{\text{image}}, t)}_{\text{image}}?$

What is the size of $\nabla_x u_\theta^q(\underbrace{x}_{\text{image}}, t)$?

Empirical validation: receptive field comparison 1/2

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- Learned velocity field $u_\theta(\underbrace{x}_{\text{image}}, t)$
- Value of the velocity field at pixel q : $u_\theta^q(\underbrace{x}_{\text{image}}, t)$
 $\in \mathbb{R}$, real valued

What is a receptive field?

Question

- $\underbrace{\nabla_x u_\theta^q(\underbrace{x}_{\text{image}}, t)}_{\text{image}}?$

What is the size of $\nabla_x u_\theta^q(\underbrace{x}_{\text{image}}, t)$?

$$\underbrace{\nabla_x u_\theta^q(\underbrace{x}_{\text{image}}, t)}_{\text{image}}$$

image; receptive field at pixel q

Empirical validation: receptive field comparison 1/2

- Learned velocity field $u_\theta(x, t)$
- Learned velocity field $u_\theta(\underbrace{x}_{\text{image}}, t)$
- Value of the velocity field at pixel q : $u_\theta^q(\underbrace{x}_{\text{image}}, t)$
 $\in \mathbb{R}$, real valued

What is a receptive field?

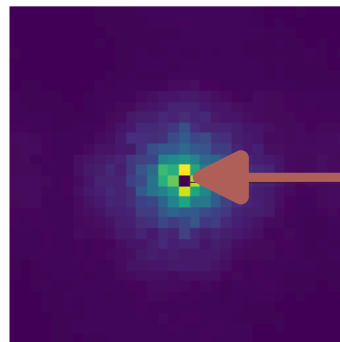
Question

- $\underbrace{\nabla_x u_\theta^q(\underbrace{x}_{\text{image}}, t)}_{\text{image}}?$

What is the size of $\nabla_x u_\theta^q(\underbrace{x}_{\text{image}}, t)$?

$$\underbrace{\nabla_x u_\theta^q(\underbrace{x}_{\text{image}}, t)}_{\text{image}}$$

image; receptive field at pixel q



Pixel q

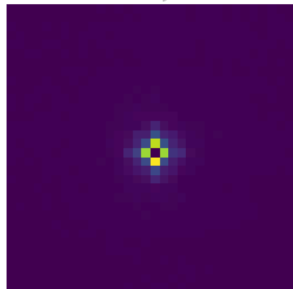
Empirical validation: receptive field comparison 2/2

Empirical validation: receptive field comparison 2/2

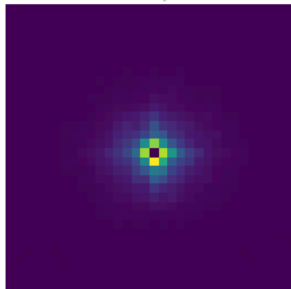
$$\begin{array}{c} \text{image} \\ \nabla_x u_\theta^q(\underbrace{x}, t) \\ \underbrace{\hspace{10em}} \\ \text{receptive field at pixel } q \end{array}$$

Empirical validation: receptive field comparison 2/2

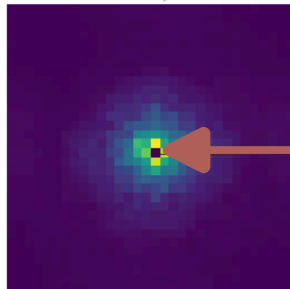
$t = 0.95$



$t = 0.5$



$t = 0$



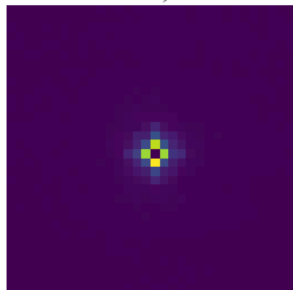
U-Net

Pixel q

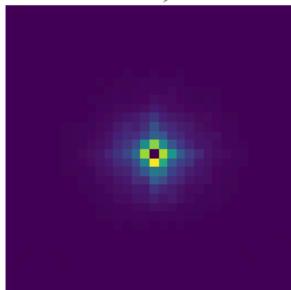
$$\underbrace{\nabla_x u_\theta^q(\overbrace{x}^{\text{image}}, t)}_{\text{receptive field at pixel } q}$$

Empirical validation: receptive field comparison 2/2

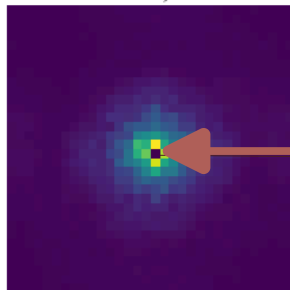
$t = 0.95$



$t = 0.5$



$t = 0$



Pixel q

image

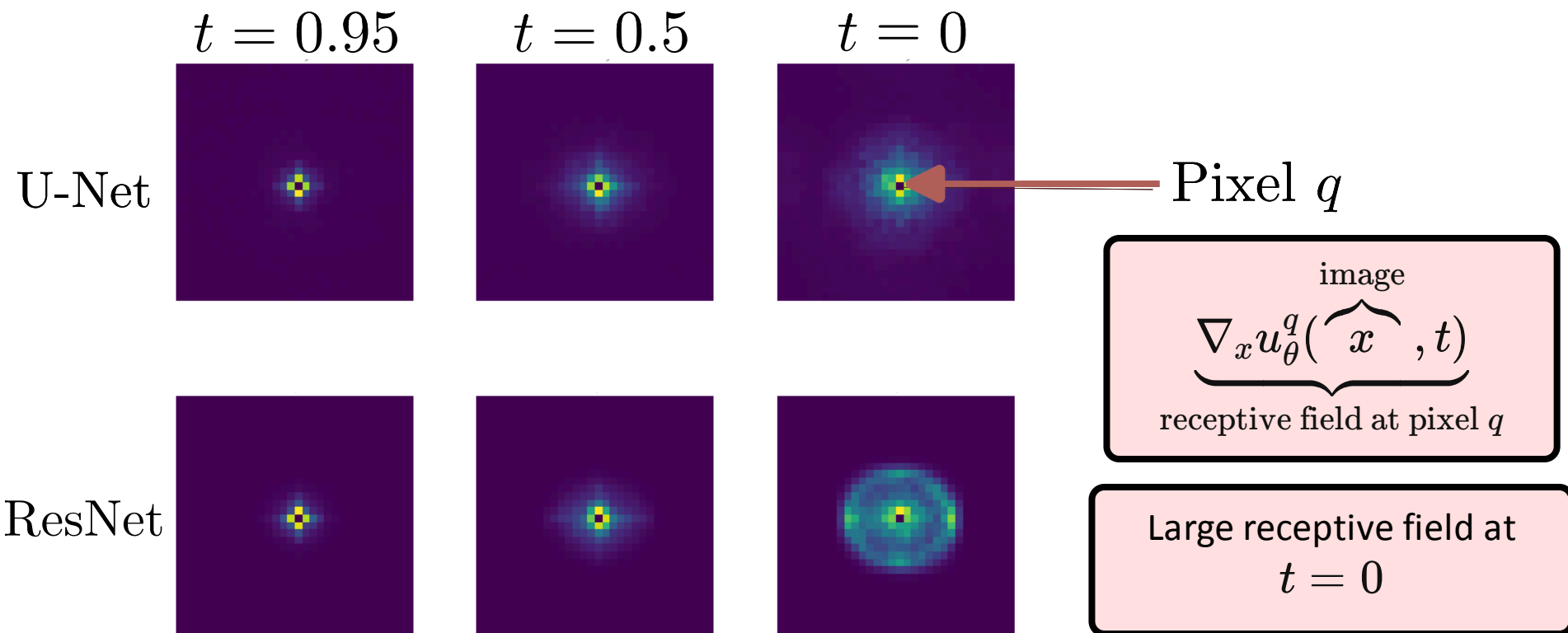
$$\nabla_x u_\theta^q(\underbrace{x}_{\text{receptive field at pixel } q}, t)$$

receptive field at pixel q

Large receptive field at
 $t = 0$

U-Net

Empirical validation: receptive field comparison 2/2



Local mask constraint limitations⁶

Locality constraint reminder

$$\begin{aligned} \min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim p_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} & \|u(tx_1 + (1-t)x_0, t) - (x_1 - x_0)\|^2 \\ \text{s.t. } & u^q(x, t) = u^q(M_t^q \odot x, t), \text{ (Loc.)} \\ & M_t^q : \text{ Binary mask centered on pixel } q \end{aligned}$$

⁶ A. Lukoianov et al., **Locality in Image Diffusion Models Emerges From Data Statistics**, In: NeurIPS, 2025.

Local mask constraint limitations⁶

Locality constraint reminder

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim p_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u(tx_1 + (1-t)x_0, t) - (x_1 - x_0)\|^2$$

Limitations:

$$\text{s.t. } u^q(x, t) = u^q(M_t^q \odot x, t), (\text{Loc.})$$

M_t^q : Binary mask centered on pixel q

⁶ A. Lukoianov et al., **Locality in Image Diffusion Models Emerges From Data Statistics**, In: NeurIPS, 2025.

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$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim p_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u(tx_1 + (1-t)x_0, t) - (x_1 - x_0)\|^2$$

Limitations:

$$\text{s.t. } u^q(x, t) = u^q(M_t^q \odot x, t), (\text{Loc.})$$

M_t^q : Binary mask centered on pixel q

How to choose the binary mask constraints M_t^q ?

⁶ A. Lukoianov et al., *Locality in Image Diffusion Models Emerges From Data Statistics*, In: NeurIPS, 2025.

Local mask constraint limitations⁶

Locality constraint reminder

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim p_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u(tx_1 + (1-t)x_0, t) - (x_1 - x_0)\|^2$$

Limitations:

$$\text{s.t. } u^q(x, t) = u^q(M_t^q \odot x, t), (\text{Loc.})$$

M_t^q : Binary mask centered on pixel q

How to choose the binary mask constraints M_t^q ?

- One mask for each pixel q

⁶ A. Lukoianov et al., *Locality in Image Diffusion Models Emerges From Data Statistics*, In: NeurIPS, 2025.

Local mask constraint limitations⁶

Locality constraint reminder

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim p_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u(tx_1 + (1-t)x_0, t) - (x_1 - x_0)\|^2$$

Limitations:

$$\text{s.t. } u^q(x, t) = u^q(M_t^q \odot x, t), (\text{Loc.})$$

M_t^q : Binary mask centered on pixel q

How to choose the binary mask constraints M_t^q ?

- One mask for each pixel q
- And for each time t

⁶ A. Lukoianov et al., *Locality in Image Diffusion Models Emerges From Data Statistics*, In: NeurIPS, 2025.

Local mask constraint limitations⁶

Locality constraint reminder

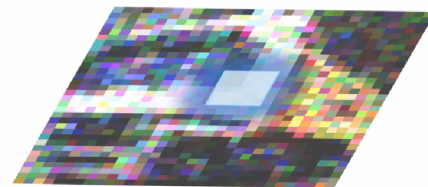
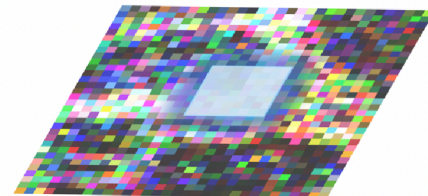
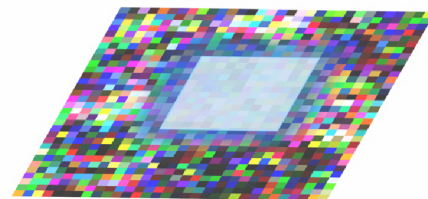
$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim p_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u(tx_1 + (1-t)x_0, t) - (x_1 - x_0)\|^2$$

Limitations:

s.t. $u^q(x, t) = u^q(M_t^q \odot x, t)$, (Loc.)
 M_t^q : Binary mask centered on pixel q

How to choose the binary mask constraints M_t^q ?

- One mask for each pixel q
- And for each time t



⁶ A. Lukoianov et al., *Locality in Image Diffusion Models Emerges From Data Statistics*, In: NeurIPS, 2025.

Local mask constraint limitations⁶

Locality constraint reminder

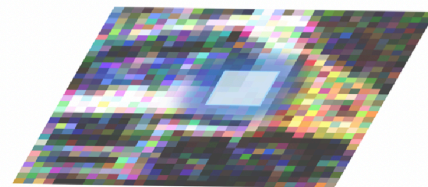
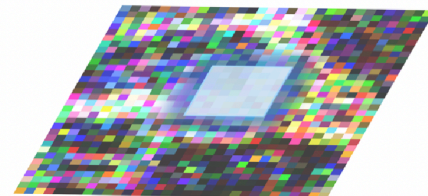
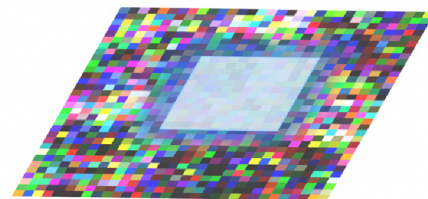
$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim p_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u(tx_1 + (1-t)x_0, t) - (x_1 - x_0)\|^2$$

Limitations:

s.t. $u^q(x, t) = u^q(M_t^q \odot x, t)$, (Loc.)
 M_t^q : Binary mask centered on pixel q

How to choose the binary mask constraints M_t^q ?

- One mask for each pixel q
- And for each time t
- Not trivial



⁶ A. Lukoianov et al., *Locality in Image Diffusion Models Emerges From Data Statistics*, In: NeurIPS, 2025.

Local mask constraint limitations⁶

Locality constraint reminder

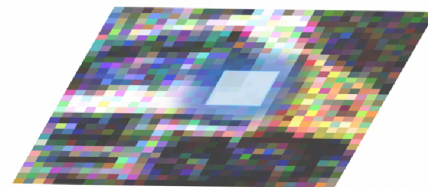
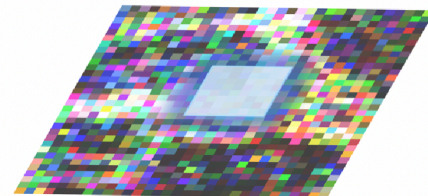
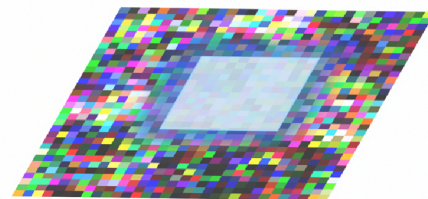
$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim p_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u(tx_1 + (1-t)x_0, t) - (x_1 - x_0)\|^2$$

Limitations:

s.t. $u^q(x, t) = u^q(M_t^q \odot x, t)$, (Loc.)
 M_t^q : Binary mask centered on pixel q

How to choose the binary mask constraints M_t^q ?

- One mask for each pixel q
- And for each time t
- Not trivial
- Cross-validated using a pre-trained U-Net u_θ



⁶ A. Lukoianov et al., *Locality in Image Diffusion Models Emerges From Data Statistics*, In: NeurIPS, 2025.

Local mask constraint limitations⁶

Locality constraint reminder

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim p_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u(tx_1 + (1-t)x_0, t) - (x_1 - x_0)\|^2$$

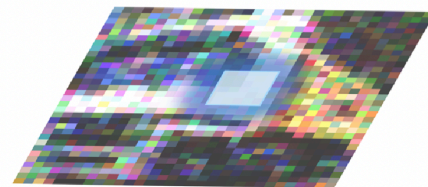
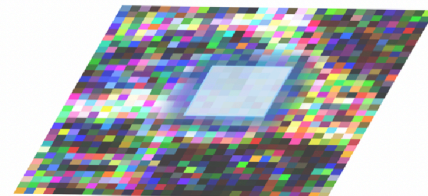
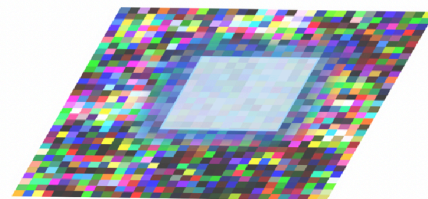
Limitations:

s.t. $u^q(x, t) = u^q(M_t^q \odot x, t)$, (Loc.)
 M_t^q : Binary mask centered on pixel q

How to choose the binary mask constraints M_t^q ?

- One mask for each pixel q
- And for each time t
- Not trivial
- Cross-validated using a pre-trained U-Net u_θ

Local receptive field: too restrictive

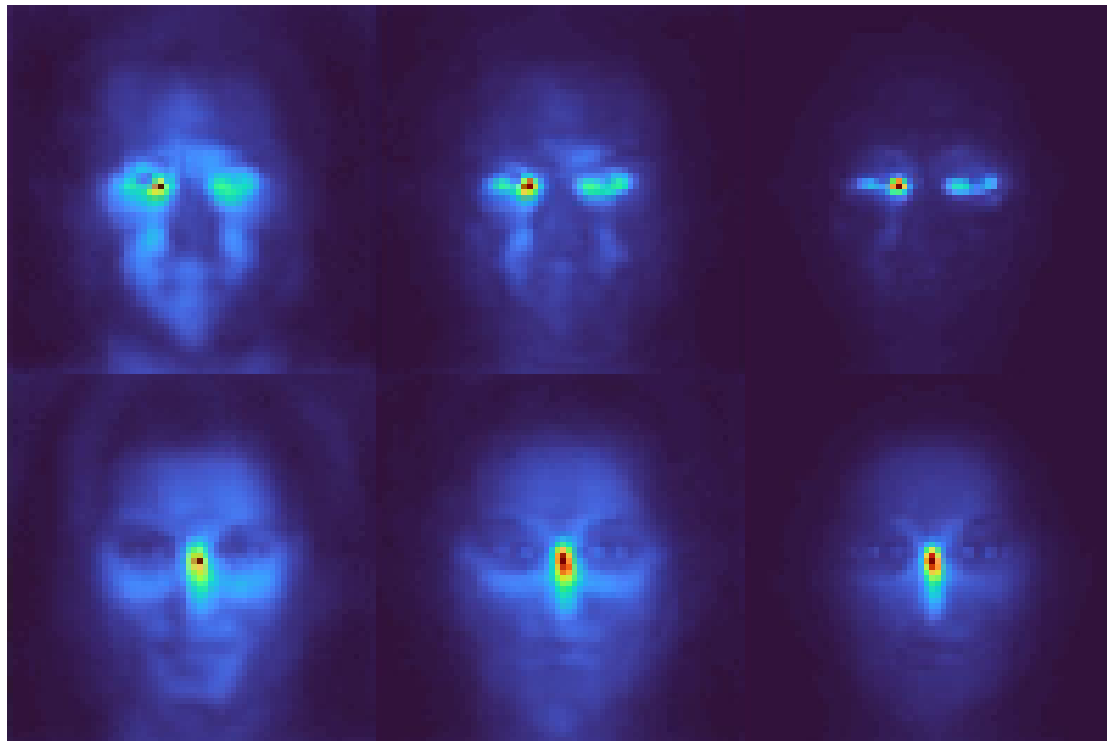


⁶ A. Lukoianov et al., Locality in Image Diffusion Models Emerges From Data Statistics, In: NeurIPS, 2025.

Example of non-local receptive field⁶

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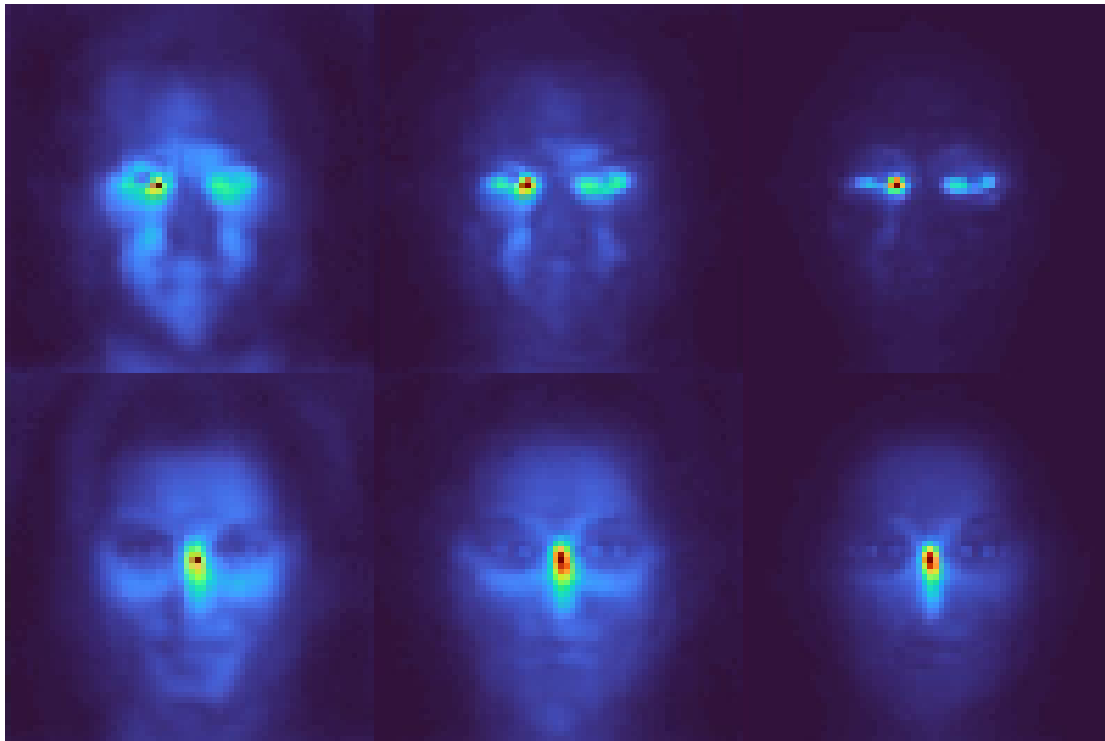
Example of non-local receptive field⁶



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Example of non-local receptive field⁶

Receptive field for the pixel in the eye: non local



⁶ A. Lukoianov et al., *Locality in Image Diffusion Models Emerges From Data Statistics*, In: NeurIPS, 2025.

Locality constraints: too restrictive?⁶

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Locality constraints: too restrictive?⁶

Main Idea 1: generalize the locality constraints

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Locality constraints: too restrictive?⁶

Main Idea 1: generalize the locality constraints

- Generalize the locality constraints M_t^q , to "correlation" constraints

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Locality constraints: too restrictive?⁶

Main Idea 1: generalize the locality constraints

- Generalize the locality constraints M_t^q , to "correlation" constraints
- Learn these correlation constraints M_t^q using a simple linear denoiser/velocity

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Main Idea 2: linear score/velocity

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \|u(tx_1 + (1-t)x_0, t) - (x_1 - x_0)\|^2$$

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What about the simple linear velocity case $u(x, t) = W_t x$?

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Linear Score/Velocity¹²

¹² B. Wang et al., **The unreasonable effectiveness of Gaussian score approximation for diffusion models and its applications**, In: TMLR, 2024.

Linear Score/Velocity¹²

$$\min_u \mathbb{E}_{\substack{x_0 \sim p_0 \\ x_1 \sim \hat{p}_{\text{data}} \\ t \sim \mathcal{U}([0,1])}} \left\| \overbrace{u((1-t)x_0 + tx_1, t)}^{\text{simple case } u(x,t)=W_t x} - (x_1 - x_0) \right\|^2$$

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Well-known result: Wiener
filter

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$$W_t = U \text{diag} \frac{(1-t) - t\lambda_i}{(1-t)^2 + t^2\lambda_i^2} U^\top \quad \text{with } \text{Cov}(X) = U \text{diag}(\lambda_1^2, \dots, \lambda_d^2) U^\top$$

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For each time t and pixel q , the most predictive pixels are given by the q -th row of W_t

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For each time t and pixel q , the most predictive pixels are given by the q -th row of W_t

The masks M_t^q are then chosen as a binarization of the q -th row of the Wiener filter W_t

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Combining all the building blocks⁶

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Combining all the building blocks⁶

W_t : Wiener filter

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$$\text{s.t. } u^q(x, t) = u^q(M_t^q \odot x, t), \text{ (Correlation)}$$

M_t^q : Binary mask centered on pixel q

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Combining all the building blocks⁶

W_t : Wiener filter

$$W_t = U \text{diag} \left((1-t) - t \lambda_i^2 \right) U^T \cdot \text{Cov}(X) = U \text{diag}(\lambda^2) U^T$$

Binary masks M_t^q : binarized q -th row of the Wiener filter
 W_t

Closed-form solution for the minimizer $u_{\text{Corr.}}^*$ with correlations

$$u_{\text{Corr.}}^*(x, t) = \sum_{i=1}^n \lambda_i(x, t) \left(\frac{x^{(i)} - x}{1-t} \right)$$

$$\lambda_i(x, t) = \text{softmax} \left(- \frac{\|M_t^q \odot (tx^{(j)} - x)\|^2}{2(1-t)^2} \right)_i$$

⁶ A. Lukoianov et al., *Locality in Image Diffusion Models Emerges From Data Statistics*, In: NeurIPS, 2025.

Empirical results⁶

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Summary and Conclusion^{4,5,6,7,8}

⁴ M. Kamb et al., **An Analytic Theory of Creativity in Convolutional Diffusion Models**, In: ICML, 2025.

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⁶ A. Lukoianov et al., **Locality in Image Diffusion Models Emerges From Data Statistics**, In: NeurIPS, 2025.

⁷ Z. Kadkhodaie et al., **Generalization in Diffusion Models Arises from Geometry-Adaptive Harmonic Representations**, In: ICLR, 2024.

⁸ Q. Bertrand et al., **On the Closed-Form of Flow Matching: Generalization Does Not Arise from Target Stochasticity**, In: NeurIPS, 2025.

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Summary and Conclusion^{4,5,6,7,8}

- Explicit regularization of the score/velocity



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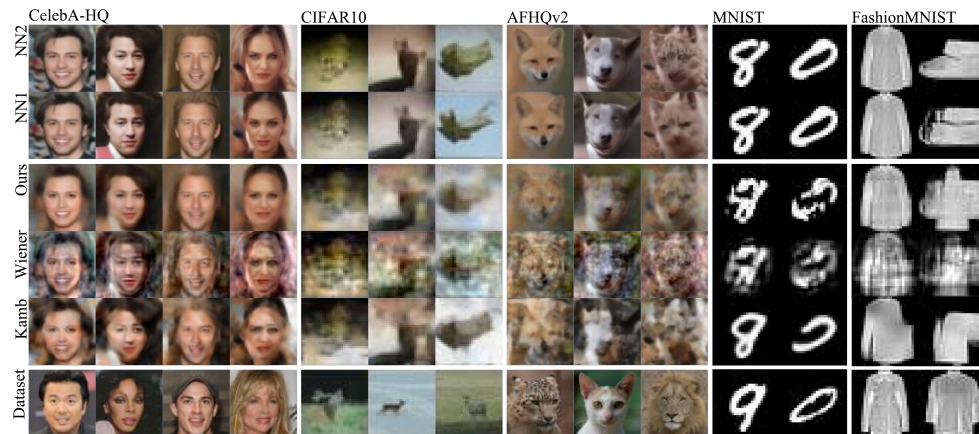
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Summary and Conclusion^{4,5,6,7,8}

- Explicit regularization of the score/velocity
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Summary and Conclusion^{4,5,6,7,8}

- Explicit regularization of the score/velocity
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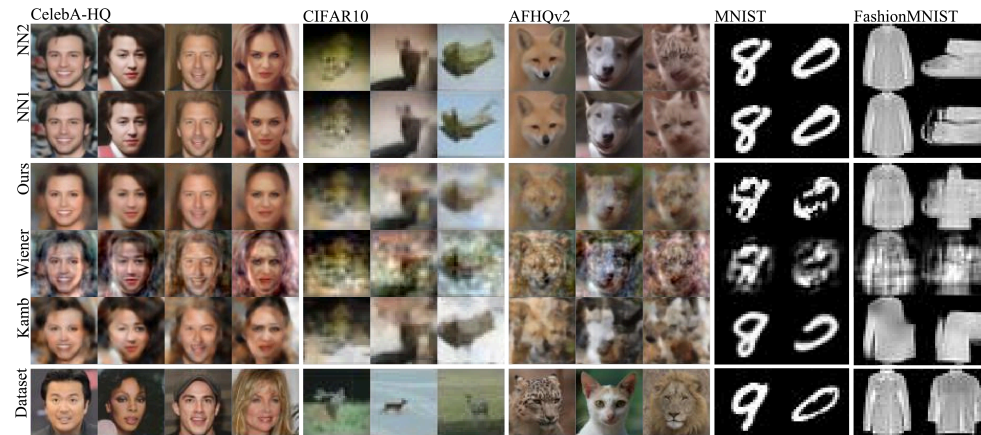
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Summary and Conclusion^{4,5,6,7,8}

- Explicit regularization of the score/velocity
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 - Generalization of locality to correlation constraints



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Summary and Conclusion^{4,5,6,7,8}

- Explicit regularization of the score/velocity
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 - Generalization of locality to correlation constraints
- Closed-form formula for the constrained problem



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Summary and Conclusion^{4,5,6,7,8}

- Explicit regularization of the score/velocity
 - Equivariance
 - Locality constraints
 - Generalization of locality to correlation constraints
- Closed-form formula for the constrained problem
 - Empirically "match well" small U-Nets



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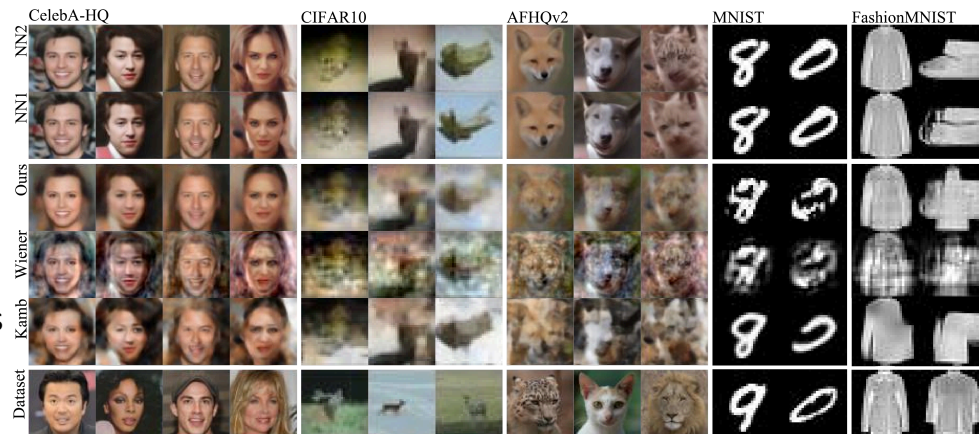
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- Explicit regularization of the score/velocity
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 - Empirically "match well" small U-Nets
 - Gives intuition on how small diffusion models works



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Thank you for your attention!

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ICML 2026 tutorial

Diffusion and Flow Matching

Part IV: Open Questions & Discussions

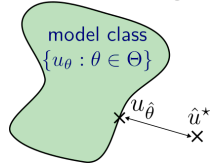
Quentin Bertrand & Mathurin Massias

<https://memorization-generalization.github.io>

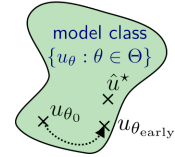
Inria | ENS Lyon | Laboratoire Hubert Curien | Mila Affiliated Member | CIFAR Global Scholar

Over- vs under-parameterized models

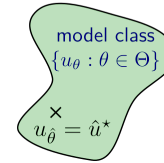
Architectural reg.



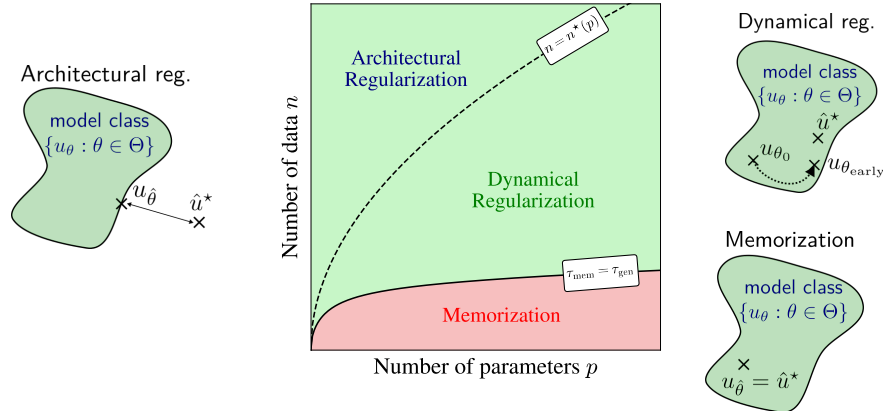
Dynamical reg.



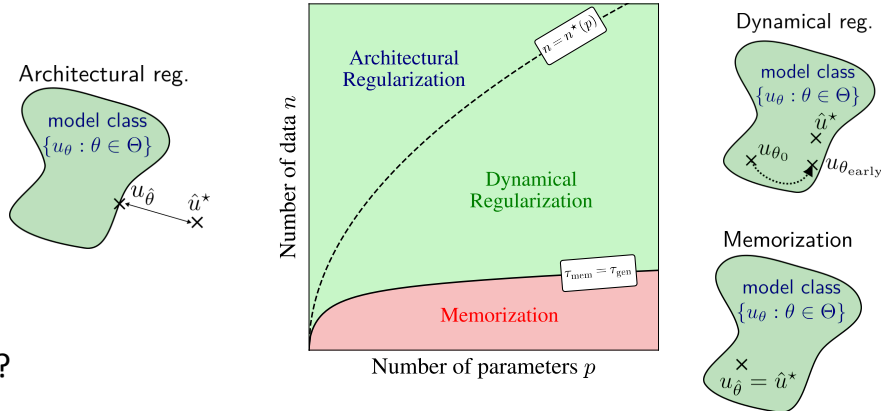
Memorization



Over- vs under-parameterized models

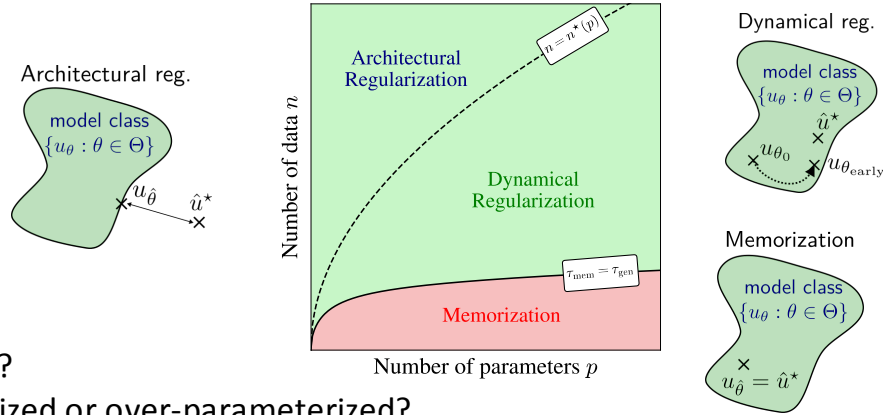


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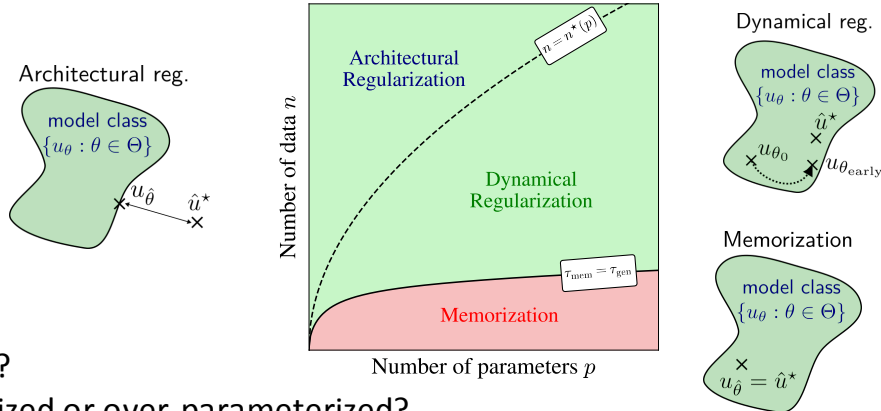
- Which regime are we in?

Over- vs under-parameterized models



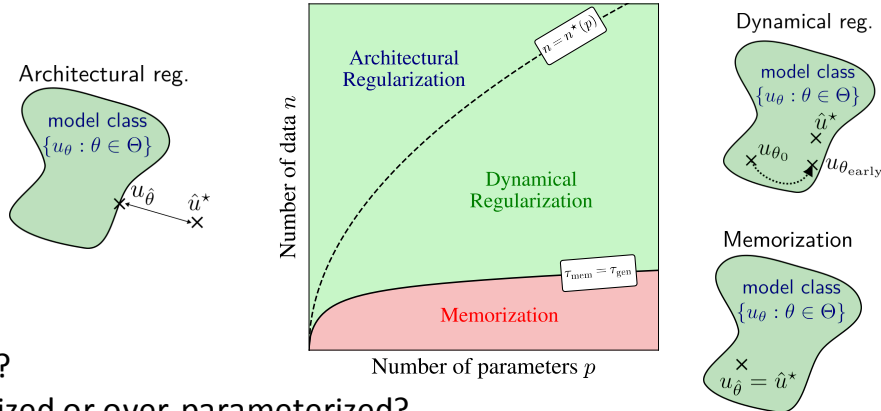
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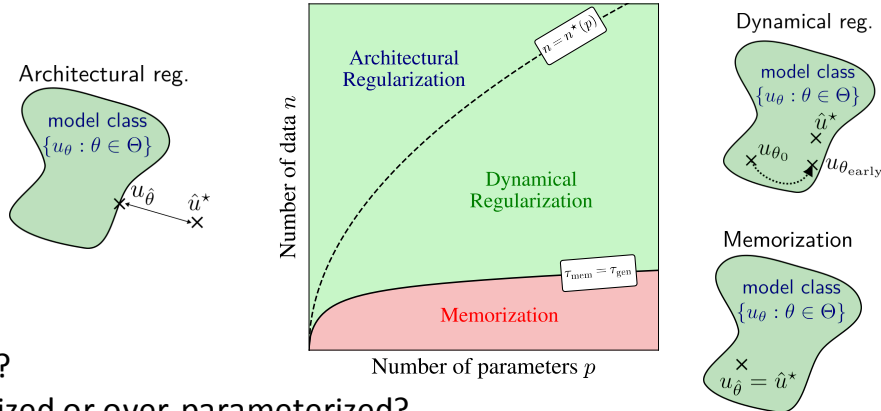
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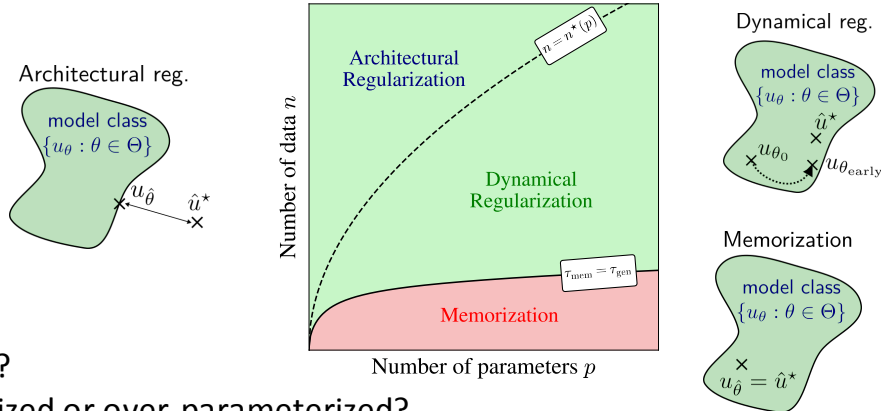
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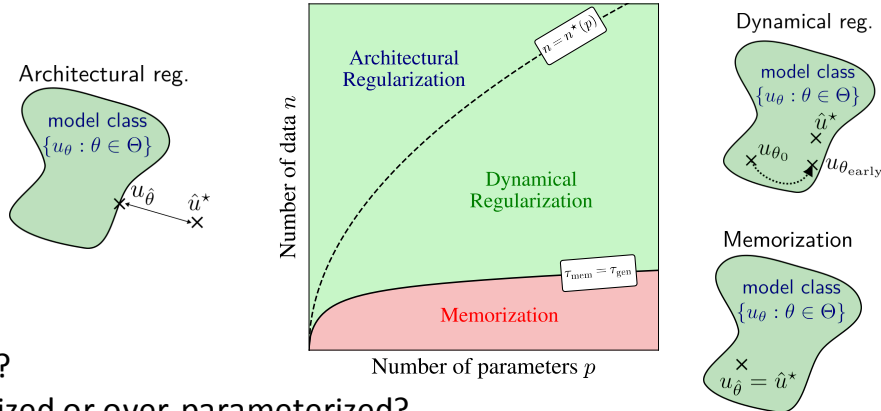
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Over- vs under-parameterized models



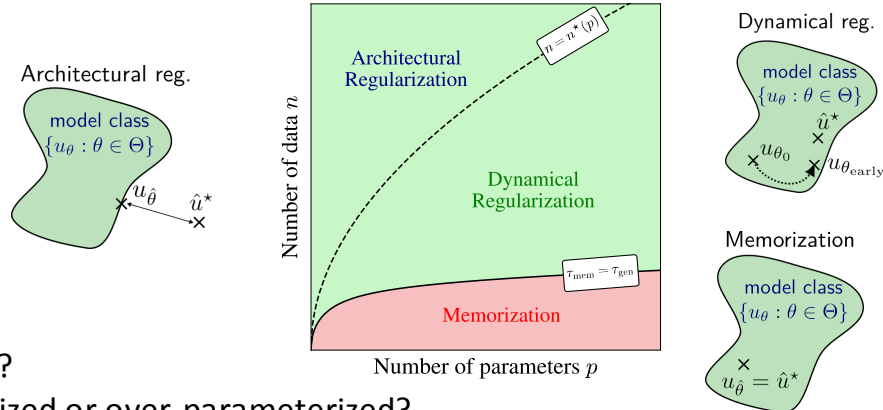
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Over- vs under-parameterized models



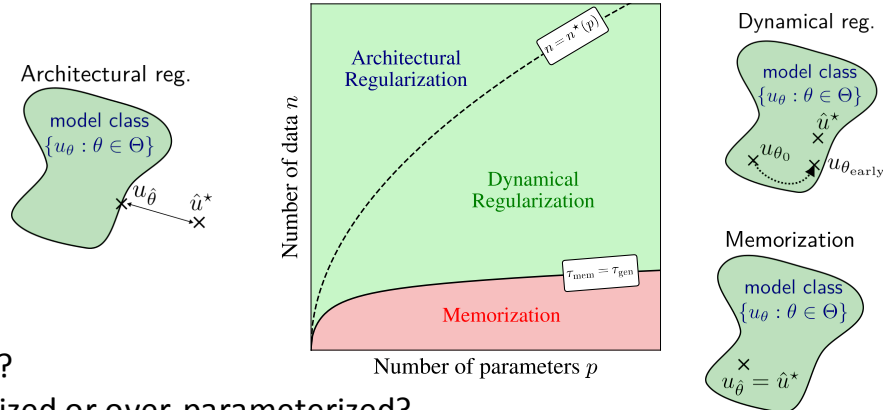
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 - Would the error vanish if we train for longer?

Over- vs under-parameterized models



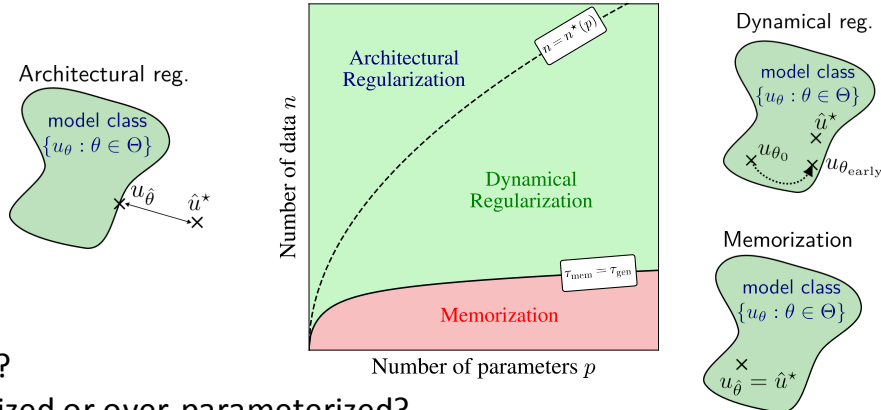
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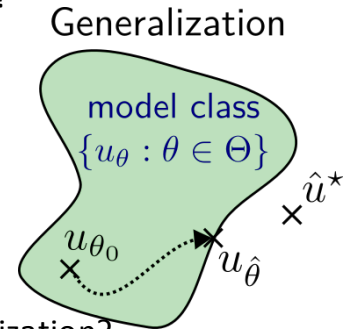


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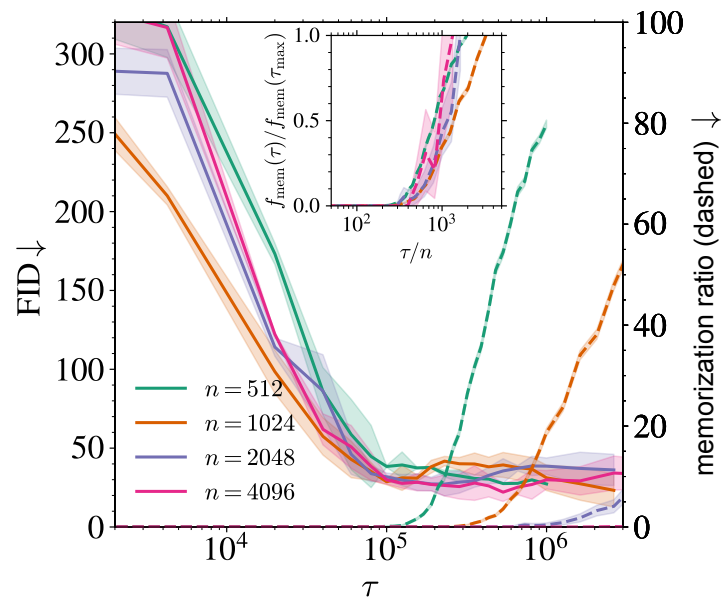
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- Can we combine the 2 points of view/analyses?
 - Interaction between architectural inductive bias + dynamical regularization of the optimization?



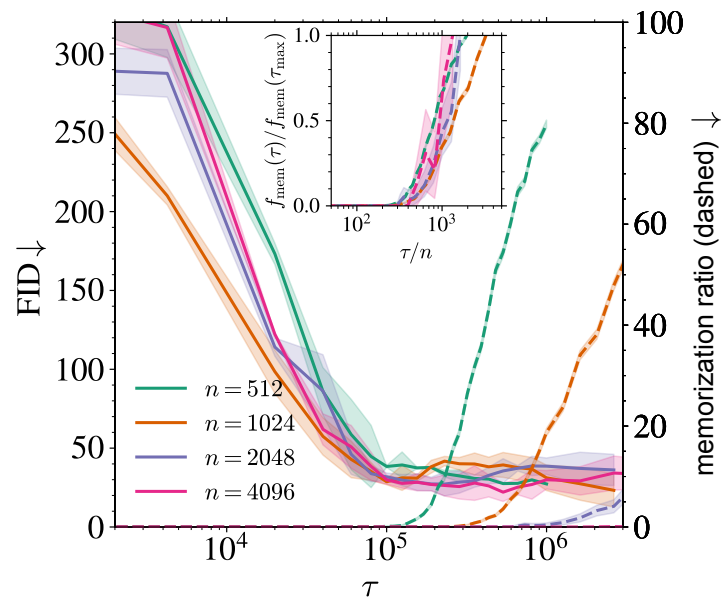
Memorization/Generalization dichotomy?



Bonnaire et al. (2025)

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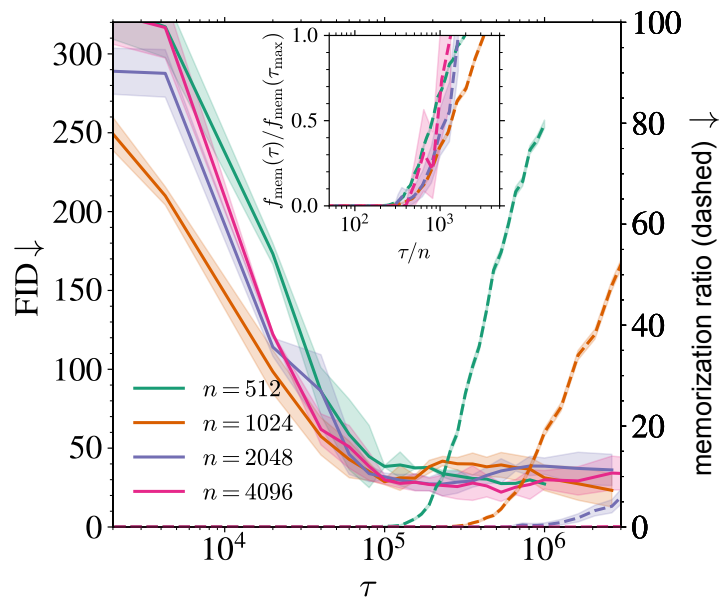
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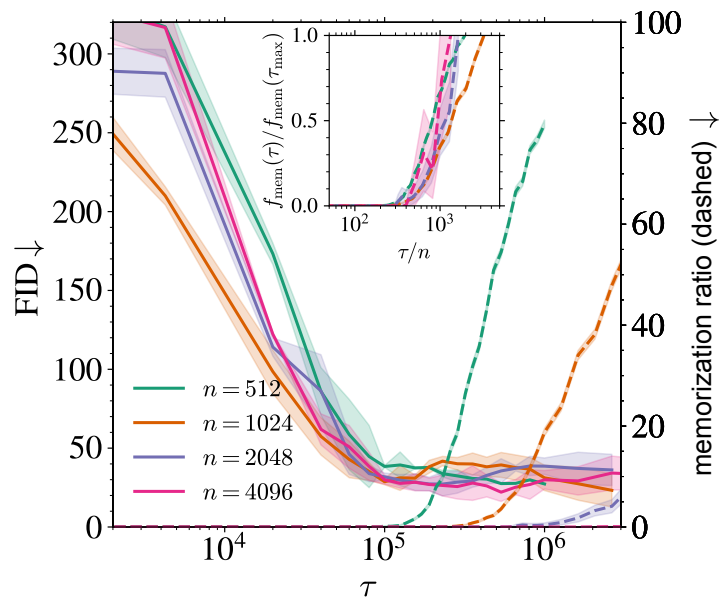
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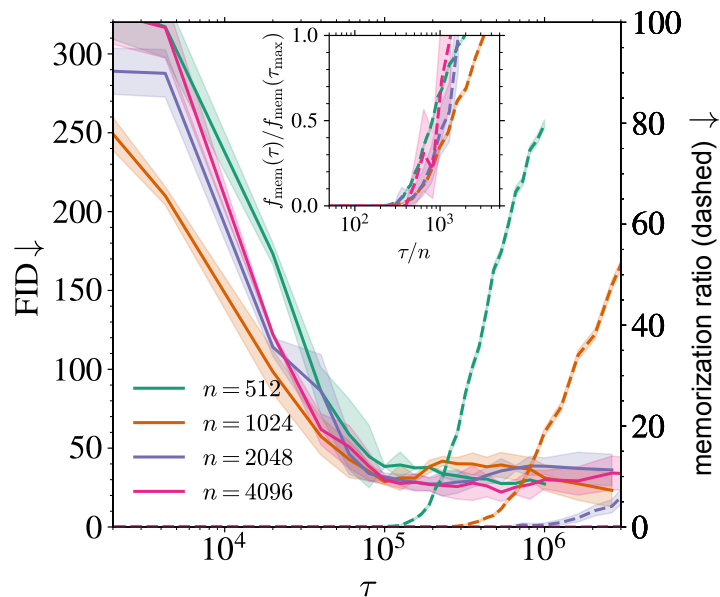
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Bonnaire et al. (2025)

Memorization/Generalization dichotomy?

- Currently: transition phase memorization vs generalization
 - In practice? How fast is the transition?
 - More complex than a transition phase?
 - Which samples are memorized? Easy to memorize?
 - Sample level memorization?
 - What about classes with a few examples?¹



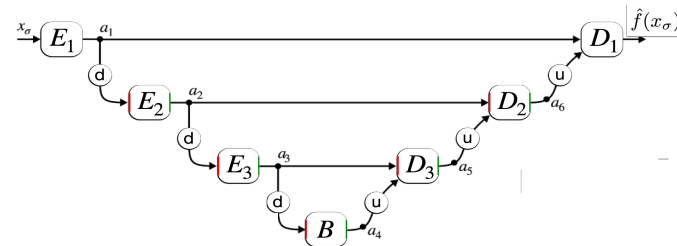
Bonnaire et al. (2025)

¹ C. Merger et al., **Local Coverage Governs Memorization in Diffusion Models**, In: arXiv preprint arXiv:2606.14390, 2026.

Beyond U-Nets?

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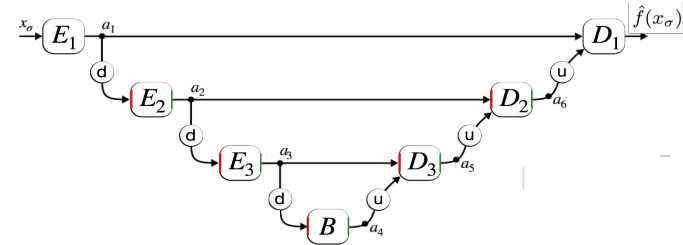
- U-Nets play a crucial in diffusion models for images



Kadkhodaie et al. (2026)

Beyond U-Nets?

- U-Nets play a crucial role in diffusion models for images
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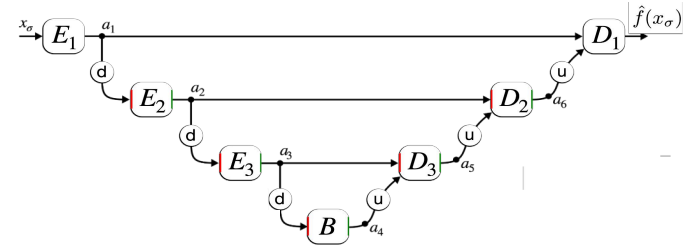
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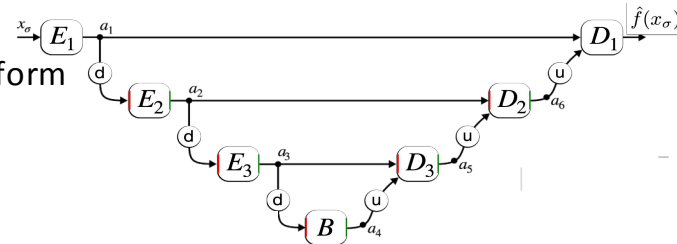
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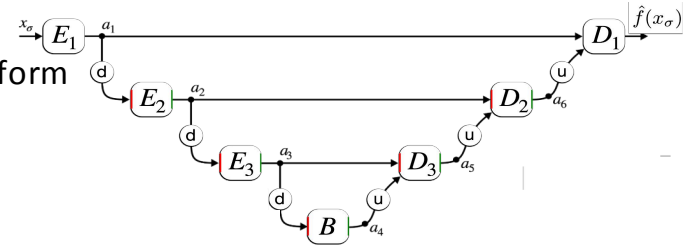
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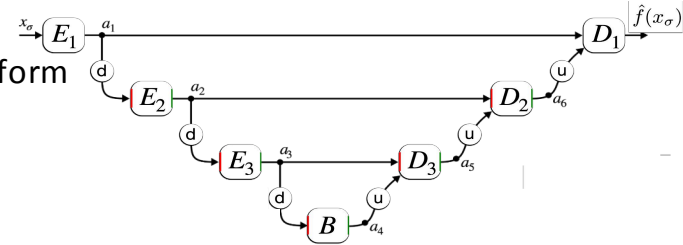
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Beyond unconditional image generation?

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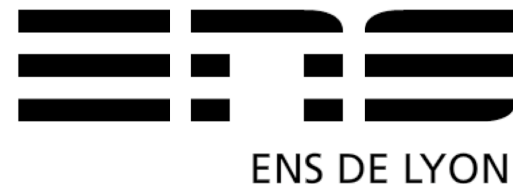
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Thank you for your attention!



Interested in discrete diffusion for LLMs? Just released speedrun!

github.com/agonon/speedrun-dlm

