Title: Architectural bias in a transport-based generative model : an asymptotic perspective

Speakers: Hugo Cui

Collection/Series: Theory + Al Workshop: Theoretical Physics for Al

Date: April 10, 2025 - 9:45 AM

URL: https://pirsa.org/25040092

Abstract:

We consider the problem of learning a generative model parametrized by a two-layer auto-encoder, and trained with online stochastic gradient descent, to sample from a high-dimensional data distribution with an underlying low-dimensional structure. We provide a tight asymptotic characterization of low-dimensional projections of the resulting generated density, and evidence how mode(I) collapse can arise. On the other hand, we discuss how in a case where the architectural bias is suited to the target density, these simple models can efficiently learn to sample from a binary Gaussian mixture target distribution.

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Architectural bias in generative models —an asymptotic viewpoint

Hugo Cui

PI Theory + AI workshop

Based on

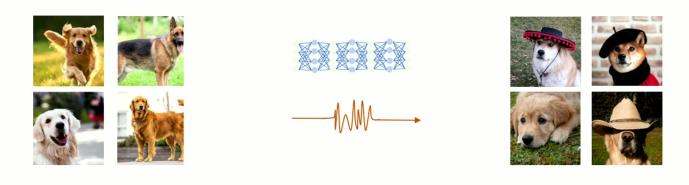
HC, Pehlevan, Lu, Precise asymptotics of learning diffusion models: theory & insights, ArXiv 2025

HC, Krzakala, Vanden-Eijnden, Zdeborová, Analysis of a learning a flow-based generative model from finite sample complexity, ICLR 2024





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Transport-based generative models learn to sample (generate) complex distributions in high-dimensions from moderate training sets.

new generated samples

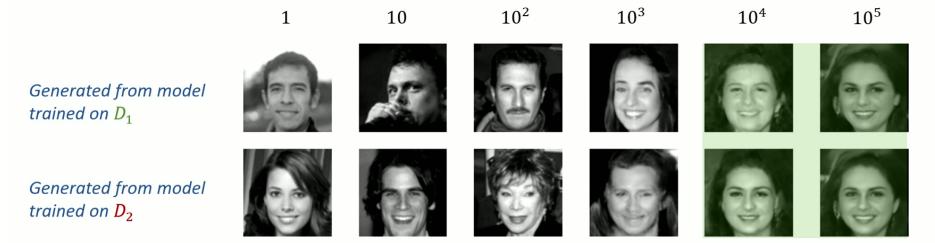
→Existence of strong *inductive biases* in the architecture.

Ho, Jain, Abbeel, *Denoising Diffusion Probabilistic Models*, NeurIPS 2020 Sohl-Dickstein et al., *unsupervised learning using nonequi-librium thermodynamics*, ICML 2015 Song and Ermon, *Generative modeling by estimating gradients of the data distribution*. NeurIPS 2019

Training set $\sim \rho$

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training samples



Kadkhodaie et al., Generalization in diffusion models arises from geometry-adaptive harmonic representation, ICLR 2024

Two models trained on disjoint training sets D_1 and D_2 generate the **same image** from a given prompt when trained with sufficiently many samples ($\sim 2-16x$ dimension).

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How is the distribution of generated samples shaped by the network architecture? $\rightarrow\!\text{Try}$ to understand in simple models.

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Chen et al,. Sampling is as easy as learning the score: theory for diffusion models with minimal data assumptions. arXiv:2209.11215, 2022. Biroli et al, Dynamical regimes of diffusion models. Nature Communications, 15(1):9957, 2024

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Chen et al,. Sampling is as easy as learning the score: theory for diffusion models with minimal data assumptions. arXiv:2209.11215, 2022. Biroli et al, Dynamical regimes of diffusion models. Nature Communications, 15(1):9957, 2024

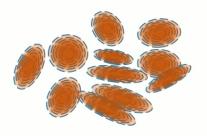
Sample bounds when density can be perfectly learnt by the model class with enough samples:

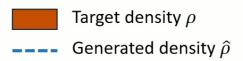
Boffi et al., Shallow diffusion networks provably learn hidden low-dimensional structure., arXiv:2410.11275, 2024.

Chen et al., Score approx-imation, estimation and distribution recovery of diffusion models on low-dimensional data, ICML 2023

Oko, Akiyama and Suzuki, Diffusion models are minimax optimal distribution estimators, ICML 2023

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Chen et al,. Sampling is as easy as learning the score: theory for diffusion models with minimal data assumptions. arXiv:2209.11215, 2022. Biroli et al, Dynamical regimes of diffusion models. Nature Communications, 15(1):9957, 2024

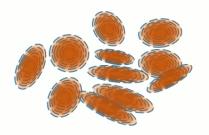
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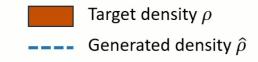
Chen et al., Score approx-imation, estimation and distribution recovery of diffusion models on low-dimensional data, ICML 2023

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Chen et al,. Sampling is as easy as learning the score: theory for diffusion models with minimal data assumptions. arXiv:2209.11215, 2022. Biroli et al, Dynamical regimes of diffusion models. Nature Communications, 15(1):9957, 2024

Sample bounds when density can be perfectly learnt by the model class with enough samples:

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Oko, Akiyama and Suzuki, Diffusion models are minimax optimal distribution estimators, ICML 2023

 \rightarrow <u>To complement these results</u>: a **tight** characterization of the generated density in the case **where** architecture and target distribution are not perfectly matched.

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Outline

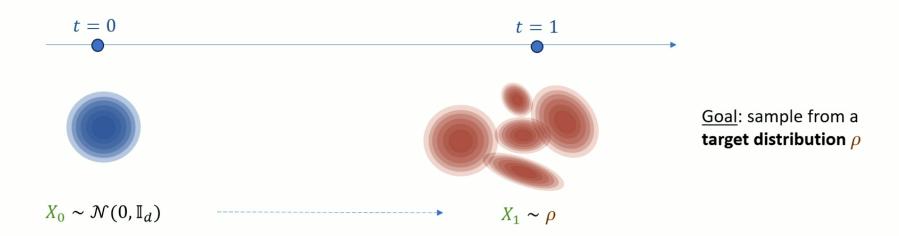
- 1. Generated density for an auto-encoder parametrized model
- 2. Failure modes : mode(I) collapse
- 3. Aligned case: binary isotropic Gaussian mixture distribution.

HC, Pehlevan, Lu, Precise asymptotics of learning diffusion models: theory & insights, ArXiv 2025

HC, Krzakala, Vanden-Eijnden, Zdeborová, Analysis of a learning a flow-based generative model from finite sample complexity, ICLR 2024

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Albergo, Boffi, and Vanden-Eijnden, Stochastic interpolants: A unifying framework for flows and diffusions. arXiv:2303.08797, 2023.

Transport-based generative models: reminders, notations

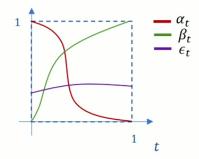
Generated density



The sampling can be done by transporting X_0 through the SDE for $t \in [0,1]$

$$\frac{d}{dt}X_t = \left(\beta_t - \frac{\dot{\alpha}_t}{\alpha_t}\beta_t + \epsilon_t \frac{\beta_t}{\alpha_t^2}\right) f(t, X_t) + \left(\frac{\dot{\alpha}_t}{\alpha_t} - \frac{\epsilon_t}{\alpha_t^2}\right) X_t + \sqrt{2\epsilon_t} dW_t$$

For any choice of $\alpha, \beta \in \mathcal{C}^2([0,1])$ interpolation schedules st: $\alpha_0 = \beta_1 = 1, \alpha_1 = \beta_0 = 0$ $\epsilon_t \geq 0$



Albergo, Boffi, and Vanden-Eijnden, Stochastic interpolants: A unifying framework for flows and diffusions. arXiv:2303.08797, 2023.

Transport-based generative models: reminders, notations

1. Generated density



The sampling can be done by transporting X_0 through the SDE for $t \in [0,1]$

$$\frac{d}{dt}X_t = \left(\beta_t - \frac{\dot{\alpha}_t}{\alpha_t}\beta_t + \epsilon_t \frac{\beta_t}{\alpha_t^2}\right) f(t, X_t) + \left(\frac{\dot{\alpha}_t}{\alpha_t} - \frac{\epsilon_t}{\alpha_t^2}\right) X_t + \sqrt{2\epsilon_t} dW_t$$

Denoising function is the minimizer of a denoising objective

$$f = \min_{h} \int_{0}^{1} \mathbb{E}_{x_{1} \sim \rho, x_{0} \sim \mathcal{N}(0, \mathbb{I}_{d})} \|h(t, \alpha_{t} x_{0} + \beta_{t} x_{1}) - x_{1}\|^{2} dt$$

Learnable from data

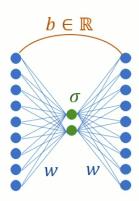
Empirical average Network param.

Albergo, Boffi, and Vanden-Eijnden, Stochastic interpolants: A unifying framework for flows and diffusions. arXiv:2303.08797, 2023.

$$\forall x \in \mathbb{R}^d$$
, $\left[f_{b,w}(x) = \frac{b}{v} x + \frac{w}{\sqrt{d}} \sigma \left(\frac{w^{\mathsf{T}} x}{\sqrt{d}} \right) \right]$

Trainable skip connection $b \in \mathbb{R}$

Weight matrix $w \in \mathbb{R}^{d \times r}$



Vincent et al., Stacked denoising AEs:Learning useful representations in a deep net. with a local denoising criterion, JMLR 2010

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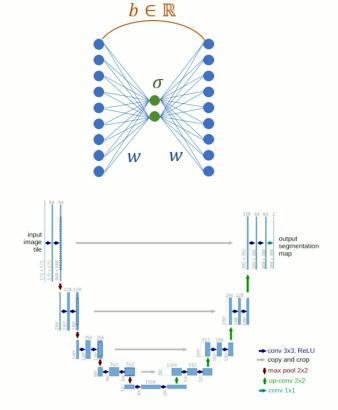
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Remark: U-Nets are used in practice.

- skip connections
- bottlenecks
- convolutional layers



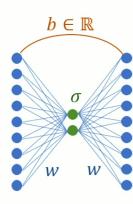
Ronneberger, Fischer, and Brox U-net: Convolutional networks for biomedical image segmentation. MICCAI 2015

Vincent et al., Stacked denoising AEs:Learning useful representations in a deep net. with a local denoising criterion, JMLR 2010

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Given a training set of n i.i.d samples $\left\{x_1^{\mu} \sim \rho, x_0^{\mu} \sim \mathcal{N}(0, \mathbb{I}_d)\right\}_{\mu=1}^n$ one can train the network $f_{b,w}\left(x\right)$ with <u>online SGD</u>

$$b_{\mu+1} - b_{\mu} = -\frac{\eta}{d^2} \left(\partial_b \mathbb{E}_t \left\| x_1^{\mu} - f_{b_{\mu}, w_{\mu}} \left(\alpha_t x_0^{\mu} + \beta_t x_1^{\mu} \right) \right\|^2 \right)$$

$$w_{\mu+1} - w_{\mu} = -\eta \left(\nabla_w \mathbb{E}_t \left\| x_1^{\mu} - f_{b_{\mu}, w_{\mu}} \left(\alpha_t x_0^{\mu} + \beta_t x_1^{\mu} \right) \right\|^2 + \lambda / dw_{\mu} \right)$$

Note $\tau = 2\eta^n/_d$ and w_{τ} , b_{τ} the trained parameters.

Vincent et al., Stacked denoising AEs:Learning useful representations in a deep net. with a local denoising criterion, JMLR 2010

Generated density

1. Generated density



$$\frac{d}{dt}X_t = \left(\beta_t - \frac{\dot{\alpha}_t}{\alpha_t}\beta_t + \epsilon_t \frac{\beta_t}{\alpha_t^2}\right) f(t, X_t) + \left(\frac{\dot{\alpha}_t}{\alpha_t} - \frac{\epsilon_t}{\alpha_t^2}\right) X_t + \sqrt{2\epsilon_t} dW_t$$

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Generated density

1. Generated density



$$\frac{d}{dt}X_t = \left(\dot{\beta_t} - \frac{\dot{\alpha_t}}{\alpha_t}\beta_t + \epsilon_t \frac{\beta_t}{\alpha_t^2}\right) f(t, X_t) + \left(\frac{\dot{\alpha_t}}{\alpha_t} - \frac{\epsilon_t}{\alpha_t^2}\right) X_t + \sqrt{2\epsilon_t} dW_t$$

$$\frac{d}{dt}X_t = \left(\beta_t - \frac{\dot{\alpha}_t}{\alpha_t}\beta_t + \epsilon_t \frac{\beta_t}{\alpha_t^2}\right) f_{b_{\tau}, w_{\tau}}(X_t) + \left(\frac{\dot{\alpha}_t}{\alpha_t} - \frac{\epsilon_t}{\alpha_t^2}\right) X_t + \sqrt{2\epsilon_t} dW_t$$

Using the trained AE in the generative SDE

$$\widehat{
ho}_{ au}(t) = \operatorname{Law}[X_t]$$
 ?

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Gaussian mixture supported on a low-dimensional latent manifold

$$ho = \int\limits_{\mathbb{R}^{\kappa}} d\pi(c) \mathcal{N}(\mu(c), \Sigma(c))$$

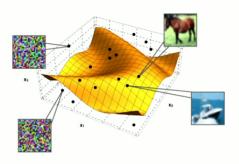


Figure from Goldt et al., Modelling the influence of data structure in learning in neural networks: the hidden manifold model, PRX 2020.

Tenenbaum., Silva and Langford, A global geometric framework for nonlinear dimensionality reduction. science, 2000 Weinberger and Saul, Unsupervised learning of image manifolds by semidefinite programming. Int. journal of computer vision, 2006.

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Gaussian mixture supported on a low-dimensional latent manifold

$$\rho = \int_{\mathbb{R}^{\kappa}} d\pi(c) \mathcal{N}(\mu(c), \Sigma(c))$$

centroids

$$\mu: \mathbb{R}^{\kappa} \to \mathbb{R}^d$$

 $\exists D > 0$, w.p. 1, $\|\mu(c)\| \le D$

 $K = \dim \operatorname{span}\{\mu(c)\}_c$ is low

covariances

$$\Sigma: \mathbb{R}^{\kappa} \to \mathcal{S}^d(\mathbb{R})$$

assumed jointly diagonalizable, with a well-defined joint limiting spectral density.

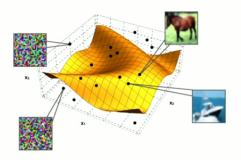


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1. Generated density

Gaussian mixture supported on a low-dimensional latent manifold

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covariances

$$\Sigma: \mathbb{R}^{\kappa} \to \mathcal{S}^d(\mathbb{R})$$

assumed jointly diagonalizable, with a well-defined joint limiting spectral density.

Average extension of the $\Lambda = \int d\pi(c) \frac{1}{d} \text{Tr}[\Sigma(c)]$ density

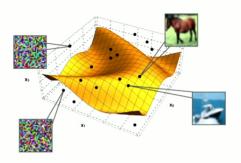


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Problem formulation: recap

1. Generated density

Target density
$$\rho = \int_{\mathbb{R}^{\kappa}} d\pi(c) \mathcal{N}(\mu(c), \Sigma(c))$$

Architecture
$$f_{b,w}(x) = {}^{b}x + {}^{w}{\sqrt{d}}\sigma\left({}^{w}{\sqrt{d}}\right)$$

Learning
$$b_{\mu+1} - b_{\mu} = -\frac{\eta}{d^2} \left(\partial_b \mathbb{E}_t \left\| x_1^{\mu} - f_{b_{\mu},w_{\mu}} \left(\alpha_t x_0^{\mu} + \beta_t x_1^{\mu} \right) \right\|^2 \right)$$
 for a time $\boldsymbol{\tau}$
$$w_{\mu+1} - w_{\mu} = -\eta \left(\nabla_w \mathbb{E}_t \left\| x_1^{\mu} - f_{b_{\mu},w_{\mu}} \left(\alpha_t x_0^{\mu} + \beta_t x_1^{\mu} \right) \right\|^2 + \lambda / dw_{\mu} \right)$$

Sampling
$$\frac{d}{dt}X_t = \Gamma_t \frac{w_{\mathbf{T}}}{\sqrt{d}} \sigma \left(\frac{w_{\mathbf{T}}^{\mathsf{T}} X_t}{\sqrt{d}} \right) + \Delta_t^{\mathsf{T}} X_t + \sqrt{2\epsilon_t} dW_t \qquad \text{for a time } t$$

with
$$\Gamma_t = \left(\dot{\beta_t} - \frac{\dot{\alpha_t}}{\alpha_t} \beta_t + \epsilon_t \frac{\beta_t}{\alpha_t^2} \right) \qquad \Delta_t^{\tau} = b_{\tau} \Gamma_t + \frac{\dot{\alpha_t}}{\alpha_t} - \frac{\epsilon_t}{\alpha_t^2}$$

Generated density
$$\hat{\rho}_{\tau}(t) = \text{Law}[X_t]$$

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Asymptotic limit

$$n, d \to \infty$$
 with $n/d, \kappa, r, D, K = \Theta_d(1)$

Finite width, large amount of data, large dimension

Saad and Solla, Exact solution for on-line learning in multilayer neural networks, PRL 1995,

Gabrié, Mean-Field inference methods for neural networks, J. Phys. A 2020. **HC**, High-dimensional learning of narrow networks, J.Stat Mech 2025

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Main result (informal)

1. Generated density

<u>Tight characterization of low-dimensional projections of the generated density</u> $\hat{\rho}_{\tau}(t)$

Consider a low-dimensional subspace $\mathcal{E} \subset \mathbb{R}^d$, with $\dim \mathcal{E} = R = \Theta_d(1)$. The distribution of the R -dimensional projection $\Pi_{\mathcal{E}} X_t$ is given by

$$\left(\Pi_{\varepsilon} X_t = ^d \Theta_{\tau}^{\top} Q_{\tau}^{+} Z_t + Y_t \right)$$

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Where:

 $extbf{Y}_t \in \mathbb{R}^R$ is Gaussian

$$\mathbf{Y}_{t} \sim \mathcal{N}\left(\mathbf{0}_{R}, e^{2\int_{0}^{t} \Delta_{S}^{\tau} ds} \left[1 + 2\int_{0}^{t} \epsilon_{S} e^{-2\int_{0}^{s} \Delta_{Z}^{\tau} dz} ds\right] (\mathbb{I}_{R} - \Theta_{\tau}^{\mathsf{T}} \mathbf{Q}_{\tau}^{\mathsf{+}} \Theta_{\tau})\right)$$

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<u>Tight characterization of low-dimensional projections of the generated density</u> $\hat{\rho}_{\tau}(t)$

Consider a low-dimensional subspace $\mathcal{E} \subset \mathbb{R}^d$, with $\dim \mathcal{E} = R = \Theta_d(1)$. The distribution of the R -dimensional projection $\Pi_{\mathcal{E}} X_t$ is given by

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$$Y_{t} \sim \mathcal{N}\left(0_{R}, e^{2\int_{0}^{t} \Delta_{S}^{\tau} ds} \left[1 + 2\int_{0}^{t} \epsilon_{S} e^{-2\int_{0}^{s} \Delta_{Z}^{\tau} dz} ds\right] (\mathbb{I}_{R} - \Theta_{\tau}^{\mathsf{T}} Q_{\tau}^{\mathsf{+}} \Theta_{\tau})\right)$$

 $Z_t \in \mathbb{R}^r$ is distributed as the solution of the SDE

$$\frac{d}{dt}Z_t = \Delta_t^{\tau} Z_t + \Gamma_t Q_{\tau} \sigma(Z_t) + \sqrt{2\epsilon_t} Q_{\tau}^{1/2} W_t$$

From initialization $Z_0 \sim \mathcal{N}(0_r, \mathbf{Q_\tau})$

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Tight characterization of low-dimensional projections of the generated density $\hat{\rho}_{\tau}(t)$

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From initialization $Z_0 \sim \mathcal{N}(0_r, Q_\tau)$

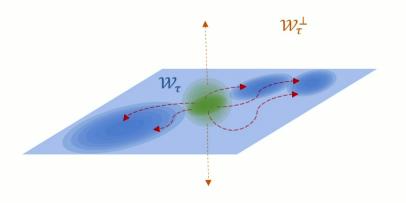
The parameters $\Theta_{\tau} \in \mathbb{R}^{r \times R}$, $Q_{\tau} \in \mathbb{R}^{r \times r}$ are the solutions of a set of 5 coupled **low-dimensional** deterministic **ODEs**.

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Sketch of derivation 1. Generated density

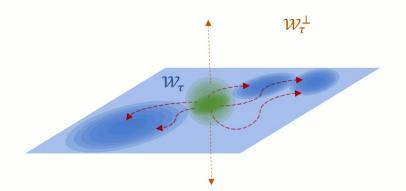


$$\frac{d}{dt}X_t = \left[\Gamma_t \frac{w_{\tau}}{\sqrt{d}} \sigma \left(\frac{w_{\tau}^{\mathsf{T}} X_t}{\sqrt{d}} \right) + \Delta_t^{\tau} X_t + \sqrt{2\epsilon_t} dW_t \right]$$

Non-linear transport in $W_{\tau} = \text{span}(\{w_i\}_{i=1}^r)$

Linear in $\mathcal{W}_{ au}^{\perp}$

Generated density Sketch of derivation



$$\frac{d}{dt}X_t = \Gamma_t \frac{w_{\mathbf{\tau}}}{\sqrt{d}} \sigma \left(\frac{w_{\mathbf{\tau}}^{\mathsf{T}} X_t}{\sqrt{d}}\right) + \Delta_t^{\mathsf{T}} X_t + \sqrt{2\epsilon_t} dW_t$$

Non-linear transport in $W_{\tau} = \operatorname{span}(\{w_i\}_{i=1}^r)$

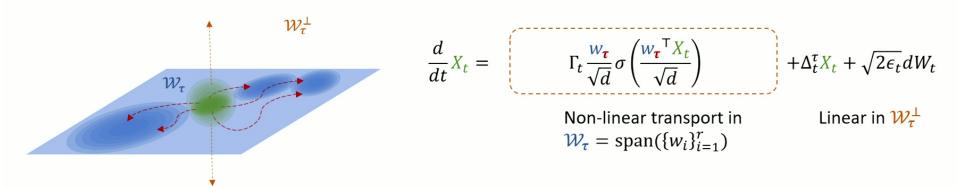
Linear in $\mathcal{W}_{\tau}^{\perp}$

Dynamics of
$$Z_t = \frac{w_{\tau}^{\mathsf{T}} X_t}{\sqrt{d}}$$

Dynamics of
$$Z_t = \frac{w_{\mathbf{r}}^{\mathsf{T}} X_t}{\sqrt{d}}$$

$$\frac{d}{dt} Z_t = \Delta_t^{\mathsf{T}} Z_t + \Gamma_t \frac{w_{\mathbf{r}}^{\mathsf{T}} w_{\mathbf{r}}}{d} \sigma(Z_t) + \sqrt{2\epsilon_t} \left(\frac{w_{\mathbf{r}}^{\mathsf{T}} w_{\mathbf{r}}}{d}\right)^{\frac{1}{2}} W_t$$

Sketch of derivation 1. Generated density



Dynamics of
$$Z_t = \frac{w_{\tau}^{\mathsf{T}} X_t}{\sqrt{d}}$$

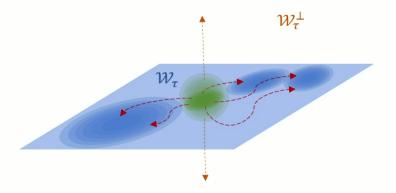
$$\frac{d}{dt} Z_t = \Delta_t^{\mathsf{T}} Z_t + \Gamma_t \frac{w_{\tau}^{\mathsf{T}} w_{\tau}}{d} \sigma(Z_t) + \sqrt{2\epsilon_t} \left(\frac{w_{\tau}^{\mathsf{T}} w_{\tau}}{d}\right)^{\frac{1}{2}} W_t$$

The SGD dynamics of the summary statistic $Q_{\tau} = \frac{w_{\tau}^{\mathsf{T}} w_{\tau}}{d}$ (and others) self-average and can be characterized in closed-form by a set of low-dimensional ODEs.

Saad and Solla, Exact solution for on-line learningin multilayer neural networks, PRL 1995

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Intuition:

- The network **identifies** a r -dimensional \mathcal{W}_{τ} subspace where the target ρ has important structure, and implements a non-linear transport.
- It approximates ρ in the orthogonal space by an **isotropic Gaussian**, whose variance is tuned by the skip connection strength.

Special case: linear networks $\sigma(x) = x$

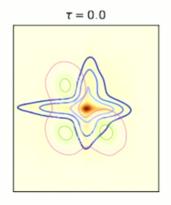
• Linear networks approximately learn \approx **principal components** $\mathcal{W}_{\tau} \approx \mathrm{PCA}_{r}\big[\{x_{1}^{\mu}\}_{\mu}\big]$ Pretorius et al,. Learning dynamics of linear denoising autoencoders. ICML, 2018. ,

• The linear diffusion model does a Gaussian approximation in the principal space. In the orthogonal space, approximates by an isotropic Gaussian.

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 $\sigma = \text{ReLU}$ activation, r = 4 hidden units

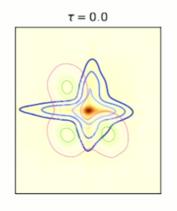


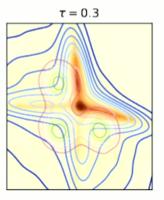
Target density ρ (theory) Generated density $\hat{\rho}$ (exp) Generated density $\hat{\rho}$

31

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 $\sigma = \text{ReLU}$ activation, r = 4 hidden units





 $lue{}$ Target density ho

___ (t

(**theory**) Generated density $\hat{
ho}$

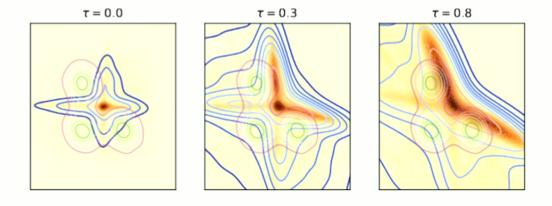


(**exp**) Generated density $\hat{
ho}$

32

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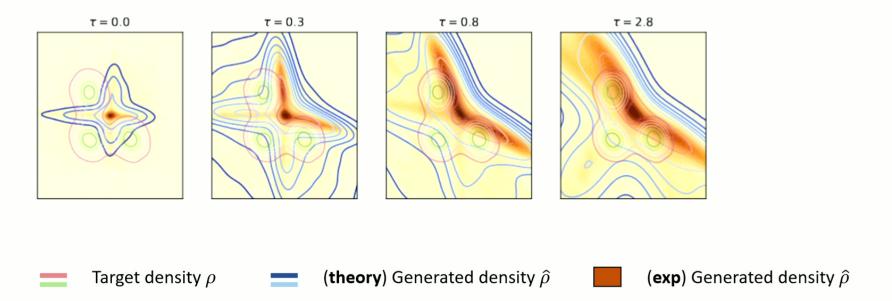




Target density ho (theory) Generated density $\hat{
ho}$ (exp) Generated density $\hat{
ho}$

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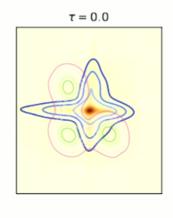


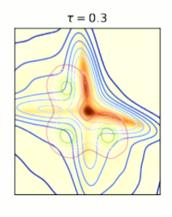


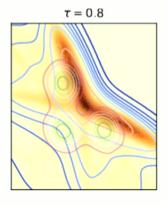
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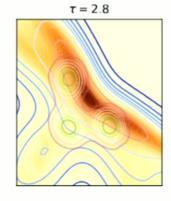


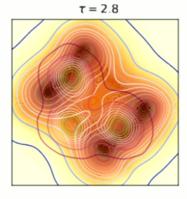
 σ = tanh activation, r = 2 hidden units











 $lue{}$ Target density ho



(theory) Generated density $\hat{\rho}$

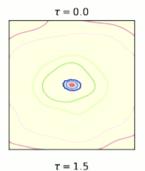


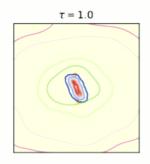
(**exp**) Generated density $\hat{\rho}$

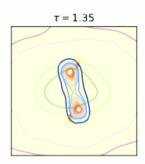
35

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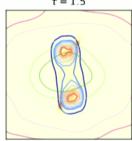
1. Generated density







 $\sigma=$ tanh activation, r=2 hidden units Gaussian ho with MNIST covariance



 $lue{}$ Target density ho

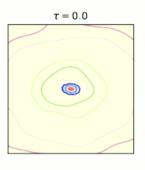
(theory) Generated density $\widehat{
ho}$

(exp) Generated density $\hat{
ho}$

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 $\sigma = \tanh \arctan$ r = 2 hidden units Gaussian ρ with MNIST covariance

Target density ho

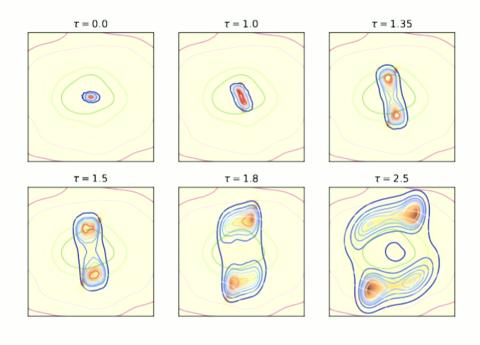
(theory) Generated density $\hat{
ho}$

(**exp**) Generated density $\hat{\rho}$

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1. Generated density

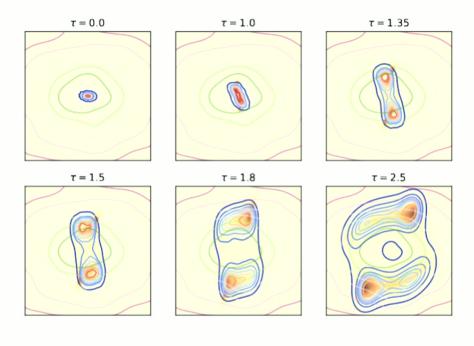


 $\sigma=$ tanh activation, r=2 hidden units Gaussian ho with MNIST covariance

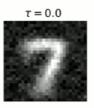
Target density ho (theory) Generated density $\hat{
ho}$ (exp) Generated density $\hat{
ho}$

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1. Generated density



 $\sigma=$ tanh activation, r=2 hidden units Gaussian ho with MNIST covariance



 $lue{}$ Target density ho

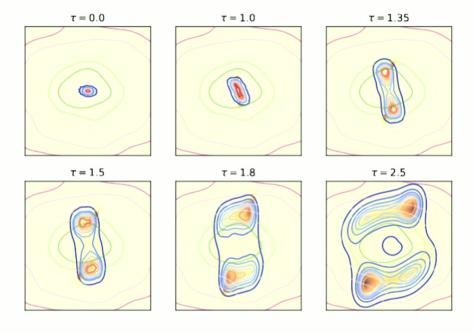
(theory)

(theory) Generated density $\widehat{
ho}$

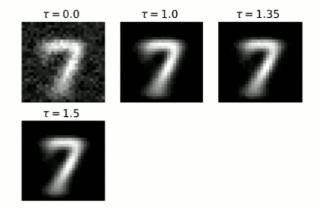
(**exp**) Generated density $\hat{\rho}$

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 $\sigma=$ tanh activation, r=2 hidden units Gaussian ho with MNIST covariance



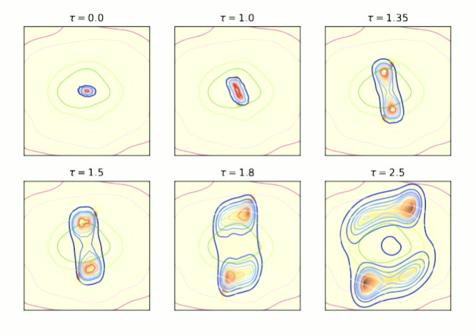
 $lue{}$ Target density ho

(theory) Generated density $\hat{
ho}$

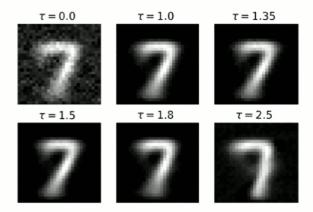
(exp) Generated density $\hat{\rho}$

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 $\sigma=$ tanh activation, r=2 hidden units Gaussian ho with MNIST covariance



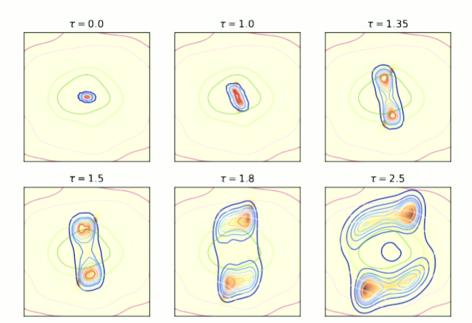
ullet Target density ho

(theory) Generated density $\hat{
ho}$

(exp) Generated density $\hat{\rho}$

Mode collapse

2. Failure modes



Closed-form expression for the trained skip connection

$$b_{\tau} = \frac{\Lambda \mathbb{E}_{t}[\beta_{t}] \left[1 - (1 - b_{0}) e^{-\left(\Lambda \mathbb{E}_{t}[\beta_{t}^{2}] + \mathbb{E}_{t}[\alpha_{t}^{2}]\right)\tau} \right]}{\Lambda \mathbb{E}_{t}[\beta_{t}^{2}] + \mathbb{E}_{t}[\alpha_{t}^{2}]}$$

Average cov. eigenvalue $\Lambda = \int d\pi(c) \frac{1}{d} \text{Tr}[\Sigma(c)]$

is typically **small** in real datasets, causing ≈ **mode collapse**

Goodfellow et al., Generative adversarial nets. NeurIPS 2014.

 $lue{}$ Target density ho

(theory) Generated density $\hat{
ho}$

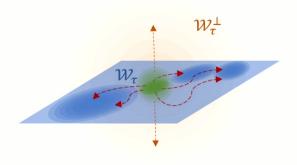
(**exp**) Generated density $\hat{
ho}$

Can this bias be *aggravated* when using synthetic data to train a new generative model?

$$\rho \to \hat{\rho}^{(1)} \to \hat{\rho}^{(2)} \to \cdots \to \hat{\rho}^{(g)}$$

Can this bias be aggravated when using synthetic data to train a new generative model?

$$\rho \to \hat{\rho}^{(1)} \to \hat{\rho}^{(2)} \to \cdots \to \hat{\rho}^{(g)}$$



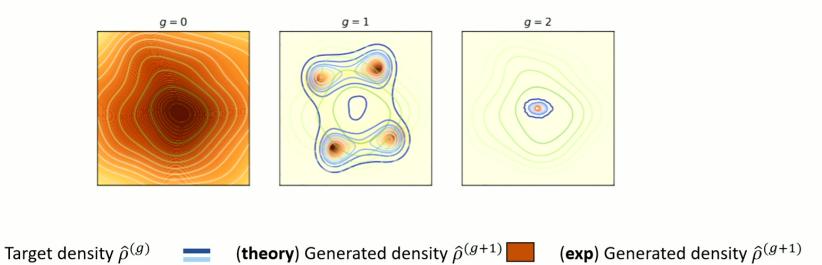
Remark: Manifold form of the generated density

 $\hat{
ho}^{(1)}$ is still of the form $\int d\pi(c) \mathcal{N} ig(\mu(c), \Sigma(c) ig)$, with $\mu(c) = c$ and

$$\begin{bmatrix} \pi = \Pi_{\mathcal{W}_{\tau}} \, \hat{\rho}^{(1)} \\ \Sigma(c) = e^{2 \int_0^t \Delta_s^{\tau} ds} \left[1 + 2 \int_0^t \epsilon_s e^{-2 \int_0^s \Delta_z^{\tau} dz} ds \right] \Pi_{\mathcal{W}_{\tau}^{\perp}} \end{bmatrix}$$

Thus the analysis *carries over iteratively* to generations $\hat{\rho}^{(2)}$, ...

Model collapse 2. Failure modes

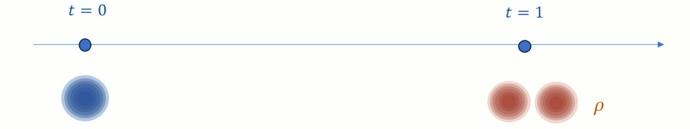


Shumailov et al., Ai models collapse when trained onrecursively generated data. Nature, 2024

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Binary, isotropic Gaussian mixture $\rho = 1/2 \mathcal{N}(-\mu, \sigma^2 \mathbb{I}_d) + 1/2 \mathcal{N}(+\mu, \sigma^2 \mathbb{I}_d)$



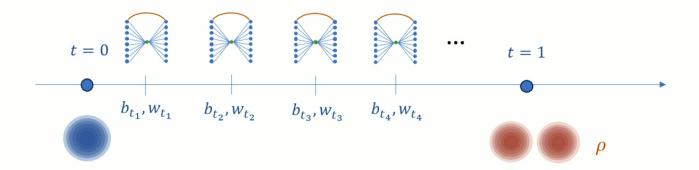
Aligned case

3. Aligned bias

Binary, isotropic Gaussian mixture $\rho = \frac{1}{2} \mathcal{N}(-\mu, \sigma^2 \mathbb{I}_d) + \frac{1}{2} \mathcal{N}(+\mu, \sigma^2 \mathbb{I}_d)$

At $\it each \ sampling \ time$, train a $\it separate$ AE with r=1 hidden unit and $\sigma={\rm sign} \ {\rm activation}$

$$b_t, w_t = \operatorname{argmin}_{\theta \in \mathbb{R}^{d \times r}} \sum_{\mu=1}^n \| f_{b,w} (\alpha_t x_0^{\mu} + \beta_t x_1^{\mu}) - x_1^{\mu} \|_2^2 + \lambda \|w\|^2$$



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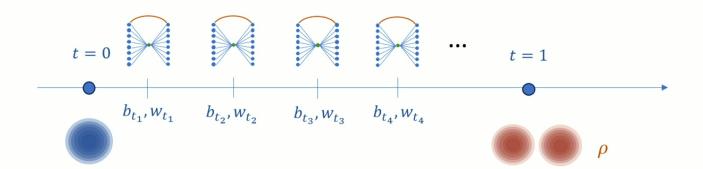
3. Aligned bias

Binary, isotropic Gaussian mixture $\rho = 1/2 \mathcal{N}(-\mu, \sigma^2 \mathbb{I}_d) + 1/2 \mathcal{N}(+\mu, \sigma^2 \mathbb{I}_d)$

At each sampling time, train a separate AE with r=1 hidden unit and $\sigma=\mathrm{sign}$ activation

$$b_t, w_t = \operatorname{argmin}_{\theta \in \mathbb{R}^{d \times r}} \sum_{\mu=1}^n \left\| f_{b,w} \left(\alpha_t x_0^{\mu} + \beta_t x_1^{\mu} \right) - x_1^{\mu} \right\|_2^2 + \lambda \|w\|^2$$

Sampling: $\frac{d}{dt}X_t = \left(\beta_t - \frac{\dot{\alpha}_t}{\alpha_t}\beta_t\right) f_{b_t,w_t}(X_t) + \frac{\dot{\alpha}_t}{\alpha_t}X_t$



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Closed form characterization of the dynamics

In the asymptotic limit $d \to \infty$ with $n = \Theta_d(1)$, $\|\mu\| = \Theta_d(\sqrt{d})$, the sampling dynamic is non-linear in $\mathrm{span}(\mu, \xi, \eta)$ where

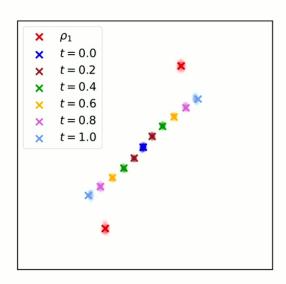
$$oldsymbol{\xi} \equiv \sum_{\mu=1}^n s^\mu oldsymbol{x}_0^\mu, \qquad \qquad oldsymbol{\eta} \equiv \sum_{\mu=1}^n s^\mu (oldsymbol{x}_1^\mu - s^\mu oldsymbol{\mu}),$$

The coordinates M_t , Q_t^{ξ} , Q_t^{η} of a sample X_t follow the ODEs

$$\begin{cases} \frac{d}{dt}M_t = \frac{\left(\dot{\beta}(t)\beta(t)(\lambda(1+\sigma^2)+(n-1)\sigma^2)+\dot{\alpha}(t)\alpha(t)(\lambda+n-1)\right)M_t + \left(\alpha(t)\dot{\beta}(t)-\dot{\alpha}(t)\beta(t)\right)\frac{n\alpha(t)(\lambda+n-1)}{\lambda+n}}{\alpha(t)^2(\lambda+n-1)+\beta(t)^2(\lambda(1+\sigma^2)+(n-1)\sigma^2)} \\ \frac{d}{dt}Q_t^\xi = \frac{\left(\dot{\beta}(t)\beta(t)(\lambda(1+\sigma^2)+(n-1)\sigma^2)+\dot{\alpha}(t)\alpha(t)(\lambda+n-1)\right)Q_t^\xi - \left(\alpha(t)\dot{\beta}(t)-\dot{\alpha}(t)\beta(t)\right)\frac{\beta(t)(\lambda(1+\sigma^2)+(n-1)\sigma^2)}{\lambda+n}}{\alpha(t)^2(\lambda+n-1)+\beta(t)^2(\lambda(1+\sigma^2)+(n-1)\sigma^2)} \\ \frac{d}{dt}Q_t^\eta = \frac{\left(\dot{\beta}(t)\beta(t)(\lambda(1+\sigma^2)+(n-1)\sigma^2)+\dot{\alpha}(t)\alpha(t)(\lambda+n-1)\right)Q_t^\eta + \left(\alpha(t)\dot{\beta}(t)-\dot{\alpha}(t)\beta(t)\right)\frac{\alpha(t)(\lambda+n-1)}{\lambda+n}}{\alpha(t)^2(\lambda+n-1)+\beta(t)^2(\lambda(1+\sigma^2)+(n-1)\sigma^2)} \end{cases}$$

The component X_t^{\perp} orthogonal to span (μ, ξ, η) evolves linearly

$$\frac{d}{dt}X_t^{\perp} = \frac{\left(\dot{\beta}(t)\beta(t)(\lambda(1+\sigma^2)+(n-1)\sigma^2)+\dot{\alpha}(t)\alpha(t)(\lambda+n-1))\right)}{\alpha(t)^2(\lambda+n-1)+\beta(t)^2(\lambda(1+\sigma^2)+(n-1)\sigma^2)}X_t^{\perp}$$



HC, Krzakala, Vanden-Eijnden, Zdeborová, Analysis of a learning a flow-based generative model from finite sample complexity, ICLR 2024

Corollary

The *mixture Wasserstein distance* between the target ho and the generated density $\hat{
ho}$ decays as

$$\left\{\mathsf{M}\mathcal{W}_2[\rho,\hat{\rho}] = O\left(\frac{1}{n}\right)\right\}$$

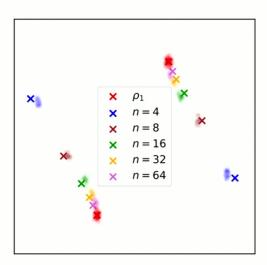
HC, Krzakala, Vanden-Eijnden, Zdeborová, Analysis of a learning a flow-based generative model from finite sample complexity, ICLR 2024

3. Aligned bias

Corollary

The mixture Wasserstein distance between the target ho and the generated density $\hat{
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$$\left\{\mathsf{M}\mathcal{W}_2[\rho,\hat{\rho}] = O\left(\frac{1}{n}\right)\right\}$$



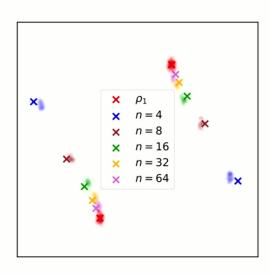
HC, Krzakala, Vanden-Eijnden, Zdeborová, Analysis of a learning a flow-based generative model from finite sample complexity, ICLR 2024

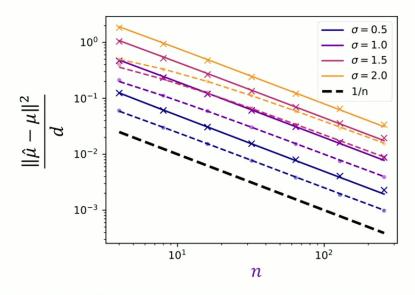
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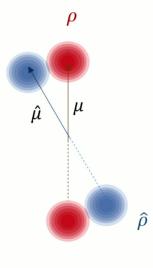
<u>Corollary</u>

The mixture Wasserstein distance between the target ho and the generated density $\hat{
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$$\left\{\mathsf{M}\mathcal{W}_2[\rho,\widehat{\rho}] = O\left(\frac{1}{n}\right)\right\}$$







HC, Krzakala, Vanden-Eijnden, Zdeborová, Analysis of a learning a flow-based generative model from finite sample complexity, ICLR 2024

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<u>Intuition</u>: The optimal denoising function follows from *Tweedie's formula* (Empirical Bayes) and is of the <u>same</u> functional form as the AE

$$f_t^{\star}(x) = \frac{\beta(t)\sigma^2}{\alpha(t)^2 + \beta(t)^2 \sigma^2} x + \frac{\alpha(t)^2}{\alpha(t)^2 + \beta(t)^2 \sigma^2} \mu \times \tanh\left(\frac{\beta(t)}{\alpha(t)^2 + \beta(t)^2 \sigma^2} \mu^{\top} x\right)$$

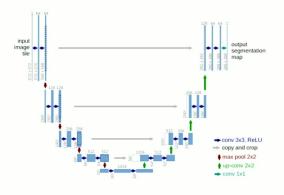
 \rightarrow The architectural bias is **aligned** with the target distribution.

Bradley Efron. *Tweedie's formula and selection bias*. Journal of the American Statistical Association, 2011
Robbins, Proceedings of the Third Berkeley Symposium on Mathematical Statistics and Probability, vol. 1: Contributions to the Theory of Statistics. Koichi Miyasawa. *An empirical Bayes estimator of the mean of a normal population*. Bulletin of the International Statistical Institute, 1961

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Perspectives



Inductive bias of Unets?

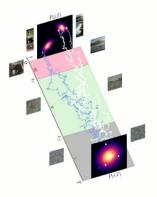
U-nets are suited to data with a hierarchical structure

Kadkhodaie et al., Generalization in diffusion models arises from geometry-adaptive harmonic representation, ICLR 2024

Mei, S. U-nets as belief propagation: Efficient classification, denoising, and diffusion in generative hierarchical models, arXiv:2404.18444, 2024.

(Recall also Alessandro's talk!)

Ronneberger, Fischer, and Brox U-net: Convolutional networks for biomedical image segmentation. MICCAI 2015



For infinitely expressive networks who can perfectly overfit the data, dynamical transitions in the sampling process.

Biroli et al, Dynamical Regimes of Diffusion Models, Nature Comm. 2024

How are they altered for networks with finite expressivity?

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Collaborators



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Florent Krzakala (EPFL)



Eric Vanden-Eijnden (NYU)

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Thank you for your attention!

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