A Precise Examination of Diffusion Models via Their Application to Gaussian Distributions

Émile Pierret[a], work supervised by Bruno Galerne[b,c]
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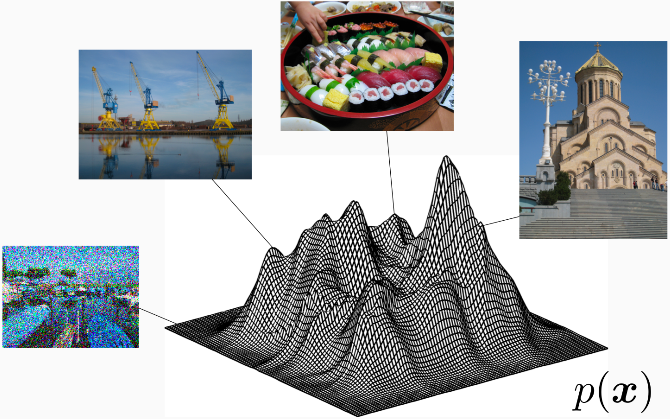
[c] Institut universitaire de France (IUF)

Introduction

What is a generative model ?

Goal: Sample from a data distribution of images.



CelebA dataset

Dataset samples

50K samples

CelebA dataset

Dataset samples

50K samples

Generated (Fake) samples

Style GAN, (Karras et al., 2018) (NVIDIA)

Challenge: Given a model $G(\cdot;\Theta)$, find $\Theta^\star$ such that $G(\mathcal{N}(\mathbf{0}, \boldsymbol{I}_N), \Theta^\star) \approx p$

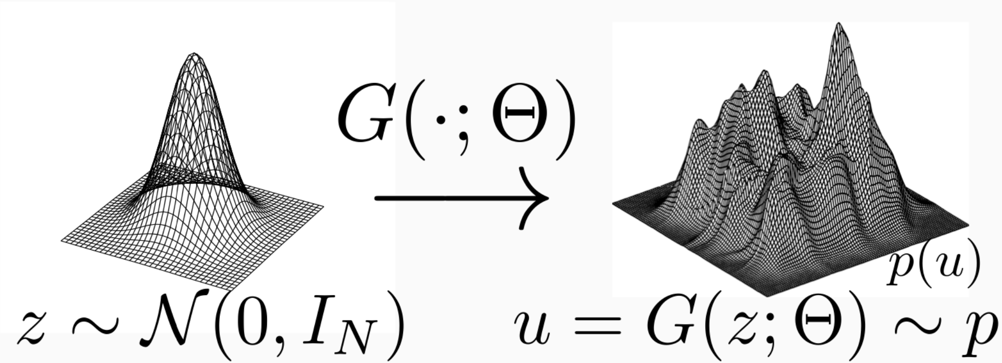


Image extracted from Bruno Galerne's slides

Diffusion models through SDE

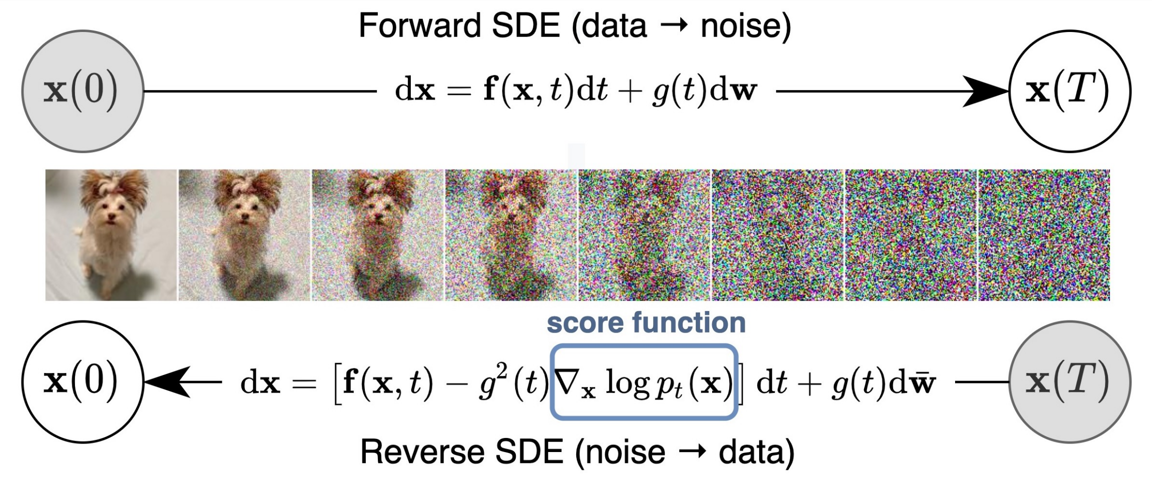
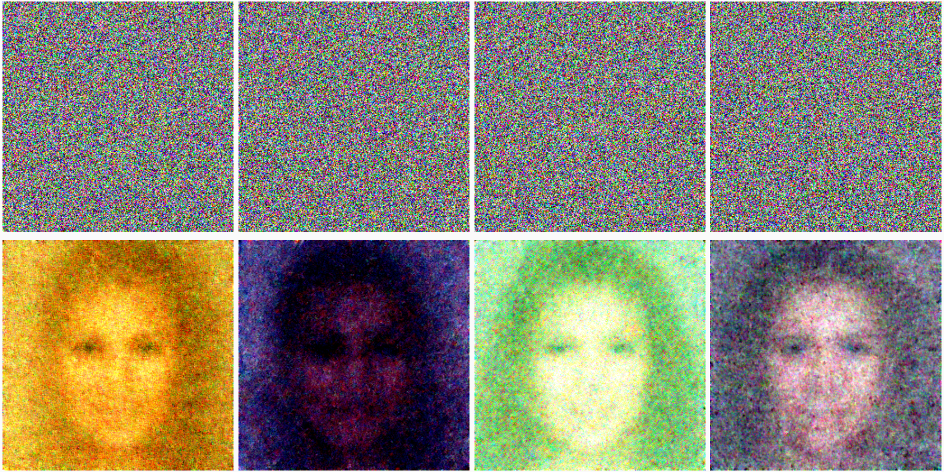


Image extracted from [Song et al. 2021]

Examples (generated with [Lugmayr et al. 2022][1])



t = 249

[1] Andreas Lugmayr et al. (2022). "RePaint: Inpainting using Denoising Diffusion Probabilistic Models". In: *2022 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 11451–11461. URL: `https://api.semanticscholar.org/CorpusID:246240274`

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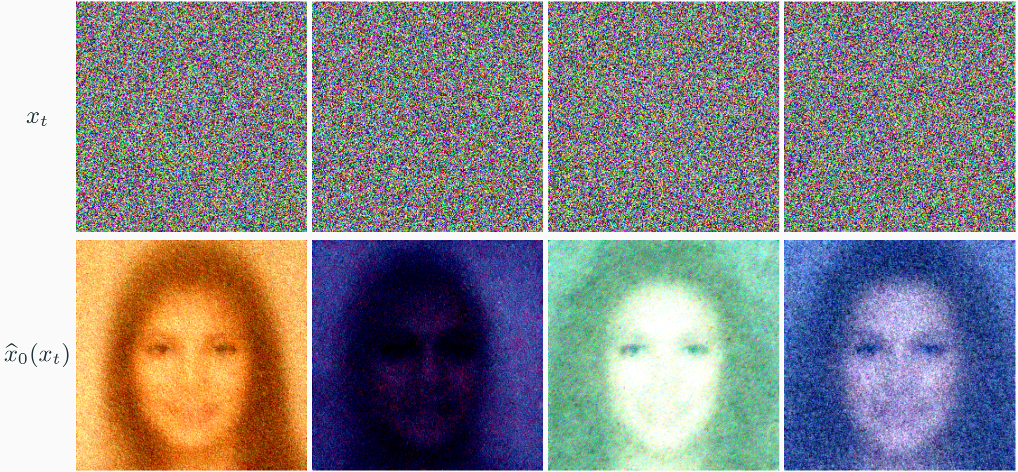

t = 230

[1] Andreas Lugmayr et al. (2022). "RePaint: Inpainting using Denoising Diffusion Probabilistic Models". In: *2022 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 11451–11461. URL: https://api.semanticscholar.org/CorpusID:246240274

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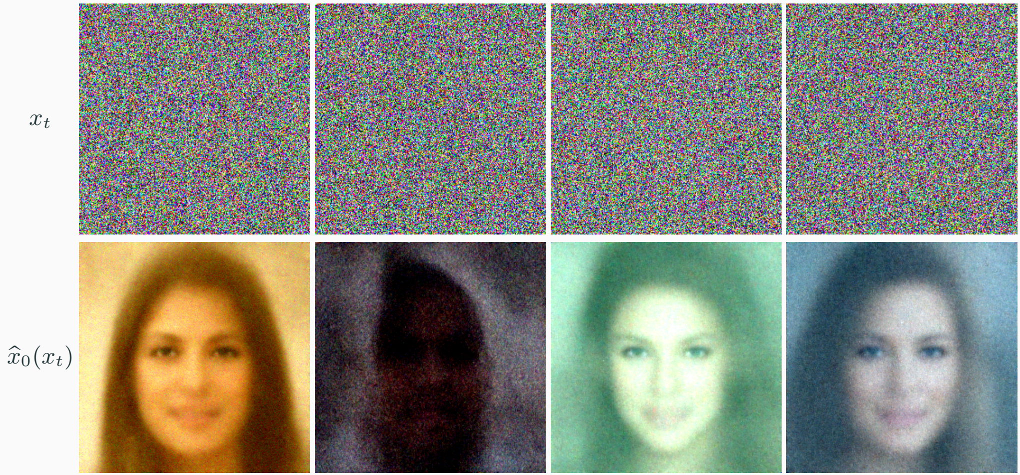

t = 210

[1] Andreas Lugmayr et al. (2022). "RePaint: Inpainting using Denoising Diffusion Probabilistic Models". In: *2022 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 11451–11461. URL: https://api.semanticscholar.org/CorpusID:246240274

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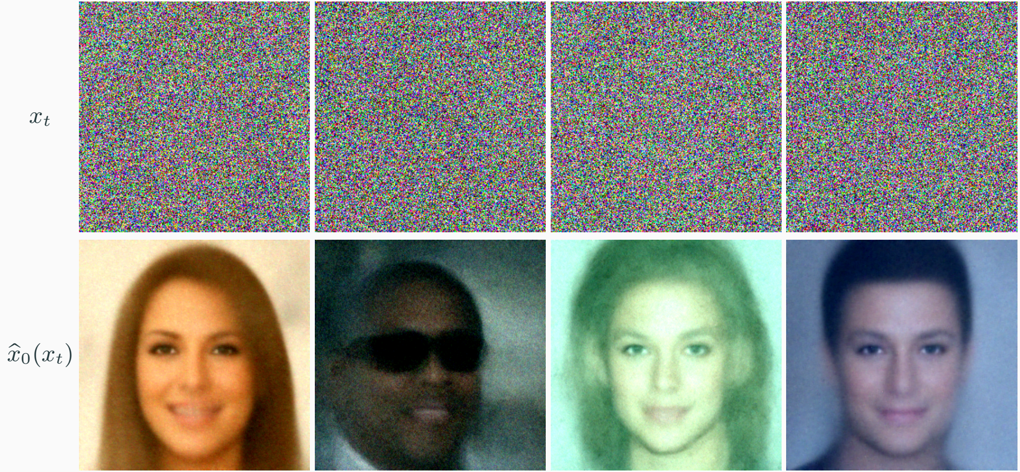


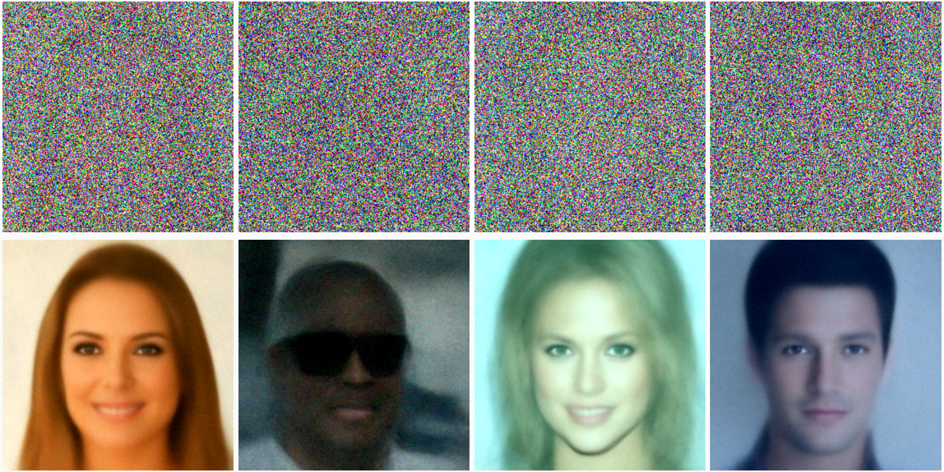
$t = 190$

[1] Andreas Lugmayr et al. (2022). "RePaint: Inpainting using Denoising Diffusion Probabilistic Models". In: *2022 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 11451–11461. URL: `https://api.semanticscholar.org/CorpusID:246240274`

Examples (generated with [Lugmayr et al. 2022][1])

x_t

$\widehat{x}_0(x_t)$



t = 170

[1] Andreas Lugmayr et al. (2022). "RePaint: Inpainting using Denoising Diffusion Probabilistic Models". In: *2022 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 11451–11461. URL: https://api.semanticscholar.org/CorpusID:246240274

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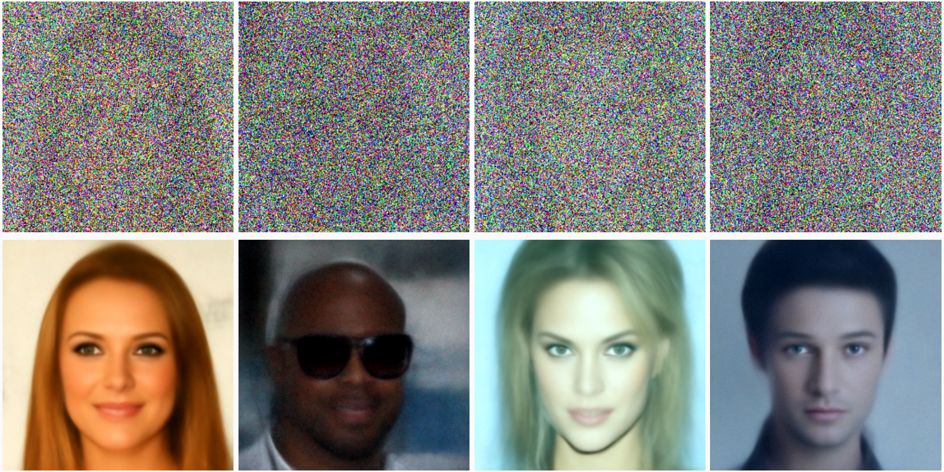

t = 150

[1] Andreas Lugmayr et al. (2022). "RePaint: Inpainting using Denoising Diffusion Probabilistic Models". In: *2022 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 11451–11461. URL: https://api.semanticscholar.org/CorpusID:246240274

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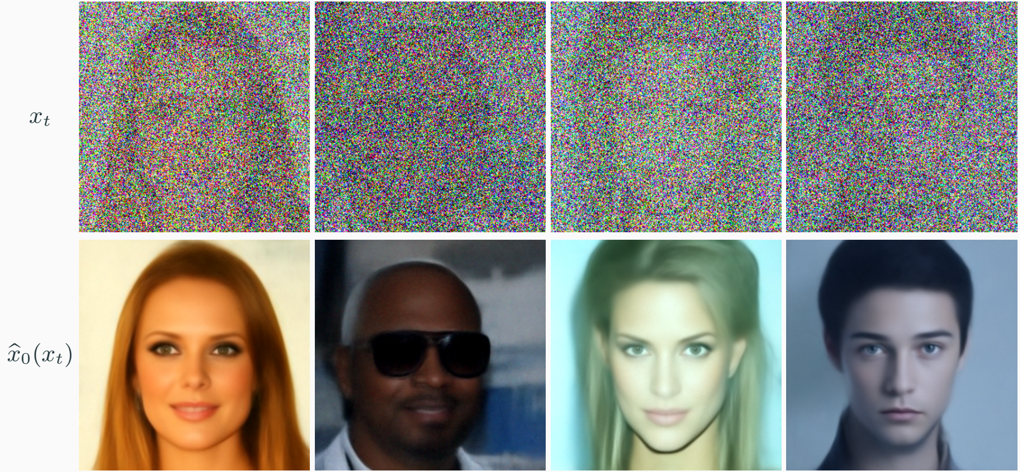

t = 130

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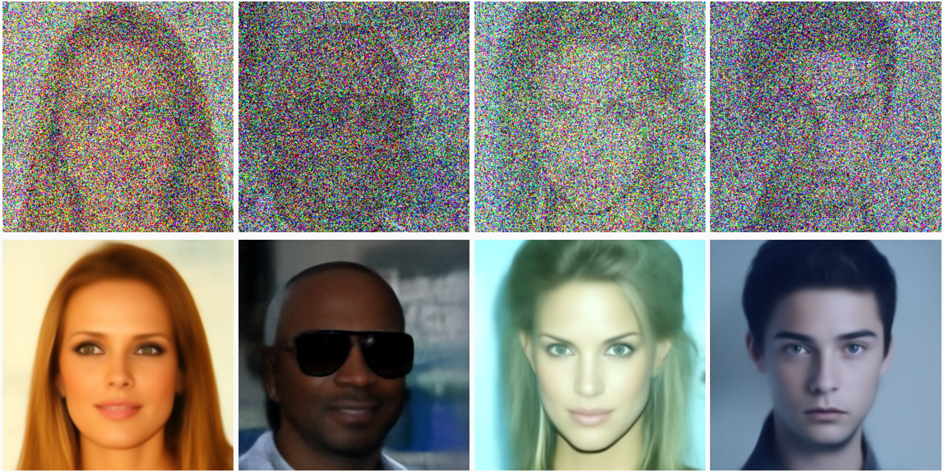

$t = 110$

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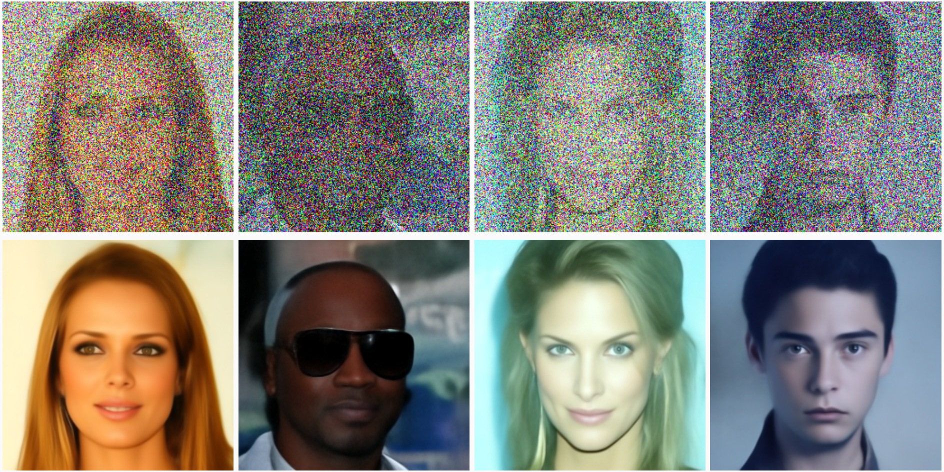


x_t

$\widehat{x}_0(x_t)$

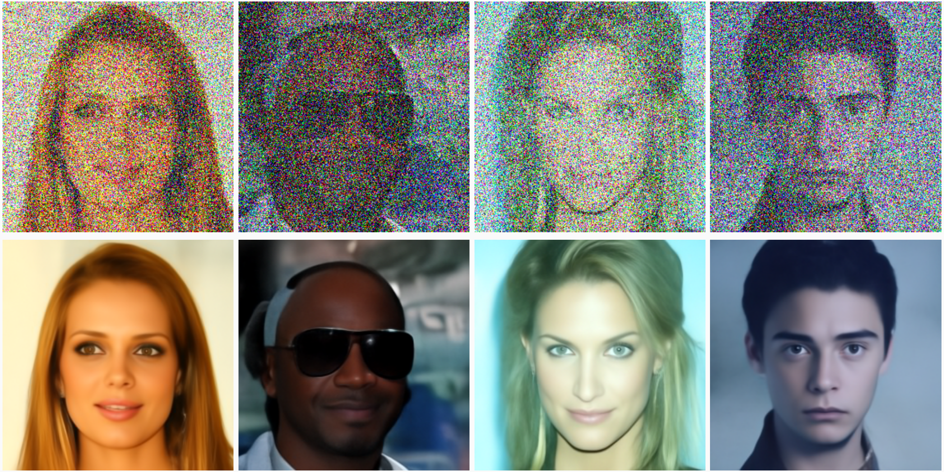
t = 90

[1] Andreas Lugmayr et al. (2022). "RePaint: Inpainting using Denoising Diffusion Probabilistic Models". In: *2022 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 11451–11461. URL: https://api.semanticscholar.org/CorpusID:246240274

Examples (generated with [Lugmayr et al. 2022][1])

x_t

$\widehat{x}_0(x_t)$

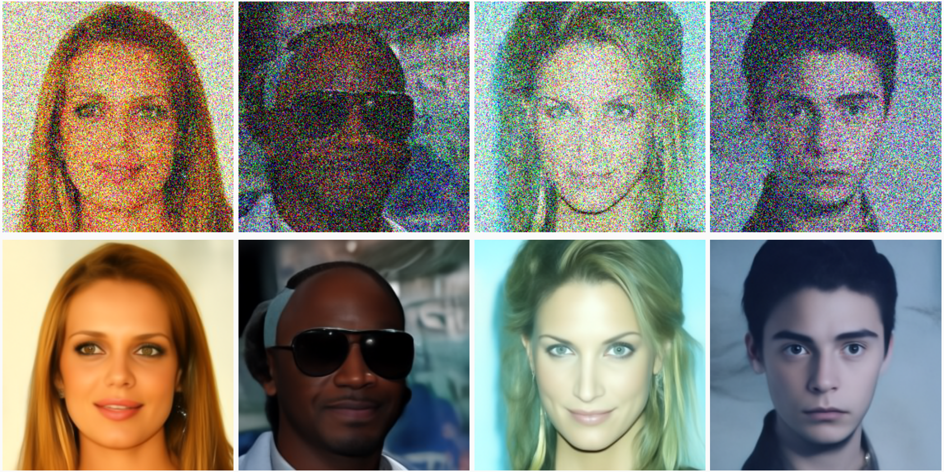


t = 70

[1] Andreas Lugmayr et al. (2022). "RePaint: Inpainting using Denoising Diffusion Probabilistic Models". In: *2022 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 11451–11461. URL: https://api.semanticscholar.org/CorpusID:246240274

x_t

$\widehat{x}_0(x_t)$



t = 50

[1] Andreas Lugmayr et al. (2022). "RePaint: Inpainting using Denoising Diffusion Probabilistic Models". In: *2022 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 11451–11461. URL: https://api.semanticscholar.org/CorpusID:246240274

Examples (generated with [Lugmayr et al. 2022][1])

x_t

$\widehat{x}_0(x_t)$

t = 30

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Examples (generated with [Lugmayr et al. 2022][1])

x_t

$\widehat{x}_0(x_t)$

$t = 10$

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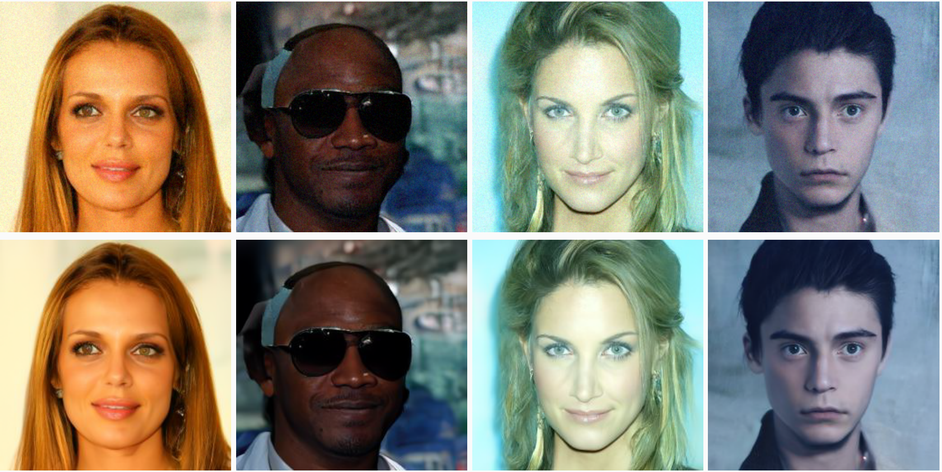
Examples (generated with [Lugmayr et al. 2022][1])

x_t

$\widehat{x}_0(x_t)$



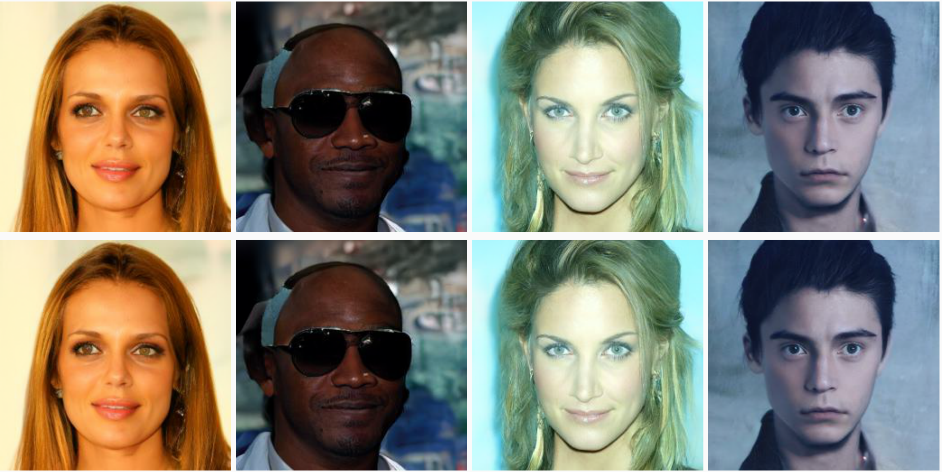
$t = 5$

[1] Andreas Lugmayr et al. (2022). "RePaint: Inpainting using Denoising Diffusion Probabilistic Models". In: *2022 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 11451–11461. URL: https://api.semanticscholar.org/CorpusID:246240274

Examples (generated with [Lugmayr et al. 2022][1])

x_t

$\widehat{x}_0(x_t)$



t = 0

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Introduction to diffusion models through SDEs

Focus on the VP-SDE: the forward process

$$dx_t = -\beta_t x_t dt + \sqrt{2\beta_t} dw_t, \quad 0 \leqslant t \leqslant T, \quad x_0 \sim p_{\text{data}}$$

The strong solution of this equation is:

$$x_t = e^{-B_t} x_0 + \boldsymbol{\eta}_t, \quad 0 \leqslant t \leqslant T, \text{ with } \eta_t \sim \mathcal{N}(\mathbf{0}, \left(1 - e^{-2B_t}\right) \boldsymbol{I}), B_t = \int_0^t \beta_u du.$$

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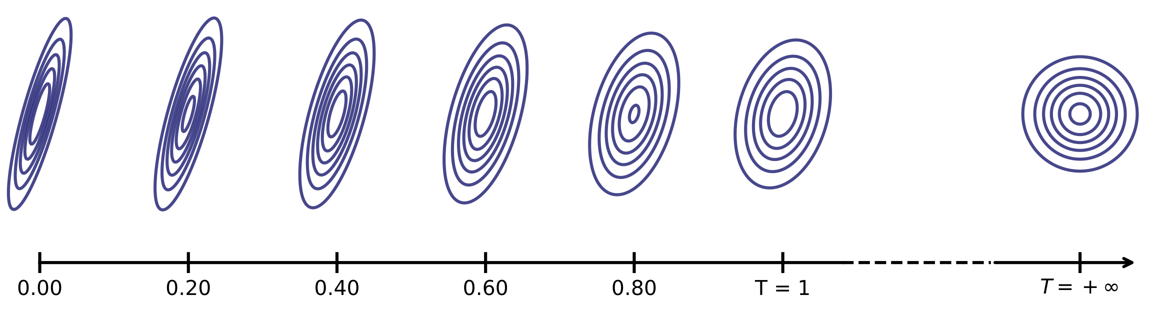


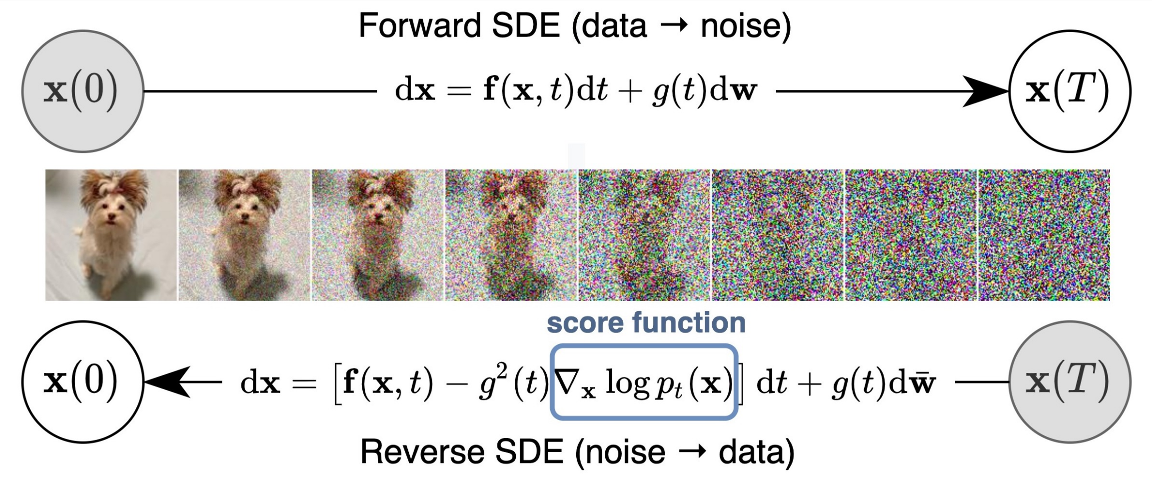


Image extracted from [Song et al. 2021]

Forward equation

$$dx_t = -\beta_t x_t + \sqrt{2\beta_t} dw_t, \quad 1 \leqslant t \leqslant T$$

↓ via p_t density distribution of x_t

Fokker-Planck equation

$$\partial_t p_t(x) = -\operatorname{div}(f(x,t)p_t(x)) + \frac{1}{2}\Delta_x p_t(x), \quad 1 \leqslant t \leqslant T$$

↓ Reversed in time

"Reversed" Fokker-Planck equation

$$\partial_t q_t(x) = -\operatorname{div}_x\left[\left(-f(x,T-t) + g(T-t)^2\nabla_x \log q_t(x)\right) q_t(x)\right] + \frac{(g(T-t))^2}{2} q_t(x), \quad 1 \leqslant t \leqslant T$$

↓

A family of backward equations

$$dy_t = \left[-\beta_{T-t} y_t + (1+\alpha)\beta_t \nabla_y \log p_{T-t}(y_t)\right] dt + \sqrt{2\alpha\beta_{T-t}} dw_t, \quad 1 \leqslant t \leqslant T.$$

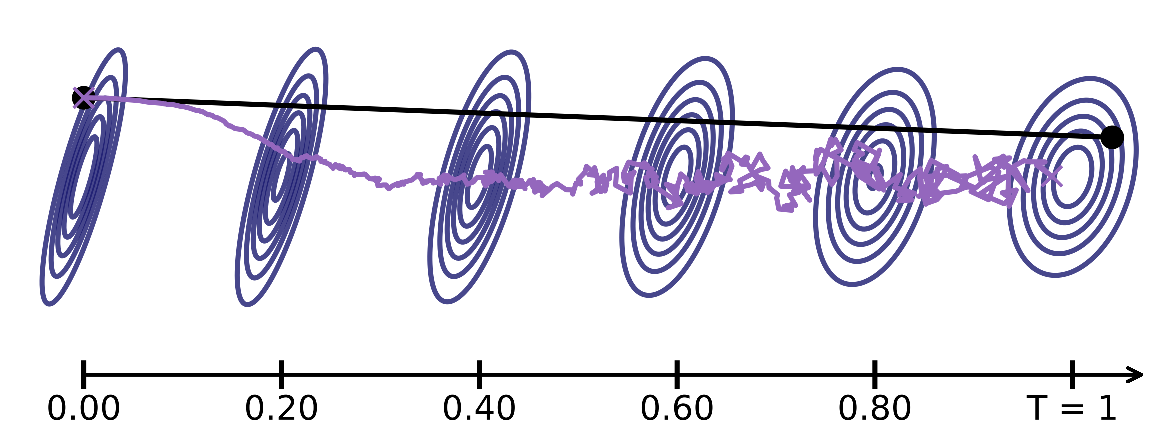
SDE ($\alpha = 1$):

$$dy_t = \left[-\beta_{T-t} y_t + 2\beta_t \nabla_y \log p_{T-t}(y_t)\right] dt + \sqrt{2\beta_{T-t}} dw_t.$$

ODE ($\alpha = 0$):

$$dy_t = \left[-\beta_{T-t} y_t + \beta_t \nabla_y \log p_{T-t}(y_t)\right] dt.$$

SDE ($\alpha = 1$), ODE ($\alpha = 0$)



Study of the convergence of diffusion models

Illustration of the different error types

Theoretical setting

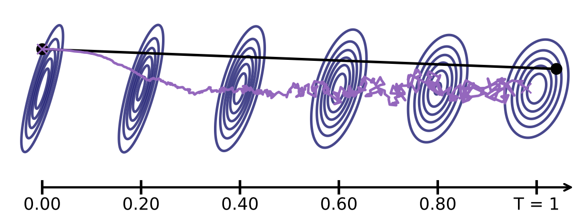
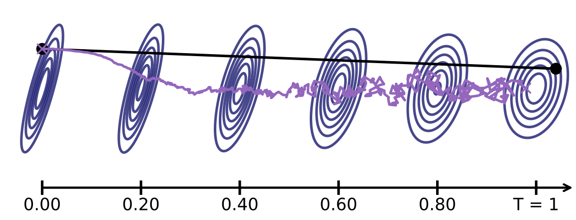
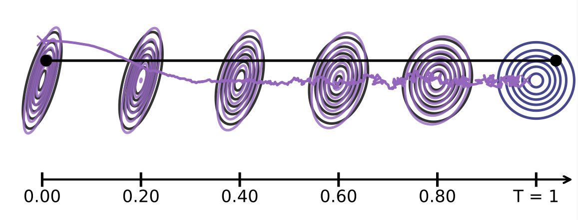


Illustration of the different error types

Theoretical setting



Initialization error



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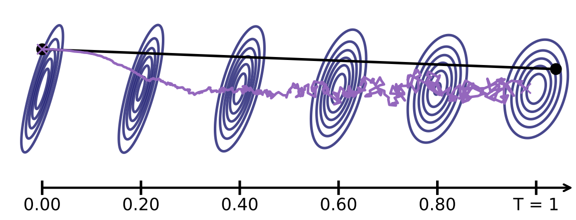
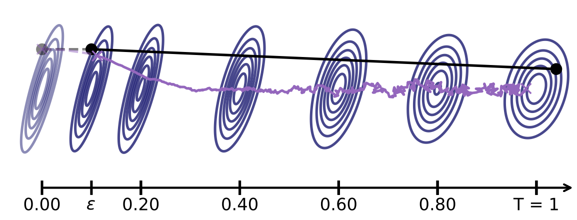
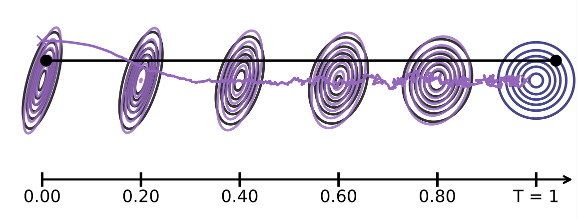


Truncation error



Initialization error



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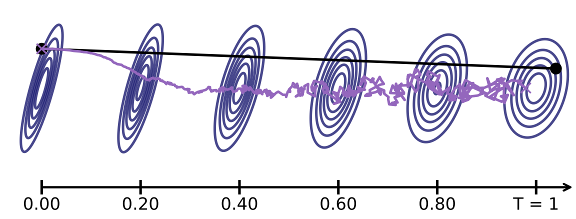
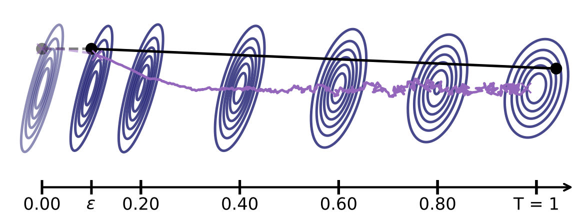
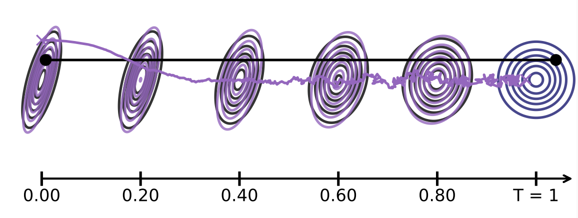


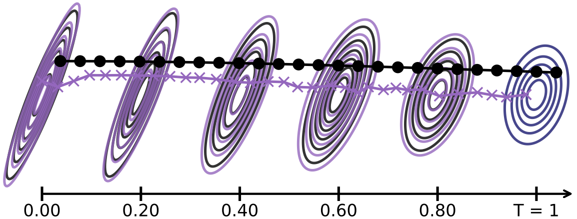
Truncation error



Initialization error



Discretization error



$$dy_t = \left[\beta_t y_t + (1+\alpha)\beta_t \nabla_y \log p_t(y_t)\right] dt + \sqrt{2\alpha\beta_t} dw_t, \quad 0 \leqslant t \leqslant T, \quad y_T \sim p_T.$$

Sampling a distribution using diffusion models implies different choices and error types:

Sampling through diffusion models

$$dy_t = [-\beta_t y_t + (1+\alpha)\beta_t \nabla_y \log p_t(y_t)]\, dt + \sqrt{2\alpha\beta_t} dw_t, \quad 0 \leqslant t \leqslant T, \quad y_T \sim \underbrace{\cancel{y_T \sim p_T}}_{y_T \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})} .$$

Sampling a distribution using diffusion models implies different choices and error types:

- p_T, which is unknown, is replaced by $\mathcal{N}(\mathbf{0}, \boldsymbol{I})$ $\rightarrow$ **initialization error**

Sampling through diffusion models

$$dy_t = \left[-\beta_t y_t + (1+\alpha)\beta_t \nabla_y \log p_t(y_t)\right] dt + \sqrt{2\alpha\beta_t} dw_t, \quad \underset{\varepsilon}{\not{0}} \leqslant t \leqslant T, \quad y_T \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}).$$

Sampling a distribution using diffusion models implies different choices and error types:

- p_T, which is unknown, is replaced by $\mathcal{N}(\mathbf{0}, \boldsymbol{I})$ $\rightarrow$ **initialization error**
- In fact, another time ε to consider them on $[\varepsilon, T]$ $\rightarrow$ **truncation error**

Sampling through diffusion models

$$dy_t = \left[-\beta_t y_t + (1+\alpha)\beta_t \nabla_y \log p_t(y_t)\right] dt + \sqrt{2\alpha\beta_t} dw_t, \quad \varepsilon \leqslant t \leqslant T, \quad y_T \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}).$$

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- p_T, which is unknown, is replaced by $\mathcal{N}(\mathbf{0}, \boldsymbol{I})$ → **initialization error**
- In fact, another time ε to consider them on $[\varepsilon, T]$ → **truncation error**
- A scheme to discretize the equations → **discretization error**

Sampling through diffusion models

$$dy_t = \left[-\beta_t y_t + (1+\alpha)\beta_t \underbrace{\nabla_y \log p_t(y_t)}_{s_\theta(t,y_t)} \right] dt + \sqrt{2\alpha\beta_t} dw_t, \quad \varepsilon \leqslant t \leqslant T, \quad y_T \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}).$$

Sampling a distribution using diffusion models implies different choices and error types:

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- In fact, another time ε to consider them on $[\varepsilon, T]$ → **truncation error**
- A scheme to discretize the equations → **discretization error**
- A model/neural network s_θ to learn the score → **score approximation error**

Sampling through diffusion models

$$dy_t = [-\beta_t y_t + (1+\alpha)\beta_t s_\theta(t, y_t)]\, dt + \sqrt{2\alpha\beta_t} dw_t, \quad \varepsilon \leqslant t \leqslant T, \quad y_T \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}).$$

Sampling a distribution using diffusion models implies different choices and error types:

- p_T, which is unknown, is replaced by $\mathcal{N}(\mathbf{0}, \boldsymbol{I})$ $\rightarrow$ **initialization error**
- In fact, another time ε to consider them on $[\varepsilon, T]$ $\rightarrow$ **truncation error**
- A scheme to discretize the equations $\rightarrow$ **discretization error**
- A model/neural network s_θ to learn the score $\rightarrow$ **score approximation error**

$\Longrightarrow$ Let us focus on the **initialization error** and the **discretization error**.

Restriction to the Gaussian case

Gaussian assumption

Gaussian assumption: p_{data} is a centered Gaussian distribution $\mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$. ($\boldsymbol{\Sigma}$ is not necessarily invertible)

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$$\nabla_x \log p_t(x) = -\mathbf{\Sigma}_t^{-1} x, \quad 0 < t \leqslant T$$

with $\mathbf{\Sigma}_t = e^{-2B_t}\mathbf{\Sigma} + (1 - e^{-2B_t})\boldsymbol{I}$.

Gaussian assumption

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with $\mathbf{\Sigma}_t = e^{-2B_t}\mathbf{\Sigma} + (1 - e^{-2B_t})\boldsymbol{I}$.

Proposition 3: Lineartiy of the score

he three following propositions are equivalent:

(i) $x_0 \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$ for some covariance $\mathbf{\Sigma}$.

(ii) $\forall t > 0, \nabla_x \log p_t(x)$ is linear w.r.t x.

(iii) $\exists t > 0, \nabla_x \log p_t(x)$ is linear w.r.t x.

Initialization error

Explicit solution of the backward equations

$$dy_t = \left[-\beta_t y_t + (1+\alpha)\beta_t \nabla \log p_t(y_t)\right] dt + \sqrt{2\alpha\beta_t} dw_t, \quad \varepsilon \leqslant t \leqslant T, \quad y_T \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}). \qquad (1_\alpha)$$

Gaussian assumption: p_{data} is a centered Gaussian distribution $\mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$. ($\mathbf{\Sigma}$ is not necessarily invertible)

Explicit solution of the backward equations

$$dy_t = \left[-\beta_t y_t + (1+\alpha)\beta_t \nabla \log p_t(y_t)\right] dt + \sqrt{2\alpha\beta_t} dw_t, \quad \varepsilon \leqslant t \leqslant T, \quad y_T \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}). \tag{1_α}$$

Gaussian assumption: p_{data} is a centered Gaussian distribution $\mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$. ($\boldsymbol{\Sigma}$ is not necessarily invertible)

Proposition 4: Solution to the backward equations under Gaussian assumption

For $\alpha \in \mathbb{R}^+$, the strong solution of Equation (1_α) is

$$y_t = e^{-\alpha(B_T - B_{T-t})} \boldsymbol{\Sigma}_{T-t}^{\frac{1+\alpha}{2}} \boldsymbol{\Sigma}_T^{-\frac{1+\alpha}{2}} y_0 + \boldsymbol{\xi}_t \text{ with } \operatorname{Cov}(\boldsymbol{\xi}_t) = \boldsymbol{\Sigma}_{T-t} - e^{-2\alpha(B_T - B_{T-t})} \boldsymbol{\Sigma}_{T-t}^{1+\alpha} \boldsymbol{\Sigma}_T^{-\alpha}$$

Explicit solution of the backward equations

$$dy_t = [-\beta_t y_t + (1+\alpha)\beta_t \nabla \log p_t(y_t)]\, dt + \sqrt{2\alpha\beta_t} dw_t, \quad \varepsilon \leqslant t \leqslant T, \quad y_T \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}). \qquad (1_\alpha)$$

Gaussian assumption: p_{data} is a centered Gaussian distribution $\mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$. ($\mathbf{\Sigma}$ is not necessarily invertible)

Proposition 5: Solution to the equations under Gaussian assumption

If $\text{Cov}(y_T)\mathbf{\Sigma} = \mathbf{\Sigma}\,\text{Cov}(y_T)$, for $0 \leqslant t \leqslant T$,

$$\begin{aligned}
\mathbf{\Sigma}_t^{\mathsf{SDE}} &= \text{Cov}(y_t^{\mathsf{SDE}}) = \mathbf{\Sigma}_t + e^{-2(B_T - B_t)} \mathbf{\Sigma}_t^2 \mathbf{\Sigma}_T^{-2} \left[\text{Cov}(y_T) - \mathbf{\Sigma}_T\right], \\
\mathbf{\Sigma}_t^{\mathsf{ODE}} &= \text{Cov}(y_t^{\mathsf{ODE}}) = \mathbf{\Sigma}_t \mathbf{\Sigma}_T^{-1}\,\text{Cov}(y_T),
\end{aligned}$$

Explicit solution of the backward equations

$$dy_t = [-\beta_t y_t + (1+\alpha)\beta_t \nabla \log p_t(y_t)]\, dt + \sqrt{2\alpha\beta_t} dw_t, \quad \varepsilon \leqslant t \leqslant T, \quad y_T \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}). \qquad (1_\alpha)$$

Gaussian assumption: p_{data} is a centered Gaussian distribution $\mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$. ($\boldsymbol{\Sigma}$ is not necessarily invertible)

Proposition 6: Solution to the equations under Gaussian assumption

If $\operatorname{Cov}(y_T)\boldsymbol{\Sigma} = \boldsymbol{\Sigma}\operatorname{Cov}(y_T)$, for $0 \leqslant t \leqslant T$,

$$\boldsymbol{\Sigma}_t^{\mathsf{SDE}} = \operatorname{Cov}(y_t^{\mathsf{SDE}}) = \boldsymbol{\Sigma}_t + e^{-2(B_T - B_t)} \boldsymbol{\Sigma}_t^2 \boldsymbol{\Sigma}_T^{-2} \left[\operatorname{Cov}(y_T) - \boldsymbol{\Sigma}_T\right],$$
$$\boldsymbol{\Sigma}_t^{\mathsf{ODE}} = \operatorname{Cov}(y_t^{\mathsf{ODE}}) = \boldsymbol{\Sigma}_t \boldsymbol{\Sigma}_T^{-1} \operatorname{Cov}(y_T),$$

If $y_T \sim p_T = \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_T)$,

$$\boldsymbol{\Sigma}_t^{\mathsf{SDE}} = \boldsymbol{\Sigma}_t^{\mathsf{ODE}} = \boldsymbol{\Sigma}_t, \quad 0 \leqslant t \leqslant T.$$

Explicit solution of the backward equations

$$dy_t = [-\beta_t y_t + (1+\alpha)\beta_t \nabla \log p_t(y_t)]\, dt + \sqrt{2\alpha\beta_t} dw_t, \quad \varepsilon \leqslant t \leqslant T, \quad y_T \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}). \tag{1_α}$$

Gaussian assumption: p_{data} is a centered Gaussian distribution $\mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$. ($\boldsymbol{\Sigma}$ is not necessarily invertible)

Proposition 7: Solution to the equations under Gaussian assumption

If $\operatorname{Cov}(y_T)\boldsymbol{\Sigma} = \boldsymbol{\Sigma} \operatorname{Cov}(y_T)$, for $0 \leqslant t \leqslant T$,

$$\begin{aligned}
\boldsymbol{\Sigma}_t^{\text{SDE}} &= \operatorname{Cov}(y_t^{\text{SDE}}) = \boldsymbol{\Sigma}_t + e^{-2(B_T - B_t)} \boldsymbol{\Sigma}_t^2 \boldsymbol{\Sigma}_T^{-2} \left[\operatorname{Cov}(y_T) - \boldsymbol{\Sigma}_T\right], \\
\boldsymbol{\Sigma}_t^{\text{ODE}} &= \operatorname{Cov}(y_t^{\text{ODE}}) = \boldsymbol{\Sigma}_t \boldsymbol{\Sigma}_T^{-1} \operatorname{Cov}(y_T),
\end{aligned}$$

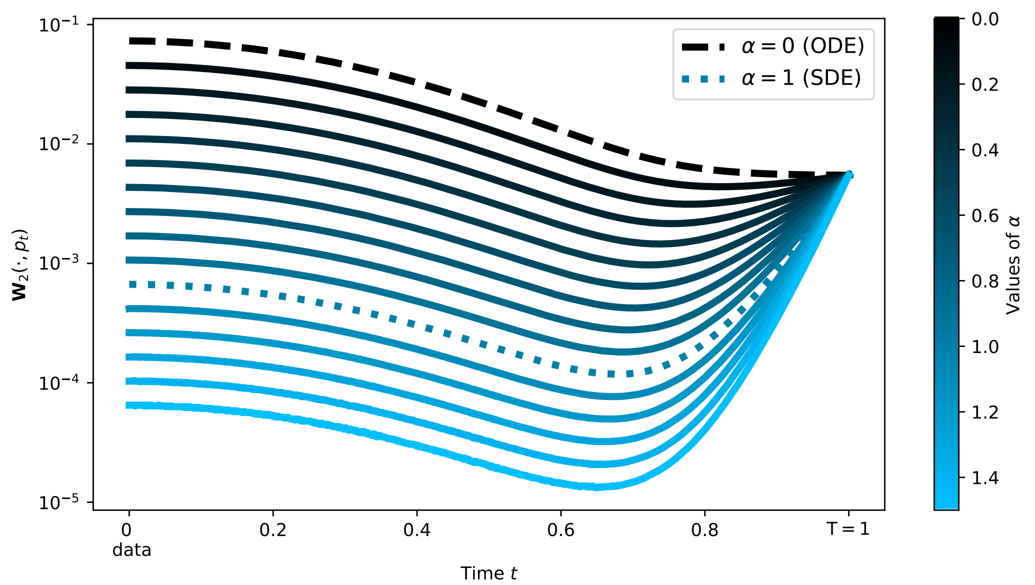
If $y_T \sim p_T = \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_T)$,

$$\boldsymbol{\Sigma}_t^{\text{SDE}} = \boldsymbol{\Sigma}_t^{\text{ODE}} = \boldsymbol{\Sigma}_t, \quad 0 \leqslant t \leqslant T.$$

If $y_T \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$, (with intialization error)

$$\boldsymbol{\Sigma}_t^{\text{SDE}} = \boldsymbol{\Sigma}_t + e^{-2(B_T - B_t)} \boldsymbol{\Sigma}_t^2 \boldsymbol{\Sigma}_T^{-2} (\boldsymbol{I} - \boldsymbol{\Sigma}_T), \quad 0 \leqslant t \leqslant T.$$

Initialization error: exact Wasserstein error



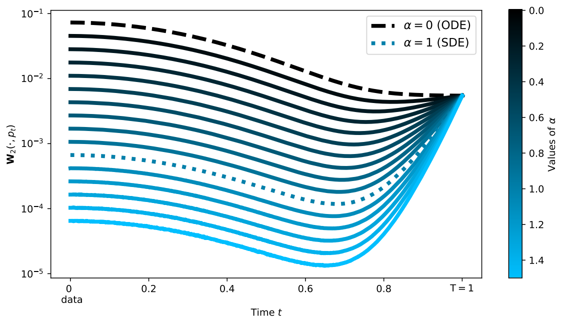
By considering p_t^α the marginals of the backward Equation (1_α),

$$dy_t = \left[-\beta_t y_t + (1+\alpha)\beta_t \nabla \log p_t(y_t)\right] dt + \sqrt{2\alpha\beta_t} dw_t, \quad \varepsilon \leqslant t \leqslant T, \quad y_T \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}). \tag{1_α}$$

Proposition 8: Marginals of the generative processes under Gaussian assumption

Under Gaussian assumption, for all $0 \leqslant t \leqslant T$,

$$\mathcal{W}_2(p_t^{\alpha'}, p_t^{\text{Forward}}) \leqslant \mathcal{W}_2(p_t^{\alpha}, p_t^{\text{Forward}}).$$



Exponential forgetting of the initial condition

Under Gaussian assumption, the strong solution to backward SDEs can be written as:

$$y_t = e^{-\alpha(B_T - B_{T-t})} \boldsymbol{\Sigma}_{T-t}^{\frac{1+\alpha}{2}} \boldsymbol{\Sigma}_T^{-\frac{1+\alpha}{2}} y_T + \boldsymbol{\xi}_t, 0 \leqslant t \leqslant T.$$

Under Gaussian assumption, the solution to ODE can be written as:

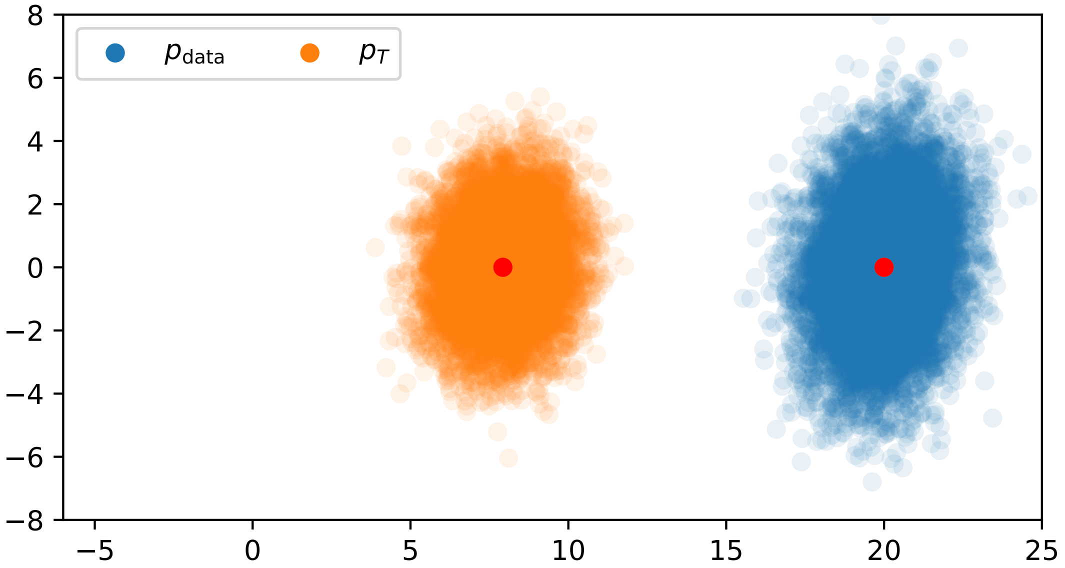
$$y_t^{\text{ODE}} = \boldsymbol{\Sigma}_T^{-1/2} \boldsymbol{\Sigma}_t^{1/2} y_T, \quad 0 \leqslant t \leqslant T,$$

- $y \mapsto \boldsymbol{\Sigma}_T^{-1/2} \boldsymbol{\Sigma}_t^{1/2} y$ is the transport map between p_T and p_t.
- False in general:, see [Lavenant and Santambrogio 2022][2]
- However, used in [Khrulkov et al. 2023][3]

[2] Hugo Lavenant and Filippo Santambrogio (2022). "The flow map of the Fokker–Planck equation does not provide optimal transport". In: *Applied Mathematics Letters* 133, p. 108225. ISSN: 0893-9659. DOI: https://doi.org/10.1016/j.aml.2022.108225. URL: https://www.sciencedirect.com/science/article/pii/S089396592200180X

[3] Valentin Khrulkov et al. (2023). "Understanding DDPM Latent Codes Through Optimal Transport". In: *The Eleventh International Conference on Learning Representations*. URL: https://openreview.net/forum?id=6PIrhAx1j4i

Initialization error: Focus on the ODE



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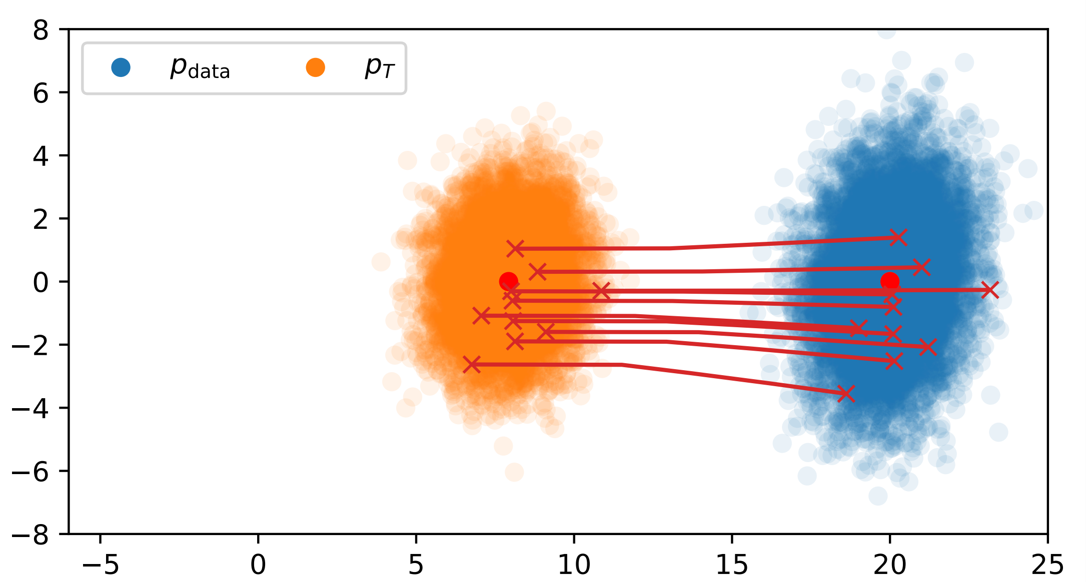

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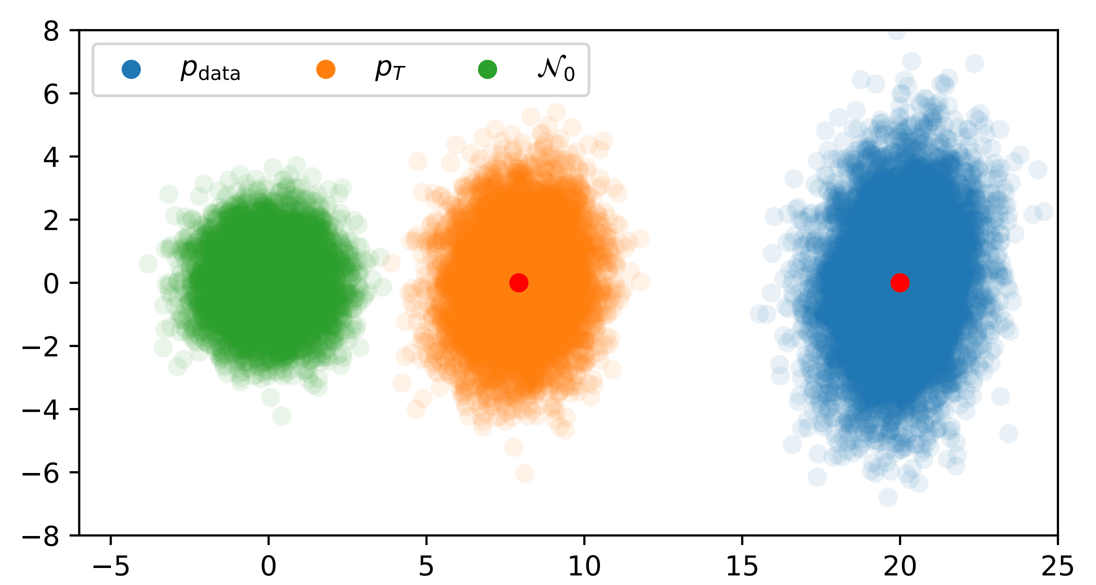

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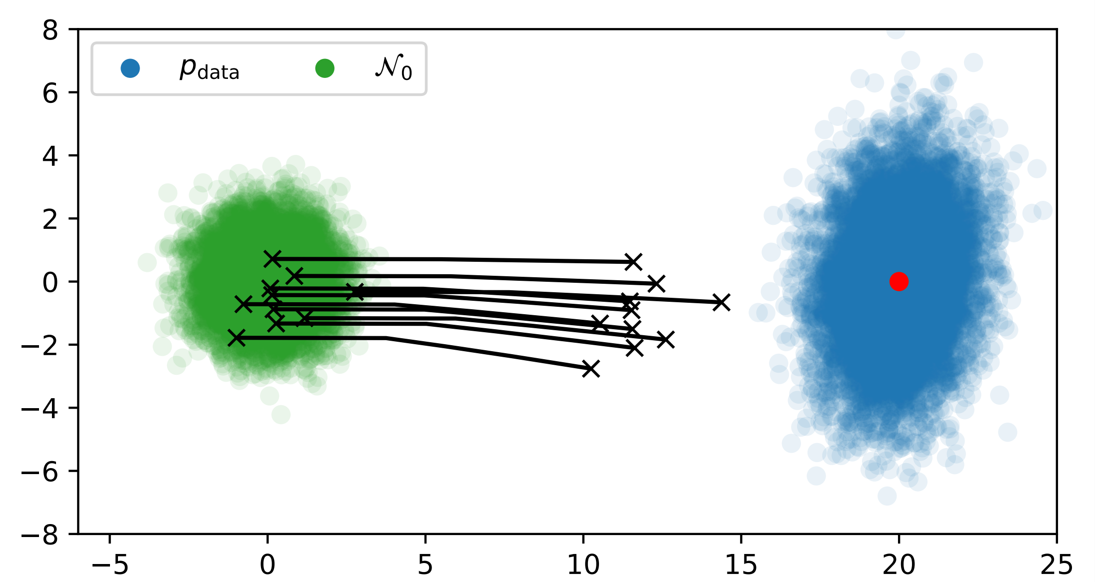
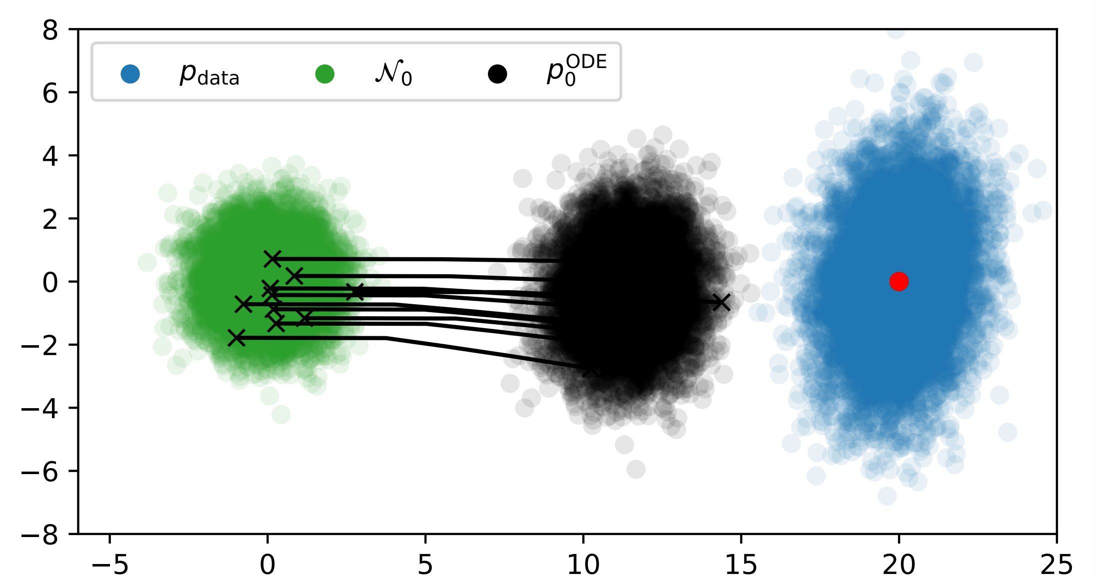
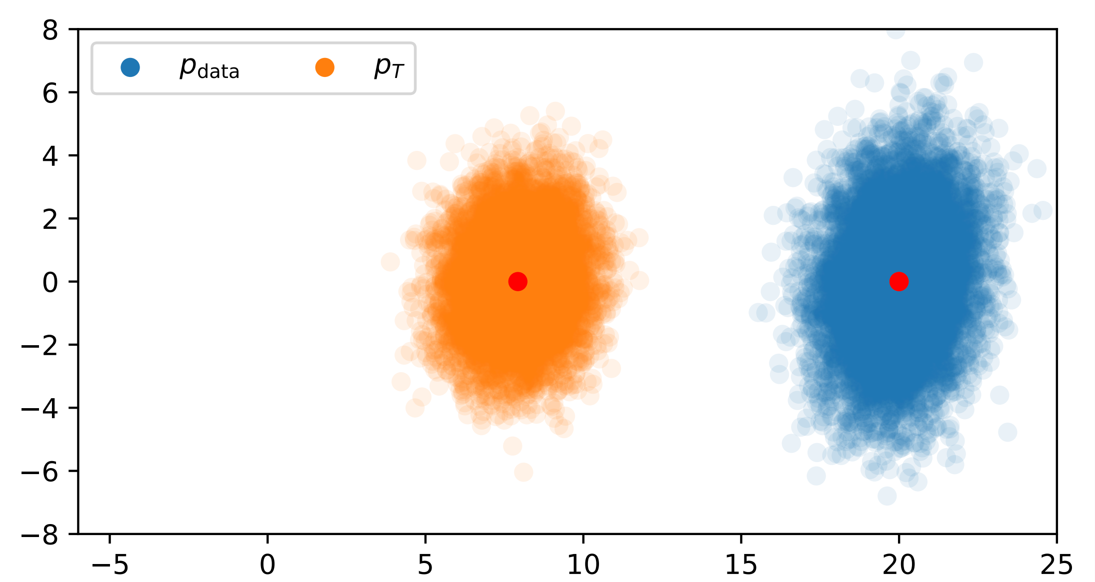


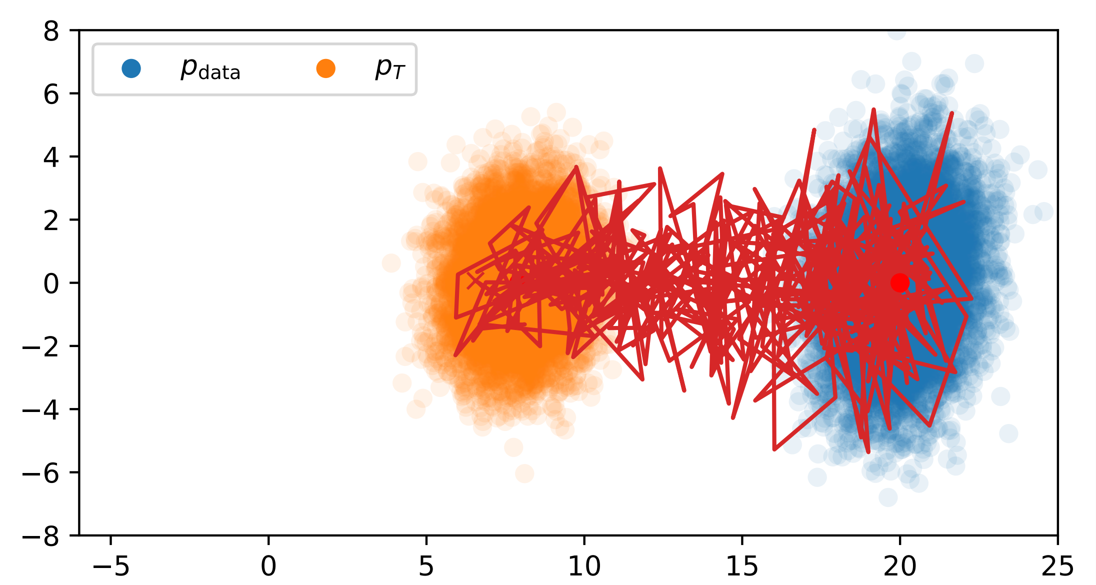
Initialization error: Focus on the ODE



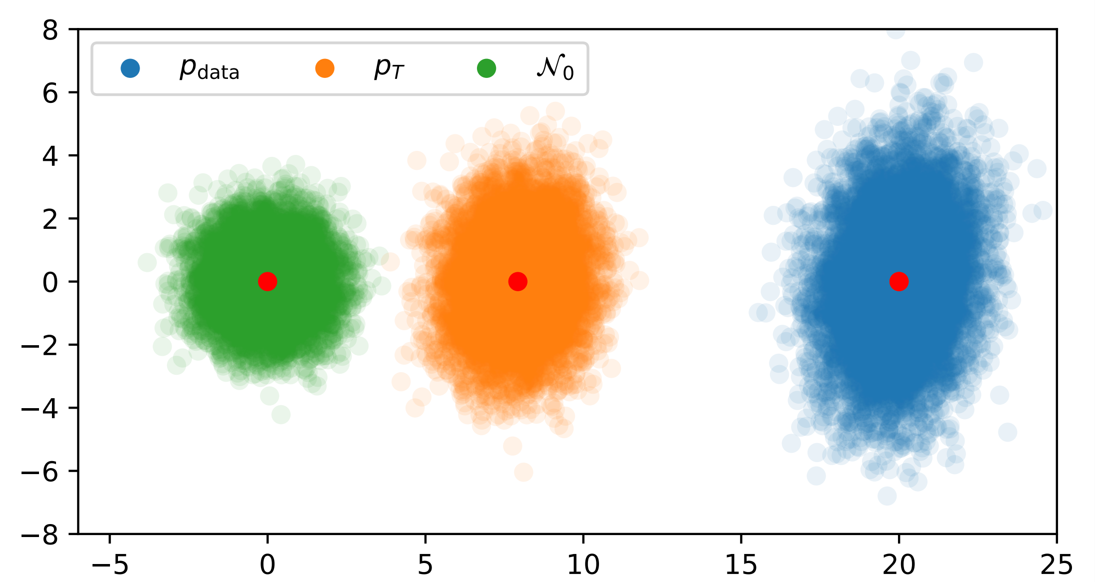
Initialization error: Focus on the SDE



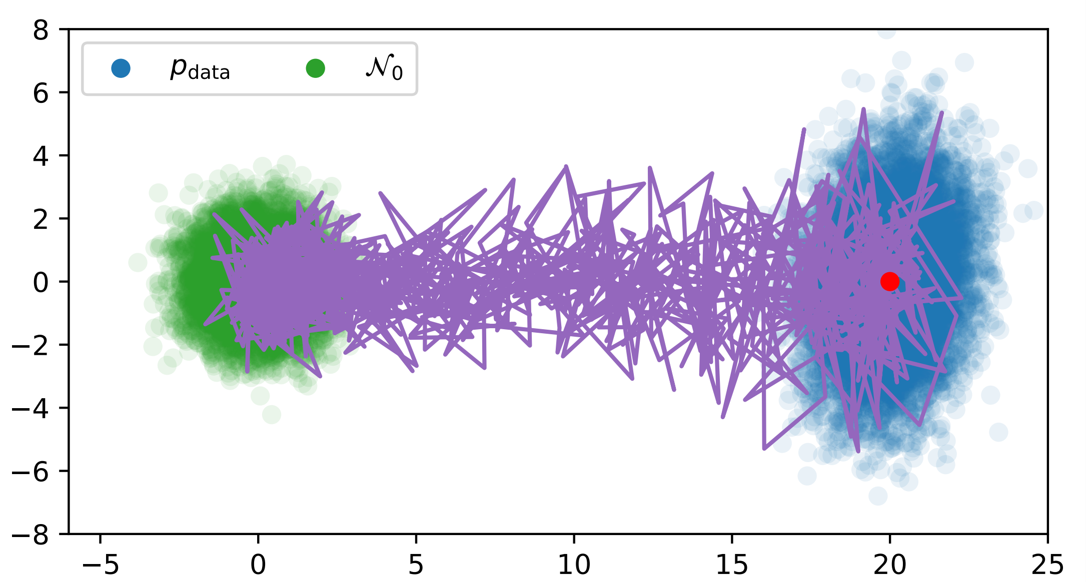
Initialization error: Focus on the SDE



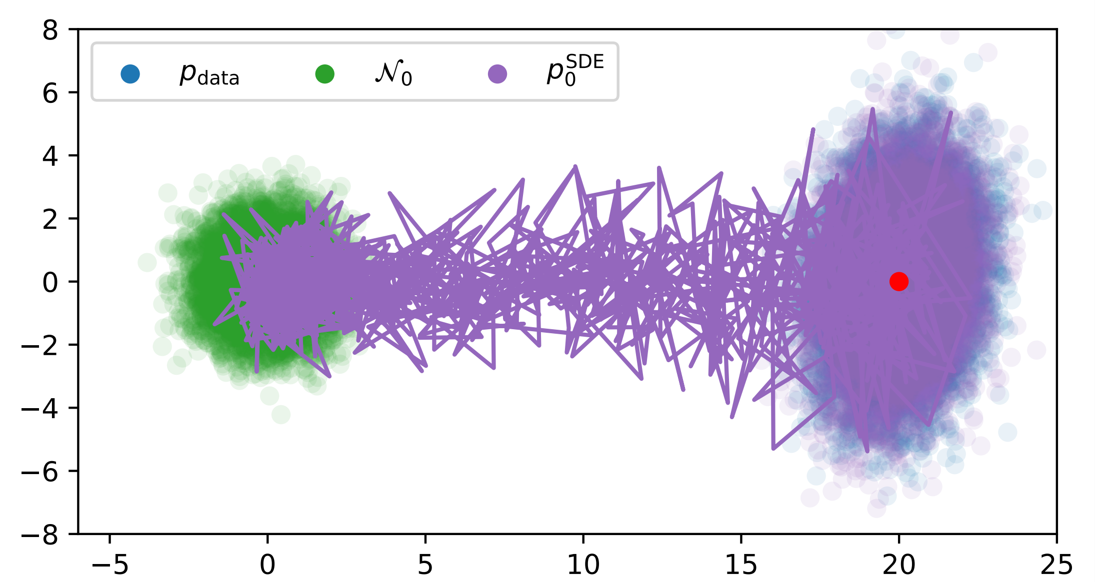
Initialization error: Focus on the SDE



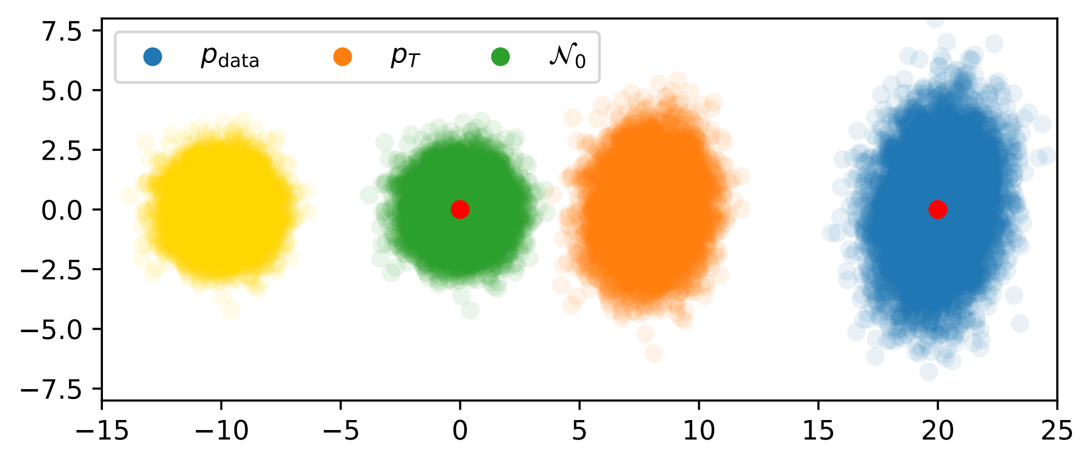
Initialization error: Focus on the SDE



Initialization error: Focus on the SDE



Initialization error: Focus on the SDE



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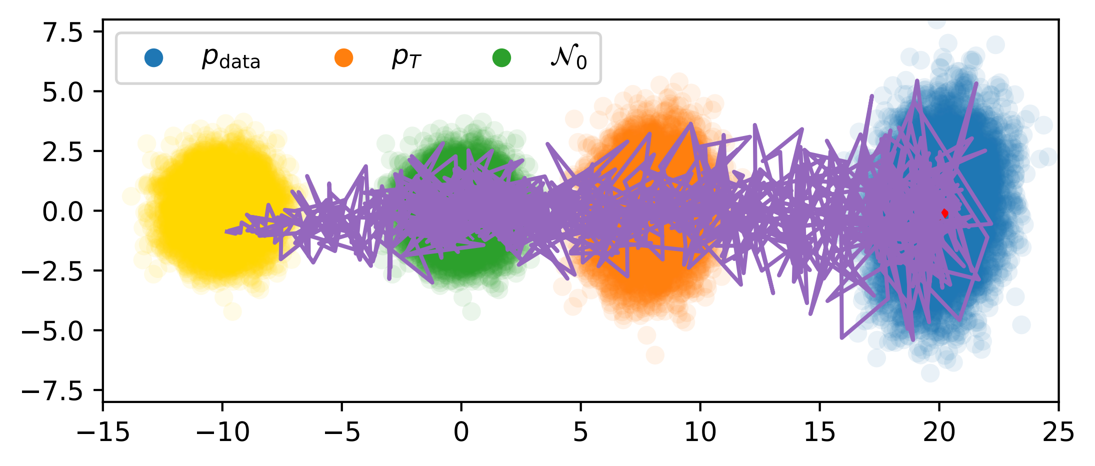

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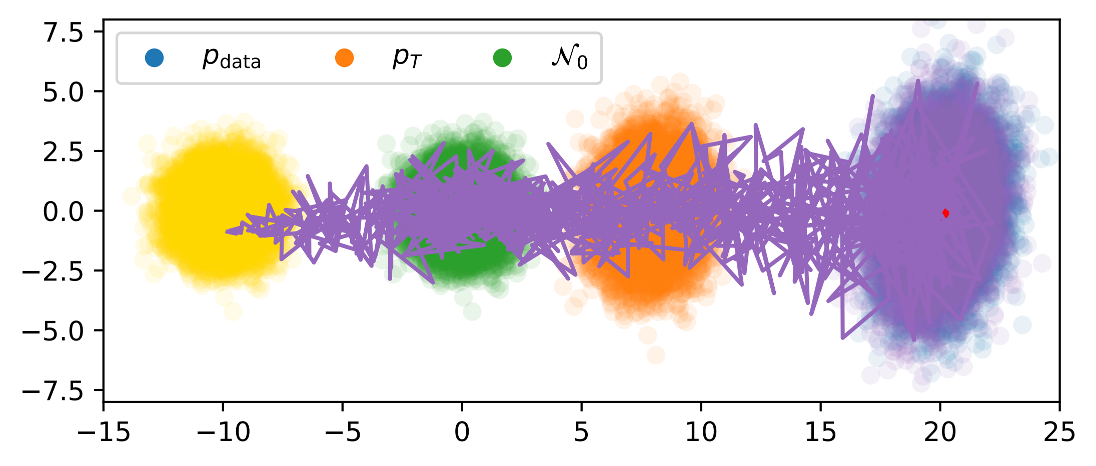


Study of the discretization error

The Euler-Maruyama scheme

We propose to discretize the backward equations with the Euler-Maruyama scheme.

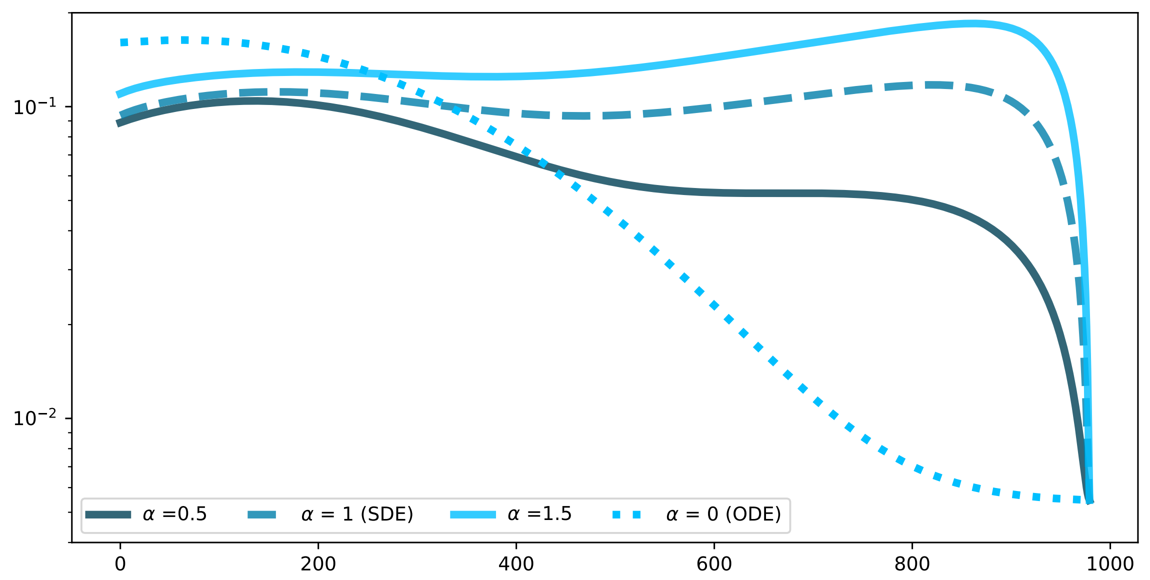
$$dy_t = [-\beta_t y_t + (1+\alpha)\beta_t s_\theta(t, y_t)]\, dt + \sqrt{2\alpha\beta_t} dw_t, \quad \varepsilon \leqslant t \leqslant T, \quad y_T \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}). \tag{1_α}$$

becomes

$$\begin{cases} y_N & \sim \mathcal{N}(0, \boldsymbol{I}) \text{ (initialization error)} \\ y_{k-1} & = [-\beta_{t_k} y_k + 1 + \alpha)\beta_{t_k} \nabla \log p_{t_k}(y_k)]\, \Delta_t + 2\alpha\beta_{t_{k-1}} z_k, z_k \sim \mathcal{N}(0, I) \end{cases}$$

We observe the behavior with respect to α with the adding of initialization error and discretization error.

Discretization of the SDEs: exact Wasserstein error



Conclusion

There is a trade-off between initialization error and discretization error to modelize

$$y_t = e^{-\alpha(B_T - B_{T-t})} \boldsymbol{\Sigma}_{T-t}^{\frac{1+\alpha}{2}} \boldsymbol{\Sigma}_T^{-\frac{1+\alpha}{2}} y_0 + \boldsymbol{\xi}_t, 0 \leqslant t \leqslant T.$$

- The exponential decrease is beneficial for the initialization error.
- However, it is difficult to capture it with a discretization scheme.
- Consequently, optimal α seems to be in $]0, 1[$ wrt these two error types.

A bridge to Flow matching

Another direction to avoid initialization error

As a generative model, Flow Matching aims to learn a velocity field v_t such that by using

$$dx_t = v_t(x_t)dt, x_0 \sim \mathcal{N}(0, I),$$

we have

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

There is a direct link with the "ODE of diffusion models. But how is it possible to avoid initialization error ?

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$$dx_t = v_t(x_t)dt, x_0 \sim \mathcal{N}(0, I),$$

we have

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

There is a direct link with the "ODE of diffusion models. But how is it possible to avoid initialization error ?
The corresponding forward process to Flow Mathing is

$$dx_t = -\frac{1}{1-t} x_t dt + \sqrt{\frac{2t}{1-t}} dw_t \tag{1}$$

with $\frac{1}{1-t} \underset{t \longrightarrow 1}{\longrightarrow} +\infty$.

Link with memoryless stochastic process? (reading group of tuesday).

Conclusion

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- Extension to GMM ?

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- Extension to GMM ?
  - Exact solutions are not known.
  - A closed form for the $\mathbf{W}_2$ distance is not known.
  - The discretized processes are no more GMM.
- Add theoretical score approximation ?
  → Samuel Hurault et al. (2025). *From Denoising Score Matching to Langevin Sampling: A Fine-Grained Error Analysis in the Gaussian Setting*. arXiv: 2503.11615 [cs.LG]. URL: https://arxiv.org/abs/2503.11615

Thank you for your attention !

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To the restoration problems ?

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My thesis title: Stochastic super resolution using deep generative models

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→ We need to use **conditional** diffusion model !

How to perform conditional simulation ?

What is the link with solving inverse problems $\boldsymbol{v} = \boldsymbol{A}x + \sigma\boldsymbol{\varepsilon}$?

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A large literature [Song et al. 2021[4],Lugmayr et al. 2022[5],Chung et al. 2022[6],Choi et al. 2021[7]] uses the Bayes formula

$$\nabla_x \log p_t(x_t \mid \boldsymbol{v}) = \nabla_x \log p_t(\boldsymbol{v} \mid x_t) + \nabla_x \log p_t(x_t). \quad (2)$$

where $\nabla_x \log p_t(x_t)$ is the unconditional score. Consequently, studying the unconditional case provides information for the conditional one.

[4] Yang Song et al. (2021). "Score-Based Generative Modeling through Stochastic Differential Equations". In: *International Conference on Learning Representations*. URL: https://openreview.net/forum?id=PxTIG12RRHS

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Ablation study

		Continuous		$N=50$		$N=250$		$N=500$		$N=1000$	
		p_T	$\mathcal{N}_0$	p_T	$\mathcal{N}_0$	p_T	$\mathcal{N}_0$	p_T	$\mathcal{N}_0$	p_T	$\mathcal{N}_0$
EM	$\varepsilon=0$	0	6.7E-4	4.77	4.77	0.65	0.65	0.31	0.31	0.15	0.16
	$\varepsilon=10^{-5}$	2.5E-3	2.6E-3	4.77	4.77	0.65	0.65	0.31	0.31	0.16	0.16
	$\varepsilon=10^{-3}$	0.17	0.17	4.67	4.67	0.69	0.69	0.39	0.39	0.27	0.27
	$\varepsilon=10^{-2}$	1.35	1.35	4.56	4.56	1.69	1.69	1.50	1.50	1.42	1.42
EI	$\varepsilon=0$	0	6.7E-4	2.81	2.81	0.57	0.57	0.30	0.30	0.16	0.16
	$\varepsilon=10^{-5}$	2.5E-3	2.6E-3	2.81	2.81	0.57	0.57	0.30	0.30	0.16	0.16
	$\varepsilon=10^{-3}$	0.17	0.17	2.91	2.91	0.66	0.66	0.41	0.41	0.28	0.28
	$\varepsilon=10^{-2}$	1.35	1.35	3.93	3.93	1.76	1.76	1.55	1.55	1.45	1.45
Euler	$\varepsilon=0$	0	0.07	1.72	1.78	0.38	0.44	0.19	0.26	0.10	0.17
	$\varepsilon=10^{-5}$	2.5E-3	0.07	1.72	1.78	0.38	0.44	0.20	0.26	0.10	0.17
	$\varepsilon=10^{-3}$	0.17	0.19	1.72	1.78	0.42	0.48	0.27	0.32	0.21	0.25
	$\varepsilon=10^{-2}$	1.35	1.36	2.21	2.25	1.41	1.43	1.37	1.38	1.36	1.37
Heun	$\varepsilon=0$	0	0.07	7.09	7.09	0.72	0.73	0.21	0.22	0.05	0.09
	$\varepsilon=10^{-5}$	2.5E-3	0.07	6.48	6.48	0.64	0.65	0.18	0.20	0.05	0.09
	$\varepsilon=10^{-3}$	0.17	0.19	0.56	0.57	0.13	0.15	0.16	0.18	0.17	0.19
	$\varepsilon=10^{-2}$	1.35	1.36	1.37	1.38	1.35	1.36	1.35	1.36	1.35	1.36