

Diffusion models for Gaussian distributions: Exact solutions and Wasserstein errors

Émile Pierret^a, supervised by Bruno Galerne^{a,b}

Séminaire Imaging in Paris

January 6th 2025

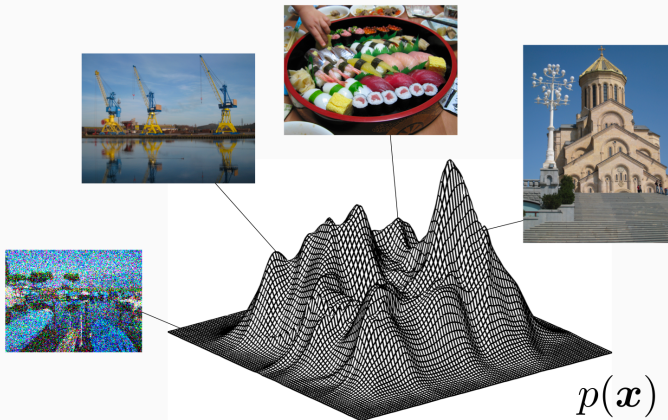
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^b Institut universitaire de France (IUF)

Introduction

What is a generative model ?

Goal: Sample from a data distribution of images.



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 Θ^* such that $G(\mathcal{N}(\mathbf{0}, \mathbf{I}_N), \Theta^*) \approx p$

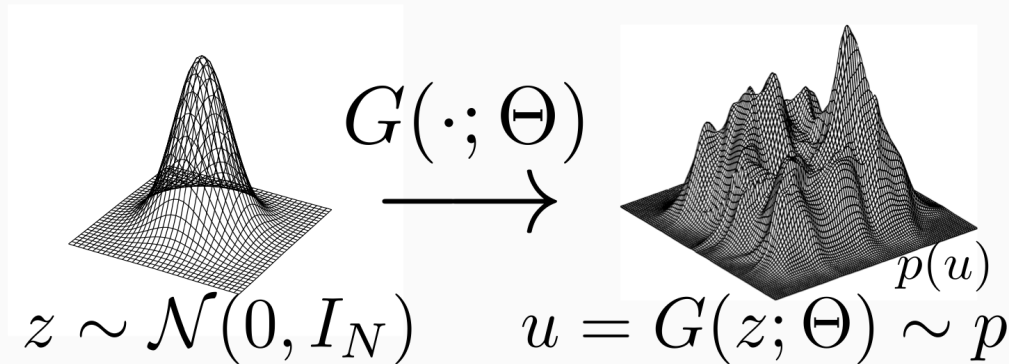


Image extracted from Bruno Galerne's slides

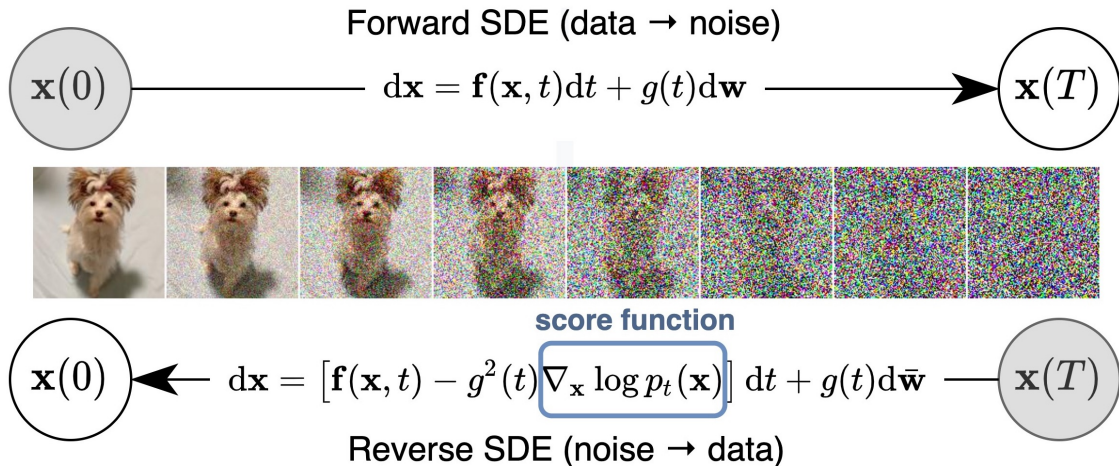


Image extracted from [Song et al. 2021]

$$dx_t = -\beta_t x_t dt + \sqrt{2\beta_t} dw_t, \quad 0 \leq t \leq T, \quad x_0 \sim p_{\text{data}} \quad (1)$$

where β_t is an affine non-decreasing function. We denote $(p_t)_{0 \leq t \leq T}$ the density of x_t .

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The strong solution of Equation (1) is:

$$x_t = e^{-B_t} x_0 + \boldsymbol{\eta}_t, \quad 0 \leq t \leq T. \quad (2)$$

with $\boldsymbol{\eta}_t \sim \mathcal{N}(\mathbf{0}, (1 - e^{-2B_t}) \mathbf{I})$, $B_t = \int_0^t \beta_u du$.

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Consequently, if $t \rightarrow +\infty$, $x_\infty \sim \mathcal{N}_0$.

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Furthermore, denoting $\boldsymbol{\Sigma}_t = \text{Cov}(x_t)$,

$$d\boldsymbol{\Sigma}_t = 2\beta_t(\mathbf{I} - \boldsymbol{\Sigma}_t)dt, \quad 0 < t \leq T. \quad (3)$$

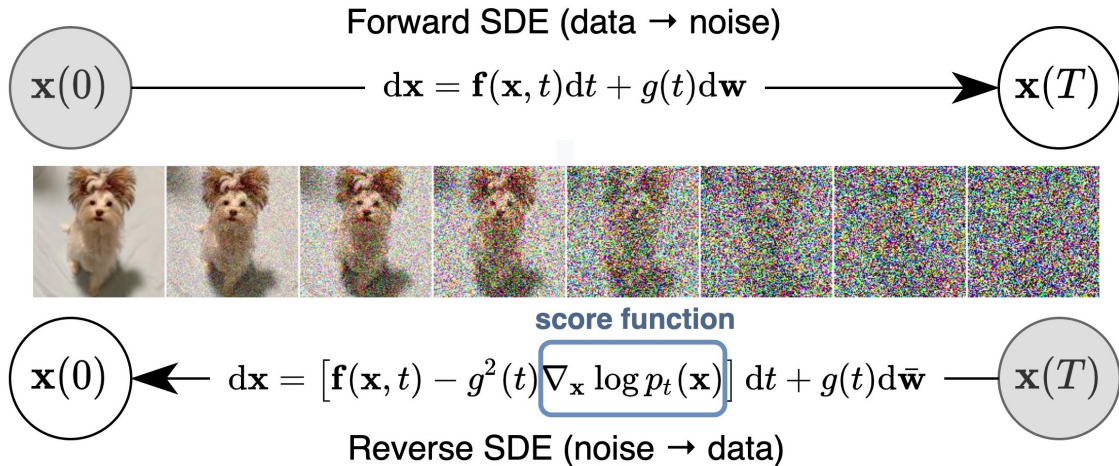


Image extracted from [Song et al. 2021]

If X_t solution of

$$d\mathbf{X}_t = b(t, \mathbf{X}_t)dt + \sigma(t, \mathbf{X}_t)d\mathbf{W}_t \quad (4)$$

Under assumptions

1. **(H1)** $\exists K > 0$ s.t. $\forall (t, x, y) \in [0, 1] \times \mathbb{R}^d \times \mathbb{R}^d$,

$$|b(t, x) - b(t, y)| + |\sigma(t, x) - \sigma(t, y)| \leq K|x - y|$$

$$|b(t, x)| + |\sigma(t, x)| \leq K(1 + |x|).$$

2. **(H2)** p_{data} has a density distribution in $L^2\left(\mathbb{R}^d, \frac{dx}{1+|x|^k}\right)$ for a certain $k \in \mathbb{N}$.
3. **(H3)** $\frac{\partial^2 \sigma^2}{\partial x_i \partial x_j}(t, x) \in L^\infty(]0, 1[\times \mathbb{R}^d)$ for $1 \leq i, j \leq d$.

then $\overline{\mathbf{X}}_t = \mathbf{X}_{1-t}$ is solution of

$$d\overline{\mathbf{X}}_t = \overline{b}(t, \overline{\mathbf{X}}_t)dt + \overline{\sigma}(t, \overline{\mathbf{X}}_t)d\overline{\mathbf{W}}_t \quad (5)$$

In our case, $b(t, x) = -\beta_t x, \sigma(t, x) = \sqrt{2\beta_t}$

¹E. Pardoux (1986). "Grossissement d'une filtration et retournement du temps d'une diffusion". In: *Séminaire de Probabilités XX 1984/85*. Ed. by Jacques Azéma and Marc Yor. Berlin, Heidelberg: Springer Berlin Heidelberg, pp. 48–55. ISBN: 978-3-540-39860-8

Study of the backward process [Pardoux 1986]²

Under some assumptions on the distribution p_{data} [Pardoux 1986], the backward process $(x_{T-t})_{0 \leq t \leq T}$ verifies the backward SDE

$$dy_t = \beta_{T-t}(y_t + 2\nabla \log p_{T-t}(y_t))dt + \sqrt{2\beta_{T-t}}d\bar{w}_t, \quad 0 \leq t < T, \quad y_0 \sim p_T. \quad (6)$$

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- The backward Brownian motion $\bar{w}$ is not defined on the same filtration than the forward w :

$$\bar{w}_t = w_t - w_T + \int_t^T \frac{1}{p(s, x_s)} \operatorname{div}(\sigma p)(s, x_s) ds. \quad (7)$$

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- We are unable to derive the score function: **No closed-form solution !**
- Learn $s_\theta(x, t) \approx \nabla \log p_t(x)$

$$dy_t = \beta_{T-t}(y_t + 2s_\theta(y_t, T - t))dt + \sqrt{2\beta_{T-t}}d\bar{w}_t, \quad 0 \leq t < T, \quad y_0 \sim p_T. \quad (8)$$

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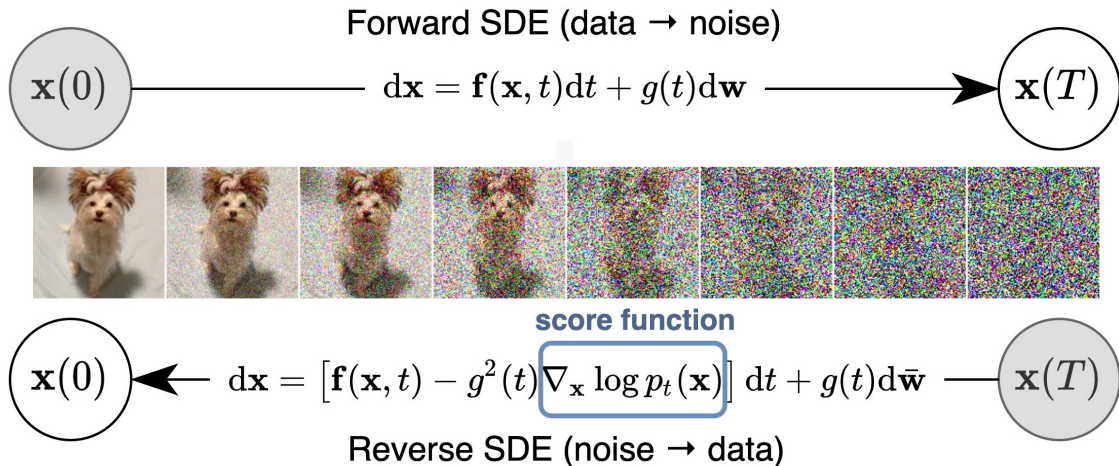


Image extracted from [Song et al. 2021]

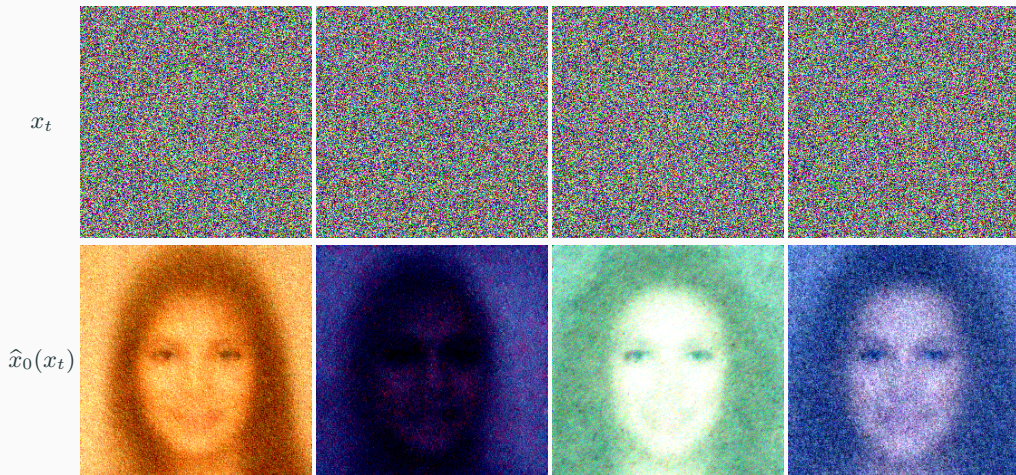
Examples (generated with [Lugmayr et al. 2022]³)



$t = 249$

³Andreas 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>

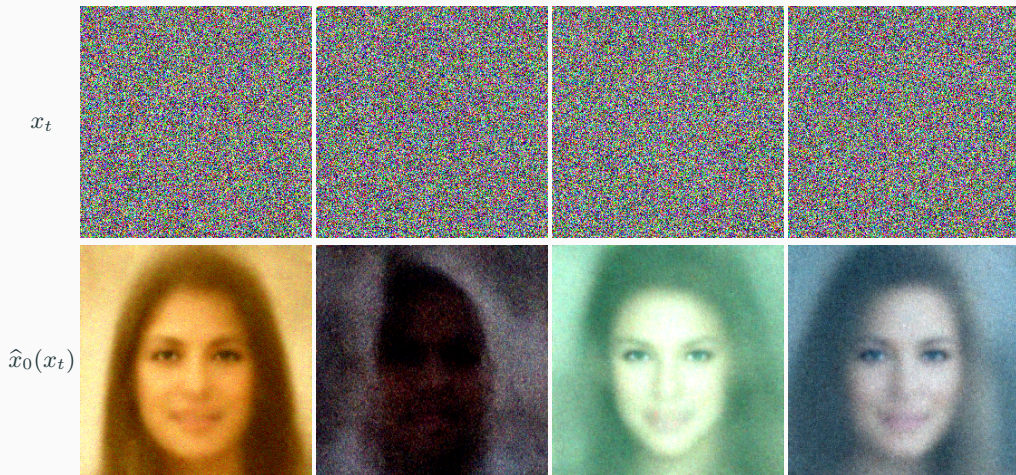
Examples (generated with [Lugmayr et al. 2022]³)



$t = 230$

³Andreas 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>

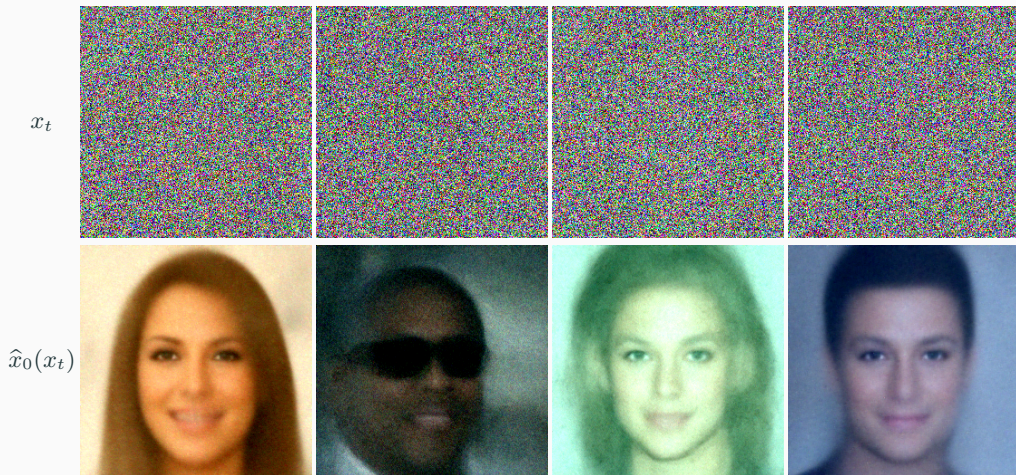
Examples (generated with [Lugmayr et al. 2022]³)



$t = 210$

³Andreas 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>

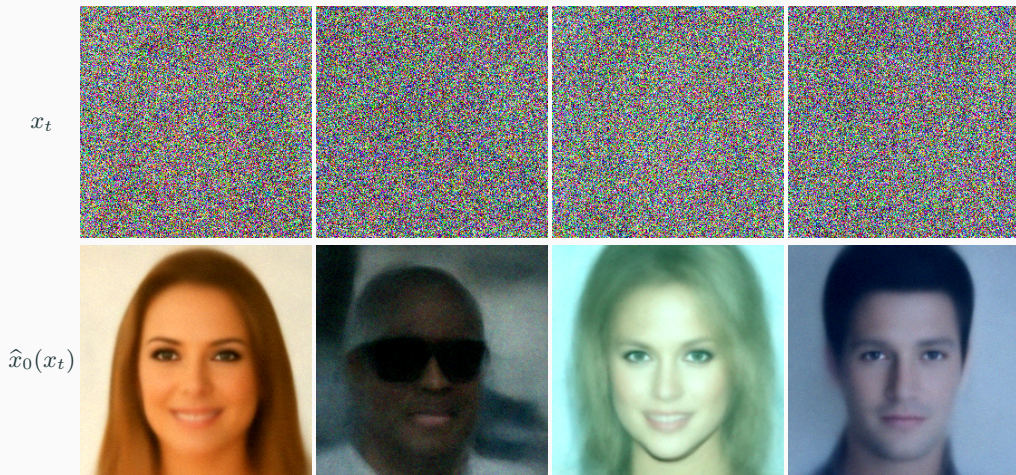
Examples (generated with [Lugmayr et al. 2022]³)



$t = 190$

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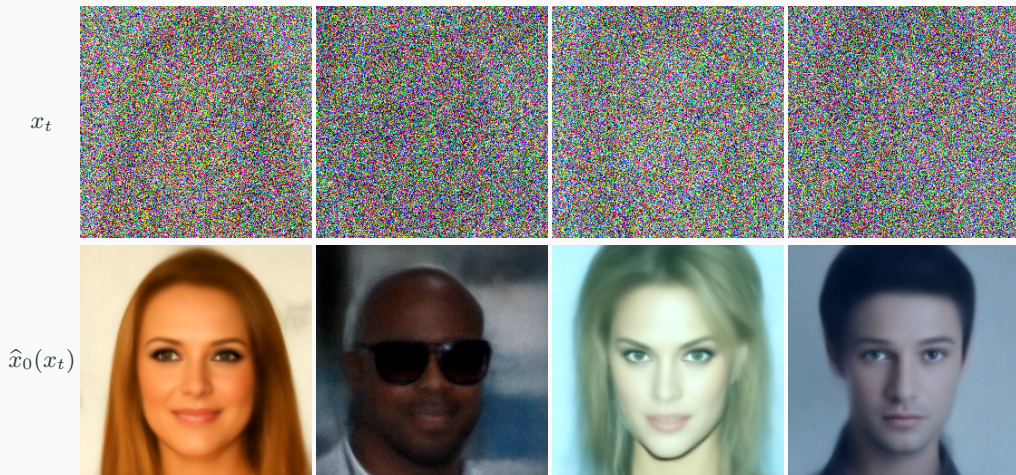
Examples (generated with [Lugmayr et al. 2022]³)



$t = 170$

³Andreas 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>

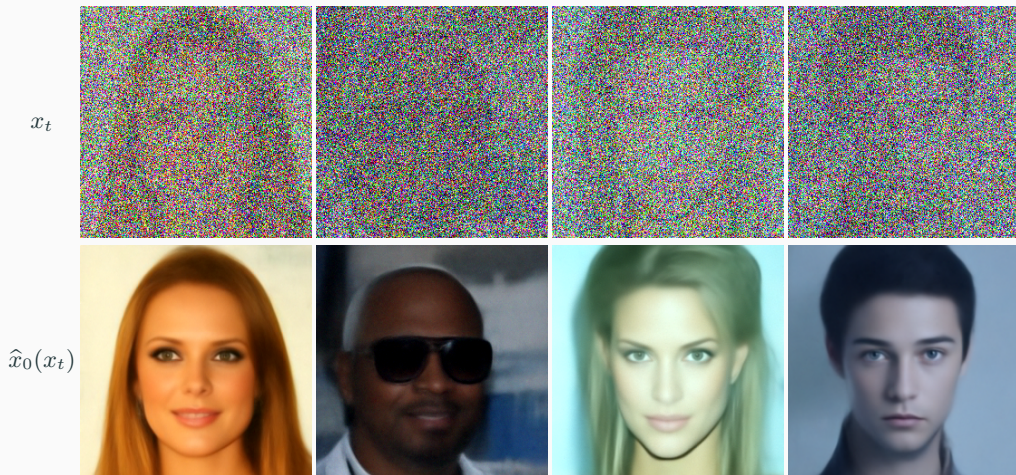
Examples (generated with [Lugmayr et al. 2022]³)



$t = 150$

³Andreas 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>

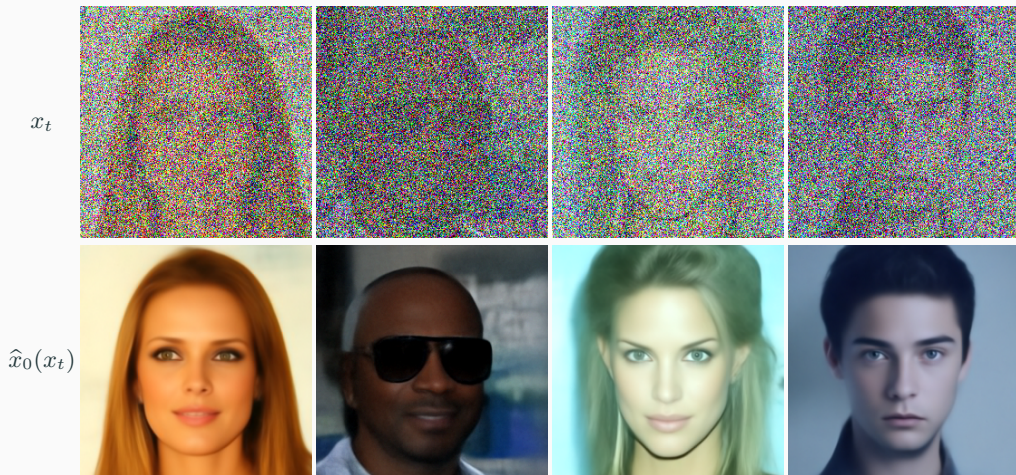
Examples (generated with [Lugmayr et al. 2022]³)



$t = 130$

³Andreas 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>

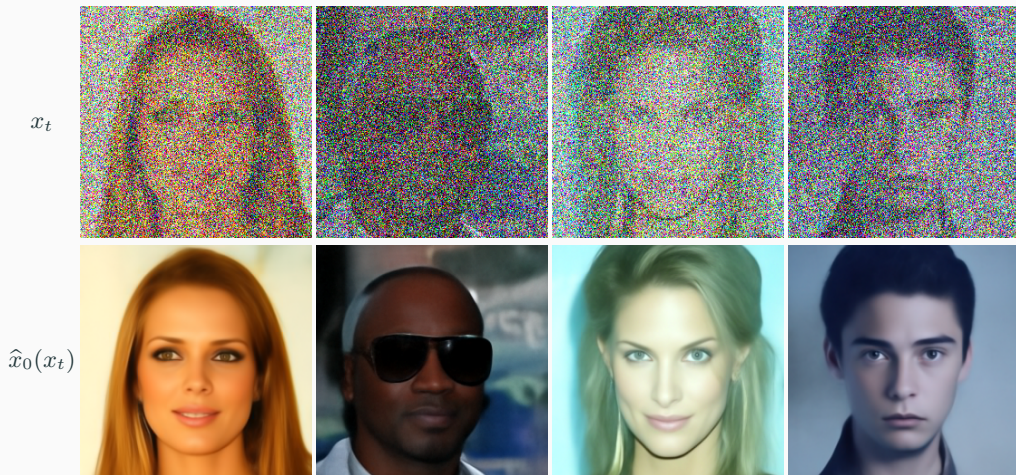
Examples (generated with [Lugmayr et al. 2022]³)



$t = 110$

³Andreas 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>

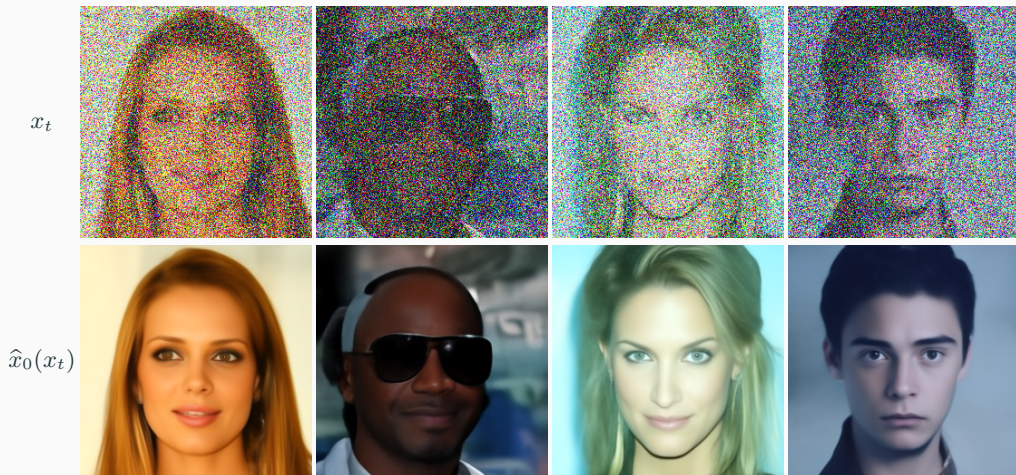
Examples (generated with [Lugmayr et al. 2022]³)



$t = 90$

³Andreas 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]³)

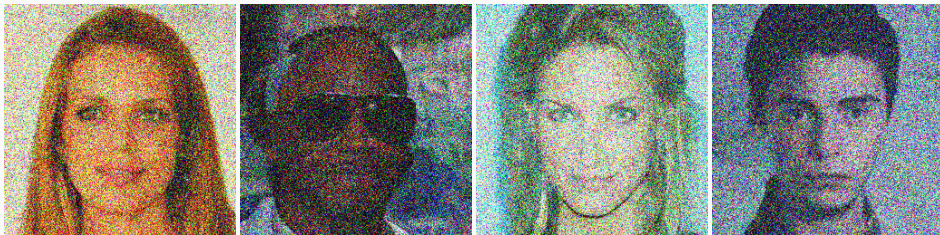


$t = 70$

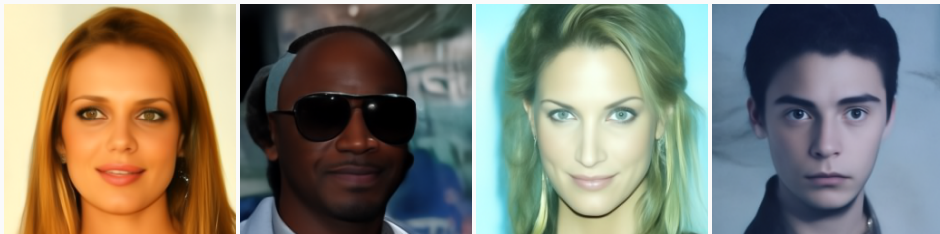
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Examples (generated with [Lugmayr et al. 2022]³)

x_t



$\hat{x}_0(x_t)$

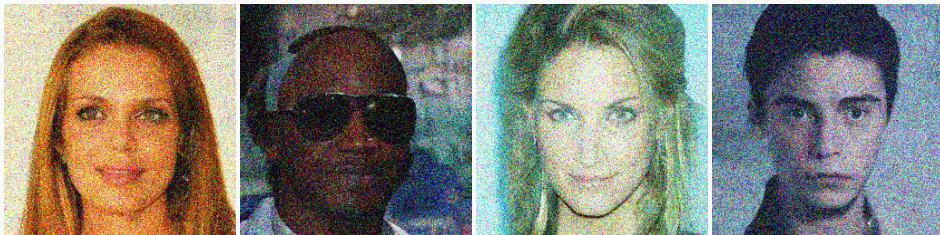


$t = 50$

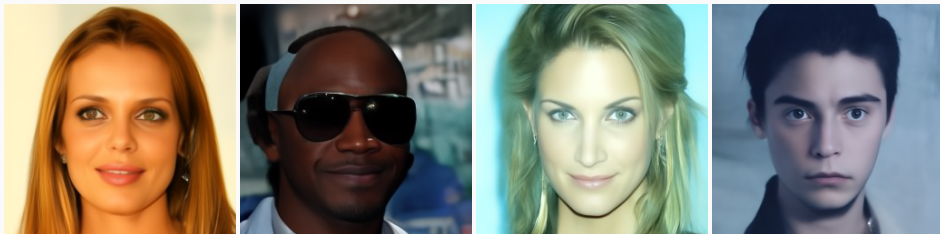
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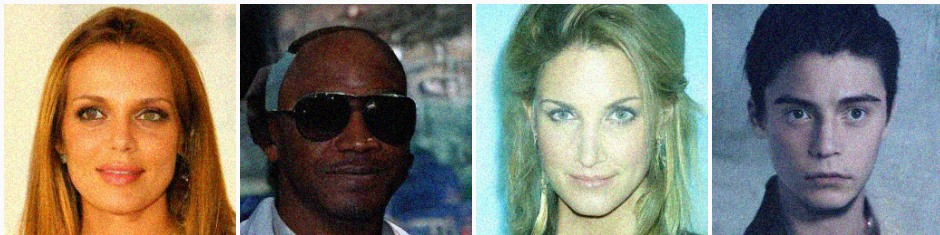


$t = 30$

³Andreas 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]³)

x_t



$\hat{x}_0(x_t)$



$t = 10$

³Andreas 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]³)

x_t



$\hat{x}_0(x_t)$



$t = 5$

³Andreas 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]³)

x_t



$\hat{x}_0(x_t)$



$t = 0$

³Andreas 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>

To the probability flow-ODE: the Fokker-Planck equation

$$dx_t = f(x_t, t)dt + g(t)dw_t \quad (9)$$

The marginals $(p_t)_{0 \leq t \leq T}$ follow the Fokker-Planck Equation:

$$\partial_t p_t(x) = -\operatorname{div}_x [f(x, t)p_t(x)] + \frac{1}{2}g(t)^2 \Delta_x p_t(x). \quad (10)$$

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By denoting $q_t = p_{T-t}$, we search for a Fokker-Planck equation associated with q_t .

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$$\begin{aligned} \partial_t q_t(x) &= -\partial_t p_{T-t}(x) \\ &= \operatorname{div}_x [f(x, T-t)q_t(x)] + \left(-1 + \frac{1}{2}\right)g(T-t)^2 \Delta_x q_t(x) \\ &= -\operatorname{div}_x \left[(-f(x, T-t) + g(T-t)^2 \nabla_x \log q_t(x)) q_t(x)\right] + \frac{1}{2}g(T-t)^2 \Delta_x q_t(x). \end{aligned}$$

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The marginals $(p_t)_{0 \leq t \leq T}$ associated with the backward SDE

$$dy_t = -\beta_t [y_t + 2\nabla_y \log p_t(y_t)] dt + \sqrt{2\beta_t} d\bar{w}_t, \quad 0 \leq t \leq T, \quad y_T \sim p_T \quad (11)$$

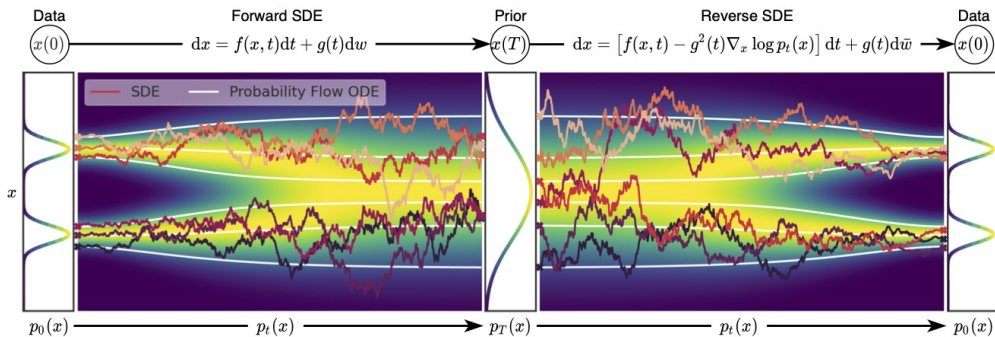
Probability-flow ODE

The marginals $(p_t)_{0 \leq t \leq T}$ associated with the backward SDE

$$dy_t = -\beta_t [y_t + 2\nabla_y \log p_t(y_t)] dt + \sqrt{2\beta_t} d\bar{w}_t, \quad 0 \leq t \leq T, \quad y_T \sim p_T \quad (11)$$

are the same as those of this ODE

$$dy_t = -\beta_t [y_t + \nabla_y \log p_t(y_t)] dt, \quad 0 \leq t \leq T, \quad y_T \sim p_T. \quad (12)$$



Study of the convergence

$$\begin{aligned} dy_t &= -\beta_t [y_t + 2\nabla_y \log p_t(y_t)] dt + \sqrt{2\beta_t} d\bar{w}_t, \\ \text{or} \qquad \qquad \qquad & \text{where } 0 \leq t \leq T, \quad y_T \sim p_T. \\ dy_t &= -\beta_t [y_t + \nabla_y \log p_t(y_t)] dt, \end{aligned} \tag{13}$$

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

$$dy_t = -\beta_t [y_t + 2\nabla_y \log p_t(y_t)] dt + \sqrt{2\beta_t} d\bar{w}_t,$$

or

$$dy_t = -\beta_t [y_t + \nabla_y \log p_t(y_t)] dt,$$

where $0 \leq t \leq T$, ~~$y_T \sim p_T$~~ . $y_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$. (13)

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

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

$$dy_t = -\beta_t [y_t + 2\nabla_y \log p_t(y_t)] dt + \sqrt{2\beta_t} d\bar{w}_t,$$

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$$dy_t = -\beta_t [y_t + \nabla_y \log p_t(y_t)] dt,$$

$$\text{where } \underset{\varepsilon}{0} \leq t \leq T, \quad y_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I}). \quad (13)$$

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

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

$$dy_t = -\beta_t [y_t + 2\nabla_y \log p_t(y_t)] dt + \sqrt{2\beta_t} d\bar{w}_t,$$

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$$dy_t = -\beta_t [y_t + \nabla_y \log p_t(y_t)] dt,$$

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$$dy_t = -\beta_t[y_t + 2 \underbrace{\nabla_y \log p_t(y_t)}_{s_\theta(t, y_t)}]dt + \sqrt{2\beta_t}d\bar{w}_t,$$

or

$$dy_t = -\beta_t[y_t + \underbrace{\nabla_y \log p_t(y_t)}_{s_\theta(t, y_t)}]dt,$$

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$$dy_t = -\beta_t[y_t + 2s_\theta(t, y_t)]dt + \sqrt{2\beta_t}d\bar{w}_t,$$

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Theorem 1. Assume **A1**, **A2**, **A3**, **A4** that $T \geq 2\bar{\beta}(1 + \log(1 + \text{diam}(\mathcal{M})))$, $\gamma_K = \varepsilon$ and $\varepsilon, \mathbf{M}, \delta \leq 1/32$. Then, there exists $\mathbf{D}_0 \geq 0$ such that

$$\mathbf{W}_1(\mathcal{L}(Y_K), \pi) \leq \mathbf{D}_0(\exp[\kappa/\varepsilon](\mathbf{M} + \delta^{1/2})/\varepsilon^2 + \exp[\kappa/\varepsilon] \exp[-T/\bar{\beta}] + \varepsilon^{1/2}),$$

with $\kappa = \text{diam}(\mathcal{M})^2(1 + \bar{\beta})/2$ and

$$\mathbf{D}_0 = D(1 + \bar{\beta})^7(1 + d + \text{diam}(\mathcal{M})^4)(1 + \log(1 + \text{diam}(\mathcal{M}))), \quad (7)$$

and D is a numerical constant.

Theorem 3. Assume **A1**, **A2**, **A3**, **A4** that $T \geq 2\beta(1 + \log(1 + \text{diam}(\mathcal{M})))$, $\gamma_K = \varepsilon$ and $\varepsilon, \mathbf{M}, \delta \leq 1/32$. In addition, assume that there exists $\Gamma \geq 0$ such that for any $t \in (0, T]$ and $x_t \in \mathbb{R}^d$

$$\|\nabla^2 \log p_t(x_t)\| \leq \Gamma/\sigma_t^2. \quad (9)$$

Then, there exists $\mathbf{D}_0 \geq 0$ such that

$$\mathbf{W}_1(\mathcal{L}(Y_K), \pi) \leq \mathbf{D}_0((\mathbf{M} + \delta^{1/2})/\varepsilon^{\Gamma+2} + \exp[-T/\bar{\beta}]/\varepsilon^\Gamma + \varepsilon^{1/2}),$$

From Valentin De Bortoli (2022). “Convergence of denoising diffusion models under the manifold hypothesis”.

In: *Transactions on Machine Learning Research*. ISSN: 2835-8856. URL:

<https://openreview.net/forum?id=MhK5aXo3gB>

Restriction to the Gaussian case

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

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$$\nabla \log p_t(x) = -\Sigma_t^{-1}x, \quad 0 < t \leq T \quad (14)$$

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Proposition 3: Linearity of the score

The three following propositions are equivalent:

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

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Proposition 4: Solution to the equations under Gaussian assumption

Under Gaussian assumption, the strong solution to SDE (6) can be written as:

$$y_t^{\text{SDE}} = e^{-(B_T - B_t)} \Sigma_t \Sigma_T^{-1} y_T + \xi_t, \quad 0 \leq t \leq T \quad (15)$$

Under Gaussian assumption, the solution to ODE (12) can be written as:

$$y_t^{\text{ODE}} = \Sigma_T^{-1/2} \Sigma_t^{1/2} y_T, \quad 0 \leq t \leq T, \quad (16)$$

with $\Sigma_t = e^{-2Bt} \Sigma + (1 - e^{-2Bt}) I$.

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

Proposition 5: Solution to the equations under Gaussian assumption

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

$$\Sigma_t^{\text{SDE}} = \text{Cov}(y_t^{\text{SDE}}) = \Sigma_t + e^{-2(B_T - B_t)} \Sigma_t^2 \Sigma_T^{-2} [\text{Cov}(y_T) - \Sigma_T], \quad (15)$$

$$\Sigma_t^{\text{ODE}} = \text{Cov}(y_t^{\text{ODE}}) = \Sigma_t \Sigma_T^{-1} \text{Cov}(y_T), \quad (16)$$

Explicit solution of the backward equations

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

Proposition 6: Solution to the equations under Gaussian assumption

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

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$$\Sigma_t^{\text{ODE}} = \text{Cov}(y_t^{\text{ODE}}) = \Sigma_t \Sigma_T^{-1} \text{Cov}(y_T), \quad (16)$$

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

$$\Sigma_t^{\text{SDE}} = \Sigma_t^{\text{ODE}} = \Sigma_t, \quad 0 \leq t \leq T.$$

Explicit solution of the backward equations

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

Proposition 7: Solution to the equations under Gaussian assumption

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

$$\Sigma_t^{\text{SDE}} = \text{Cov}(y_t^{\text{SDE}}) = \Sigma_t + e^{-2(B_T - B_t)} \Sigma_t^2 \Sigma_T^{-2} [\text{Cov}(y_T) - \Sigma_T], \quad (15)$$

$$\Sigma_t^{\text{ODE}} = \text{Cov}(y_t^{\text{ODE}}) = \Sigma_t \Sigma_T^{-1} \text{Cov}(y_T), \quad (16)$$

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

$$\Sigma_t^{\text{SDE}} = \Sigma_t^{\text{ODE}} = \Sigma_t, \quad 0 \leq t \leq T.$$

If $y_T \sim \mathcal{N}(\mathbf{0}, I)$,

$$\Sigma_t^{\text{SDE}} = \Sigma_t + e^{-2(B_T - B_t)} \Sigma_t^2 \Sigma_T^{-2} (I - \Sigma_T), \quad 0 \leq t \leq T.$$

$$\Sigma_t^{\text{ODE}} = \Sigma_t \Sigma_T^{-1}$$

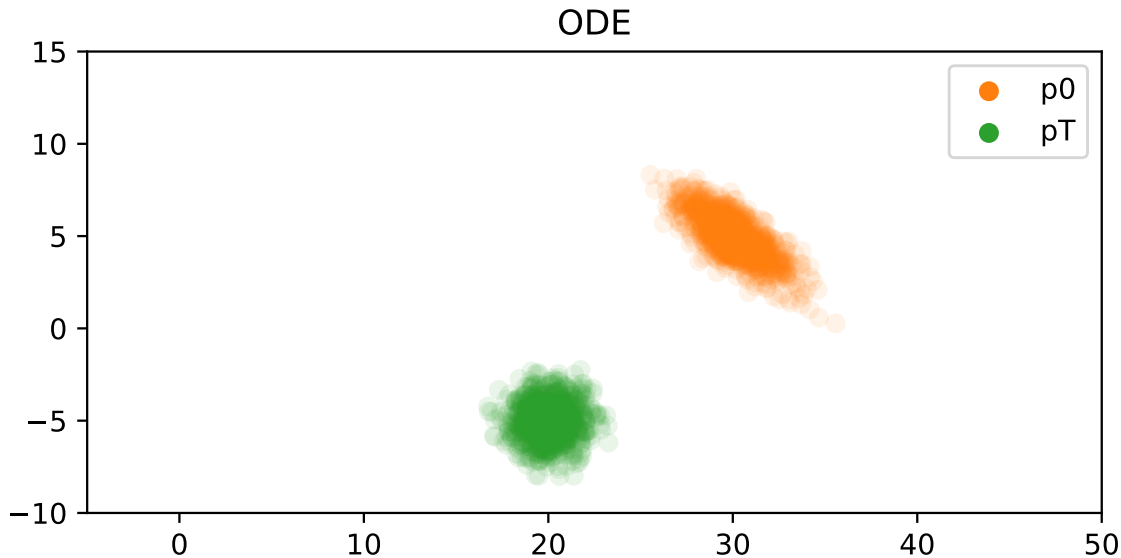
Under Gaussian assumption, the solution to ODE (12) can be written as:

$$y_t^{\text{ODE}} = \Sigma_T^{-1/2} \Sigma_t^{1/2} y_T, \quad 0 \leq t \leq T, \quad (17)$$

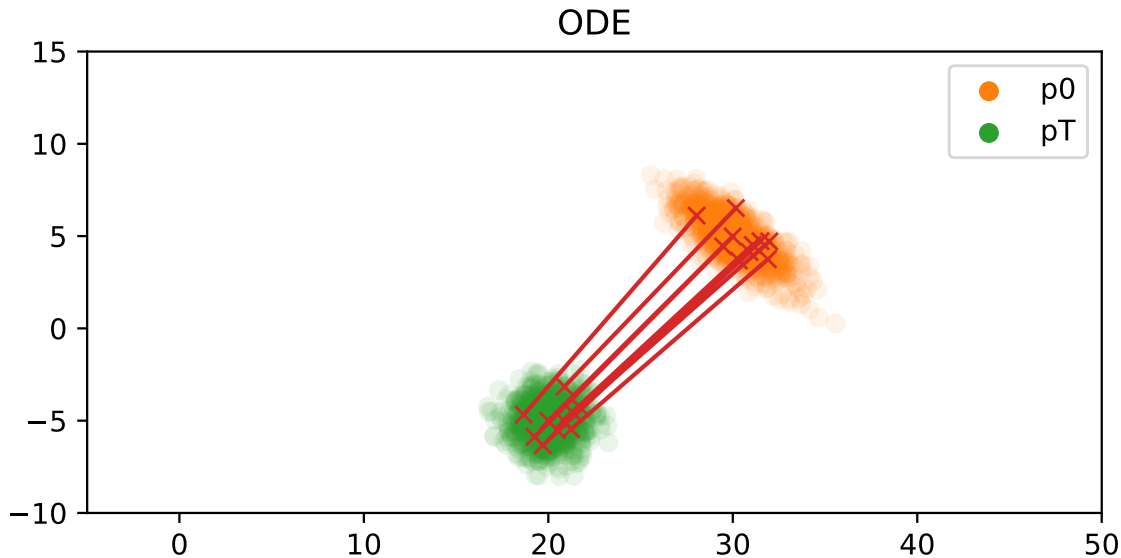
- $y \mapsto \Sigma_T^{-1/2} \Sigma_t^{1/2} y$ is the transport map between p_T and p_t .
- False in general:, see [Lavenant and Santambrogio 2022]⁴
- However, used in [Khrulkov et al. 2023]⁵

⁴Hugo 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>

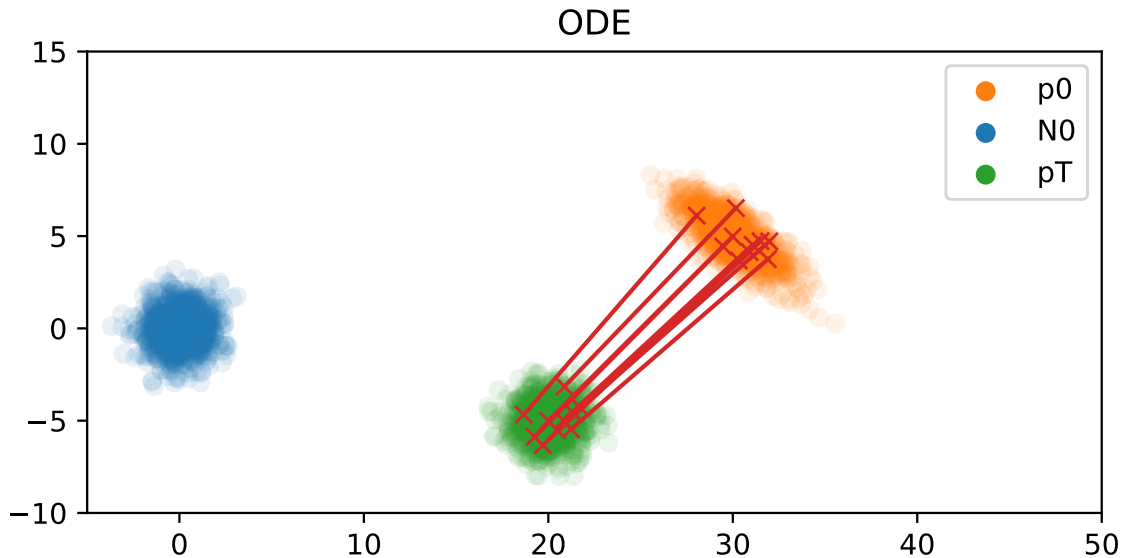
⁵Valentin Khrulkov et al. (2023). “Understanding DDPM Latent Codes Through Optimal Transport”. In: *The Eleventh International Conference on Learning Representations*. URL: <https://openreview.net/forum?id=6PIrhAx1j4i>

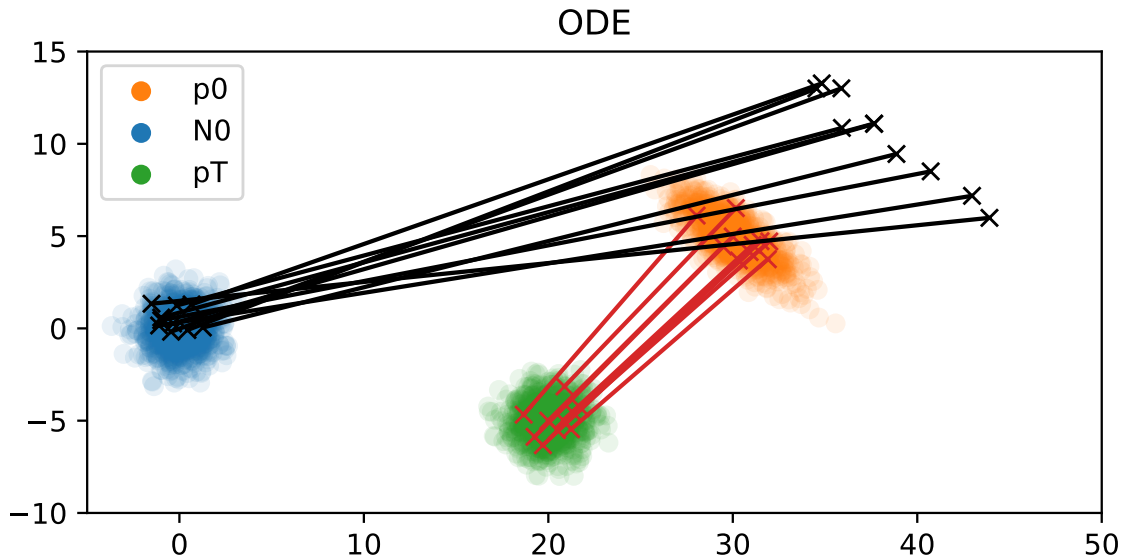


Initialization error: Focus on the ODE

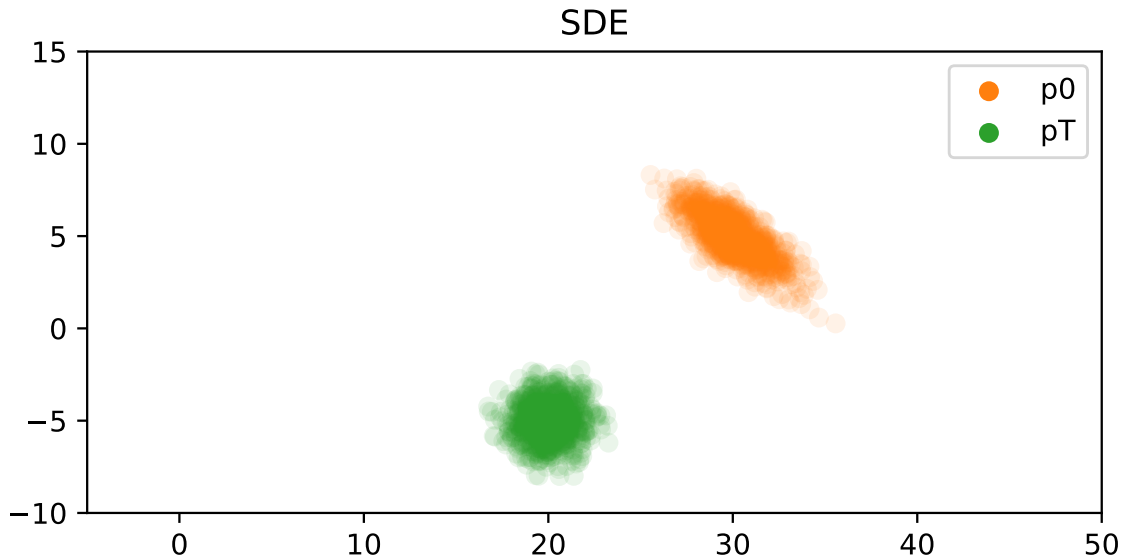


Initialization error: Focus on the ODE

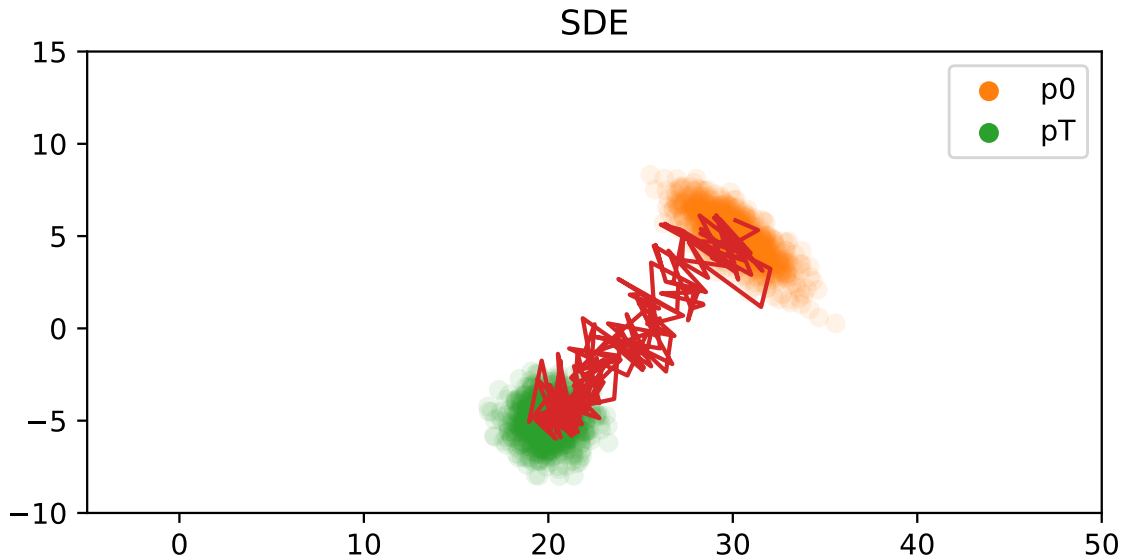




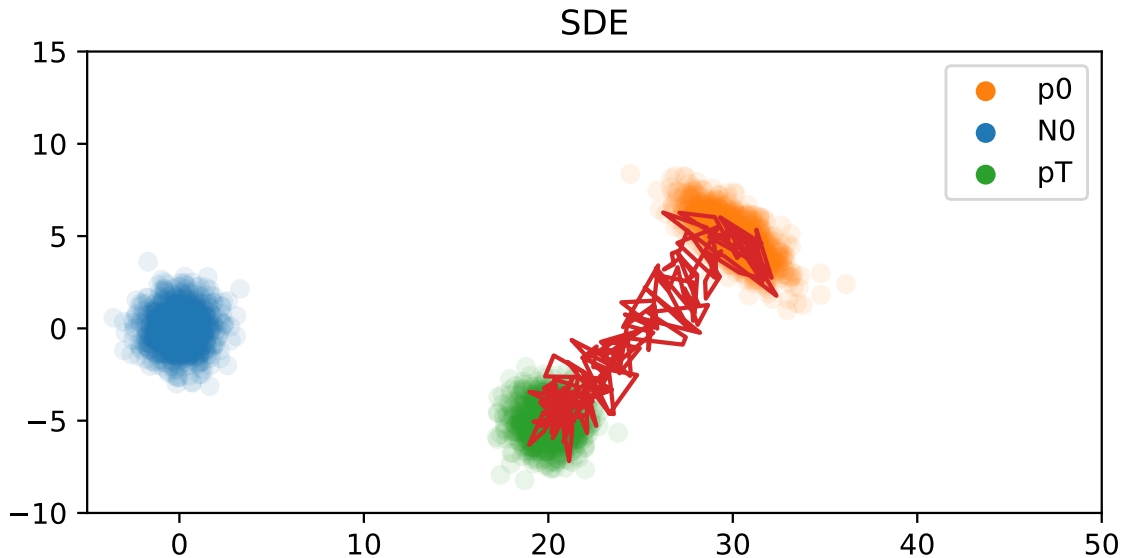
Initialization error: Focus on the SDE



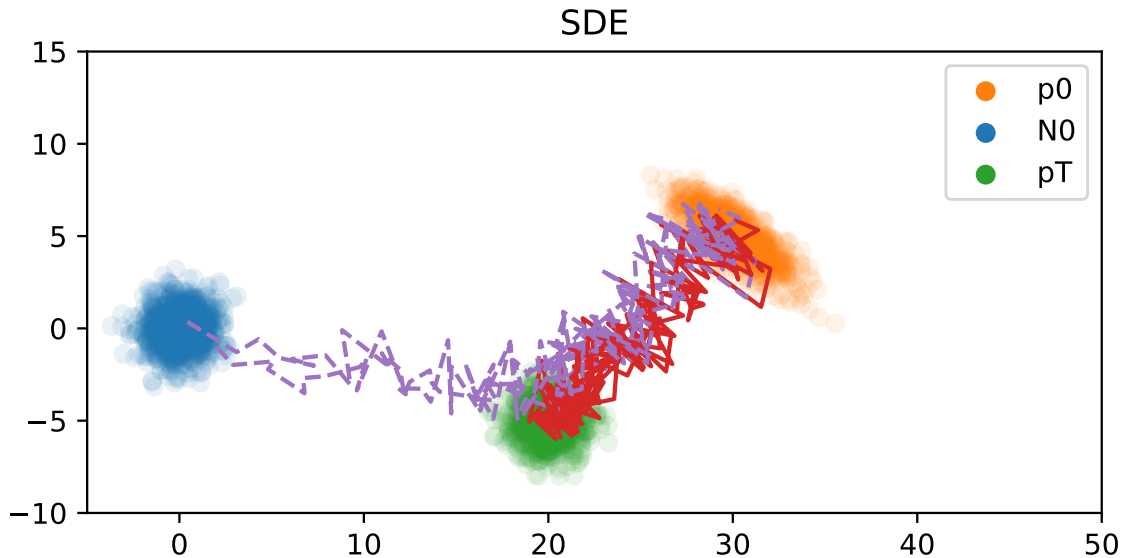
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Initialization error: Focus on the SDE



Under Gaussian assumption, the strong solution to SDE (6) can be written as:

$$y_t^{\text{SDE}} = e^{-(B_T - B_t)} \Sigma_t \Sigma_T^{-1} y_T + \xi_t, \quad 0 \leq t \leq T \quad (18)$$

with $\text{Cov}(\xi_t) = \Sigma_t - e^{-2(B_T - B_t)} \Sigma_t^2 \Sigma_T^{-1}$.

Finally,

$$\text{Cov}(y_t) = \Sigma_t + e^{-2(B_T - B_t)} \Sigma_{T-t}^2 \Sigma_T^{-2} [\text{Cov}(y_0) - \Sigma_T]. \quad (19)$$

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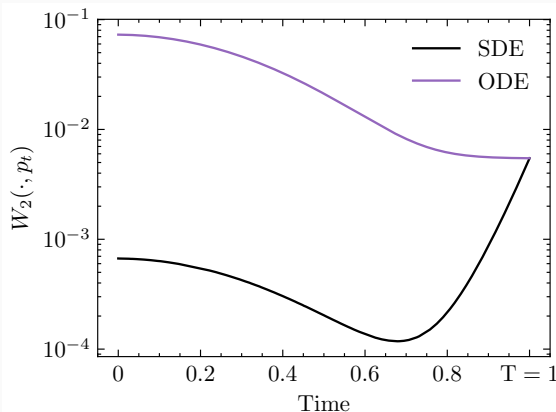
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Proposition 8: Marginals of the generative processes under Gaussian assumption

Under Gaussian assumption,

$$\mathbf{W}_2(p_t^{\text{SDE}}, p_t) \leq \mathbf{W}_2(p_t^{\text{ODE}}, p_t) \quad (20)$$

which shows that at each time $0 \leq t \leq T$ and in particular for $t = 0$ which corresponds to the desired outputs of the sampler, the SDE sampler is a better sampler than the ODE sampler when the exact score is known.



Truncation error

$$\begin{aligned} dy_t &= -\beta_t[y_t + 2s_\theta(t, y_t)]dt + \sqrt{2\beta_t}d\bar{w}_t, \\ \text{or} \qquad \qquad \qquad & \text{where } \varepsilon \leq t \leq T, \quad y_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I}). \\ dy_t &= -\beta_t[y_t + s_\theta(t, y_t)]dt, \end{aligned} \tag{21}$$

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- p_T , which is unknown, is replaced by $\mathcal{N}(\mathbf{0}, \mathbf{I})$ → **initialization error**
- In fact, another time ε to consider them on $[\varepsilon, T]$ → **truncation error**
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Gaussian assumption: p_{data} is a centered Gaussian distribution $\mathcal{N}(\mathbf{0}, \Sigma)$. (Σ is not necessarily invertible) In this case,

$$\nabla \log p_t(x) = -\Sigma_t^{-1}x, \quad 0 < t \leq T \quad (22)$$

with $\Sigma_t = e^{-2Bt}\Sigma + (1 - e^{-2Bt})I$.

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$$\Sigma_0 = \Sigma$$

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Consequently, $\nabla \log p_0(x)$ is not defined in general.

$\implies$ The truncation error is vital.

Discretization error

$$\begin{aligned} dy_t &= -\beta_t[y_t + 2s_\theta(t, y_t)]dt + \sqrt{2\beta_t}d\bar{w}_t, \\ \text{or} \qquad \qquad \qquad & \text{where } \varepsilon \leq t \leq T, \quad y_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I}). \\ dy_t &= -\beta_t[y_t + s_\theta(t, y_t)]dt, \end{aligned} \tag{23}$$

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$$\begin{cases} \tilde{\mathbf{y}}_0^{\Delta, \text{EM}} & \sim \mathcal{N}_0 \\ \tilde{\mathbf{y}}_{k+1}^{\Delta, \text{EM}} & = \tilde{\mathbf{y}}_k^{\Delta, \text{EM}} + \Delta_t \beta_{T-t_k} \left(\tilde{\mathbf{y}}_k^{\Delta, \text{EM}} - 2 \Sigma_{T-t_k}^{-1} \tilde{\mathbf{y}}_k^{\Delta, \text{EM}} \right) + \sqrt{2 \Delta_t \beta_{T-t_k}} z_k, \quad z_k \sim \mathcal{N}_0 \end{cases} \quad (24)$$

$$\begin{cases} \tilde{\mathbf{y}}_0^{\Delta, \text{EI}} & \sim \mathcal{N}_0 \\ \tilde{\mathbf{y}}_{k+1}^{\Delta, \text{EI}} & = \tilde{\mathbf{y}}_k^{\Delta, \text{EI}} + \gamma_{1,k} \left(\tilde{\mathbf{y}}_k^{\Delta, \text{EI}} - 2 \Sigma_{T-t_k}^{-1} \tilde{\mathbf{y}}_k^{\Delta, \text{EI}} \right) + \sqrt{2 \gamma_{2,k}} z_k, \quad z_k \sim \mathcal{N}_0 \end{cases} \quad (25)$$

where $\gamma_{1,k} = \exp(B_{T-t_k} - B_{T-t_{k+1}}) - 1$ and $\gamma_{2,k} = \frac{1}{2}(\exp(2B_{T-t_k} - 2B_{T-t_{k+1}}) - 1)$

$$\begin{cases} \hat{\mathbf{y}}_0^{\Delta, \text{Euler}} & \sim \mathcal{N}_0 \\ \hat{\mathbf{y}}_{k+1}^{\Delta, \text{Euler}} & = \hat{\mathbf{y}}_k^{\Delta, \text{Euler}} + \Delta_t f(t_k, \hat{\mathbf{y}}_k^{\Delta, \text{Euler}}) \quad \text{with } f(t, y) = \beta_{T-t} y - \beta_{T-t} \Sigma_{T-t}^{-1} y \end{cases} \quad (26)$$

$$\begin{cases} \hat{\mathbf{y}}_0^{\Delta, \text{Heun}} & \sim \mathcal{N}_0 \\ \hat{\mathbf{y}}_{k+1/2}^{\Delta, \text{Heun}} & = \hat{\mathbf{y}}_k^{\Delta, \text{Heun}} + \Delta_t f(t_k, \hat{\mathbf{y}}_k^{\Delta, \text{Heun}}) \quad \text{with } f(t, y) = \beta_{T-t} y - \beta_{T-t} \Sigma_{T-t}^{-1} y \\ \hat{\mathbf{y}}_{k+1}^{\Delta, \text{Heun}} & = \hat{\mathbf{y}}_k^{\Delta, \text{Heun}} + \frac{\Delta_t}{2} \left(f(t_k, \hat{\mathbf{y}}_k^{\Delta, \text{Heun}}) + f(t_{k+1}, \hat{\mathbf{y}}_{k+1/2}^{\Delta, \text{Heun}}) \right) \end{cases} \quad (27)$$

The EM discretized process is a Gaussian process:

$$\begin{cases} \tilde{\mathbf{y}}_0^{\Delta, \text{EM}} & \sim \mathcal{N}_0 \\ \tilde{\mathbf{y}}_1^{\Delta, \text{EM}} & = \tilde{\mathbf{y}}_0^{\Delta, \text{EM}} + \Delta_t \beta_{T-t_0} \left(\tilde{\mathbf{y}}_0^{\Delta, \text{EM}} - 2 \Sigma_{T-t_0}^{-1} \tilde{\mathbf{y}}_0^{\Delta, \text{EM}} \right) + \sqrt{2 \Delta_t \beta_{T-t_0}} z_0, \quad z_0 \sim \mathcal{N}_0 \end{cases} \quad (14)$$

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$$\Sigma_0^{\Delta, \text{EM}} = \mathbf{I} \quad (28)$$

$$\Sigma_1^{\Delta, \text{EM}} = \left(\mathbf{I} + \Delta_t \beta_{T-t_0} \left(\mathbf{I} - 2 \Sigma_{T-t_0}^{-1} \right) \right)^2 \Sigma_0^{\Delta, \text{EM}} + 2 \Delta_t \beta_{T-t_0} \mathbf{I} \quad (29)$$

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Denoting $(\mathbf{v}_i)_i$ the eigenvectors of Σ , let $1 \leq i \leq d$,

$$\Sigma_1^{\Delta, \text{EM}} \mathbf{v}_i = \left[\left(1 + \Delta_t \beta_{T-t_0} \left(\mathbf{I} - \frac{2}{\lambda_{i, T-t_0}} \right) \right)^2 \lambda_{i, 0}^{\Delta, \text{EM}} + 2 \Delta_t \beta_{T-t_0} \right] \mathbf{v}_i \quad (30)$$

The EM discretized process is a Gaussian process:

$$\begin{cases} \tilde{\mathbf{y}}_0^{\Delta, \text{EM}} & \sim \mathcal{N}_0 \\ \tilde{\mathbf{y}}_1^{\Delta, \text{EM}} & = \tilde{\mathbf{y}}_0^{\Delta, \text{EM}} + \Delta_t \beta_{T-t_0} \left(\tilde{\mathbf{y}}_0^{\Delta, \text{EM}} - 2\boldsymbol{\Sigma}_{T-t_0}^{-1} \tilde{\mathbf{y}}_0^{\Delta, \text{EM}} \right) + \sqrt{2\Delta_t \beta_{T-t_0}} z_0, \quad z_0 \sim \mathcal{N}_0 \end{cases} \quad (14)$$

$$\boldsymbol{\Sigma}_0^{\Delta, \text{EM}} = \mathbf{I} \quad (28)$$

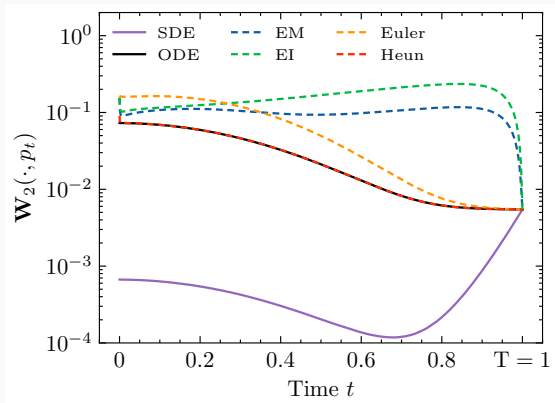
$$\boldsymbol{\Sigma}_1^{\Delta, \text{EM}} = \left(\mathbf{I} + \Delta_t \beta_{T-t_0} (\mathbf{I} - 2\boldsymbol{\Sigma}_{T-t_0}^{-1}) \right)^2 \boldsymbol{\Sigma}_0^{\Delta, \text{EM}} + 2\Delta_t \beta_{T-t_0} \mathbf{I} \quad (29)$$

Denoting $(\mathbf{v}_i)_i$ the eigenvectors of $\boldsymbol{\Sigma}$, let $1 \leq i \leq d$,

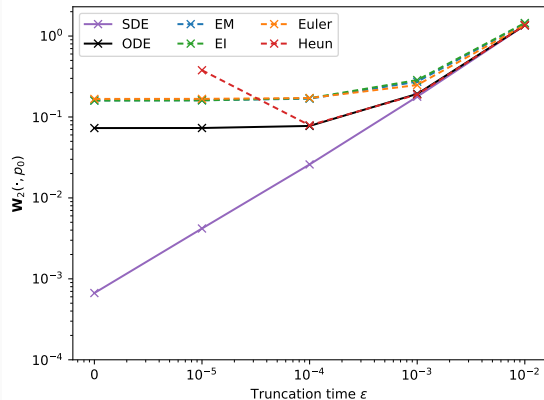
$$\boldsymbol{\Sigma}_1^{\Delta, \text{EM}} \mathbf{v}_i = \left[\left(1 + \Delta_t \beta_{T-t_0} \left(\mathbf{I} - \frac{2}{\lambda_{i, T-t_0}} \right) \right)^2 \lambda_{i, 0}^{\Delta, \text{EM}} + 2\Delta_t \beta_{T-t_0} \right] \mathbf{v}_i \quad (30)$$

$$\lambda_{i, 1}^{\Delta, \text{EM}} = \left(1 + \Delta_t \beta_{T-t_0} \left(\mathbf{I} - \frac{2}{\lambda_{i, T-t_0}} \right) \right)^2 \lambda_{i, 0}^{\Delta, \text{EM}} + 2\Delta_t \beta_{T-t_0}, \quad 1 \leq i \leq d. \quad (31)$$

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



Initialization + discretization



Truncature + Initialization

$$\begin{cases} \tilde{\mathbf{y}}_0^{\Delta, \text{EM}} & \sim \mathcal{N}_0 \\ \tilde{\mathbf{y}}_{k+1}^{\Delta, \text{EM}} & = \tilde{\mathbf{y}}_k^{\Delta, \text{EM}} + \Delta_t \beta_{T-t_k} \left(\tilde{\mathbf{y}}_k^{\Delta, \text{EM}} - 2 \Sigma_{T-t_k}^{-1} \tilde{\mathbf{y}}_k^{\Delta, \text{EM}} \right) + \sqrt{2 \Delta_t \beta_{T-t_k}} z_k, \quad z_k \sim \mathcal{N}_0 \end{cases} \quad (32)$$

$$\begin{cases} \tilde{\mathbf{y}}_0^{\Delta, \text{EI}} & \sim \mathcal{N}_0 \\ \tilde{\mathbf{y}}_{k+1}^{\Delta, \text{EI}} & = \tilde{\mathbf{y}}_k^{\Delta, \text{EI}} + \gamma_{1,k} \left(\tilde{\mathbf{y}}_k^{\Delta, \text{EI}} - 2 \Sigma_{T-t_k}^{-1} \tilde{\mathbf{y}}_k^{\Delta, \text{EI}} \right) + \sqrt{2 \gamma_{2,k}} z_k, \quad z_k \sim \mathcal{N}_0 \end{cases} \quad (33)$$

where $\gamma_{1,k} = \exp(B_{T-t_k} - B_{T-t_{k+1}}) - 1$ and $\gamma_{2,k} = \frac{1}{2}(\exp(2B_{T-t_k} - 2B_{T-t_{k+1}}) - 1)$

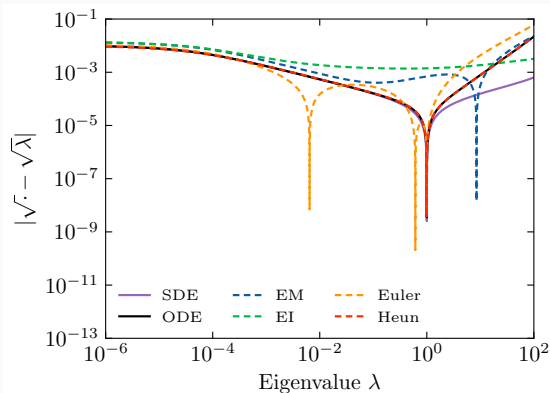
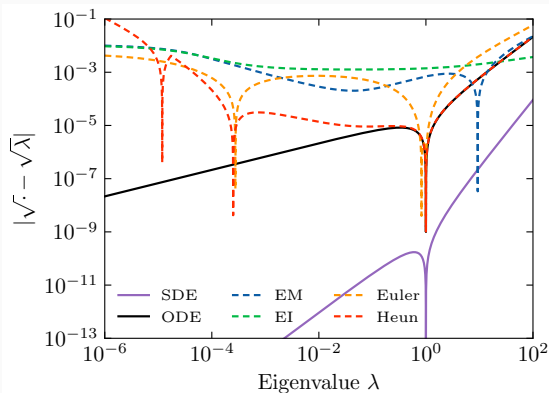
$$\begin{cases} \hat{\mathbf{y}}_0^{\Delta, \text{Euler}} & \sim \mathcal{N}_0 \\ \hat{\mathbf{y}}_{k+1}^{\Delta, \text{Euler}} & = \hat{\mathbf{y}}_k^{\Delta, \text{Euler}} + \Delta_t f(t_k, \hat{\mathbf{y}}_k^{\Delta, \text{Euler}}) \quad \text{with } f(t, y) = \beta_{T-t} y - \beta_{T-t} \Sigma_{T-t}^{-1} y \end{cases} \quad (34)$$

$$\begin{cases} \hat{\mathbf{y}}_0^{\Delta, \text{Heun}} & \sim \mathcal{N}_0 \\ \hat{\mathbf{y}}_{k+1/2}^{\Delta, \text{Heun}} & = \hat{\mathbf{y}}_k^{\Delta, \text{Heun}} + \Delta_t f(t_k, \hat{\mathbf{y}}_k^{\Delta, \text{Heun}}) \quad \text{with } f(t, y) = \beta_{T-t} y - \beta_{T-t} \Sigma_{T-t}^{-1} y \\ \hat{\mathbf{y}}_{k+1}^{\Delta, \text{Heun}} & = \hat{\mathbf{y}}_k^{\Delta, \text{Heun}} + \frac{\Delta_t}{2} \left(f(t_k, \hat{\mathbf{y}}_k^{\Delta, \text{Heun}}) + f(t_{k+1}, \hat{\mathbf{y}}_{k+1/2}^{\Delta, \text{Heun}}) \right) \end{cases} \quad (35)$$

Separable 2-Wasserstein distance

For two centered Gaussians $\mathcal{N}(\mathbf{0}, \Sigma_1)$ and $\mathcal{N}(\mathbf{0}, \Sigma_2)$ such that Σ_1, Σ_2 are simultaneously diagonalizable with respective eigenvalues $(\lambda_{i,1})_{1 \leq i \leq d}, (\lambda_{i,2})_{1 \leq i \leq d}$,

$$\mathbf{W}_2(\mathcal{N}(\mathbf{0}, \Sigma_1), \mathcal{N}(\mathbf{0}, \Sigma_2))^2 = \sum_{1 \leq i \leq d} (\sqrt{\lambda_{i,1}} - \sqrt{\lambda_{i,2}})^2 \quad (36)$$



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-04	4.78	4.78	0.65	0.66	0.32	0.32	0.16	0.16
	$\varepsilon = 10^{-5}$	4.1E-03	4.2E-03	4.77	4.77	0.66	0.66	0.32	0.32	0.16	0.16
	$\varepsilon = 10^{-4}$	0.03	0.03	4.76	4.76	0.66	0.66	0.32	0.32	0.17	0.17
	$\varepsilon = 10^{-3}$	0.18	0.18	4.68	4.68	0.70	0.70	0.40	0.40	0.27	0.27
EI	$\varepsilon = 0$	0	6.7E-04	2.81	2.81	0.57	0.57	0.30	0.30	0.16	0.16
	$\varepsilon = 10^{-5}$	4.1E-03	4.2E-03	2.81	2.81	0.57	0.57	0.30	0.30	0.16	0.16
	$\varepsilon = 10^{-4}$	0.03	0.03	2.82	2.82	0.58	0.58	0.31	0.31	0.17	0.17
	$\varepsilon = 10^{-3}$	0.18	0.18	2.91	2.91	0.67	0.67	0.41	0.41	0.29	0.29
Euler	$\varepsilon = 0$	0	0.07	1.72	1.78	0.38	0.44	0.20	0.26	0.10	0.17
	$\varepsilon = 10^{-5}$	4.1E-03	0.07	1.72	1.78	0.38	0.44	0.20	0.26	0.10	0.17
	$\varepsilon = 10^{-4}$	0.03	0.08	1.72	1.78	0.38	0.44	0.20	0.26	0.11	0.17
	$\varepsilon = 10^{-3}$	0.18	0.19	1.73	1.79	0.42	0.48	0.27	0.32	0.21	0.25
Heun	$\varepsilon = 0$	0	0.07	-	-	-	-	-	-	-	-
	$\varepsilon = 10^{-5}$	4.1E-03	0.07	23.42	23.42	2.86	2.87	1.05	1.06	0.37	0.38
	$\varepsilon = 10^{-4}$	0.03	0.08	4.68	4.68	0.43	0.44	0.12	0.14	0.03	0.08
	$\varepsilon = 10^{-3}$	0.18	0.19	0.58	0.59	0.13	0.15	0.16	0.18	0.17	0.19

Score approximation error

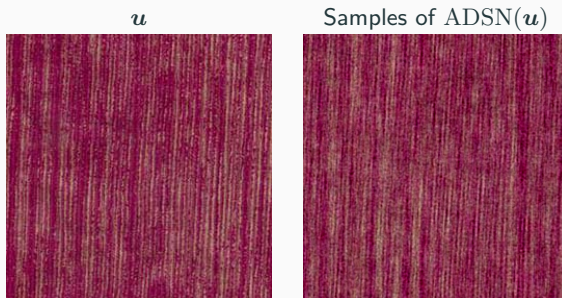
$$\begin{aligned} dy_t &= -\beta_t[y_t + 2s_\theta(t, y_t)]dt + \sqrt{2\beta_t}d\bar{w}_t, \\ \text{or} \qquad \qquad \qquad & \text{where } \varepsilon \leq t \leq T, \quad y_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I}). \\ dy_t &= -\beta_t[y_t + s_\theta(t, y_t)]dt, \end{aligned} \tag{37}$$

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

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

The Asymptotic Discrete Spot Noise (ADSN) model [Galerne, Gousseau, and Morel 2011] ⁶

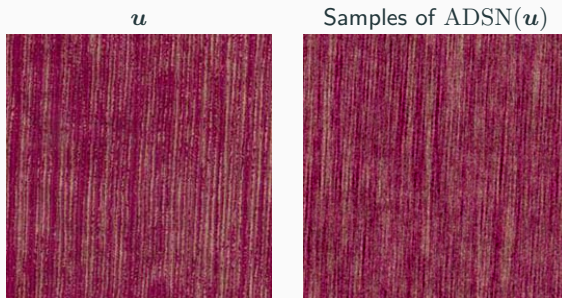
A Gaussian distribution, named $\text{ADSN}(u)$, can be associated with a texton u



⁶Bruno Galerne, Yann Gousseau, and Jean-Michel Morel (2011). "Random Phase Textures: Theory and Synthesis". In: *IEEE Transactions on Image Processing* 20.1, pp. 257–267. DOI: 10.1109/TIP.2010.2052822

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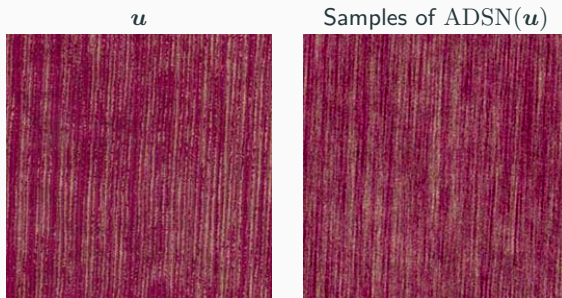
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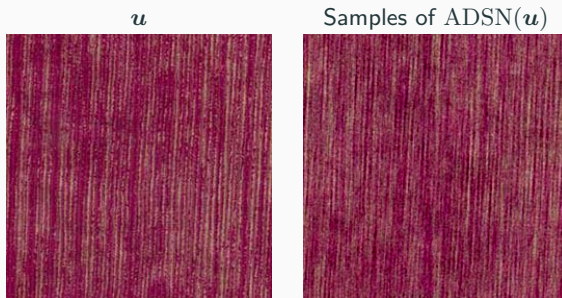
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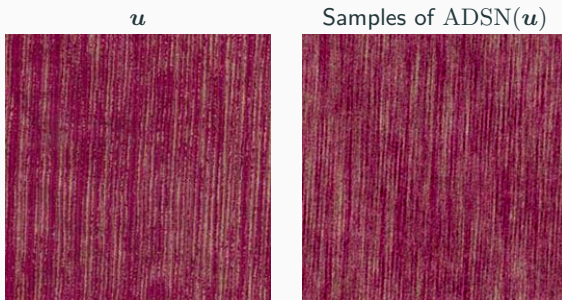
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We learn $s_\theta \approx \nabla_x \log p_t(x)$ for the previous ADSN model by score matching, using *DDPM continuous* [Song et al. 2021]⁷.

$$\theta^* = \operatorname{argmin}_\theta \mathbb{E}_t \left\{ \lambda(t) \mathbb{E}_{x_0} \mathbb{E}_{x_t|x_0} [s_\theta(x_t, t) - \nabla_{x_t} \log p_t(x_0 | x_t)] \right\} \quad (38)$$

x_0 is sampled during the training.

⁷Yang 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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Then, we apply the EM scheme and the Heun's scheme with this learned network.

⁷Yang 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>

u



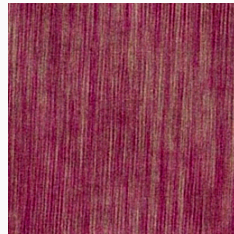
Gaussian samples



p_{θ}^{EM}



p_{θ}^{Heun}



u



Gaussian samples



p_{θ}^{EM}



p_{θ}^{Heun}



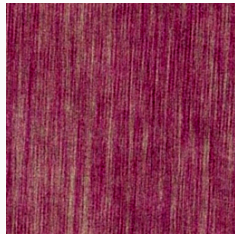
u



Gaussian samples



p_{θ}^{EM}



p_{θ}^{Heun}



u



Gaussian samples



p_{θ}^{EM}



p_{θ}^{Heun}



u



Gaussian samples



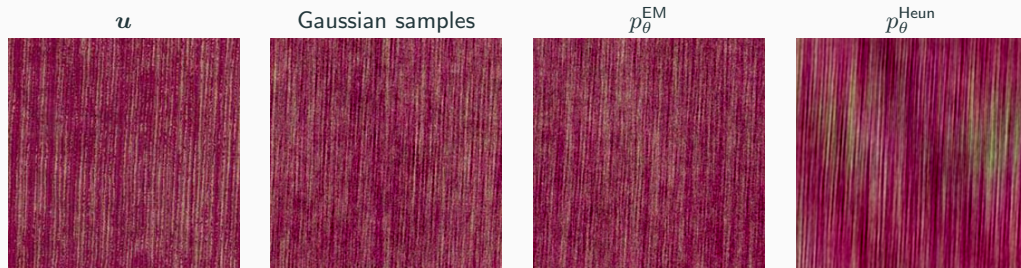
p_{θ}^{EM}



p_{θ}^{Heun}



Score approximation



	Exact score distribution			Learned score distribution	
p	$\mathbf{W}_2(p, p_{\text{data}}) \downarrow$	$\mathbf{W}_2^{\text{emp.}}(p^{\text{emp.}}, p_{\text{data}}) \downarrow$	$\text{FID}(p^{\text{emp.}}, p_{\text{data}}^{\text{emp.}}) \downarrow$	$\mathbf{W}_2^{\text{emp.}}(p_{\theta}^{\text{emp.}}, p_{\text{data}}^{\text{emp.}}) \downarrow$	$\text{FID}(p_{\theta}^{\text{emp.}}, p_{\text{data}}^{\text{emp.}}) \downarrow$
EM	5.16	5.1630	0.0891	15.6	1.02
Heun	3.73	3.7323	0.0447	56.7	19.4

Conclusion

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- Extension to GMM ?

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 - Exact solutions are not known.

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(in progress) → Stanislas Strasman et al. (2024). *An analysis of the noise schedule for score-based generative models*. arXiv: 2402.04650 [math.ST]. URL: <https://arxiv.org/abs/2402.04650>

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- Extension to conditional diffusion models ?
(in progress) → Joël Greffier et al. (2024). "Photon-counting CT systems: A technical review of current clinical possibilities". In: *Diagnostic and Interventional Imaging*. ISSN: 2211-5684. DOI: <https://doi.org/10.1016/j.diii.2024.09.002>. URL: <https://www.sciencedirect.com/science/article/pii/S2211568424001955>

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 $\boldsymbol{v} = \boldsymbol{A}x + \sigma\boldsymbol{\varepsilon}$?

How to perform conditional simulation ?

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

A large literature [Song et al. 2021⁸, Lugmayr et al. 2022⁹, Chung et al. 2022¹⁰, Choi et al. 2021¹¹] uses the Bayes formula

$$\nabla_x \log p_t(x_t \mid \boldsymbol{v}) = \nabla_x \log p_t(\boldsymbol{v} \mid x_t) + \nabla_x \log p_t(x_t). \quad (39)$$

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

⁸Yang 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
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	$\varepsilon = 10^{-3}$	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