AdjointDEIS: Efficient Gradients for Diffusion Models

On the use of the continuous adjoint equations with diffusion models

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2025.01.15

Outline

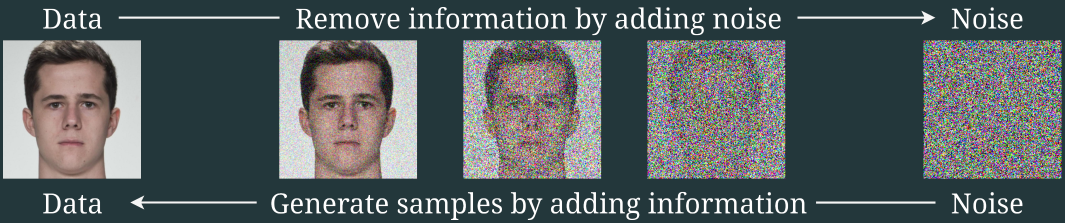
Introduction

AdjointDEIS

Remarks about using the continuous adjoint equations with diffusion models

Introduction

Diffusion models



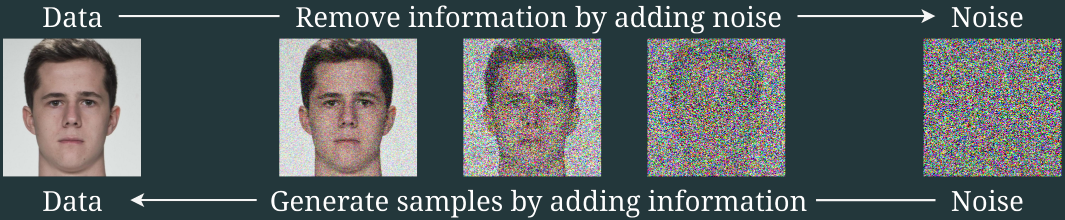
- Forward diffusion process is governed by the Itô SDE

$$d\mathbf{x}_t = f(t)\mathbf{x}_t \, dt + g(t) \, d\mathbf{w}_t, \tag{1}$$

where $\{\mathbf{w}_t\}_{t \in [0,T]}$ is the standard Wiener process on $[0, T]$.

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

Diffusion models



- The diffusion equation can be reversed with

$$d\mathbf{x}_t = [f(t)\mathbf{x}_t - g^2(t)\nabla_{\mathbf{x}} \log p_t(\mathbf{x}_t)]\, dt + g(t)\, d\bar{\mathbf{w}}_t, \tag{2}$$

  where $\bar{\mathbf{w}}_t$ is the *reverse* Wiener process and 'dt' is a *negative* timestep.
- The marginal distributions $p_t(\mathbf{x})$ follow the *probability flow* ODE[1]

$$\frac{d\mathbf{x}_t}{dt} = f(t)\mathbf{x}_t - \frac{1}{2} g^2(t)\nabla_{\mathbf{x}} \log p_t(\mathbf{x}_t). \tag{3}$$

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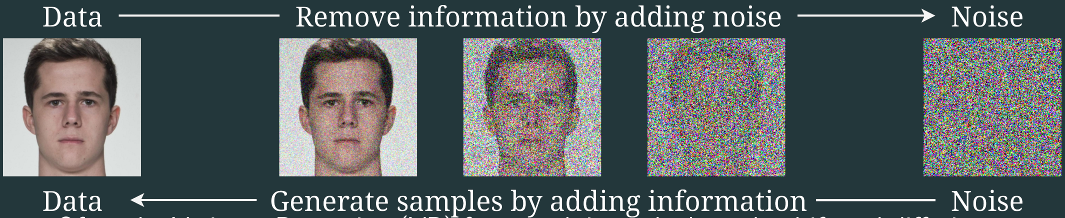
Diffusion models



- Often the Variance Preserving (VP) framework is used where the drift and diffusion coefficients are

$$f(t) = \frac{\mathrm{d}\log \alpha_t}{\mathrm{d}t}, \qquad g^2(t) = \frac{\mathrm{d}\sigma_t^2}{\mathrm{d}t} - 2\frac{\mathrm{d}\log \alpha_t}{\mathrm{d}t}\sigma_t^2, \tag{4}$$

  for some noise schedule α_t, σ_t

- Sampling the forward trajectory then simplifies to

$$\mathbf{x}_t = \alpha_t \mathbf{x}_0 + \sigma_t \boldsymbol{\epsilon}_t \qquad \boldsymbol{\epsilon}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \tag{5}$$

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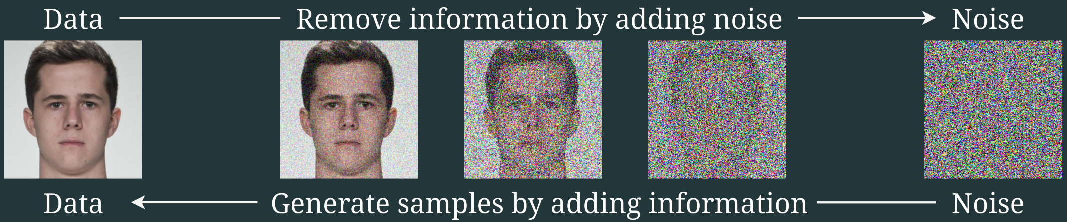

- Train the model via score-matching to learn $\nabla_{\mathbf{x}} \log p_t(\mathbf{x}_t)$.
- This is similar to learning the noise ϵ, *i.e.*,

$$\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \approx -\sigma_t \nabla_{\mathbf{x}} \log p_t(\mathbf{x}_t). \tag{6}$$

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Problem statement

- Solve the following optimization problem:

$$\arg\min_{\mathbf{x}_T,\mathbf{z},\theta} \mathcal{L}\left(\mathbf{x}_T + \int_T^0 f(t)\mathbf{x}_t + \frac{g^2(t)}{2\sigma_t}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t,\mathbf{z},t)\;\mathrm{d}t\right). \tag{7}$$

- Or in the SDE case:

$$\arg\min_{\mathbf{x}_T,\mathbf{z},\theta} \mathcal{L}\left(\mathbf{x}_T + \int_T^0 f(t)\mathbf{x}_t + \frac{g^2(t)}{\sigma_t}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t,\mathbf{z},t)\;\mathrm{d}t + \int_T^0 g(t)\;\mathrm{d}\bar{\mathbf{w}}_t\right). \tag{8}$$

- To backpropagate through an ODE/SDE solve we solve the continuous adjoint equations.

Continuous adjoint equations

- Let $\boldsymbol{f}_\theta$ describe a parameterized neural field of the probability flow ODE, defined as

$$\boldsymbol{f}_\theta(\mathbf{x}_t, \mathbf{z}, t) = f(t)\mathbf{x}_t + \frac{g^2(t)}{2\sigma_t}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, \mathbf{z}, t). \tag{9}$$

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- Then $\boldsymbol{f}_\theta(\mathbf{x}_t, \mathbf{z}, t)$ describes a neural ODE which admits an adjoint state, $\mathbf{a}_\mathbf{x} := \partial\mathcal{L}/\partial\mathbf{x}_t$ (and likewise for $\mathbf{a}_\mathbf{z}(t)$ and $\mathbf{a}_\theta(t)$), which solve the continuous adjoint equations [7, Theorem 5.2] in the form of the following Initial Value Problem (IVP):

$$\begin{aligned}
\mathbf{a}_\mathbf{x}(0) &= \frac{\partial\mathcal{L}}{\partial\mathbf{x}_0}, & \frac{\mathrm{d}\mathbf{a}_\mathbf{x}}{\mathrm{d}t}(t) &= -\mathbf{a}_\mathbf{x}(t)^\top\frac{\partial\boldsymbol{f}_\theta(\mathbf{x}_t, \mathbf{z}, t)}{\partial\mathbf{x}_t},\\
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\end{aligned} \tag{10}$$

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AdjointDEIS

The continuous adjoint equations are also semi-linear

- Like diffusion ODEs the adjoint diffusion ODE is also semi-linear

$$\frac{\mathrm{d}\mathbf{a}_{\mathbf{x}}}{\mathrm{d}t}(t) = -\underbrace{f(t)\mathbf{a}_{\mathbf{x}}(t)}_{\text{Linear}} - \frac{g^2(t)}{2\sigma_t}\mathbf{a}_{\mathbf{x}}(t)^\top \frac{\partial \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, \mathbf{z}, t)}{\partial \mathbf{x}_t}. \tag{11}$$

[2] Cheng Lu et al. "DPM-Solver: A Fast ODE Solver for Diffusion Probabilistic Model Sampling in Around 10 Steps". In: *Advances in Neural Information Processing Systems*. Ed. by S. Koyejo et al. Vol. 35. Curran Associates, Inc., 2022, pp. 5775–5787. URL: https://proceedings.neurips.cc/paper_files/paper/2022/file/260a14acce2a89dad36adc8eefe7c59e-Paper-Conference.pdf.

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- Then, the exact solution at time s given time $t < s$ is found to be

$$\mathbf{a}_{\mathbf{x}}(s) = \underbrace{e^{\int_s^t f(\tau)\,\mathrm{d}\tau}\mathbf{a}_{\mathbf{x}}(t)}_{\text{linear}} - \underbrace{\int_t^s e^{\int_s^u f(\tau)\,\mathrm{d}\tau}\frac{g^2(u)}{2\sigma_u}\mathbf{a}_{\mathbf{x}}(u)^\top \frac{\boldsymbol{\epsilon}_\theta(\mathbf{x}_u, \mathbf{z}, u)}{\partial \mathbf{x}_u}\,\mathrm{d}u\,.}_{\text{non-linear}} \tag{12}$$

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$$\frac{\mathrm{d}\mathbf{a_x}}{\mathrm{d}t}(t) = -f(t)\mathbf{a_x}(t) - \frac{g^2(t)}{2\sigma_t}\mathbf{a_x}(t)^\top \frac{\partial \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, \mathbf{z}, t)}{\partial \mathbf{x}_t}. \tag{11}$$

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- Use the log-SNR trick[2] to further simplify the exact solution with $\lambda_t \coloneqq \log(\alpha_t/\sigma_t)$.

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Simplified exact solutions

Proposition 1 (Exact solution of adjoint diffusion ODEs[3])

Given initial values $[\mathbf{a}_{\mathbf{x}}(t), \mathbf{a}_{\mathbf{z}}(t), \mathbf{a}_{\theta}(t)]$ *at time* $t \in (0, T)$*, the solution* $[\mathbf{a}_{\mathbf{x}}(s), \mathbf{a}_{\mathbf{z}}(s), \mathbf{a}_{\theta}(s)]$ *at time* $s \in (t, T]$ *of adjoint diffusion ODEs in Eq.* (10) *is*

$$\mathbf{a}_{\mathbf{x}}(s) = \frac{\alpha_t}{\alpha_s}\mathbf{a}_{\mathbf{x}}(t) + \frac{1}{\alpha_s}\int_{\lambda_t}^{\lambda_s} \alpha_\lambda^2 e^{-\lambda}\mathbf{a}_{\mathbf{x}}(\lambda)^\top \frac{\partial \boldsymbol{\epsilon}_\theta(\mathbf{x}_\lambda, \mathbf{z}, \lambda)}{\partial \mathbf{x}_\lambda}\,\mathrm{d}\lambda, \tag{13}$$

$$\mathbf{a}_{\mathbf{z}}(s) = \mathbf{a}_{\mathbf{z}}(t) + \int_{\lambda_t}^{\lambda_s} \alpha_\lambda e^{-\lambda}\mathbf{a}_{\mathbf{x}}(\lambda)^\top \frac{\partial \boldsymbol{\epsilon}_\theta(\mathbf{x}_\lambda, \mathbf{z}, \lambda)}{\partial \mathbf{z}}\,\mathrm{d}\lambda, \tag{14}$$

$$\mathbf{a}_{\theta}(s) = \mathbf{a}_{\theta}(t) + \int_{\lambda_t}^{\lambda_s} \alpha_\lambda e^{-\lambda}\mathbf{a}_{\mathbf{x}}(\lambda)^\top \frac{\partial \boldsymbol{\epsilon}_\theta(\mathbf{x}_\lambda, \mathbf{z}, \lambda)}{\partial \theta}\,\mathrm{d}\lambda. \tag{15}$$

[3] Zander W. Blasingame and Chen Liu. "AdjointDEIS: Efficient Gradients for Diffusion Models". In: *The Thirty-eighth Annual Conference on Neural Information Processing Systems*. 2024. URL: https://openreview.net/forum?id=fAlcxvrOEX.

Designing bespoke ODE solvers

- We denote the n-th derivative of the *scaled* vector-Jacobian product by

$$\mathbf{V}^{(n)}(\mathbf{x};\lambda_t) = \frac{\mathrm{d}^n}{\mathrm{d}\lambda^n}\left[\alpha_\lambda^2 \mathbf{a}_\mathbf{x}(\lambda)^\top \frac{\partial \boldsymbol{\epsilon}_\theta(\mathbf{x}_\lambda, \mathbf{z}, \lambda)}{\partial \mathbf{x}_\lambda}\right]_{\lambda=\lambda_t}. \tag{16}$$

- Use Taylor Expansion on Eq. (13) to obtain and letting $h = \lambda_s - \lambda_t$ yields

$$\mathbf{a}_\mathbf{x}(s) = \underbrace{\frac{\alpha_t}{\alpha_s}\mathbf{a}_\mathbf{x}(t)}_{\substack{\text{Linear term} \\ \textbf{Exactly computed}}} + \frac{1}{\alpha_s}\sum_{n=0}^{k-1} \mathbf{V}^{(n)}(\mathbf{x};\lambda_t) \int_{\lambda_t}^{\lambda_s} \frac{(\lambda-\lambda_t)^n}{n!} e^{-\lambda}\,\mathrm{d}\lambda + \mathcal{O}(h^{k+1}). \tag{17}$$

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- And analogously for $\mathbf{a}_\mathbf{z}(t)$ and $\mathbf{a}_\theta(t)$.

AdjointDEIS

Theorem 1 (AdjointDEIS-k as a k-th order solver)

Assume the function $\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, \mathbf{z}, t)$ and its associated vector-Jacobian products follow the regularity conditions detailed in Appendix B of the main paper, then for $k = 1, 2$, AdjointDEIS-k is a k-th order solver for adjoint diffusion ODEs, i.e., for the sequence $\{\tilde{\mathbf{a}}_\mathbf{x}(t_i)\}_{i=1}^M$ computed by AdjointDEIS-k, the global truncation error at time T satisfies $\tilde{\mathbf{a}}_\mathbf{x}(t_M) - \mathbf{a}_\mathbf{x}(T) = \mathcal{O}(h_{max}^2)$, where $h_{max} = \max_{1 \leq j \leq M}(\lambda_{t_i} - \lambda_{t_{i-1}})$. Likewise, AdjointDEIS-$k$ is a k-th order solver for the estimated gradients w.r.t. $\mathbf{z}$ and θ.

Certain adjoint SDEs are actually ODEs

Theorem 2

Let $\boldsymbol{f} : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}^d$ *be in* $\mathcal{C}_b^{\infty,1}$ *and* $\boldsymbol{g} : \mathbb{R} \to \mathbb{R}^{d\times w}$ *be in* $\mathcal{C}_b^1$*. Let* $\mathcal{L} : \mathbb{R}^d \to \mathbb{R}$ *be a scalar-valued differentiable function. Let* $\mathbf{w}_t : [0,T] \to \mathbb{R}^w$ *be a* w*-dimensional Wiener process. Let* $\mathbf{x} : [0,T] \to \mathbb{R}^d$ *solve the Stratonovich SDE*

$$\mathrm{d}\mathbf{x}_t = \boldsymbol{f}(\mathbf{x}_t, t)\,\mathrm{d}t + \boldsymbol{g}(t) \circ \mathrm{d}\mathbf{w}_t,$$

with initial condition $\mathbf{x}_0$*. Then the adjoint process* $\mathbf{a}_{\mathbf{x}}(t) \coloneqq \partial\mathcal{L}(\mathbf{x}_T)/\partial\mathbf{x}_t$ *is a strong solution to the backwards-in-time ODE*

$$\mathrm{d}\mathbf{a}_{\mathbf{x}}(t) = -\mathbf{a}_{\mathbf{x}}(t)^\top \frac{\partial \boldsymbol{f}}{\partial \mathbf{x}_t}(\mathbf{x}_t, t)\,\mathrm{d}t. \tag{18}$$

ODE solvers for the adjoint diffusion SDE

- Probability Flow ODEs are related to diffusion SDEs by the manipulations of the Kolmogorov equations[4].
- The drift term is identical to the vector field of the ODE, sans a factor of two:

$$\underbrace{\mathrm{d}\mathbf{x}_t = f(t)\mathbf{x}_t + 2\frac{g^2(t)}{2\sigma_t}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, \mathbf{z}, t)\;\mathrm{d}t}_{\text{Probabilty Flow ODE}} + g(t)\;\mathrm{d}\bar{\mathbf{w}}_t. \tag{19}$$

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- By Theorem 2 the adjoint SDE evolves with an ODE with vector field $-\mathbf{a}_\mathbf{x}(t)^\top \partial \boldsymbol{f}_\theta(\mathbf{x}_t, \mathbf{z}, t)/\partial \mathbf{x}_t$.

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- Therefore, we can use the *same* bespoke ODE solvers for adjoint diffusion ODEs with the added factor of 2!

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

Experiment - face morphing

(a) Identity a **(b)** Face morphing with AdjointDEIS **(c)** Identity b

Figure 1: Create a morphed face which causes a Face Recognition (FR) system to accept it with **both** identities.

Experiment - face morphing

- Goal is to adversarially attack an FR system by finding the $\mathbf{x}_T, \mathbf{z}$ which creates the optimal morph.
- Optimality is defined with respect to an identity loss which is simply the average distance between the embeddings in the FR space.
- Using AdjointDEIS massively improves the performance of Diffusion Morphs (DiM).

Table 1: Vulnerability of different FR systems across different morphing attacks on the SYN-MAD 2022 dataset. FMR $= 0.1\%$.

		MMPMR [17](↑)		
Morphing Attack	**NFE(↓)**	**AdaFace** [10]	**ArcFace** [5]	**ElasticFace** [4]
Webmorph [6]	-	97.96	96.93	98.36
MIPGAN-I [19]	-	72.19	77.51	66.46
MIPGAN-II [19]	-	70.55	72.19	65.24
DiM-A [3]	350	92.23	90.18	93.05
Fast-DiM [2]	300	92.02	90.18	93.05
Morph-PIPE [20]	2350	95.91	92.84	95.5
DiM + AdjointDEIS-1 (ODE)	2250	**99.8**	**98.77**	**99.39**
DiM + AdjointDEIS-1 (SDE)	2250	98.57	97.96	97.75

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- What if the conditioning signal changed with the timestep, *i.e.*, $\mathbf{z}_t$?
- Question is then how do we find $\partial\mathcal{L}/\partial\mathbf{z}_t \coloneqq \mathbf{a}_\mathbf{z}(t)$?
- Fortunately, it reduces to a simple integral.

Gradients of scheduled conditional information

Theorem 3

Suppose there exists a function $\mathbf{z} : [0, T] \to \mathbb{R}^z$ *which can be defined as a càdlàg piecewise function where* $\mathbf{z}$ *is continuous on each partition of* $[0, T]$ *given by* $\Pi = \{0 = t_0 < t_1 < \cdots < t_n = T\}$ *and whose right derivatives exist for all* $t \in [0, T]$*. Let* $\boldsymbol{f}_\theta : \mathbb{R}^d \times \mathbb{R}^z \times \mathbb{R} \to \mathbb{R}^d$ *be continuous in* t*, uniformly Lipschitz in* $\mathbf{x}$*, and continuously differentiable in* $\mathbf{x}$*. Let* $\mathbf{x} : \mathbb{R} \to \mathbb{R}^d$ *be the unique solution for the ODE*

$$\frac{\mathrm{d}\mathbf{x}_t}{\mathrm{d}t} = \boldsymbol{f}_\theta(\mathbf{x}_t, \mathbf{z}_t, t),$$

with initial condition $\mathbf{x}_0$*. Let* $\mathcal{L} : \mathbb{R}^d \to \mathbb{R}$ *be a scalar-valued loss function defined on the output of the neural ODE. Then* $\partial\mathcal{L}/\partial\mathbf{z}_t := \mathbf{a}_\mathbf{z}(t)$ *and there exists a unique solution* $\mathbf{a}_\mathbf{z} : \mathbb{R} \to \mathbb{R}^z$ *to the following IVP:*

$$\mathbf{a}_\mathbf{z}(T) = \mathbf{0}, \qquad \frac{\mathrm{d}\mathbf{a}_\mathbf{z}}{\mathrm{d}t}(t) = -\mathbf{a}_\mathbf{x}(t)^\top \frac{\partial \boldsymbol{f}_\theta(\mathbf{x}_t, \mathbf{z}_t, t)}{\partial \mathbf{z}_t}.$$

Gradients of the conditional information are still a mere integral

- As the vector fields of the ODE are independent of $\mathbf{a}_{\mathbf{z}}$ we have a mere integral,

$$\mathbf{a}_{\mathbf{z}}(t) = -\int_T^t \mathbf{a}_{\mathbf{x}}(\tau)^\top \frac{\partial \boldsymbol{f}_\theta(\mathbf{x}_\tau, \mathbf{z}_\tau, \tau)}{\partial \mathbf{z}_\tau} \, \mathrm{d}\tau. \tag{20}$$

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- We can simply replace our $\mathbf{z}$ with $\mathbf{z}_t$ when performing guided generation.
- Enables us to update time-dependent conditioning signal.
- We have the flexibility to only update back to a certain $t \in [0, T)$.

What about neural CDEs?

- Kidger [9, Theorem C.1] showed that any equation of the form

$$\mathbf{x}_t = \mathbf{x}_0 + \int_0^t \boldsymbol{h}_\theta(\mathbf{x}_s, \mathbf{z}_s, s)\,\mathrm{d}s, \tag{21}$$

can be rewritten as a neural *controlled differential equation* (CDE) of the form

$$\mathbf{x}_t = \mathbf{x}_0 + \int_0^t \boldsymbol{f}_\theta(\mathbf{x}_s, s)\,\mathrm{d}\mathbf{z}_s, \tag{22}$$

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  where $\int \,\mathrm{d}\mathbf{z}_s$ is the Riemann-Stieltjes integral.
- Note, the converse is not true.
- Neural CDEs used $\mathbf{z}_t$ as an additional control signal, but were not interested in **updating** $\mathbf{z}_t$.

Time scheduled conditional information in practice

- Suppose we have a fully observed, but irregularly sampled time series $\{\mathbf{z}_{t_i}\}_{i=1}^{N}$ with $0 = t_0 < \cdots < t_n = T$.
- Define $\mathbf{Z} : [0, T] \to \mathbb{R}^z$ as the natural cubic spline with knots at $t_0, \ldots, t_n$ such that $\mathbf{Z}(t_i) = \mathbf{z}_{t_i}$.
- Can use this with adaptive step size solvers for $\mathbf{a}_{\mathbf{x}}(t)$.

Remarks about using the continuous adjoint equations with diffusion models

Approaches for guided generation

- We will broadly categorize approaches into two categories:
  - **Solution Optimization** - Only cares about finding the optimal output, $\mathbf{x}_0$,
  - **End-to-End Optimization** - Cares about finding the optimal *entire* solution trajectory and associated variables, $(\{\mathbf{x}_{t_i}\}_{i=1}^{n}, \mathbf{z}, \theta)$.

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- For this later category we need to backpropogate through an ODE/SDE solve of the diffusion model

Backpropagation through neural differential equations

- **Discretize-then-optimize** (DTO)
  - Simplest approach, just backprop through the solver.
  - Pros: Accuracy of gradients, fast, and easy to implement.
  - Cons: Memory intensive, optimization w.r.t. discretization and not continuous ideal.

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  - Cons: Computational cost, truncation errors.
- **Reversible solvers**
  - Possible best of both worlds.
  - Pros: Memory efficient and accurate gradients.
  - Cons: Low-order and poor stability (recent work has started to address this).
- For more details we refer to Patrick Kidger's monograph on neural differential equations[5].

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Techniques for OTD optimization of diffusion models

Table 2: Overview of different OTD methods for diffusion models.

Method	**ODE**	**SDE**	**Key Idea**
DiffPure [15]	✗	✓	First to consider OTD for diffusion models
AdjointDPM [16]	✓	✗	Exponential integrators with OTD
Implicit Diffusion [12]	✓	✓	Time parallelization of OTD
AdjointDEIS [1]	✓	✓	Bespoke solvers for ODE/SDE

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- Area of future research, can we get away with less “accurate” gradients in practice?
- Different solvers for the underlying state $\{\mathbf{x}_t\}$ and gradients $\{\mathbf{a}_{\mathbf{x}}(t)\}$.

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- Consider a first-order solver (DDIM, DPM-Solver-1) then given

$$\hat{\mathbf{x}}_0 = \frac{\alpha_0}{\alpha_t}\mathbf{x}_t - \sigma_0(e^h - 1)\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t), \quad h = \lambda_0 - \lambda_t, \tag{23}$$

$$\hat{\mathbf{x}}_t = \frac{\alpha_t}{\alpha_0}\hat{\mathbf{x}}_0 - \sigma_t(e^{-h} - 1)\boldsymbol{\epsilon}_\theta(\hat{\mathbf{x}}_0, 0), \tag{24}$$

it is not necessary that for all $t \in [0, T]$ and $\mathbf{x}_t \in \mathbb{R}^d$ that

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holds.

- This can be mitigated with small step sizes at the cost of increased compute.

Stability of OTD

- Consider a simple ODE on $t \in [0, T]$ given by

$$\frac{\mathrm{d}y}{\mathrm{d}t}(t) = \lambda y(t), \quad y(0) = y_0, \quad \lambda < 0. \tag{26}$$

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- However, for backwards in time solve from $y(T)$ the errors will grow exponentially.
- The adjoint ODE has the same stability properties as y.

Reversible solvers

- Let Φ be a numerical scheme which iteratively computes $(\mathbf{x}_{t_i}, \alpha_{t_i}) \mapsto (\mathbf{x}_{t_{i+1}}, \alpha_{t_{i+1}})$ where α_{t_i} is extra auxillary information.

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- We will review several non-symplectic[6] reversible solvers.
- Consider a neural ODE on the time interval $[0, T]$ with definition

$$\mathbf{x}(0) = \mathbf{x}_0, \qquad \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}(t) = \boldsymbol{f}_\theta(\mathbf{x}(t), t). \tag{27}$$

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Asynchronous leapfrog method (ICLR 2021)

- Initially proposed by Mutze[7] and popularized by Zhuang *et al.*[8]
- Is a second-order method.

Forward pass

With $h := t_{i+1} - t_i$ the forward pass is defined as

$$\begin{aligned} \mathbf{x}_{t_i+\frac{h}{2}} &= \mathbf{x}_{t_i} + \frac{1}{2}\mathbf{v}_{t_i}h, \\ \mathbf{v}_{t_{i+1}} &= 2\boldsymbol{f}_\theta(\mathbf{x}_{t_i+\frac{h}{2}}, t_i + h/2) - \mathbf{v}_{t_i}, \\ \mathbf{x}_{t_{i+1}} &= \mathbf{x}_{t_i} + \boldsymbol{f}_\theta(\mathbf{x}_{t_i+h/2}, t_i + \frac{h}{2})h. \end{aligned}$$

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- ODE solver is a second-order method and exhibits a strong convergence of order 1 if the noise is additive.

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Note, this method is also *symmetric*.

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- The region of stability for the asynchronous leapfrog method and reversible Heun are both the complex interval $[-i, i]$.
- Could be due to an unstable step of form $2A - B$, instability is amplified when
  - $\mathbf{v}_{t_i}$ and $\boldsymbol{f}_\theta(\mathbf{x}_{t_i}, t_i)$ drift apart (asynchronous leapfrog),
  - $\mathbf{x}_{t_i}$ and $\widehat{\mathbf{x}}_{t_i}$ drift apart (reversible Heun).

McCallum-Foster method

- Recently, McCallum and Foster[10] showed that it is possible to construct an algebraically reversible solver from **any** explicit numerical ODE solver $\Phi : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}^d$.
- Suppose the explicit solver can be expressed as $\mathbf{x}_{t_{i+1}} = \mathbf{x}_{t_i} + \Phi_h(\mathbf{x}_{t_i}, t_i)$ with step size h.

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Forward pass

With $h := t_{i+1} - t_i$ the forward pass is defined as

$$\begin{aligned} \mathbf{x}_{t_{i+1}} &= \lambda \mathbf{x}_{t_i} + (1-\lambda)\widehat{\mathbf{x}}_{t_i} + \Phi_h(\widehat{\mathbf{x}}_{t_i}, t_i) \\ \widehat{\mathbf{x}}_{t_{i+1}} &= \widehat{\mathbf{x}}_{t_i} - \Phi_{-h}(\mathbf{x}_{t_{i+1}}, t_{i+1}), \end{aligned}$$

where $\lambda \in (0, 1]$ is a coupling parameter.

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Non-trivial stability

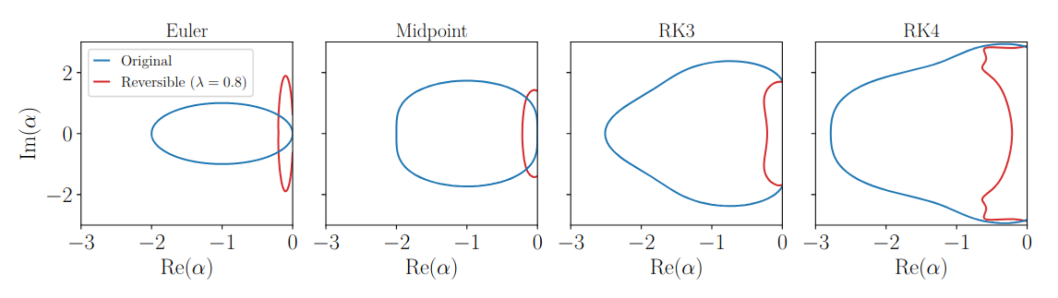

Figure 2: Stability plots from McCallum and Foster [13].

Record the solution trajectory

- A simple fix for the numerical unstability of OTD is to simply cache $\{\mathbf{x}_{t_i}\}_{i=1}^{n}$ during the forward pass.
- Note, we are not storing the internal operations of the solver and network.

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- Record $\{x_{\tau_j}\}_{j=1}^{m}$ and $\{\tau_j\}_{j=1}^{m} \subseteq \{t_i\}_{i=1}^{n}$.
- Then for any $\tau_j > t > \tau_{j+1}$ interpolate between the two samples $\mathbf{x}_{\tau_j}$ and $\mathbf{x}_{\tau_{j+1}}$ to find $\mathbf{x}_t$.

Parallel sampling and optimization

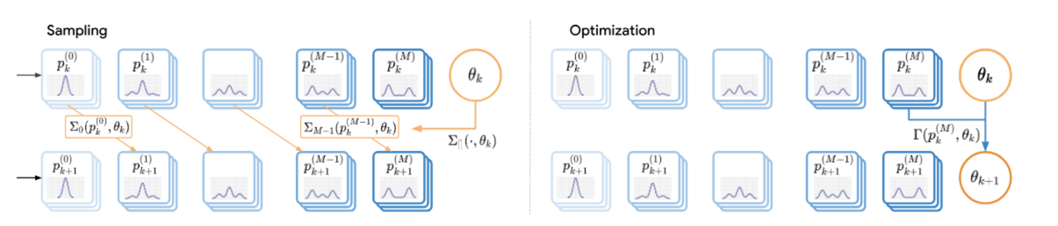

Figure 3: Implicit Diffusion by Marion *et al.*[11]

- Fill up shift register with initial sample trajectory $\{\mathbf{x}_{t_i}\}_{i=1}^n$.
- Can now sample and backpropagate in parallel.
- Because it's a shift register it still takes m steps to propagate an update to $\mathbf{x}_T$.

[11]Pierre Marion et al. "Implicit Diffusion: Efficient Optimization through Stochastic Sampling". In: *arXiv preprint arXiv:2402.05468* (2024).

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- If not, consider a reversible solver for the backward pass.
- Note, in practice OTD seems to work well enough and the gradient inaccuracy might not be a big deal in certain applications.

?

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