# A Reversible Solver for Diffusion SDEs


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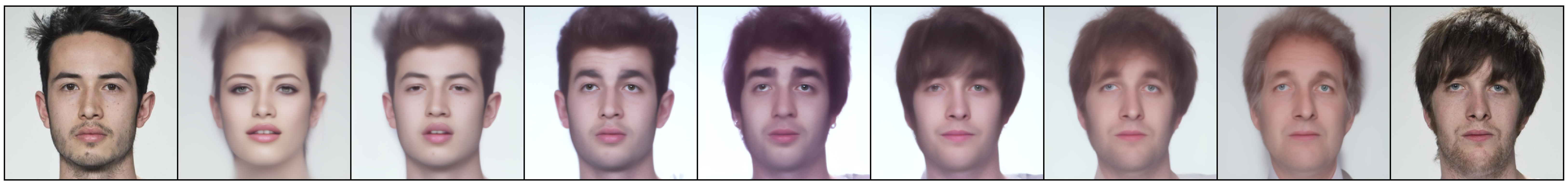
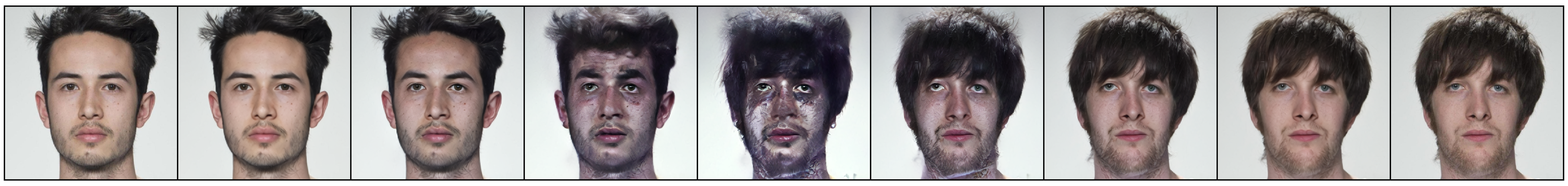
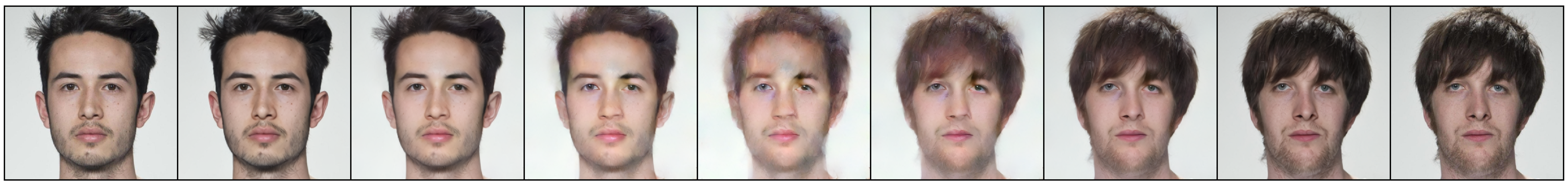


(a) DDIM inversion with 20 steps.



(b) Reversible DDIM with 20 steps.



(c) Reversible diffusion SDE with 20 steps.

Figure 1. Comparison of different solvers for diffusion models on an image interpolation task with interpolation values $0, 0.1, 0.25, 0.5, 0.75, 0.9, 1$ (from left to right). The leftmost and rightmost images are the original images: $\boldsymbol{x}_0^{(a)}$ and $\boldsymbol{x}_0^{(b)}$. The same number of steps are used for both the encoding and sampling procedure. For reversible methods $\zeta = 0.999$. Original faces from FRLL [1]. The model is an LDM trained on the CelebA-HQ dataset.

## Diffusion SDEs

Suppose we have the following Stratonovich SDE driven by $d$-dimensional Brownian motion $\{\overline{\boldsymbol{W}}_t : 0 \leq t \leq T\}$,

$$\mathrm{d}\boldsymbol{X}_t = f(t)\boldsymbol{X}_t \,\mathrm{d}t + g(t) \circ \mathrm{d}\overline{\boldsymbol{W}}_t, \tag{1}$$

where $f, g \in \mathcal{C}^1([0,T])$ form the drift and diffusion coefficients. Then with some manipulations via the Kolmogorov equations we have the *reverse-time diffusion SDE*

$$\mathrm{d}\boldsymbol{X}_t = [f(t)\boldsymbol{X}_t - g^2(t)\nabla_x \log p_t(\boldsymbol{X}_t)] \,\mathrm{d}t + g(t) \circ \mathrm{d}\boldsymbol{W}_t \tag{2}$$

where $\{\boldsymbol{W}_t : 0 \leq t \leq T\}$ is the standard Brownian motion in reverse-time and $\mathrm{d}t$ is a *negative* timestep. Let the drift and diffusion coefficients be given as

$$f(t) = \frac{\dot{\alpha}_t}{\alpha_t}, \qquad g^2(t) = \frac{\mathrm{d}}{\mathrm{d}t}\left[\sigma_t^2\right] - 2\frac{\dot{\alpha}_t}{\alpha_t}\sigma_t^2, \tag{3}$$

for the schedule $(\alpha_t, \sigma_t)$.

## Reversible solvers

**Analytic reversibility.** In a sense any numerical solver is reversible, consider the explicit Euler scheme

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + h\boldsymbol{f}(\boldsymbol{x}_n) \tag{4}$$

with vector field $\boldsymbol{f}$, then the *reverse* is the implicit Euler scheme

$$\boldsymbol{x}_n = \boldsymbol{x}_{n+1} - h\boldsymbol{f}(\boldsymbol{x}_n). \tag{5}$$

However, such schemes are undesirable in practice.

**Algebraic reversibility.** Now consider a scheme $(\boldsymbol{x}_n, \boldsymbol{\alpha}_n) \mapsto (\boldsymbol{x}_{n+1}, \boldsymbol{\alpha}_{n+1})$ where $\boldsymbol{\alpha}_n$ are additional states. The numerical scheme is *algebraically reversible* if $(\boldsymbol{x}_n, \boldsymbol{\alpha}_n)$ can be computed in closed form from $(\boldsymbol{x}_{n+1}, \boldsymbol{\alpha}_{n+1})$.

The only general reversible SDE is Kidger's reversible Heun [2] which while obtaining a strong convergence order of 1 (for additive noise) has poor stability, being nowhere linearly stable (in the ODE case).

The recently proposed McCallum-Foster method [3] has a non-trivial region of stability for ODEs and can be arbitrarily high-order.

## Exact inversion with diffusion models

Several approaches [4, 5, 6] have been proposed for the exact inversion of diffusion ODEs; however, they are all essentially the midpoint method and thus are nowhere linearly stable, along with convergence issues for [4, 5].

CycleDiffusion [7] was proposed for the inversion of diffusion SDEs however it requires storing all of $\boldsymbol{W}_t$ in memory for each step.

We propose a reversible solver for diffusion SDEs which does not require storing the entire Brownian motion in memory.

To do this, we make use of time-changed Brownian motion and the Brownian Interval [2].

## A reversible solver for diffusion SDEs

***Proposition* 1** (Exact solution of diffusion SDEs)**.** *Given an initial value $\boldsymbol{X}_s(\omega) = \boldsymbol{x}_s$ at time $s \in [0,T]$ the exact solution of Eq. (3) can be expressed as:*

$$\boldsymbol{X}_t = \underbrace{\frac{\sigma_t}{\sigma_s}e^{\lambda_s - \lambda_t}\boldsymbol{X}_s}_{\substack{\textbf{\textit{Linear term}} \\ \textit{No truncation errors}}} + \underbrace{2\alpha_t \int_{\lambda_s}^{\lambda_t} e^{2(\lambda - \lambda_t)}\boldsymbol{x}_{\lambda_0|\lambda}(\boldsymbol{X}_\lambda)\,\mathrm{d}\lambda}_{\substack{\textbf{\textit{Approximated term}} \\ \textit{Truncation errors}}} + \underbrace{\sqrt{2}\sigma_t e^{-\lambda_t}\boldsymbol{W}_{\varsigma_t,\varsigma_s}}_{\substack{\textbf{\textit{Brownian bridge}} \\ \textit{No truncation errors}}}, \tag{6}$$

*where $\varsigma_t = \frac{1}{2}(e^{2\lambda_t} - e^{2\lambda_T})$.*

**Forward pass.** Suppose that we have a single-step solver for the exponential integral term in Eq. (6) given by $\Psi_h : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ where $h$ denotes the step size $h \coloneqq \lambda_t - \lambda_s$ and timesteps $\{t_n\}_{n=1}^N$ which is defined in *reverse-time*. Let $\zeta \in (0,1)$ be a coupling parameter that determines the stability of the forward and backward passes, and let $\hat{\boldsymbol{x}}$ be an augmented state for algebraic reversibility. For notational simplicity, let $\boldsymbol{x}_n \coloneqq \boldsymbol{x}_{t_n}$ and likewise for other variables. We then define the forward pass as

$$\begin{aligned}
\boldsymbol{x}_{n+1} &= \zeta\boldsymbol{x}_n + (1-\zeta)\hat{\boldsymbol{x}}_n + \frac{\sigma_{n+1}}{\sigma_n}e^{-h}\hat{\boldsymbol{x}}_n + 2\alpha_{n+1}\Psi_h(t_n, \hat{\boldsymbol{x}}_n) \\
&\quad + \sqrt{2}\sigma_{n+1}e^{-\lambda_{n+1}}\boldsymbol{W}_{\varsigma_{n+1},\varsigma_n}, \\
\hat{\boldsymbol{x}}_{n+1} &= \hat{\boldsymbol{x}}_n - \frac{\sigma_n}{\sigma_{n+1}}e^h\boldsymbol{x}_{n+1} - 2\alpha_n\Psi_{-h}(t_{n+1}, \boldsymbol{x}_{n+1}) + \sqrt{2}\sigma_n e^{-\lambda_n}\boldsymbol{W}_{\varsigma_{n+1},\varsigma_n}.
\end{aligned} \tag{7}$$

**Backward pass.** The backward solve can then be computed algebraically from Eq. (7) as

$$\begin{aligned}
\hat{\boldsymbol{x}}_n &= \hat{\boldsymbol{x}}_{n+1} + \frac{\sigma_n}{\sigma_{n+1}}e^h\boldsymbol{x}_{n+1} + 2\alpha_n\Psi_{-h}(t_{n+1}, \boldsymbol{x}_{n+1}) - \sqrt{2}\sigma_n e^{-\lambda_n}\boldsymbol{W}_{\varsigma_{n+1},\varsigma_n}, \\
\boldsymbol{x}_n &= \zeta^{-1}\boldsymbol{x}_{n+1} + (1-\zeta^{-1})\hat{\boldsymbol{x}}_n - \frac{\sigma_{n+1}}{\sigma_n}e^{-h}\zeta^{-1}\hat{\boldsymbol{x}}_n + 2\alpha_{n+1}\zeta^{-1}\Psi_h(t_n, \hat{\boldsymbol{x}}_n) \\
&\quad - \sqrt{2}\sigma_{n+1}e^{-\lambda_{n+1}}\zeta^{-1}\boldsymbol{W}_{\varsigma_{n+1},\varsigma_n}.
\end{aligned} \tag{8}$$

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