NEURAL INFORMATION PROCESSING SYSTEMS

Score-based Generative Modeling through Stochastic Evolution Equations in Hilbert Spaces

NeurIPS 2023 Spotlight


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Research Motivation

- Score-based generative models have shown success in various domains.
- Song et al. [1] proposes a framework for continuous-time score-based generative models that use stochastic differential equations (SDEs).
- Recently, there has been active studies on diffusion models, such as generating functional data or replacing drift coefficients with image transformation, which cannot be covered by the SDE framework in [1].
- Motivated by this problem, we propose a unified framework for the continuous-time score-based generative modeling by using the theory of stochastic evolution equations in Hilbert spaces [2].

[1] Score-based Generative Modeling through Stochastic Differential Equations, Song et al., ***ICLR*** (2020)
[2] Stochastic Evolution Equations, N. V. Krylov & B. L. Rozovskii, ***Journal of Soviet Mathematics*** (1981)

Research Question and Contribution

$$\mathbf{X}_t = \mathbf{X}_0 + \int_0^t \mathbf{B}_s(\mathbf{X}_s)\mathrm{d}s + \int_0^t \mathbf{G}_s \mathrm{d}\mathbf{W}_s$$

Forward Stochastic Equation in Hilbert Space

$$\widehat{\mathbf{X}}_t = \widehat{\mathbf{X}}_0 + \int_0^t \widehat{\mathbf{B}}_s(\widehat{\mathbf{X}}_s)\mathrm{d}s + \int_0^t \widehat{\mathbf{G}}_s \mathrm{d}\mathbf{W}_s$$

Reverse Stochastic Equation in Hilbert Space

- Can we derive a ***time-reversal formula*** for Hilbert-valued stochastic equations $\mathbf{X}_t$ and $\widehat{\mathbf{X}}_t$ which have ***time-dependent*** evolution operators?

Time-Reversal Formula in Hilbert Space

Forward Equation $$\mathbf{X}_t = \mathbf{X}_0 + \int_0^t \mathbf{B}_s(\mathbf{X}_s)\mathrm{d}s + \int_0^t \mathbf{G}_s \mathrm{d}\mathbf{W}_s$$

$(\mathcal{H}^*, \mathcal{H}_\lambda, \mathcal{H})$ Gelfand triple

$f_{\varphi_{1:m}} \in \mathcal{F}C_b^\infty$ The class of smooth cylinder functions

Kolmogorov Operator of $\mathbf{X}_t$ $$\mathcal{L}_t f_{\varphi_{1:m}}(u) := \frac{1}{2}\mathrm{Tr}_{\mathcal{H}_\lambda}(\mathbf{A}_t(u) \circ \Lambda \circ D^2 f_{\varphi_{1:m}}(u)) + \langle D f_{\varphi_{1:m}}(u), \mathbf{B}_t(u)\rangle_{\mathcal{H}_\lambda}$$

$\mathbf{A}_t(u)$: $\mathbf{G}_t\mathbf{G}_t^*$; $D^2 f_{\varphi_{1:m}}$, $D f_{\varphi_{1:m}}$: Gâteaux derivative

Reverse Equation $$\widehat{\mathbf{X}}_t = \widehat{\mathbf{X}}_0 + \int_0^t \widehat{\mathbf{B}}_s(\widehat{\mathbf{X}}_s)\mathrm{d}s + \int_0^t \widehat{\mathbf{G}}_s \mathrm{d}\mathbf{W}_s$$

Kolmogorov Operator of $\widehat{\mathbf{X}}_t$ $$\widehat{\mathcal{L}}_t f_{\varphi_{1:m}}(u) := \frac{1}{2}\mathrm{Tr}_{\mathcal{H}_\lambda}(\widehat{\mathbf{A}}_t \circ \Lambda \circ D^2 f_{\varphi_{1:m}}(u)) + \langle D f_{\varphi_{1:m}}(u), \widehat{\mathbf{B}}_t(u)\rangle_{\mathcal{H}_\lambda},$$

$D^2 f_{\varphi_{1:m}}$, $D f_{\varphi_{1:m}}$: Gâteaux derivative

Time-Reversal Formula in Hilbert Space

Forward Equation $$\mathbf{X}_t = \mathbf{X}_0 + \int_0^t \mathbf{B}_s(\mathbf{X}_s)\mathrm{d}s + \int_0^t \mathbf{G}_s \mathrm{d}\mathbf{W}_s$$

$(\mathcal{H}^*, \mathcal{H}_\lambda, \mathcal{H})$ Gelfand triple

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Kolmogorov Operator of $\mathbf{X}_t$ $$\mathscr{L}_t f_{\varphi_{1:m}}(u) := \frac{1}{2}\mathrm{Tr}_{\mathcal{H}_\lambda}(\mathbf{A}_t(u) \circ \Lambda \circ D^2 f_{\varphi_{1:m}}(u)) + \langle D f_{\varphi_{1:m}}(u), \mathbf{B}_t(u)\rangle_{\mathcal{H}_\lambda}$$

$\widehat{\mathbf{A}}_t = \mathbf{A}_{T-t}$

Time-Reversal Formula

$$\widehat{\mathbf{B}}_t(u) = -\mathbf{B}_{T-t}(u) + \mathbf{S}_\lambda(T-t, u)$$

$$\mathbf{S}_\lambda(t, u) = \mathbf{G}_t \mathbf{G}_t^* \rho_{\mathcal{H}_\lambda}^{\mu_t}(u)$$

Score operator

Vector logarithmic derivative of μ_t

Reverse Equation $$\widehat{\mathbf{X}}_t = \widehat{\mathbf{X}}_0 + \int_0^t \widehat{\mathbf{B}}_s(\widehat{\mathbf{X}}_s)\mathrm{d}s + \int_0^t \widehat{\mathbf{G}}_s \mathrm{d}\mathbf{W}_s$$

Kolmogorov Operator of $\widehat{\mathbf{X}}_t$ $$\widehat{\mathscr{L}}_t f_{\varphi_{1:m}}(u) := \frac{1}{2}\mathrm{Tr}_{\mathcal{H}_\lambda}(\widehat{\mathbf{A}}_t \circ \Lambda \circ D^2 f_{\varphi_{1:m}}(u)) + \langle D f_{\varphi_{1:m}}(u), \widehat{\mathbf{B}}_t(u)\rangle_{\mathcal{H}_\lambda},$$

Research Question and Contribution

$$\mathbf{X}_t = \mathbf{X}_0 + \int_0^t \mathbf{B}_s(\mathbf{X}_s)\mathrm{d}s + \int_0^t \mathbf{G}_s \mathrm{d}\mathbf{W}_s$$

Forward Stochastic Equation in Hilbert Space

$$\widehat{\mathbf{X}}_t = \widehat{\mathbf{X}}_0 + \int_0^t \widehat{\mathbf{B}}_s(\widehat{\mathbf{X}}_s)\mathrm{d}s + \int_0^t \widehat{\mathbf{G}}_s \mathrm{d}\mathbf{W}_s$$

Reverse Stochastic Equation in Hilbert Space

- Can we derive a ***time-reversal formula*** for Hilbert-valued stochastic equations $\mathbf{X}_t$ and $\widehat{\mathbf{X}}_t$ which have ***time-dependent*** evolution operators? ✓

Research Question and Contribution

$$\mathbf{X}_t = \mathbf{X}_0 + \int_0^t \mathbf{B}_s(\mathbf{X}_s)\mathrm{d}s + \int_0^t \mathbf{G}_s \mathrm{d}\mathbf{W}_s$$

Forward Stochastic Equation in Hilbert Space

$$\widehat{\mathbf{X}}_t = \widehat{\mathbf{X}}_0 + \int_0^t \widehat{\mathbf{B}}_s(\widehat{\mathbf{X}}_s)\mathrm{d}s + \int_0^t \widehat{\mathbf{G}}_s \mathrm{d}\mathbf{W}_s$$

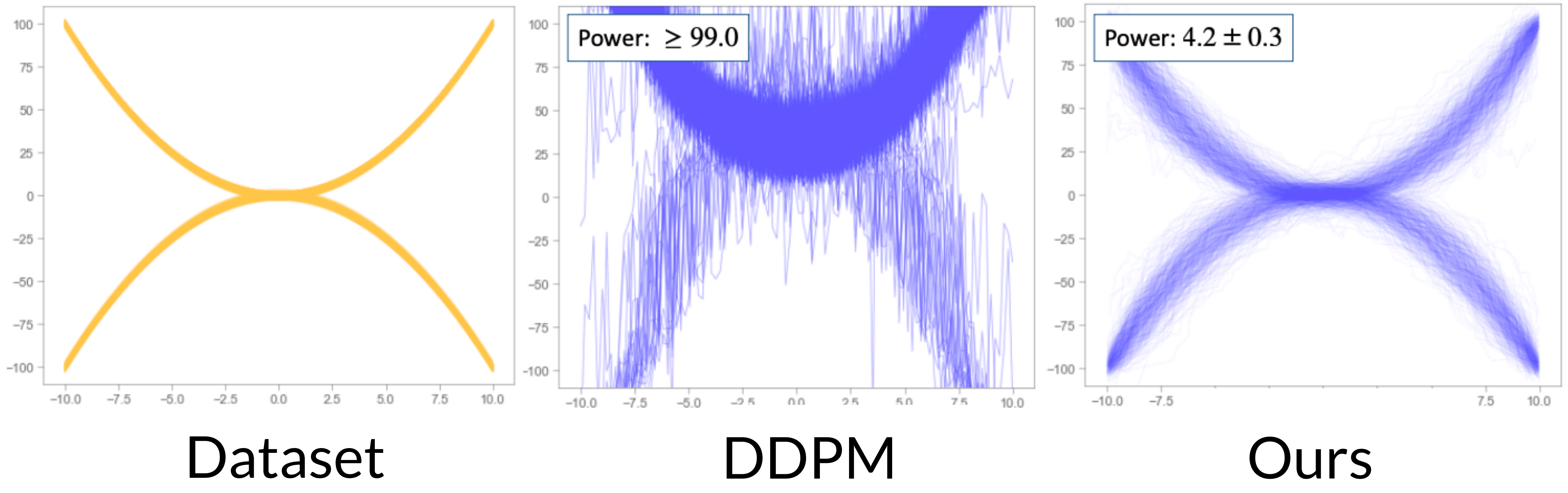
Reverse Stochastic Equation in Hilbert Space

- Can we derive a ***time-reversal formula*** for Hilbert-valued stochastic equations $\mathbf{X}_t$ and $\widehat{\mathbf{X}}_t$ which have ***time-dependent*** evolution operators? ✓
- Can we compute ***score operators*** exactly for training generative models? ✓
- Can we unify the SDE framework with stochastic equations in Hilbert spaces and propose a new class of continuous-time score-based models? ✓
- Can we build a bridge between the proposed framework and diffusion models using image transformations, e.g., heat dissipation [3]? ✓

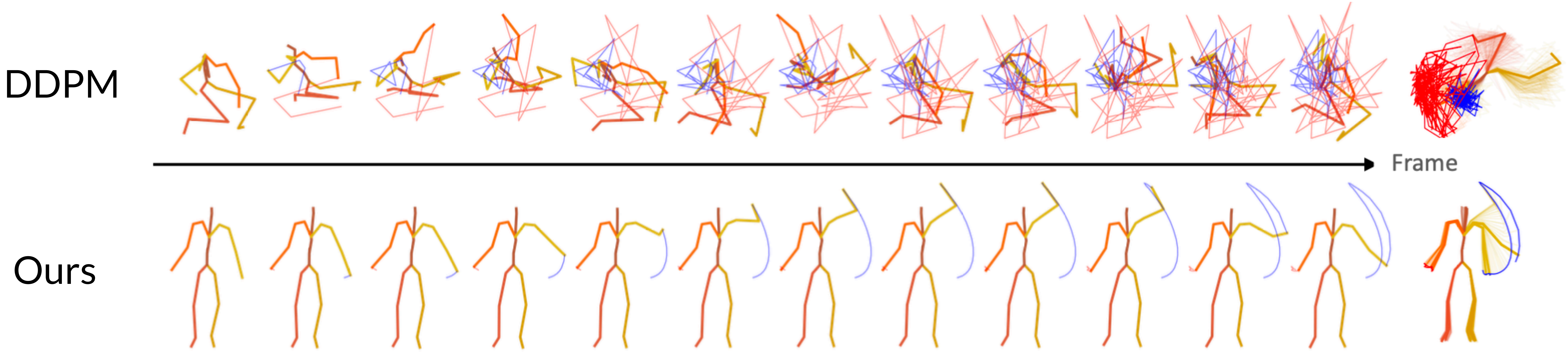
[3] Generative Modelling with Inverse Heat Dissipation, Rissanen et al., ***ICLR*** (2023)

Empirical Results: HDM-SDE

(a) HDM-SDE: 1D Function Generation



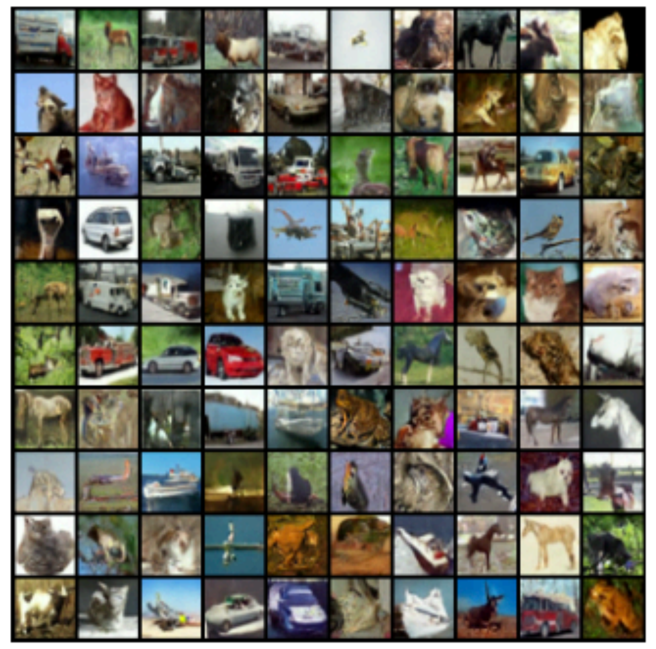
(b) HDM-SDE: Motion Generation



Empirical Results: HDM-SPDE

(a) HDM-SPDE: Image Generation

MNIST



CIFAR10

(IHDM) 18.96 → **17.84** (HDM)

LSUN-Church

45.06 → **29.09**

AFHQ

41.39 → **17.94**

FFHQ

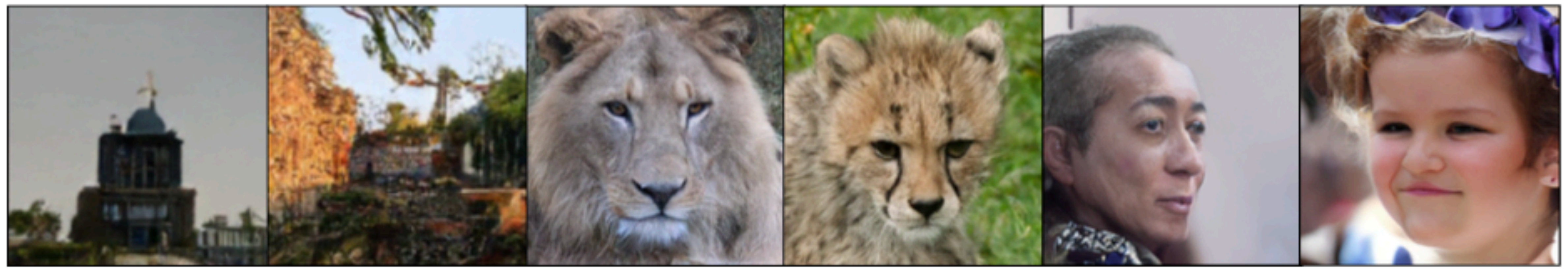
64.91 → **15.21**

(b) Connection between HDM-SPDE and IHDM [3]

LSUN | AFHQ | FFHQ

HDM Prior

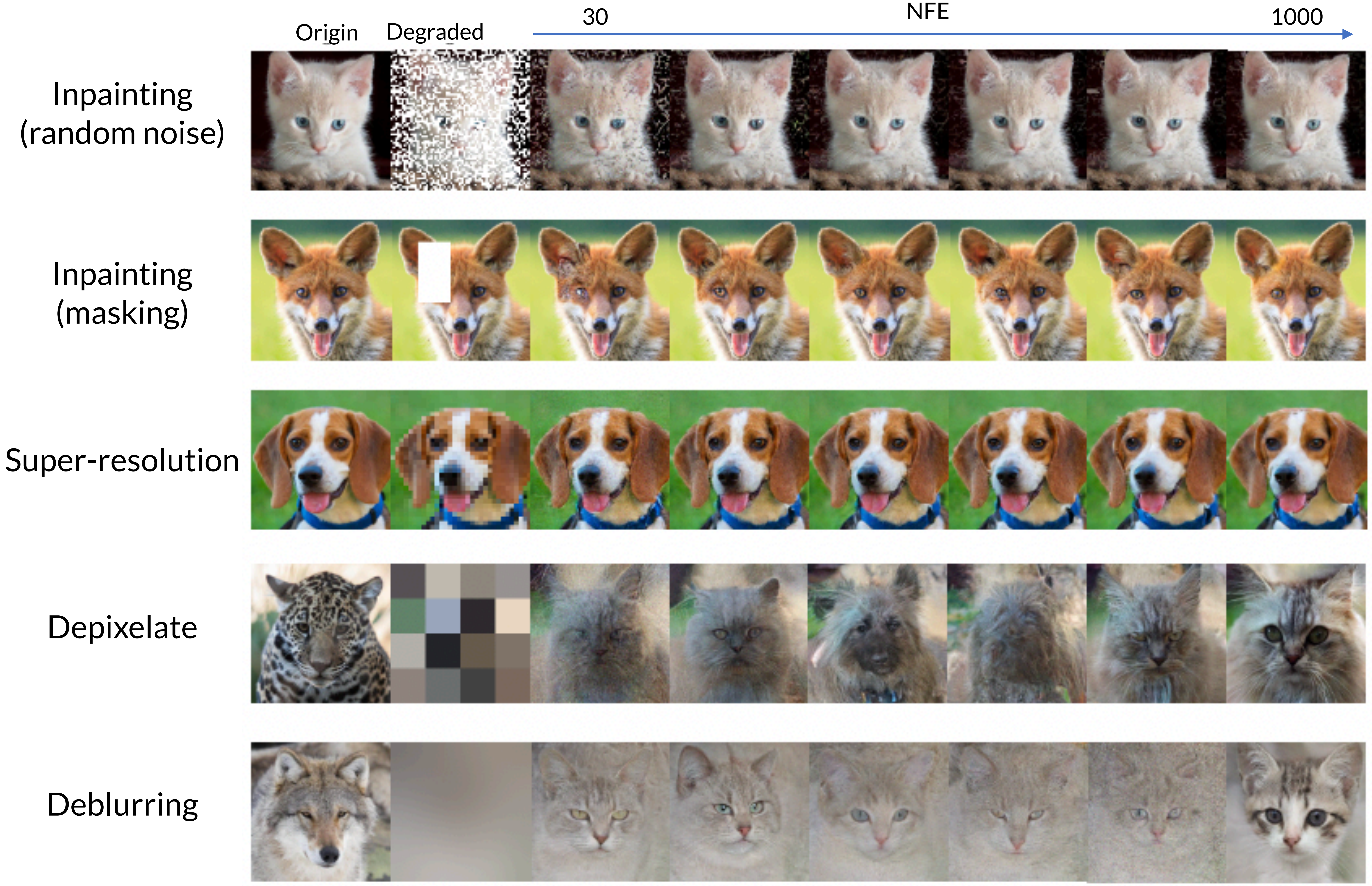
IHDM [3] Prior

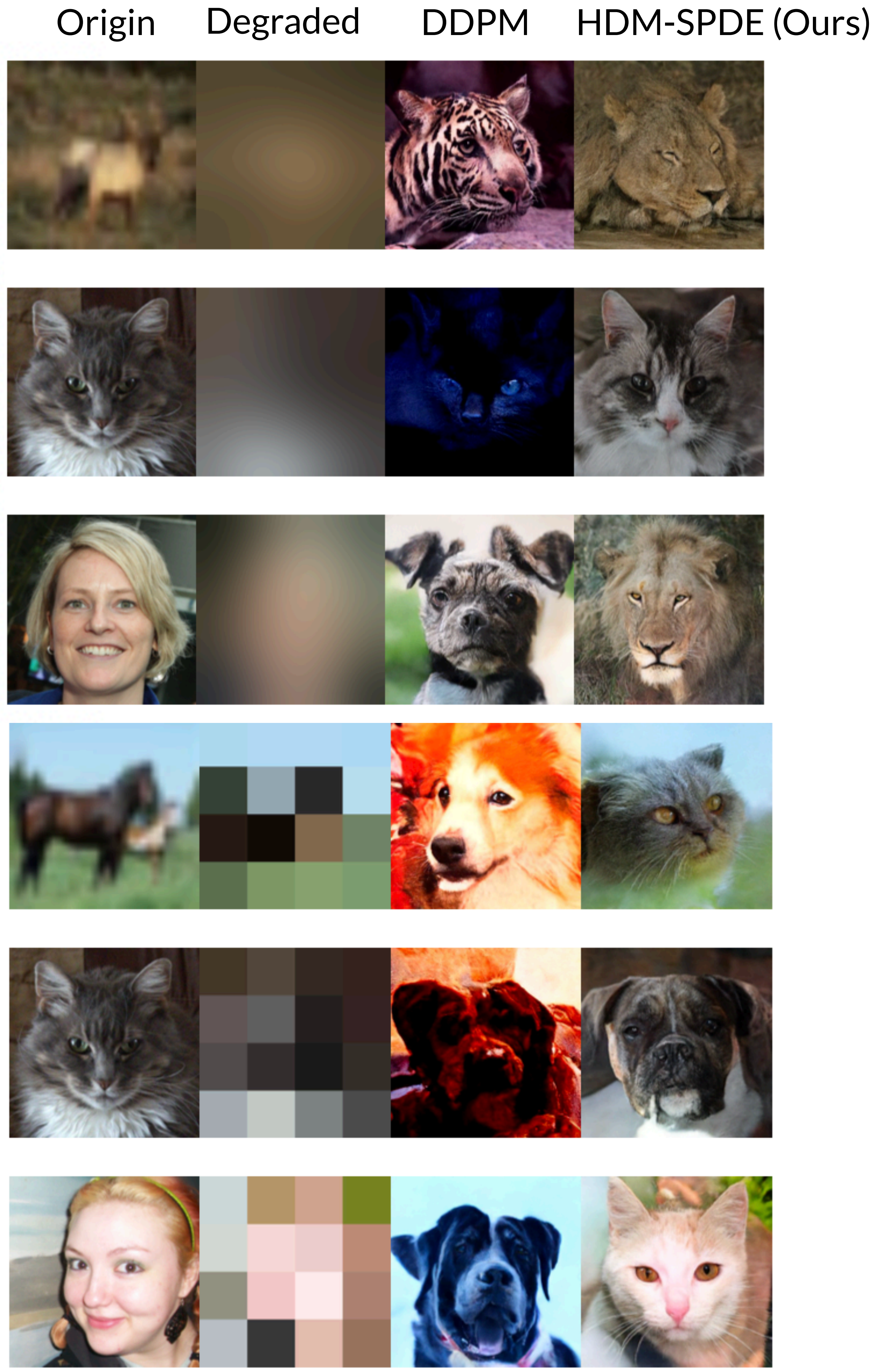


Gaussian Prior

[3] Generative Modelling with Inverse Heat Dissipation, Rissanen et al., ***ICLR*** (2023)

Experiment: Conditional Generation





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