Fractional Diffusion Bridge Models

Gabriel Nobis⋆, Maximilian Springenberg⋆,
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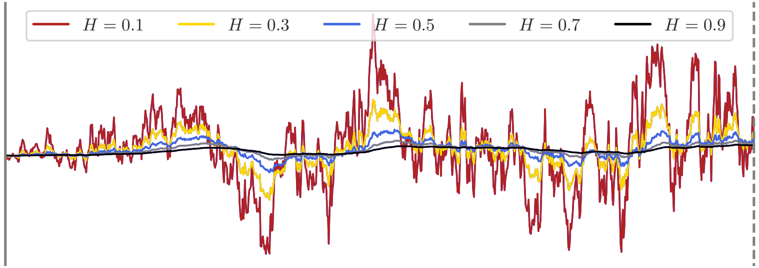
* Equal contribution; † Shared senior authorship

Generative Fractional Diffusion Models (NeurIPS 2024)

PAPER

$$X_0 \xrightarrow{\mathrm{d}X_t = \mu(t)X_t\mathrm{d}t + g(t)\mathrm{d}\hat{B}_t^H} X_T$$



$$X_0 \xleftarrow[\mathrm{d}\overline{Z}_t = \left[\overline{F}(t)\overline{Z}_t - \overline{G}(t)\overline{G}(t)^T\overline{p}_t(\overline{Z}_t)\right]\mathrm{d}t + \overline{G}(t)\mathrm{d}\overline{B}_t]{} X_T$$

CODE

We extend generative fractional diffusion models to diffusion bridges.

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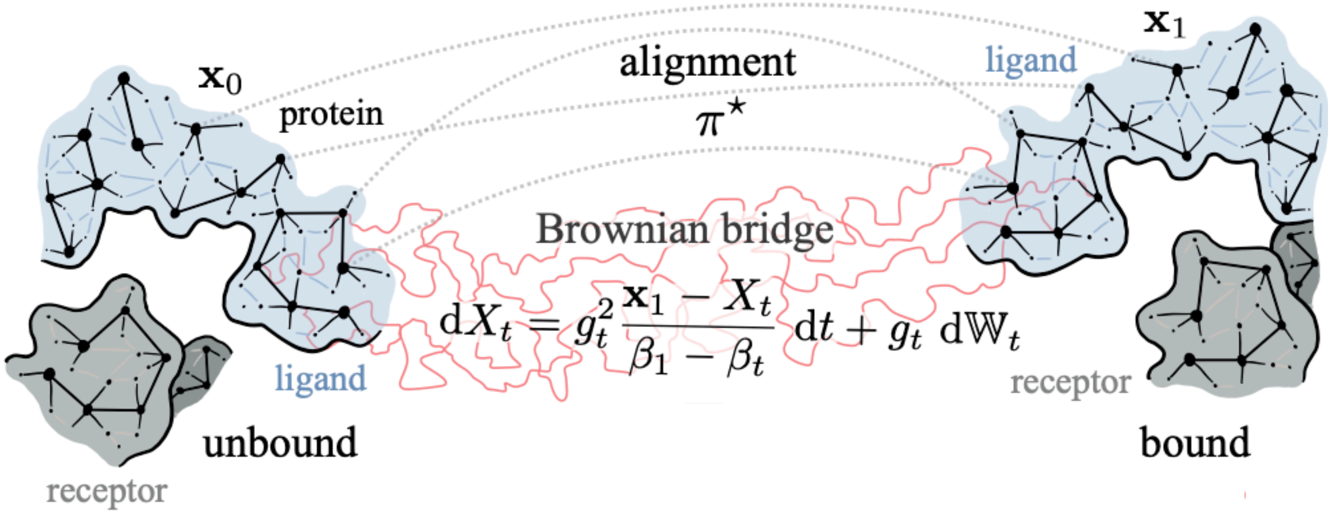
Figure from Somnath et al. (2023), Aligned Diffusion Schrödinger Bridges, UAI 2023 (MIT license).



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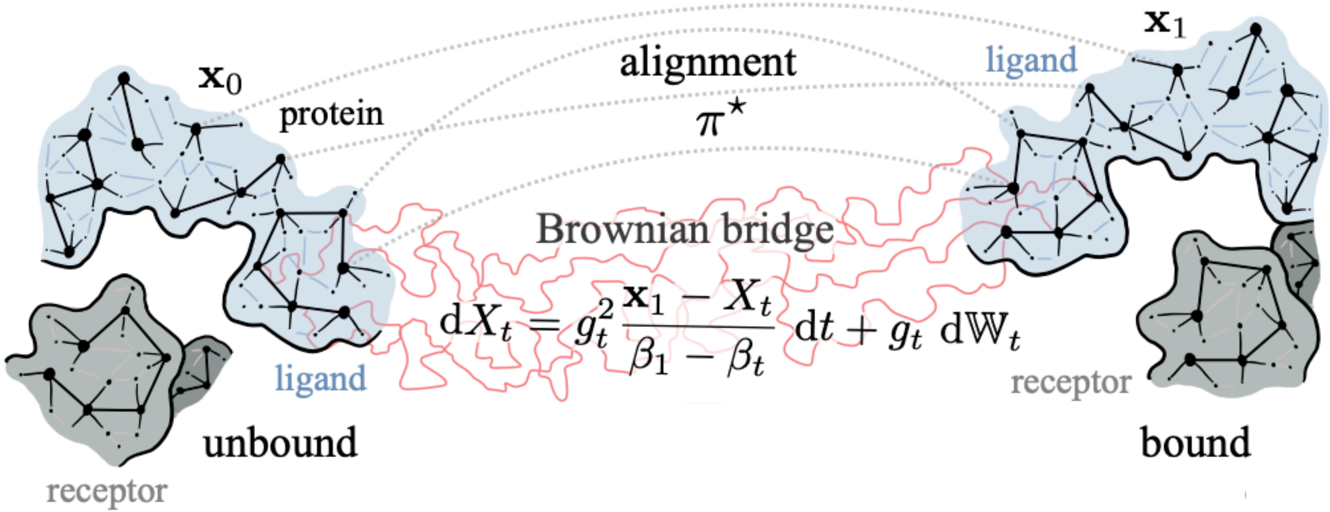

Can diffusion bridges be driven by fractional Brownian motion instead of Brownian motion?

Brownian motion (BM)

Brownian motion $B = (B_t)_{t\in[0,T]}$ is a centered Gaussian process with *independent increments*.

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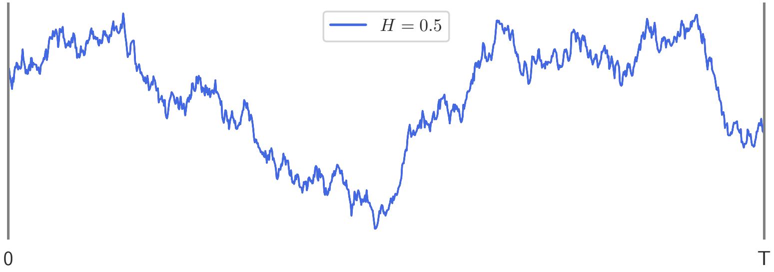
Fractional Brownian motion (fBM)



Fractional Brownian motion $B^H = (B_t^H)_{t\in[0,T]}$ with Hurst index $H \in (0,1)$ is a centered Gaussian process that posses *correlated increments* where we have for

$H = 0.5$: Brownian motion

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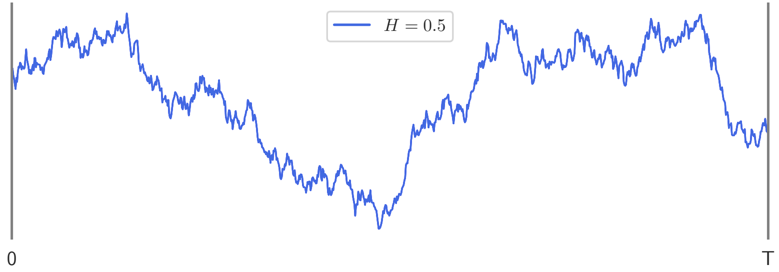

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$H > 0.5$: positively correlated increments

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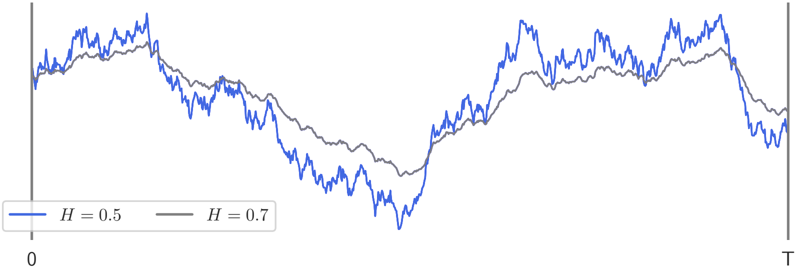

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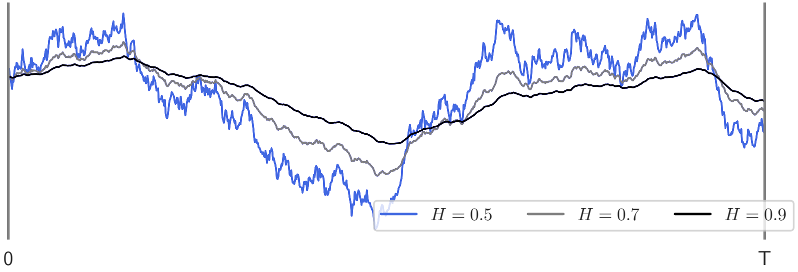

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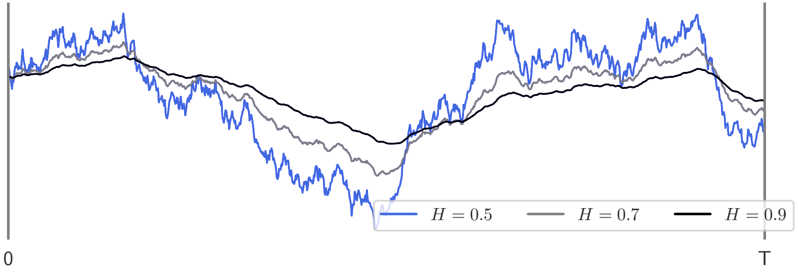

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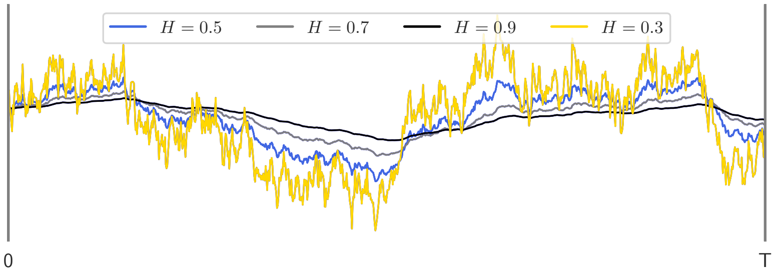

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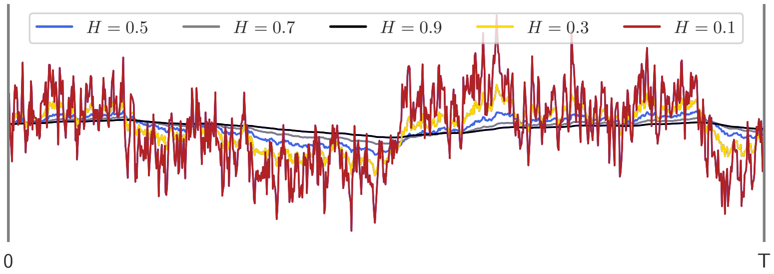

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Markovian approximation of fBM (MA-fBM)

Define for every $\gamma \in (0, \infty)$ the Ornstein-Uhlenbeck process Y^γ following

$$\mathrm{d}Y_t^\gamma = -\gamma Y_t^\gamma \mathrm{d}t + \mathrm{d}B_t, \quad Y_0^\gamma = 0.$$

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Given a Hurst index H and a geometrically spaced grid $\gamma_k = r^{k-n}$, define

$$B_t^H = \begin{cases} \int_0^\infty \left(Y_t^\gamma - Y_0^\gamma\right) \nu_1(\gamma) \mathrm{d}\gamma \\ -\int_0^\infty \partial_\gamma \left(Y_t^\gamma - Y_0^\gamma\right) \nu_2(\gamma) \mathrm{d}\gamma \end{cases}$$

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Markov-approximate fractional Brownian bridge (MA-fBB)

Let $X = \sqrt{\varepsilon}\hat{B}_t$ be the non-Markovian reference process and $Z = (X, Y^1 \ldots Y^K)$ the augmented reference process. We call the partially pinned process $Z_{|x_0,x_1} := Z|(X_0 = x_0, X_1 = x_1)$ a *Markov-approximate fractional Brownian bridge (MA-fBB)*.

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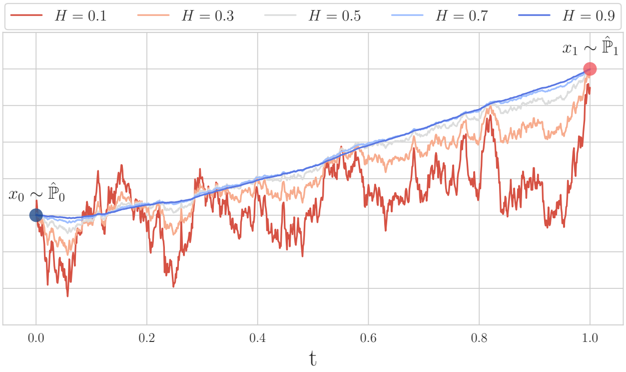

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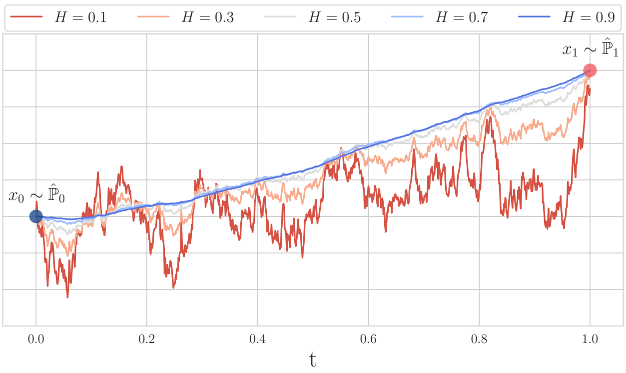

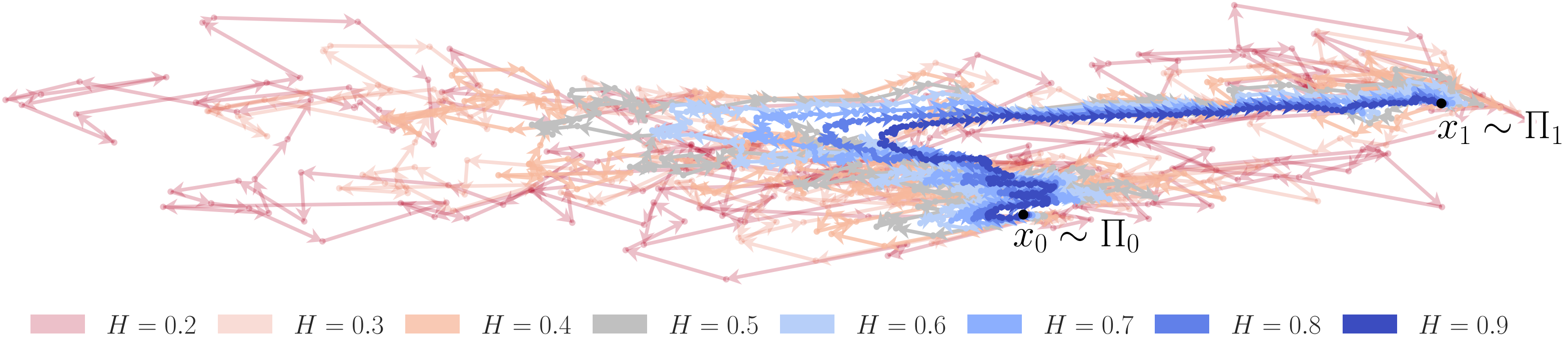

A coupling preserving stochastic bridge driven by MA-fBM

The goals of paired data translation:

A coupling preserving stochastic bridge driven by MA-fBM

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- Transform an unknown distribution Π_0 to another unknown distribution Π_1

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A coupling preserving stochastic bridge driven by MA-fBM

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- Transform an unknown distribution Π_0 to another unknown distribution Π_1
- Preserve the coupling $\Pi_{0,1}$ given in the paired training data

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Proposition: *Let $X = \sqrt{\varepsilon}\hat{B}^H$ be the non-Markovian with associated path measure $\mathbb{Q}$. We write $\mathbb{S}^1_{1|t}$ for the conditional distribution of $X_1|Z_t$. Assuming that $\mathbb{P} = \Pi_{0,1}\mathbb{Q}_{|0,1}$ is absolutely continuous with respect to $\mathbb{Q}$ we can lift the path measure $\mathbb{P}$ to a coupling preserving path measure $\mathbb{P}^\star$ on the augmented space and the SDE*

$$\mathrm{d}Z^\star_t = FZ^\star_t \mathrm{d}t + GG^T \mathbb{E}_{\mathbb{P}^\star_{1|0,t}}[\nabla_z \log \mathbb{Q}^H_{1|t}(X^\star_1|Z^\star_t)|Z^\star_0, Z^\star_t]\mathrm{d}t + G\mathrm{d}B_t,$$

with initial vector $Z^\star_0 = (X_0, 0 \ldots 0)$ admits a pathwise unique strong solution $Z^\star = (X^\star, Y^\star)$ with distribution $\mathbb{P}^\star$.

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$$\Rightarrow \mathrm{X}^\star_0 \sim \Pi_0,\ X^\star_1 \sim \Pi_1 \text{ and } (X^\star_0, X^\star_1) \sim \Pi_{0,1}$$

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Fractional Diffusion Bridge Models for paired data translation

We now define *Fractional Diffusion Bridge Models (FDBM)* for paired data translation as the stochastic process Z^θ associated with the path measure $\mathbb{P}^\theta$ solving

$$\mathrm{d}Z_t^\theta = FZ_t^\theta \mathrm{d}t + GG^T u^\theta(t, X_0, Z_t^\theta) + G\mathrm{d}B_t, \quad Z_0^\theta = (X_0, 0, \dots, 0),$$

$$u_i^\theta(t, x_0, z) = [1, \omega_1\zeta_1(t,1), \dots, \omega_K\zeta_K(t,1)]^T \tilde{u}_i^\theta(t, x_0, \mu_{1|t}(z)), \quad u^\theta = (u_1^\theta, \dots, u_d^\theta).$$

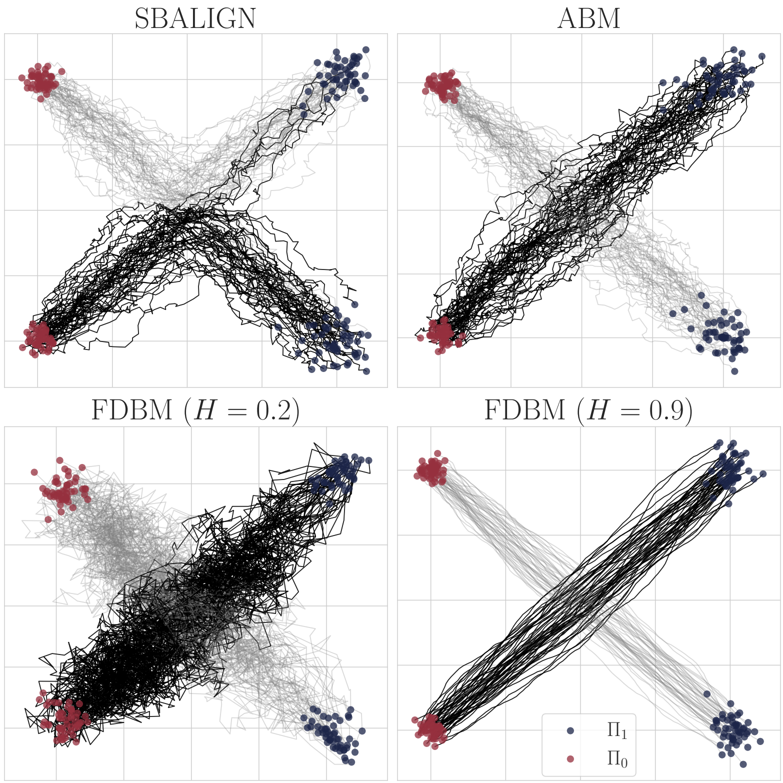
where $\tilde{u}^\theta = (\tilde{u}_1^\theta, \dots, \tilde{u}_d^\theta)$ is a time-dependent neural network-

Fractional Diffusion Bridge Models for paired data translation

To train FDBM for paired data translation, we derive the loss function as an upper bound to the KL-divergence $(\mathbb{P}^\star|\mathbb{P}^\theta)$:

$$\mathcal{L}_{\text{FDBM}}^{\text{paired}}(\theta) := \int_0^1 \mathbb{E}_{\mathbb{P}^\star}\left[\left\|\frac{X_1^\star - \mu_{1|t}(Z_t^\star)}{\sigma_{1|t}^2} - \tilde{u}^\theta(t, X_0, \mu_{1|t}(Z_t^\star))\right\|^2\right] \mathrm{d}t.$$

Fractional Diffusion Bridge Models are coupling preserving



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Predicting conformational changes in proteins

D3PM Test Set [1]	RMSD(Å) $\downarrow$			% RMSD(Å) $< \tau \uparrow$			Δ RMSD(Å) $\uparrow$		
	Median	Mean	Std	$\tau = 2$	$\tau = 5$	$\tau = 10$	Median	Mean	Std
EGNN* [1]	19.99	21.37	8.21	1%	1%	3%	-	-	-
SBALIGN$^\star_{(10,10)}$ [1]	3.80	4.98	3.95	0%	69%	93%	-	-	-
SBALIGN$^\star_{(100,100)}$ [1]	3.81	5.02	3.96	0%	70%	93%	-	-	-
SBALIGN* [2]	3.67	4.82	3.93	0%	71%	93%	1.30	1.92	2.59
Sesame* [2]	2.87	3.65	2.95	38%	82%	96%	2.15	3.11	4.26
ABM [3] (retrained)	2.40	3.49	3.54	43%	84%	96%	2.43	3.35	4.29
FDBM$(H = 0.3)$ **(ours)**	2.33	3.42	3.42	43%	85%	97%	**2.52**	**3.49**	4.39
FDBM$(H = 0.2)$ **(ours)**	**2.12**	**3.34**	3.59	**48%**	**86%**	96%	2.44	3.39	4.28
FDBM$(H = 0.1)$ **(ours)**	2.20	3.44	3.57	46%	83%	**97%**	2.47	3.45	4.29

FDBM produces on average in the rough regime the highest fraction of near-native structures.

The Schrödinger bridge problem

Given two unknown distributions Π_0 and Π_1 and the non-Markovian reference process $X = \sqrt{\epsilon}\hat{B}^H$ associated with the path measure $\mathbb{Q}$, we seek to find the solution to the dynamic Schrödinger bridge problem

$$\mathbb{T}^{SB} = \underset{\mathbb{T}\in\mathcal{P}(\mathcal{C}^d)}{\arg\min} \left\{ (\mathbb{T}|\mathbb{Q}) \ ; \ \mathbb{T}_0 = \Pi_0, \ \mathbb{T}_1 = \Pi_1 \right\}.$$

The Schrödinger bridge problem on the augmented space

Given the optimal coupling $\mathbb{T}_{0,1}^{SB}$ we can construct a coupling preserving path measure $\mathbb{P}^{\star}$. Based on the marginals of this path measre, we can define the Schrödinger bridge problem on the augmented space

$$\mathbb{V}^{SB} = \underset{\mathbb{T} \in \mathcal{P}(\mathcal{C}^d)}{\arg\min} \left\{ (\mathbb{V}|\mathbb{Q}) \ ; \ \mathbb{V}_0 = \mathbb{P}_0^{\star}, \ \mathbb{V}_1 = \mathbb{P}_1^{\star} \right\},$$

where $\mathbb{S}$ is the path measure associated with the augmented reference process $Z = (X, Y)$.

Augmented reciprocal class

Definition: We say that $\mathbb{V} \in \mathcal{P}(\mathcal{C}^{d\cdot(K+1)})$ is in the augmented reciprocal class $\mathcal{R}_a(\mathbb{S})$ of $\mathbb{S}$ if

$$\mathbb{V} = \int_{\mathbb{R}^d \times \mathbb{R}^d} \mathbb{S}_{|X_0,X_1}(\,\cdot\,|x_0, x_1)\mathrm{d}\mathbb{V}_{X_0,X_1}(x_0, x_1) =: \mathbb{V}_{X_1,X_0}\mathbb{S}_{|X_0,X_1}.$$

For any $\mathbb{V} \in \mathcal{P}(\mathcal{C}^{d\cdot(K+1)})$ we define the augmented reciprocal projection by

$$\mathrm{proj}_{\mathcal{R}_a(\mathbb{S})}(\mathbb{V}) := \mathbb{V}_{X_0,X_1|X_0,X_1}.$$

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Augmented Markovian projection

Definition: For $\mathbb{V} \in \mathcal{P}(\mathcal{C}^{d\cdot(K+1)})$ with $\mathbb{V} \in \mathcal{R}_a(\mathbb{S})$ we define the augmented Markovian projection $\mathrm{proj}_{\mathcal{M}_a}(\mathbb{V})$ by the path measure associated to $M = (M^1, M^2, \dots M^{K+1})$ solving for $M_0^1 \sim \mathbb{V}_{M_0^1}$

$$\mathrm{d}M_t = FM_t\mathrm{d}t + GG^T\mathbb{E}_{\mathbb{V}_{1|t}}\left[\nabla_{m_t}\log^1_{1|t}(M_1^1|M_t)|M_t\right]\mathrm{d}t + G\mathrm{d}B_t, \quad M_0 = (M_0^1, 0_K).$$

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Fractional Diffusion Bridge Models for unpaired data translation

We generalize Schrödinger bridge flow to a MA-fBM reference process

$$\hat{\mathbb{P}}^0 = (\Pi_0 \otimes \Pi_1)\mathbb{S}_{|X_0,X_1}, \quad \partial_s \hat{\mathbb{P}}^s = \mathrm{proj}_{\mathcal{R}_a(\mathbb{P})}(\mathrm{proj}_{\mathcal{M}_a(\mathbb{S})}(\hat{\mathbb{P}}^s)) - \hat{\mathbb{P}}^s, \quad \tilde{\mathbb{P}}^s = \mathrm{proj}_{\mathcal{M}_a(\mathbb{S})}(\hat{\mathbb{P}}^s),$$

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and propose the generalized loss function

$$\mathcal{L}^{\text{unpaired}}_{\text{FDBM}}(\theta, \tilde{\mathbb{P}}) = \int_0^1 \int_{(\mathbb{R}^{d\cdot(K+1)})} \int_{(\mathbb{R}^d)^2} \left\| \tilde{v}^\theta(t, \mu_{1|t}(z_t)) - \frac{x_1 - \mu_{1|t}(z)}{\sigma^2_{1|t}} \right\|^2 \mathrm{d}\tilde{\mathbb{P}}_{X_0,X_0}(x_0, x_1)\mathrm{d}\mathbb{S}_{t|X_0,X_1}(z_t|x_0, x_1)\mathrm{d}t.$$

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Limitations: *We do not claim convergence of the above heuristic algorithm!*

Unpaired image translation

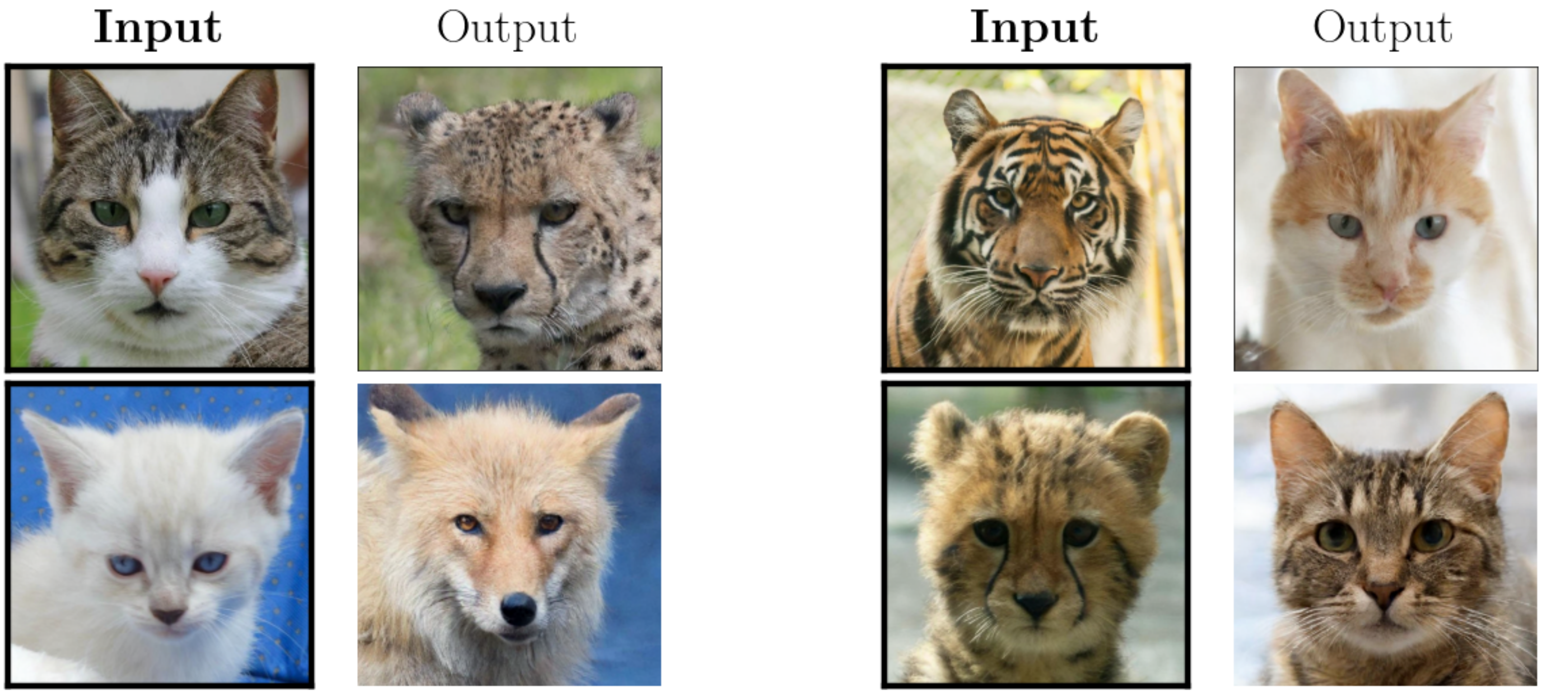
AFHQ-32 results with $H = 0.5$ and $K = 5$:

Method	Architecture	Pretraining				Online Finetuning			
		cats → wild		cats ← wild		cats → wild		cats ← wild	
		FID ↓	LPIPS ↓	FID ↓	LPIPS ↓	FID ↓	LPIPS ↓	FID ↓	LPIPS ↓
SBFlow	DiT-B/2	59.04 ±1.14	0.104 ±0.001	74.36 ±1.02	**0.151** ±0.001	43.85 ±0.48	0.083 ±0.001	64.77 ±0.78	0.107 ±0.000
SBFlow	DiT-L/2	50.68 ±0.72	0.106 ±0.001	71.77 ±0.77	0.152 ±0.001	33.92 ±0.59	0.091 ±0.000	54.10 ±0.72	0.098 ±0.001
FDBM (**ours**)	DiT-B/2	40.21 ±1.18	**0.097** ±0.001	**45.74** ±0.69	0.154 ±0.002	25.66 ±0.81	**0.073** ±0.001	28.33 ±0.35	**0.078** ±0.001
FDBM (**ours**)	DiT-L/2	**35.99** ±0.72	0.101 ±0.001	48.84 ±0.75	0.165 ±0.002	**20.26** ±0.59	0.079 ±0.001	**26.79** ±0.50	0.085 ±0.001

AFHQ-256 results with $H = 0.6$ and $K = 5$:

Method	Architecture	Pretraining				Online Finetuning			
		cats → wild		cats ← wild		cats → wild		cats ← wild	
		FID ↓	LPIPS ↓	FID ↓	LPIPS ↓	FID ↓	LPIPS ↓	FID ↓	LPIPS ↓
SBFlow	DiT-B/2	15.67 ±0.65	0.578 ±0.002	30.75 ±0.88	0.594 ±0.001	**17.50** ±0.87	**0.528** ±0.001	**25.86** ±0.32	**0.537** ±0.001
SBFlow	DiT-L/2	16.62 ±0.83	0.604 ±0.001	33.96 ±0.87	0.600 ±0.001	**16.98** ±0.53	0.560 ±0.001	27.82 ±0.41	0.547 ±0.001
FDBM (**ours**)	DiT-B/2	16.77 ±0.71	**0.530** ±0.002	**19.14** ±0.38	**0.551** ±0.001	–	–	–	–
FDBM (**ours**)	DiT-L/2	**11.62** ±0.73	0.548 ±0.002	**19.42** ±0.41	0.561 ±0.002	–	–	–	–

Unpaired image translation



AFHQ-512 cats $\leftrightarrow$ wild with $H = 0.4$ and $K = 5$.

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Fractional Diffusion Bridge Models

- We introduce a generative diffusion bridge framework driven by fractional noise
- We prove the existence of a coupling-preserving fractional diffusion bridge
- We formulate the Schrödinger bridge problem with a non-Markovian reference process and develop a heuristic to approximate its solution

Paper

Code paired

Code unpaired

Code SBFlow

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