# No Trick i, No Treat G

#### **Pursuits and Challenges Towards Simulation-free Training of Neural Samplers**

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# What are Diffusion Neural Samplers?

Learn an underlying process evolving  $p_{\text{prior}} \rightarrow \exp(-U)/Z$ :  $dX_t = f_t(X_t)dt + \sigma_t dW_t, X_0 \sim p_{\text{prior}}$ 

be time-reversal of a target process:

 $dX_t = f_t(X_t)dt + \sigma_t dW_t, X_1 \sim \exp(-U)/Z$ **Time-reversal sampler** 

 $\mathbb{P}$  map between interpolants from prior to  $\exp(-U)/Z$ .

**Escorted transport sampler** Matching the forward and backward process: KL, LV, TB, STB, DB, etc. Matching the forward with marginal interpolants:

#### Score matching, PINN, AM, etc.

### Sampling:



		Path measure alignment				Marginal alignment		
		KL	LV	(S)TB	DB	PINN	AM	Score Estimate
Time- reversal – sampler	<b>Reversal of</b>	DDS,	DDS-LV,			PINN		RDMC*,
	<b>VP/VE SDE</b>	DIS	DIS-LV					iDEM
	Reversal of PBM	PIS	PIS-LV	DGFS	DGFS			SFS*
Escorted transport sampler		CMCD	CMCD			PINN, NETS, LFIS	NETS	



# **Simulation-free Neural Samplers?**

Can we skip the expensive simulation in training? Y **Time-dependent normalizing flow** 

Same objective as DDS, and allows to jump to any time step to evaluate objective without simulation



t = 0.0 t = 0.8 t = 1.0 0.5 0.5 2.5 target 0.0 0.0 0.0 model -2.5 --0.5 -0.5 -2.5 0.0 2.5 0  $^{-1}$ 0

(a) Initialization of NF-DDS, samples generated at different time steps 0, 0.8, 1.0. As we can see, the initialization already covers all modes.

# **Trick Counts!**

(b) NF-DDS after training with Equation (13), samples generated at different time steps 0, 0.8, 1.0. Unlike DDS, NF-DDS fails to capture all modes.

Same objective as DDS, why mode collapse?

Langevin preconditioning:







mode interpolate, prior  $N(0, 30^2 I)$ mode interpolate, prior N(0, 2I)

# **Sample Efficiency Matters!**



# **Key Takeaways:**

Langevin Preconditioning is crucial for many approaches Target evaluation times are important yet not widely reported Efficiency of train-to-sample v.s. sample-to-train is worth exploring