Georgia Institute of Technology

Trivialized Momentum Facilitates Diffusion Generative Modeling on Lie Groups

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Introduction

Generative modeling of data on manifolds is an important task with wide applications in domains such as biology, robotics, physics, atmosphere, ocean sciences, etc. Diffusion models in flat spaces typically need **nontrivial adaptations** to succeed

In this work, inspired by recent progress in momentum-based optimization (Tao and Ohsawa, 2020) and sampling (Kong and Tao, 2024) on Lie groups, we develop a highly scalable and effective generative model for data on these manifolds, named **T**rivialized **D**iffusion **M**odel (TDM).

- Introduce **TDM**, using a **trivialization** technique to achieve a dramatically improved generation quality of Lie group data.
- Leverage a nontrivial **Operator Splitting Integrator** for accurate and efficient inference, further reducing generation errors.
- Achieve much better numerical results in benchmarks such as protein/RNA torsion angle generation. Present the first results on generating $\mathsf{U}(n)$ and $\mathsf{SO}(n)$ for $n > 3$.

Challenges of Manifold Diffusion Models

In Euclidean space, Diffusion models are

$$\begin{cases} \mathrm{d}X_t = -X_t\mathrm{d}t + \sqrt{2}\mathrm{d}W_t & \text{forward equation} \\ \mathrm{d}Y_t = Y_t + 2s(Y_t, T-t)\mathrm{d}t + \sqrt{2}\mathrm{d}B_t & \text{backward equation} \end{cases}$$

A naive extension to manifold G would lead to undesired consequences,

- Requirement of exact implementation of BM on the manifold $\to$ Need approximations!
- Score function $s(x,t) \approx \nabla \log p(x,t) \in T_xG \to$ Increased learning difficulty!
- Generative backward process is a manifold SDE $\to$ Hard to integrate!

Can we do better on manifolds with special structures?

Background on Lie Groups

What are Lie groups? A Lie group G is a **differentiable manifold** with an additional **group structure** (i.e., a way to define how two points multiply).

- Special Orthogonal Group $\mathsf{SO}(n) = \{R \in \mathbb{R}^{n\times n} \mid R^\top R = RR^\top = I, \det R = 1\}$
- Unitary Group $\mathsf{SU}(n) = \{U \in \mathbb{C}^{n\times n} \mid U^H U = UU^H = I\}$
- Special Euclidean Group $\mathsf{SE}(n) = \mathbb{R}^n \rtimes \mathsf{SO}(n)$

Prominent applications include.

- **Protein backbones** represented by relative orientations between rigid functioning groups (roughly speaking) $\to$ **Special Euclidean group** $\mathsf{SE}(3)$
- **Quantum Circuits** basic operations on qubits $\to$ **Unitary group** $\mathsf{U}(N)$
- ...

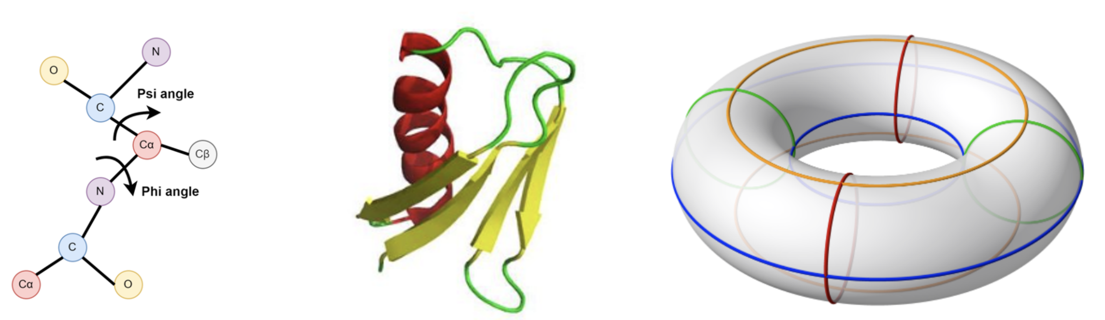
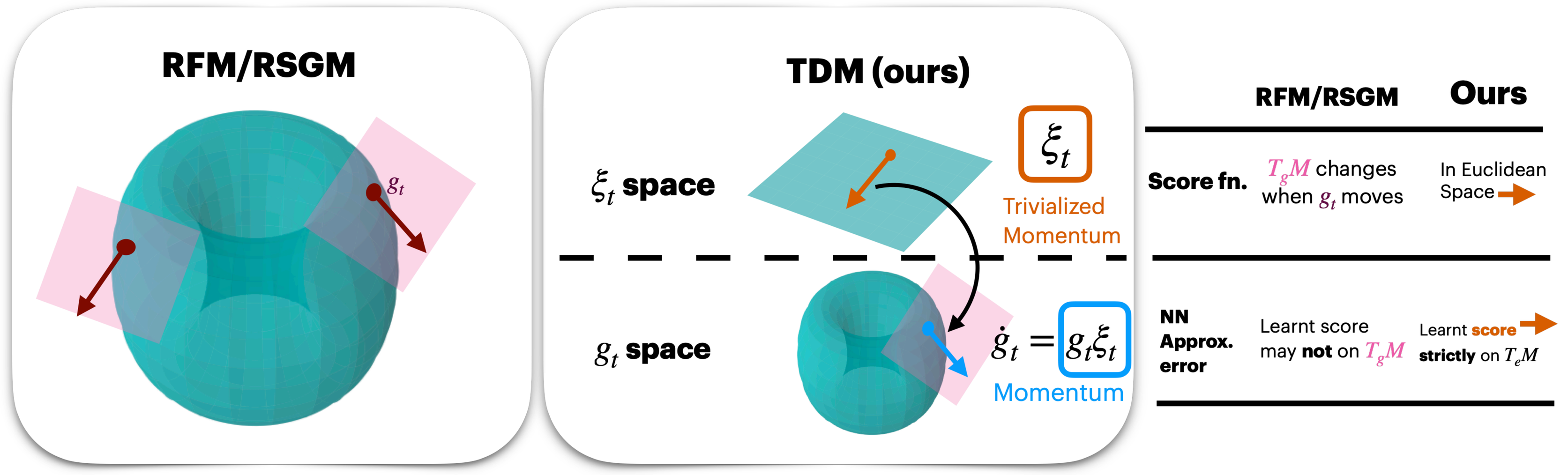


Figure 1. Left: Torsion angles. **Middle:** Protein backbone structures. **Right:** visualization of 2D Torus



Trivialized Diffusion Model

Kong and Tao (2024) shows that $(*)$ converges to the Gibbs distribution $Z^{-1}e^{-(U(g)+\|\xi\|^2)}dgd\xi$

$$\dot g = g\xi, \quad \mathrm{d}\xi = -\gamma\xi\mathrm{d}t - T_g\mathsf{L}_{g^{-1}}(\nabla U(g))\mathrm{d}t + \sqrt{2\gamma}\mathrm{d}W^{\mathfrak{g}} \qquad (*)$$

where $g(t) \in G$. This serves as Forward dynamics of TDM.
This mimics the kinetic Langevin on Euclidean space,

$$\dot q = p, \quad \mathrm{d}p = -\gamma p\mathrm{d}t - \nabla U(q)\mathrm{d}t + \sqrt{2\gamma}\mathrm{d}W$$

Except for the key differences: use of trivialization technique!

- instead of usual momentum variable $\dot g = p$, leveraging the group structure, use **trivialized momentum** $\xi = g^{-1}\dot g \Leftrightarrow$ angular momentum instead of linear momentum!
- linear momentum $\dot g \in G_{g_t}G \leftrightarrow$ A changing space dependent on g_t
- trivialized momentum $\xi \in \mathfrak{g} = T_eG \leftrightarrow$ **A fixed space!**

Moreover, $T_eG \cong \mathbb{R}^d \to \xi$ is Euclidean at any time $\to$ only require **Euclidean BM noise!**

Relevance to Diffusion Model?

- g is the **data variable** $\leftarrow$ manifold valued
- ξ is ab **auxiliary variable** $\leftarrow$ Euclidean valued, introduced for **algorithmic benefit**

Picking $U(g) = 0$ gives a forward noising dynamic,

$$\dot g_f = g_f\xi_f, \quad \mathrm{d}\xi_f = -\gamma\xi_f\mathrm{d}t + \sqrt{2\gamma}\mathrm{d}W^{\mathfrak{g}} \qquad \text{(F)}$$

(F) converges to $\mathcal{U} \times \mathcal{N}$ exponentially fast $\leftarrow \mathcal{U}$ on G implementable with random linear algebra, $\mathcal{N}(0, I)$ simple since $\mathfrak{g} \cong \mathbb{R}^d$

We shown that (F) indeed has a time reversal that serves as the backward dynamic (B)

$$\dot g_b = -g_b\xi_b, \quad \mathrm{d}\xi_b = \gamma\xi_b\mathrm{d}t + 2\gamma s(g_b, \xi_b, T-t)\mathrm{d}t + \sqrt{2\gamma}\mathrm{d}B^{\mathfrak{g}} \quad \text{(B)}$$

which satisfies $(g_b(t), \xi_b(t)) \overset{d}{=} (g_f(T-t), \xi_f(T-t))$

Only requires $s(g, \xi, t) = \nabla_\xi \log p(g, \xi, t) \leftarrow$ **Euclidean derivative, simple and familiar!**

How to do efficient inference of TDM? Operator-Splitting Integrator!

$$A_g : \begin{cases} \dot g_b = -g_b\xi_b \\ \mathrm{d}\xi_b = 0 \end{cases} + A_\xi : \begin{cases} \dot g_b = 0 \\ \mathrm{d}\xi_b = \gamma\xi_b + 2\gamma s_\theta(g_b, \xi_b, T-t)\mathrm{d}t + \sqrt{2\gamma}\mathrm{d}B^{\mathfrak{g}} \end{cases}$$

Iteratively integrate A_g and A_ξ gives a manifold-preserving, accurate numerical scheme.

$$\begin{cases} \xi_n = \exp(\gamma h)\xi_{n-1} + 2(\exp(\gamma h) - 1)s_{n-1} + \epsilon_{n-1} \\ g_n = g_{n-1}\,\mathrm{expm}(-h\xi_n) \end{cases}$$

Numerical Results

Checkerboard pattern: data distribution corresponds to $\mathbb{T}$-valued uniform distribution on the periodic, checkerboard-like region

Pacman maze: data distribution corresponds to $\mathbb{T}$-valued uniform distribution on the blue pixels (the wall in the classic Pacman game map).

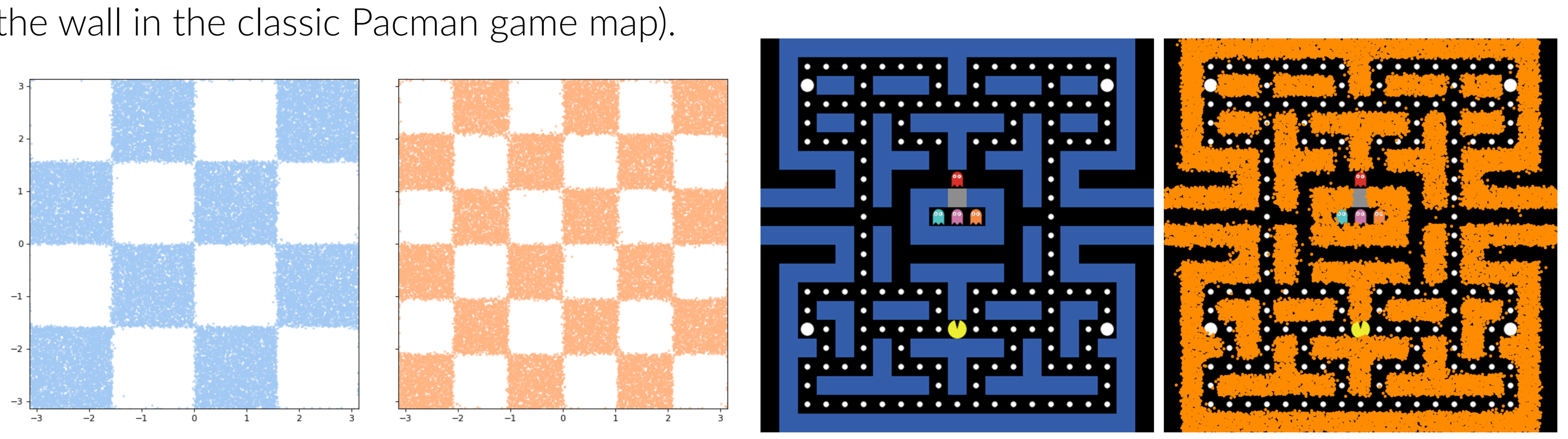
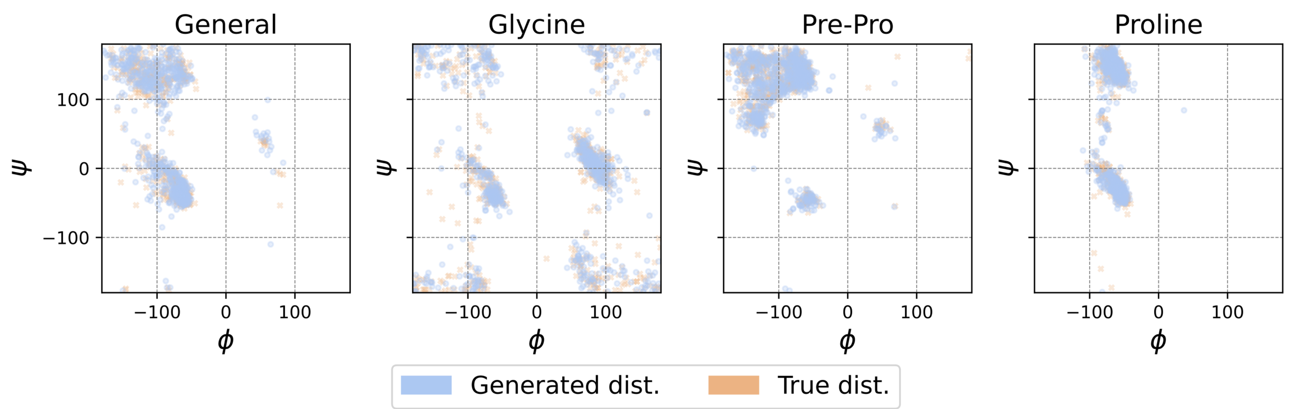


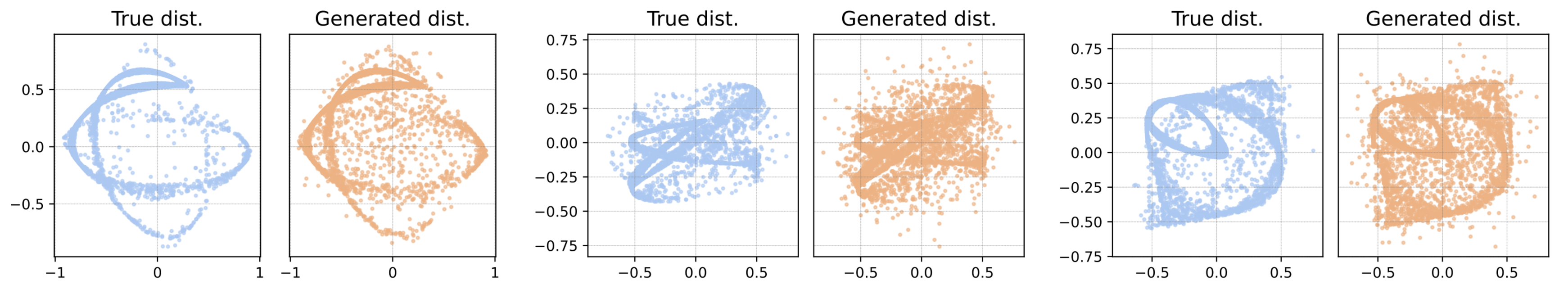
Figure 2. **Left:** Generated checkerboard pattern of different resolutions. **Right:** Learnt Pacman maze distribution

Torison angles in RNA and Proteins The data distribution corresponds to macro-molecules represented by torsion angles ($\mathbb{T}^k$-valued), which are 2D or 7D, compiled in Huang et al. (2022). Evaluated through NLL and visualization.

Model	General (2D)	Glycine (2D)	Proline (2D)	Pre-Pro (2D)	RNA (7D)
Dataset size	138208	13283	7634	6910	9478
RDM	1.04 ± 0.012	1.97 ± 0.012	0.12 ± 0.011	1.24 ± 0.004	-3.70 ± 0.592
RFM	1.01 ± 0.025	1.90 ± 0.055	0.15 ± 0.027	1.18 ± 0.055	-5.20 ± 0.067
TDM	$\mathbf{0.69 \pm 0.14}$	$\mathbf{1.04 \pm 0.27}$	$\mathbf{-0.60 \pm 0.15}$	$\mathbf{0.52 \pm 0.10}$	$\mathbf{-6.86 \pm 0.46}$



Evolution Operators of Quantum Systems The data distribution corresponds to $\mathsf{U}(N)$-valued time-evolution operators of form $e^{it\mathcal{H}}$, where $\mathcal{H}$ is the Hamiltonian for quantum oscillators, $\mathcal{H} = \Delta_h - V_h$, Δ_h is the discretized Laplacian and $V_h(x) = \frac{1}{2}\omega^2|x - x_0|^2$ is a random potential function. Newly compiled in (Zhu et al., 2024).



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