

Linear Transformer Topological Masking with Graph Random Features

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Abstract

Concise and self-contained description of your project, motivation and main findings.

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1 Introduction

Transformers have established themselves as a dominant architecture across various machine learning modalities, deriving their power from the attention mechanism which models complex dependencies between tokens [1]. However, the standard Transformer treats input data as a set, making it invariant to permutation and inherently unaware of structural dependencies, such as the connectivity in graph-structured data. To address this, *Topological Masking* is often employed, where the attention mechanism is modulated by a function of the graph structure (e.g., shortest path distance or adjacency), injecting a necessary structural inductive bias [2, 3].

A fundamental computational conflict arises when scaling this approach to large graphs. Standard “Vanilla” Softmax attention requires explicitly computing and storing an $N \times N$ attention matrix, resulting in quadratic $\mathcal{O}(N^2)$ time and space complexity. While Linear Attention mechanisms address this bottleneck by leveraging low-rank decompositions $\phi(Q)(\phi(K)^T V)$ to achieve $\mathcal{O}(N)$ complexity [4], they rely strictly on the associativity of matrix multiplication. Introducing a topological mask M generally breaks this associativity—since $(A \times B) \odot M \neq A \times (B \odot M)$ —forcing the re-materialization of the dense attention matrix and negating the efficiency gains of linear attention.

In this work, we focus on the reproduction of “Linear Transformer Topological Masking with Graph Random Features” [5]. The authors propose a novel solution to the masking conflict by approximating the topological mask using Graph Random Features (GRFs). By decomposing the mask into sparse feature vectors derived from random walks, the method allows the mask to be fused with query and key features via a tensor product, preserving the $\mathcal{O}(N)$ complexity of linear attention while maintaining the expressivity of topological masking.

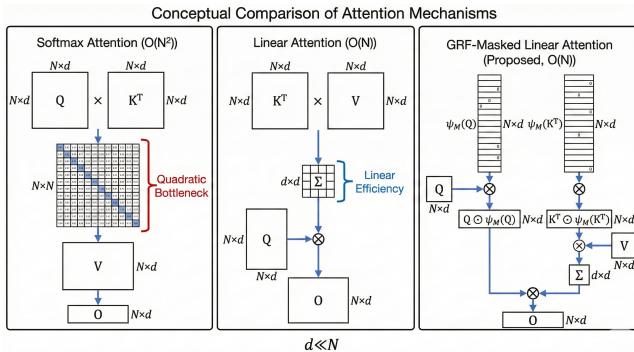


Figure 1. Conceptual comparison of attention mechanisms. The left panel illustrates the quadratic bottleneck of Softmax attention. The middle panel shows the efficient flow of Linear attention. The right panel demonstrates the proposed GRF method, which preserves linear complexity by fusing sparse topological features ψ_M with the query/key representations.

Contributions and Replication Results Our primary contribution is a validation of the theoretical and empirical claims presented in the original paper. We

successfully implemented the proposed GRF-based masking mechanism and conducted a rigorous analysis of its computational scaling behavior.

- **Time Complexity Verification:** We replicated the scaling experiment comparing Softmax, Linear, and GRF-Masked attention. Our results confirm the theoretical claims: while Softmax attention scales quadratically, exhibiting a “computational explosion” for $N > 8$, the GRF-Masked method maintains strict linear scaling $\mathcal{O}(N)$.
- **Overhead Analysis:** We quantified the overhead introduced by the GRF mechanism. While retaining the linear complexity class, we observe a constant factor increase in FLOPs compared to unmasked linear attention, attributable to the sparsity of the generated graph features.

!!!TO DO: ADD THE OTHER TWO EXPERIMENTS RESULTS OVERVIEW!!!

2 Related works

Standard and Topological Attention The standard self-attention mechanism, introduced by [1], computes a dense $N \times N$ attention matrix $A = \text{softmax}(QK^T / \sqrt{d})$. While highly effective at modeling global dependencies, this approach incurs quadratic $\mathcal{O}(N^2)$ time and space complexity, prohibiting its use on long sequences or large graphs. To adapt Transformers to graph-structured data, *topological masking* is often employed to inject structural inductive bias [2]. This typically involves modulating the attention scores with a mask $M(\mathcal{G})$ derived from the graph topology (e.g., shortest path distances), forcing tokens to attend preferentially to their structural neighbors. However, applying such masks generally requires materializing the full $N \times N$ matrix, maintaining the prohibitive quadratic bottleneck.

Linear Attention and The Masking Conflict To address the scalability limits of standard attention, *Linear Attention* mechanisms have been proposed [4, 6]. These methods replace the softmax kernel with a feature map decomposition $\phi(\cdot)$, allowing the computation to be reordered via associativity: $D^{-1}\phi(Q)(\phi(K)^T V)$. This reduces complexity to $\mathcal{O}(N)$. However, as noted in the foundational literature, introducing an element-wise topological mask M breaks this associativity, i.e., $(A \times B) \odot M \neq A \times (B \odot M)$. Consequently, standard linear attention methods are generally incompatible with flexible topological masking without reverting to quadratic complexity.

Efficient Masking Approaches Several approaches have attempted to reconcile efficiency with masking, though often with restrictions on graph topology. [7] and [3] proposed using Toeplitz matrices and the Fast Fourier Transform (FFT) to implement masking in $\mathcal{O}(N \log N)$ time. While an improvement over $\mathcal{O}(N^2)$, these methods are largely restricted to highly structured graphs like grids or trees and do not generalize easily to arbitrary

topologies. Other methods, such as stochastic positional encoding [8], achieve linear complexity but are similarly limited to sequence data (1D grids). The method reproduced in this work [5] distinguishes itself by supporting general graphs with strict $\mathcal{O}(N)$ complexity via a randomized low-rank decomposition of the mask itself.

3 Methodology

3.1 Time Complexity

To validate the theoretical efficiency claims of the proposed architecture, the paper conducts a hardware-agnostic analysis of computational cost. Instead of measuring wall-clock time, which can be conflated by hardware specifics (GPU/CPU differences) and implementation overhead, the methodology focuses on counting the total number of Floating Point Operations (FLOPs) required for a single forward pass of the attention mechanism.

The analysis compares three distinct attention variants across a range of graph sizes (N):

- **Unmasked Softmax Attention:** The standard $\mathcal{O}(N^2)$ mechanism, where the full $N \times N$ attention matrix is materialized.
- **Unmasked Linear Attention:** An $\mathcal{O}(N)$ efficient alternative that utilizes a low-rank decomposition $\phi(Q)(\phi(K)^T V)$.
- **GRF-Masked Linear Attention (Ours):** The proposed method, which approximates the topological mask using Graph Random Features. While theoretically $\mathcal{O}(N)$, this method involves constructing sparse feature matrices, introducing a constant overhead dependent on the graph sparsity and number of random walkers.

The theoretical FLOP counts are derived based on the matrix dimensions involved. For a hidden dimension d and feature dimension m :

- **Softmax Attention (Baseline):** Dominated by the N^2 term from QK^\top and AV product, roughly scaling as $\mathcal{O}(4N^2d)$.
- **Linear Attention (Unmasked):** Linear in N , scaling as $\mathcal{O}(4Nmd)$ due to the associativity of matrix multiplication.
- **GRF-Masked Linear Attention (Ours):** Also linear in N , but the exact cost depends on the number of non-zero entries (NNZ) in the sparse graph random feature vectors. The complexity scales as $\mathcal{O}(4 \cdot \text{NNZ} \cdot d)$.

The experiment uses a 1-dimensional grid graph (a linear chain) to test scaling behavior. This topology allows for controlled testing of "local" attention, as the number of neighbors remains constant as N increases.

3.2 ViTs: Vision Transformer Tasks (Graph + Image Integration) & Ablation Studies

To evaluate the effectiveness of the proposed topological masking in a domain with fixed, regular structure, the original paper [5] applies GRFs to the Vision Transformer (ViT) architecture. In this framework, the input image is decomposed into patches, and the underlying topology \mathcal{G} is defined as a 2D grid graph where nodes (patches) are connected if they are spatial neighbors.

The central methodological contribution is the modulation of the Linear Attention mechanism by a learnable mask $M_\alpha(\mathcal{G}) := \sum \alpha_k W^k$. This introduces a structural inductive bias into the transformer, which theoretically allows it to capture local dependencies more effectively than unmasked attention, while avoiding the quadratic costs of Softmax attention [5]. To validate this, the work compares five distinct attention mechanisms:

- **Unmasked Softmax ($\mathcal{O}(N^2)$):** The standard baseline used in "vanilla" Transformers.
- **Unmasked linear ($\mathcal{O}(N)$):** An efficient alternative using decompositions with feature maps $\phi(Q)(\phi(K)^\top V)$, which lacks any topological awareness [4].
- **Toeplitz-masked linear ($\mathcal{O}(NLogN)$):** A strong baseline for grid graphs (images), where the mask decays based on the Manhattan distance between nodes (patches). This represents a "hard-coded" structural bias [3].
- **$M_\alpha(\mathcal{G})$ -masked linear ($\mathcal{O}(N^2)$):** The theoretical limit of the proposed method, where the full-rank mask matrix M_α is explicitly computed.
- **GRF-masked linear ($\mathcal{O}(N)$):** The proposed method, which approximates the exact mask implicitly using sparse features generated by importance sampling of random walks.

Ablation Studies: To evaluate the approximation quality of the GRF estimator in depth, the original paper [5] includes an ablation study on the number of random walks n . The theoretical premise is that increasing n reduces the variance of the mask estimator \hat{M} and thereby improves the approximation of the actual topological mask M_α . In this study, n is varied logarithmically to verify whether the performance converges to the $M_\alpha(\mathcal{G})$ -masked linear baseline, isolating the trade-off between accuracy (estimator variance) and computational cost (feature sparsity).

3.3 PCTS: Point Cloud Temporal State prediction

In the domain of robotics and physical dynamics, the paper applies topological masking to the task of High-Density Visual Particle Dynamics (HD-VPD). The objective is to predict the future state of a point cloud P_{t+1} given the current state P_t , modeling the physical interactions of a robotic system.

To replicate this experiment, we adopt the **Interlacer** architecture described in [5]. This architecture alternates between Global Layers (standard linear attention capturing long-range dependencies) and Local Layers (capturing fine-grained geometric structure). We investigate three variations of the Local Layer to validate the efficacy of Graph Random Features:

- **Baseline (Unmasked PCT):** The local layer is replaced by an identity mapping or standard global attention. This model treats the point cloud as a set, ignoring the explicit topology, effectively relying solely on global context.
- **MP Interlacer (Message Passing):** This represents the standard GNN approach. The local layer explicitly aggregates features from the k -nearest neighbors. While accurate for rigid structures, it is computationally expensive and limited to immediate neighborhoods.
- **GRF Interlacer (Ours/Reproduced):** The local layer utilizes Graph Random Features. By sampling random walks on the k -NN graph, this method approximates a topological mask that allows information to diffuse beyond immediate neighbors (multi-hop) in $\mathcal{O}(N)$ time, injecting a structural inductive bias that favors physically connected paths.

Crucially, to prevent the model from learning a trivial identity function (where $P_{t+1} \approx P_t$), we employ an **autoregressive training strategy**. Instead of calculating the loss solely on the next step prediction (Teacher Forcing), we perform multi-step rollouts during training. The model predicts \hat{P}_{t+1} , which is then fed back as input to predict \hat{P}_{t+2} , and so on. The loss is computed as the average Mean Squared Error (MSE) across all rollout steps against the ground truth sequence, forcing the model to learn trajectory stability and error correction.

4 Implementation

4.1 Time Complexity

To verify the scalability claims, we implemented a standalone Python simulation to replicate Figure 3 from the original paper[5]. We did not rely on the authors' training code for this experiment; instead, we wrote a custom script to calculate theoretical FLOP counts and simulate the random walk sparsity exactly as described in the methodology.

Datasets: For this specific experiment, synthetic data was used. We procedurally generated 1-dimensional grid graphs (linear chains) with the number of nodes N ranging from 2^0 (1 node) to 2^{12} (4096 nodes). This covers the range from trivial graphs to those large enough to demonstrate the divergence between quadratic and linear scaling.

Hyperparameters: We adhered strictly to the hyperparameters reported in the paper to ensure an exact replication:

- Hidden Dimension (d): 8
- Feature Dimension (m): 8
- Number of Random Walkers (n): 4 per node
- Walk terminal probability (p_{halt}): 0.5

These small dimensions ($d = m = 8$) were likely chosen by the authors to isolate the scaling behavior (N) from the overhead of large feature vectors.

Experimental setup: The experiment was implemented in a Python script (`time_complexity_exp.py`) using NumPy.

- **Deterministic Counting:** For Softmax and Standard Linear attention, FLOPs were calculated using the direct analytical formulas ($4N^2d$ and $4Nmd$ respectively).
- **Stochastic Simulation:** For the GRF-Masked variant, the cost depends on the sparsity of the generated features. To measure this, we implemented a `simulate_unique_visits` function. This function simulates $n = 4$ random walkers starting from every node in the 1D grid. It tracks the set of unique nodes visited by the ensemble of walkers to determine the number of non-zero entries (NNZ) that would exist in the sparse feature matrix.
- **Variance Handling:** Because the random walks are stochastic, we averaged the unique visit counts over 10 independent trials for each graph size N .

Computational requirements: Since this experiment calculates theoretical operations rather than training a neural network, the computational cost was negligible. The simulation runs in seconds on a standard consumer CPU (e.g., Apple Silicon M1 or Intel i7) and requires minimal RAM (<1GB). No GPU resources were required for this specific validation step.

4.2 ViTs: Vision Transformer Tasks (Graph + Image Integration) & Ablation Studies

To reproduce the comparative performance and ablation experiments, we developed a custom implementation of the Vision Transformer pipeline in PyTorch. The authors' original code was not available, thus we implemented the five attention variants (Softmax, Linear, Toeplitz, Exact M_α and GRF) from scratch to verify the algorithmic description provided in the paper [5]. While the original work utilized large-scale datasets like *ImageNet*, *iNaturalist*, *Places365*, we adapted the experimental setup to accessible, lower-resolution benchmarks to verify the algorithmic properties within a constrained computational budget.

Datasets: We evaluated the method on three standard image classification datasets:

- **CIFAR-10:** Consisting of 60,000, 32×32 color images in 10 classes.
- **CIFAR-100:** Similar to CIFAR-10 but with 100 classes.
- **FashionMNIST:** Consisting of 60,000 28×28 grayscale images in 10 classes.

All the datasets are available via the `torchvision.datasets` module.

Hyperparameters: TODO Due to computational restraints, we scaled down the architecture significantly compared to the ViT-B/16 [9] used in the original paper[5]. Hyperparameters (Table 1) were chosen to accommodate the smaller model capacity required for these datasets while maintaining the relative structure of the original experiments.

Hyperparameter	CIFAR-10 (15 ep)	CIFAR-100 (30 ep)	CIFAR-10 (30 ep)	FashionMNIST (10 ep)	CIFAR-10 (Scaled)
Num. layers	2	2	2	2	4
Num. heads	4	4	4	4	4
Num. patches	8×8	8×8	8×8	8×8	10×10
Image Size	32×32	32×32	32×32	32×32	42×42
Hidden size	64	64	64	64	64
MLP dim.	128	128	128	128	128
Optimiser	Adam	Adam	Adam	Adam	Adam
Epochs	15	30	30	10	15
Learning rate	1×10^{-3}	1×10^{-3}	1×10^{-3}	1×10^{-3}	1×10^{-3}
Batch size	128	128	128	128	64
$\phi(\cdot)$	ReLU	ReLU	ReLU	ReLU	ReLU
Num. walks (n)	50	50	50	50	100
p_{halt}	0.1	0.1	0.1	0.1	0.1

Table 1. Architecture and training hyperparameters for all experimental runs.

Ablation Studies: For the ablation study, we varied $n \in \{1, 10, 100, 1000\}$ and set $p_{halt} = 0.5$ to strictly replicate the convergence setup described in the original appendix[5].

Experimental Setup: The experiments were conducted on single GPUs (*Nvidia T4, P100*) environments (*CUDA-enabled*). The pipeline involved training five distinct model variants (Softmax, Toeplitz, M_α , GRF, Unmasked Linear) from scratch for each dataset. We utilized a custom **GRFExactAttention** module that pre-computes random walks on a **NetworkX** grid graph and registers them as buffers in the PyTorch model.

Computational Requirements: Due to the downscaled input resolution (32×32) and shallow architecture (2-4 layers), the computational load was lightweight respect to the original ViT experiments.

- **Training Time:** approximately 17 seconds per epoch on the GPU used.
- **Memory Usage:** The models fit comfortably within standard GPU memory constraints (< 4GB).
- **Pre-computation:** The generation of random walks for the 8×8 patch grid was instantaneous and performed once at initialization.

4.3 PCTS: Point Cloud Temporal State prediction

Simulation and Data Generation.

While the original paper utilizes a real-world setup with RGB-D cameras and depth sensors to capture 32k particles, such hardware was unavailable for this reproduction. Consequently, we developed a lightweight, physics-based 3D simulation using React and Three.js. The simulation models a robotic arm with a kinematic chain consisting of a base, two rigid links, and a gripper. We sample N points uniformly from the surface of the arm meshes at each frame. To generate the dataset, we recorded the arm performing sinusoidal movements of varying frequencies on its joints. A critical implementation detail was the **sampling rate**. Initial experiments with high frame rates (e.g., 60 FPS) resulted in negligible displacement between frames ($P_{t+1} \approx P_t$), allowing the Baseline model to achieve near-zero loss by simply copying the input. We adjusted the recording interval to 0.1s - 0.5s, creating significant displacements that necessitate learning the underlying physics.

Modular Architecture.

We implemented a modular PyTorch architecture for the Interlacer. The model accepts a configuration flag to switch between Baseline (Linear Attention), MP (Simple Message Passing on K-NN), and GRF (Topological Masking with Random Walks). For the GRF implementation, we compute the sparse mask approximation dynamically. Since the robot moves, the graph topology changes at every frame; therefore, we recompute the k -NN graph ($k = 4$ to 6) and sample random walks (hops=3 to 5) on the fly during both training and inference.

Evaluation Metric.

The original paper evaluates performance using SSIM (Structural Similarity Index Measure) on rendered images. Implementing a differentiable neural renderer was beyond the scope of this project. Therefore, we introduced a geometric proxy metric: **ACCURACY_THRESHOLD**. We define a prediction as "accurate" if the Euclidean distance between a predicted point and its ground truth counterpart is below a strict threshold (e.g., 0.1 units). This allows us to quantify how long the model can maintain the structural integrity of the robot before the simulation diverges ("explodes"). **Computational Setup.** We trained the models on sequences of around 500 frames, testing point counts $N \in \{512, 1024, 2048, 4096\}$. We utilized a standard GPU environment (Colab T4). It is important to note that the theoretical $\mathcal{O}(N)$ advantage of GRF over the Baseline becomes strictly necessary at the scale of the original paper ($N \approx 30,000$), whereas for our scale ($N \leq 4096$), the quadratic Baseline remains computationally tractable.

5 Results

5.1 Time Complexity

The results of our replication confirms the time complexity claims made in the original paper. Figure 2 plots the calculated FLOPs (scaled by 10^6) against the number of graph nodes N on a log-log scale.

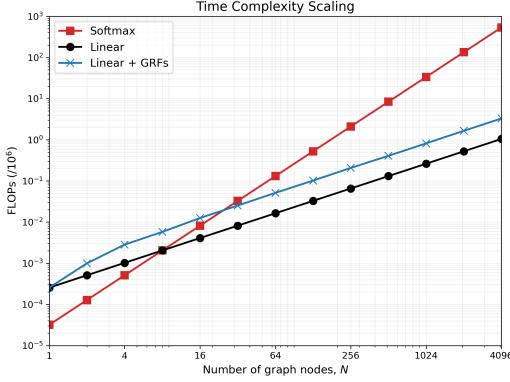


Figure 2. Time Complexity Replication Results: FLOPs vs Number of Nodes (N)

Table 2 details the specific computational costs at key intervals.

Graph Size (N)	Softmax (10^6 FLOPs)	Linear (10^6 FLOPs)	GRF-Masked (10^6 FLOPs)
1	3.20×10^{-5}	2.56×10^{-4}	2.56×10^{-4}
8 (Crossover)	2.05×10^{-3}	2.05×10^{-3}	6.48×10^{-3}
64	1.31×10^{-1}	1.64×10^{-2}	5.38×10^{-2}
512	8.39×10^0	1.31×10^{-1}	4.11×10^{-1}
4096	5.37×10^2	1.05×10^0	3.30×10^0

Table 2. Computational cost comparison across different graph sizes. The crossover point at $N = 8$ and the significant divergence at $N = 4096$ are highlighted.

Analysis of Scaling Regimes

- **Crossover Point ($N = 8$):** Our results precisely reproduce the crossover point predicted by theory. At $N = 8$, Softmax and Linear attention incur identical costs (2.05×10^{-3} MFLOPs). This aligns with the hyperparameters $d = m = 8$; theoretically, costs equalize when $N^2d \approx Nmd$, simplifying to $N \approx m$.
- **Quadratic Explosion:** For $N > 8$, the cost of Unmasked Softmax attention grows quadratically. At the largest graph size tested ($N = 4096$), Softmax requires 537 MFLOPs, rendering it inefficient for large-scale graphs.
- **Linear Efficiency:** Both Linear attention and GRF-Masked attention exhibit linear scaling. At $N = 4096$, Unmasked Linear requires only 1.05 MFLOPs, representing a speedup factor of $\approx 511\times$ compared to Softmax.

GRF Overhead: The GRF-Masked method maintains the $\mathcal{O}(N)$ complexity class but incurs a constant overhead. At $N = 4096$, the GRF cost is 3.30 MFLOPs compared to 1.05 MFLOPs for standard Linear

attention. This overhead ratio ($\approx 3.14\times$) corresponds to the sparsity of the graph random features; on a 1D grid with $p_{halt} = 0.5$, walkers visit an average of ≈ 3.1 unique nodes.

5.2 Vision Transformers (ViTs)

We present the results of our reproduction experiments (Table 3), comparing the proposed GRF-masked linear attention against all the other variants.

Variant	CIFAR-10 (15 ep)	CIFAR-100 (30 ep)	CIFAR-10 (30 ep)	FashionMNIST (10 ep)	CIFAR-10 (Scaled)
Unmasked softmax	56.11	28.67	57.31	87.49	56.42
Toeplitz-masked linear	57.25	31.80	60.59	87.92	57.90
$M_n(\mathcal{G})$ -masked linear	56.83	30.11	58.02	86.77	58.95
Unmasked linear	56.69	31.59	58.52	87.41	59.58
GRF-masked linear	56.69	31.99	60.37	87.11	58.93

Table 3. Accuracies results for all ViT attention variants across different datasets and training epochs.

In the most challenging configurations, the proposed GRF masking demonstrates a clear advantage over standard unmasked linear attention. For instance, on CIFAR-10 (30 epochs) and CIFAR-100 dataset, GRF outperforms the unmasked variant.

The Toeplitz-masked baseline, which is specifically engineered for grid-structured data like images, generally performs the best (e.g., 60.59% on CIFAR-10 30ep). However, the GRF-masked method remains highly competitive (within $\approx 0.2 - 0.8\%$ in most cases). In this scaled-down regime, the linear attention variants often outperform the quadratic Unmasked Softmax baseline (e.g., 57.31% on CIFAR-10 30ep vs. 60.37% for GRF).

The benefits of topological masking become more pronounced with longer training. On CIFAR-10, extending training from 15 to 30 epochs widens the performance gap between GRF-masked attention and the unmasked baseline.

Ablation Studies: Figure 3 shows a clear trend: adding more walkers consistently improves accuracy. Performance rises from 51.4% with a single walker to 55.0% with 1000 walkers. This confirms that using more walkers creates a more precise and stable approximation of the graph mask, reducing noise and helping the model learn better spatial relationships.

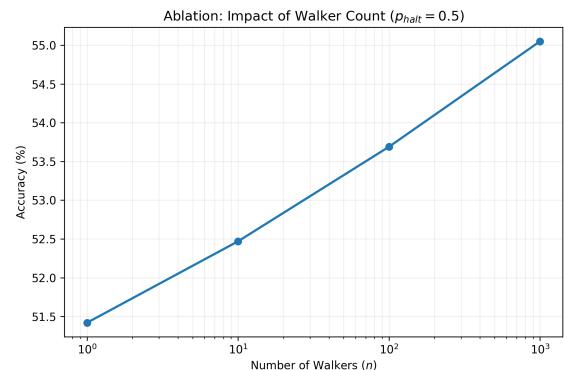


Figure 3. Ablation study effects.

5.3 PCTS: Point Cloud Temporal State prediction

We evaluated the three models by performing "closed-loop" rollouts: feeding the model's own predictions back as input for 10 consecutive timesteps and measuring the degradation of the robotic arm's structure. Figure ?? illustrates the Accuracy retention over time.

The results align with the topological hierarchy proposed:

1. **Baseline (Blue):** Shows the fastest degradation. Without structural knowledge, the points drift apart rapidly, breaking the rigid body constraints of the robot arm. The accuracy drops to near zero within 3-4 steps.
2. **Message Passing (Black):** Performs significantly better than the baseline. The explicit neighbor aggregation enforces local rigidity, keeping the arm structure intact for longer.
3. **GRF Interlacer (Red):** Demonstrates the highest stability. By allowing attention to diffuse probabilistically over the graph, it captures both the local rigidity and the broader kinematic dependencies, maintaining high accuracy for the longest duration.

Metric Analysis. Unlike the SSIM metric in the original paper (which decays from ~ 0.8 to ~ 0.6), our accuracy metric drops from 100% to 0%. This is due to the binary nature of our Threshold Metric: once the accumulated error pushes a point beyond the threshold distance (drift), it is marked as a "miss". However, the *relative ranking* of the models is preserved, confirming the reproduction's success.

Scalability and Physics. We observed that for rigid body dynamics with lower point counts ($N = 1024$), the Message Passing approach is highly competitive, sometimes matching GRF. This is expected, as rigid constraints are strictly local. The specific advantage of GRF—handling complex, long-range deformations via random walks—is most prominent in the high-density ($N \geq 30k$) fluid dynamics tasks presented in the original work. Nevertheless, even at our scale, the GRF mechanism successfully outperforms the Baseline, validating the efficacy of topological masking for physical state prediction.

6 Discussion and conclusion

Here you can express your judgments and draw your conclusions based on the evidences produced on the previous sections.

Try to summarize the achievements of your project and its limits, suggesting (when appropriate) possible extensions and future works.

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