Hyperbolic Geometric Latent Diffusion Model for Graph Generation

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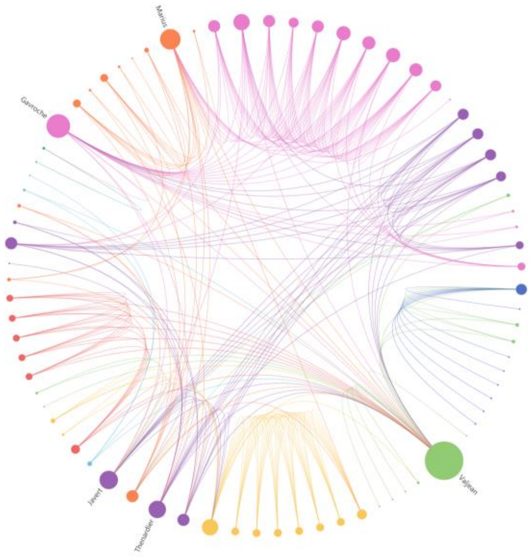
Paper: https://arxiv.org/pdf/2405.03188

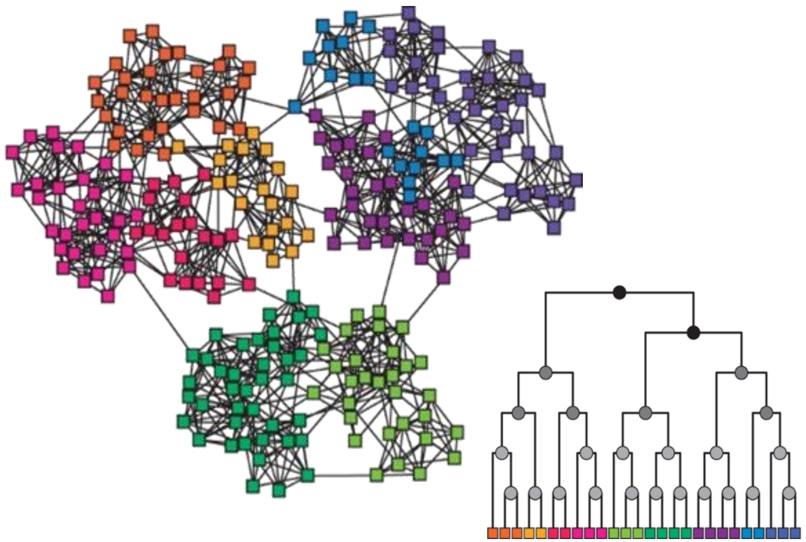
Code: https://github.com/RingBDStack/HyperDiff

Background

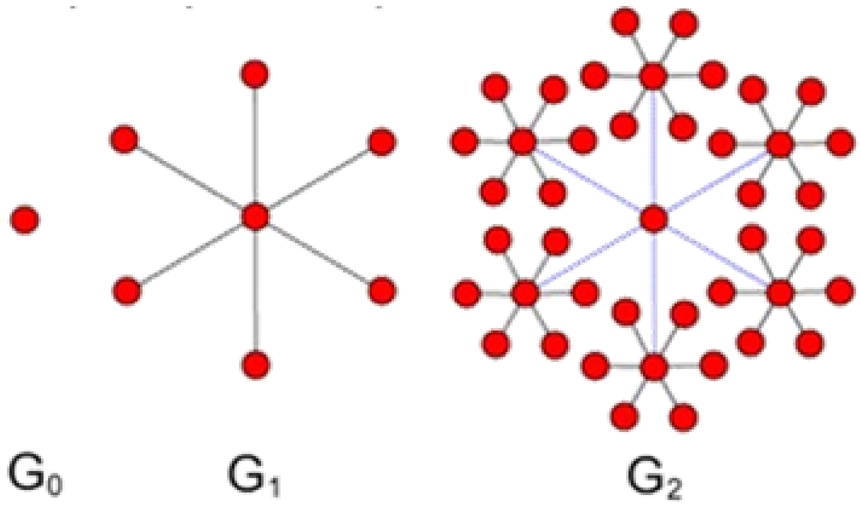
Graphs in the real world contain variety and important of topologies, and these topological properties often reflect physical laws and growth patterns.



Small-worlds



Hierarchies



Fractal structures

Graph Generation

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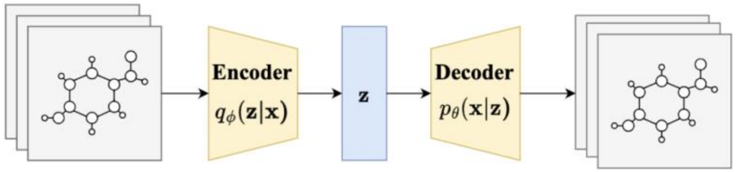
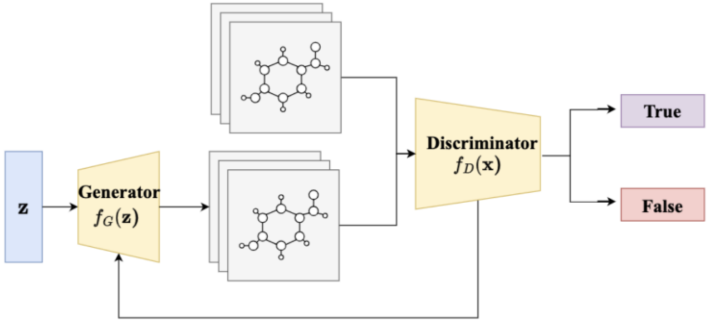
Many deep learning models have been developed for graph generation.

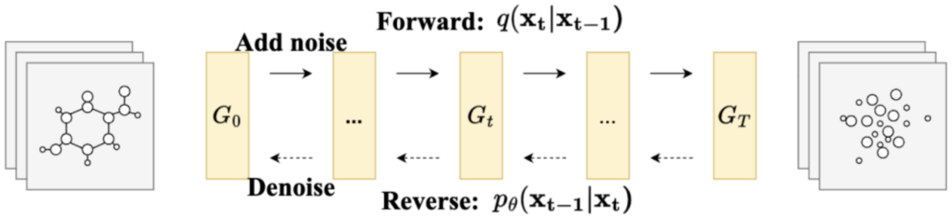
Model	Training	Quality	Generalization
VAE	Easy	Low	Good
GAN	Hard	High	Bad
Diffusion	**Easy**	**High**	**Good**



Variational AutoEncoders



Generative Adversarial Networks (GAN)



Diffusion models

[1] Liu C, Fan W, Liu Y, et al. Generative diffusion models on graphs: Methods and applications[C]. IJCAI 2023.

Graph Diffusion Model

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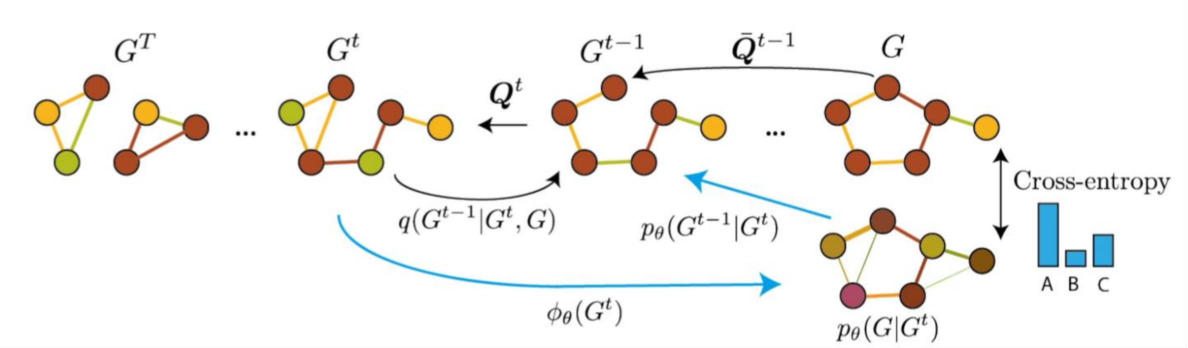
Discrete paradigm：

$$q(G^t|G^{t-1}) = \ (X^{t-1}Q_x^t, E^{t-1}Q_E^t)$$

The diffusion process is performed directly on the adjacency/Laplace matrix.

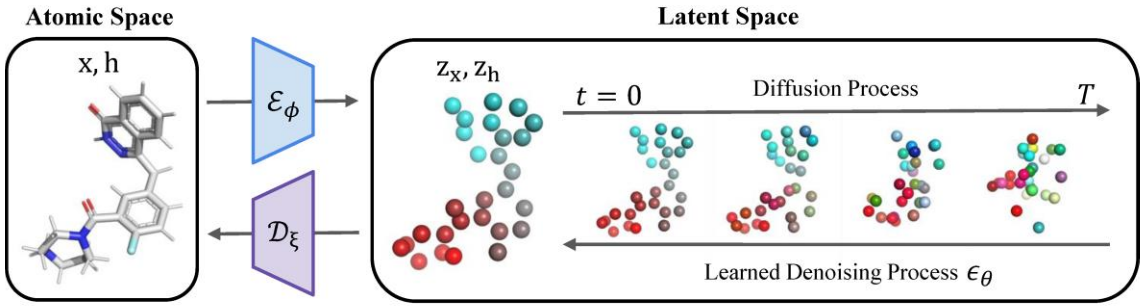


DiGress[2]

Continuous paradigm：

$$q(x^t|x^{t-1}) = N(x^t; \sqrt{1-\alpha_t}x^{t-1}, \alpha_t I)$$

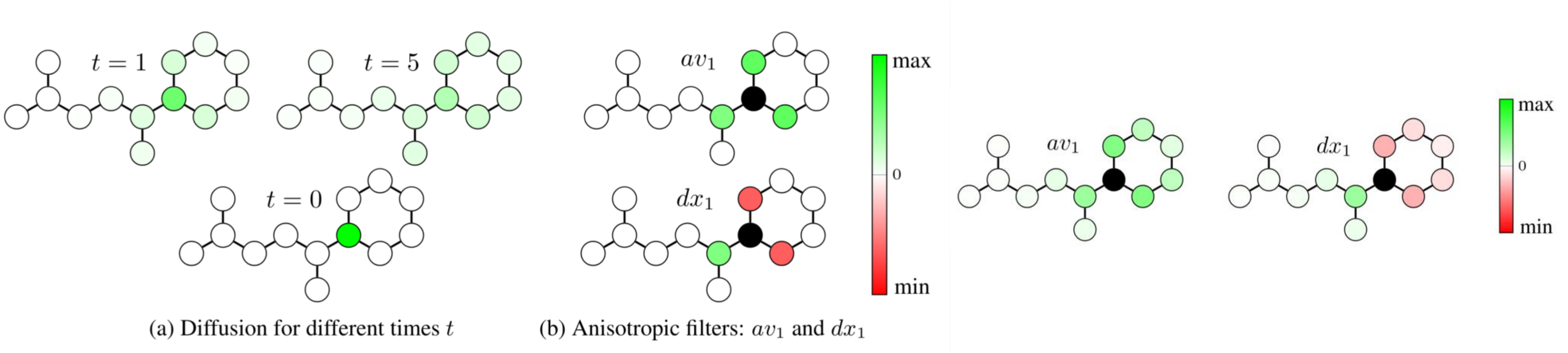
The diffusion process is performed after embedding into the continuous latent space.



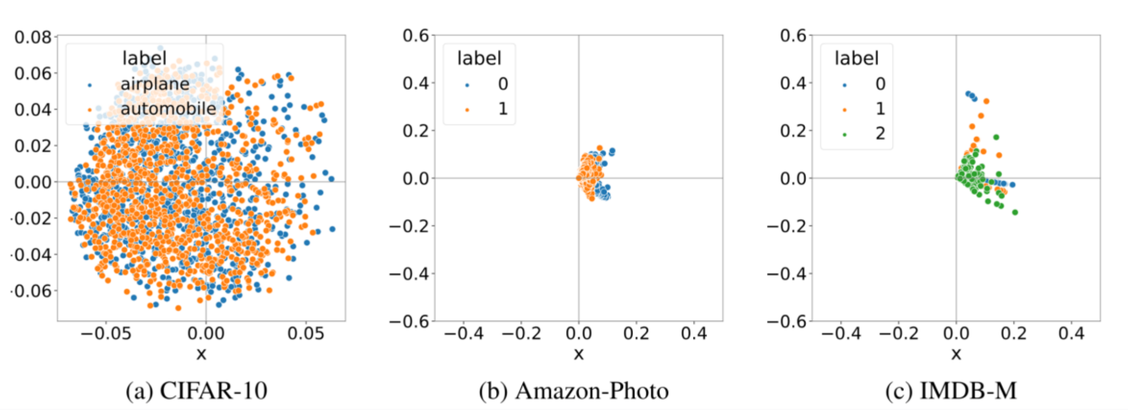
GeoLDM[3]

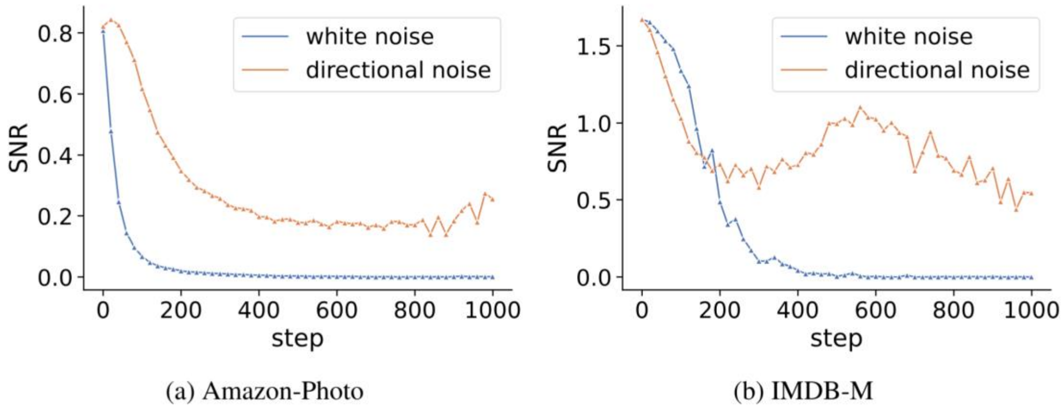
[2] Vignac C, et al. DiGress: Discrete Denoising diffusion for graph generation. ICLR 2022.
[3] Xu M, et al. Geometric latent diffusion models for 3d molecule generation. ICML 2023.

Graph Anisotropic Diffusion



Graph Anisotropic Diffusion Model[4]



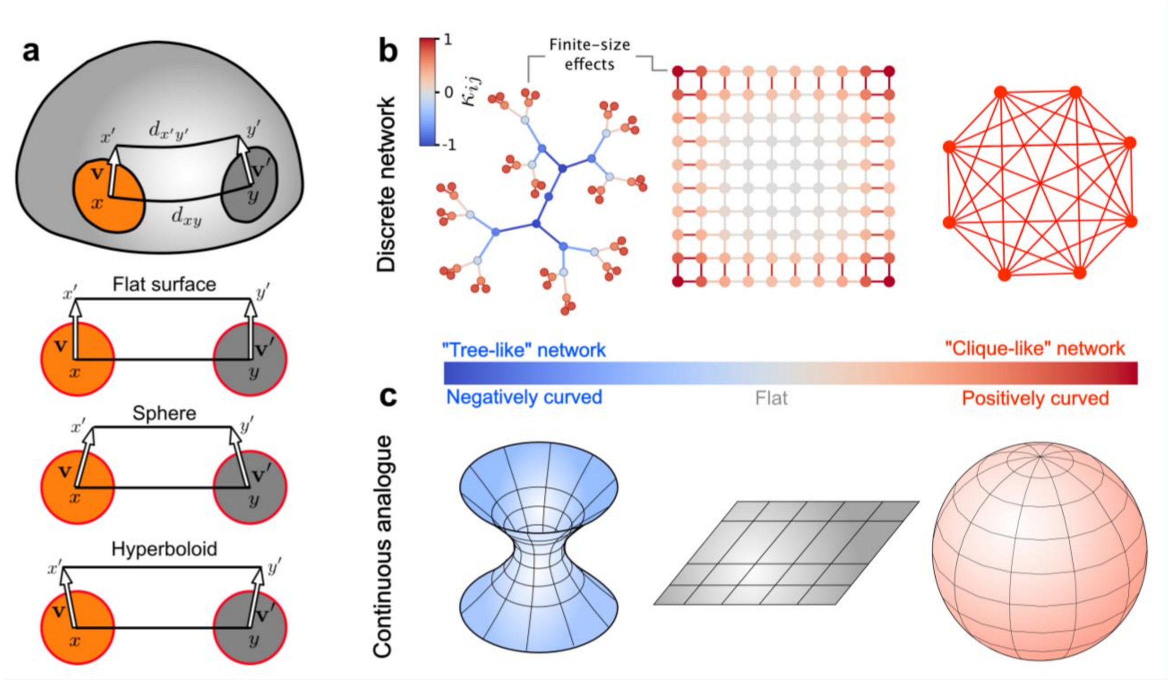


Directional Graph Diffusion Model[5]

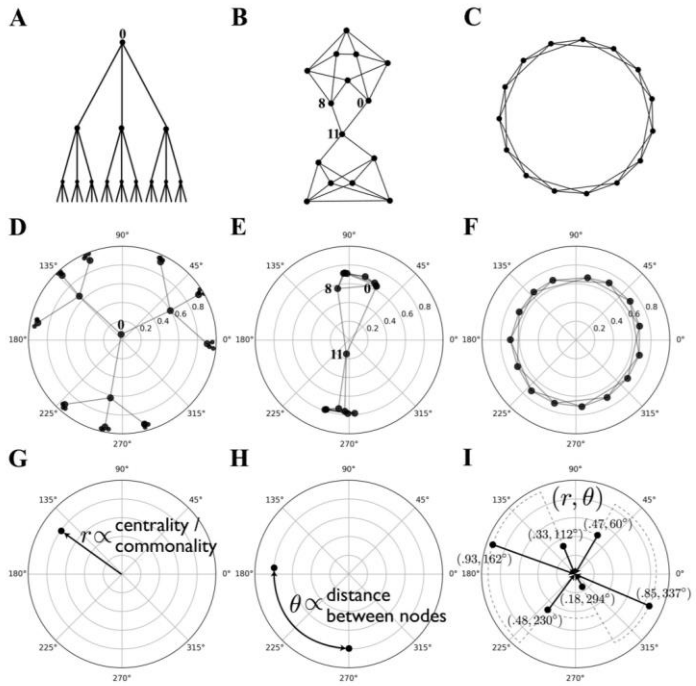
[5] Elhag, et al. Graph anisotropic diffusion for molecules. ICLR2022.
[6] Yang R, et al. Directional diffusion models for graph representation learning. NeurIPS, 2024

Geometric Prior of Graph

In Riemannian geometry, the hyperbolic geometric spaces (with negative curvature) can be intuitively understood as a continuous tree and spherical geometry spaces (with positive curvature) benefit for modeling cyclical graphs.



Riemannian Manifolds[6]



Geometric properties of hyperbolic Spaces

[6] Gosztolai A, Arnaudon A. Unfolding the multiscale structure of networks with dynamical Ollivier-Ricci curvature[J]. Nature Communications, 2021

Hyperbolic Geometry

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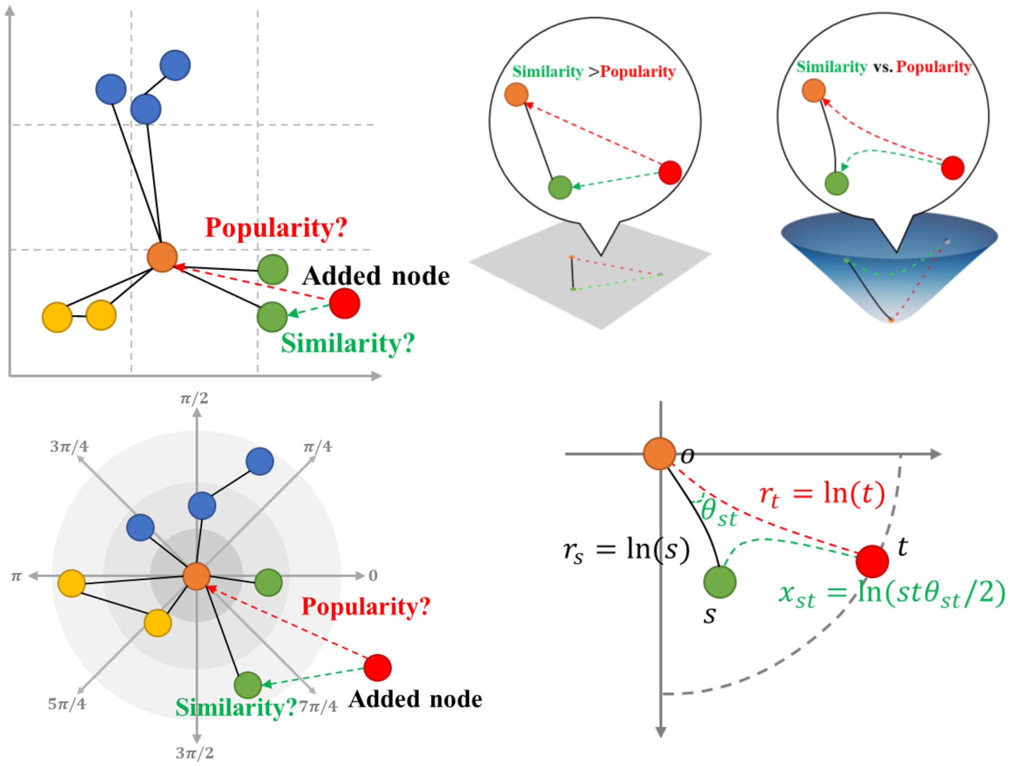
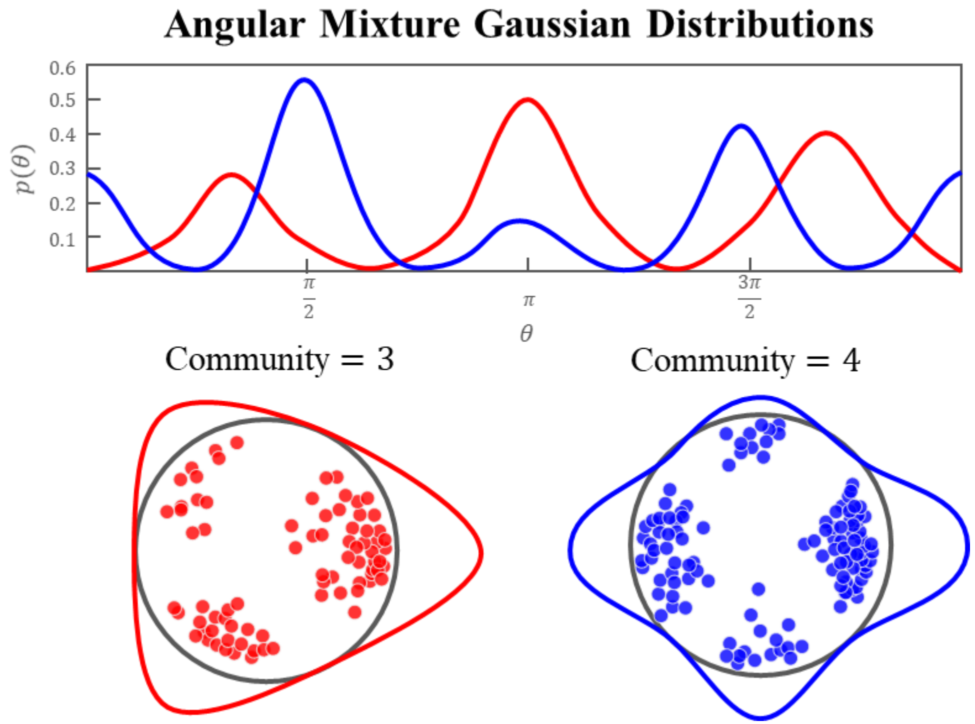
Hyperbolic geometry unifies angular and radial measures of polar coordinates and can provide geometric measures with physical semantics and interpretability.



PSO model[7] & Geometric Intuition



nPSO model[8] & Angular Distribution

[7] Papadopoulos F, et al. Popularity versus similarity in growing networks. Nature, 2012
[8] Muscoloni A, et al. A nonuniform popularity-similarity optimization. New Journal of Physics, 2018

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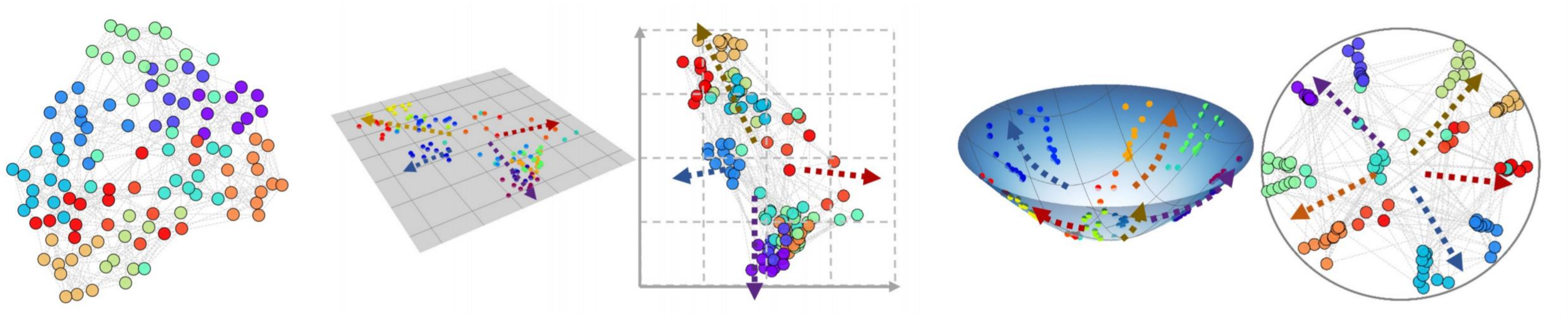
Graph Anisotropic Diffusion in Latent Space

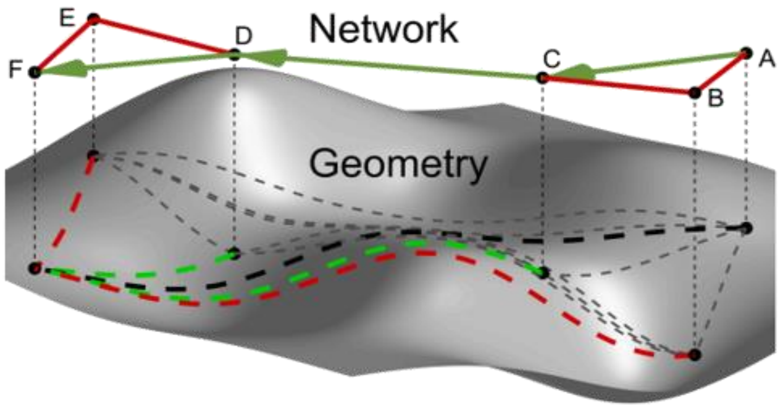
Hyperbolic geometry has great potential to address non-Euclidean structural anisotropy in graph latent diffusion processes.



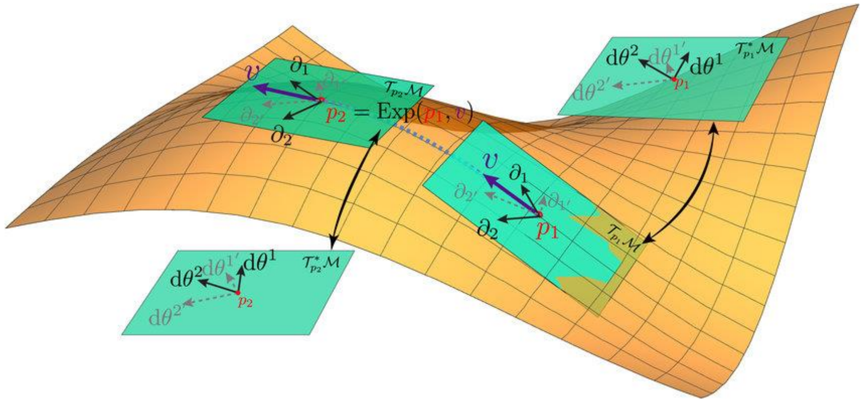
(a) Original structure. (b) Euclidean latent space. (c) Hyperbolic latent space.

Differential Geometry & Diffusion Process

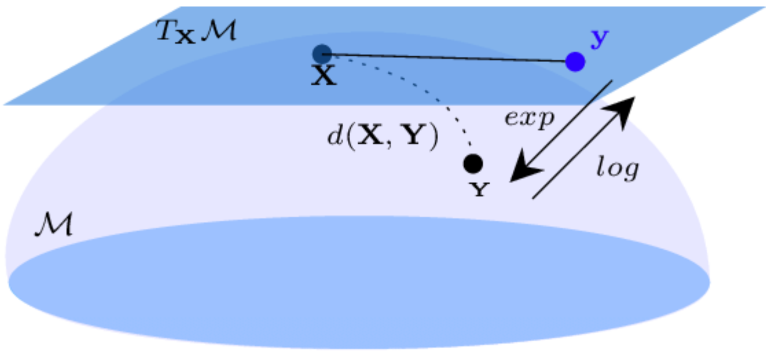
The graph can be understood as a discretization of a continuous manifold. In differential geometry, tangent planes/spaces are often used for approximate computations.



Discretized Manifold



Tangent plane/space approximation



Logmap & Expmap

Challenges

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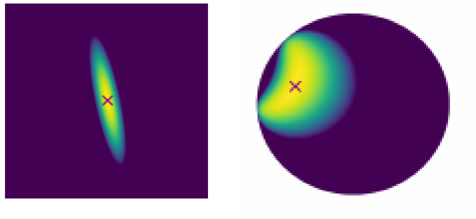
Our goal is to establish a suitable geometrically latent space based on hyperbolic geometry to design an efficient diffusion process to the non-Euclidean structure.

Challenge 1

The additivity of continuous Gaussian distributions is undefined in hyperbolic latent space.

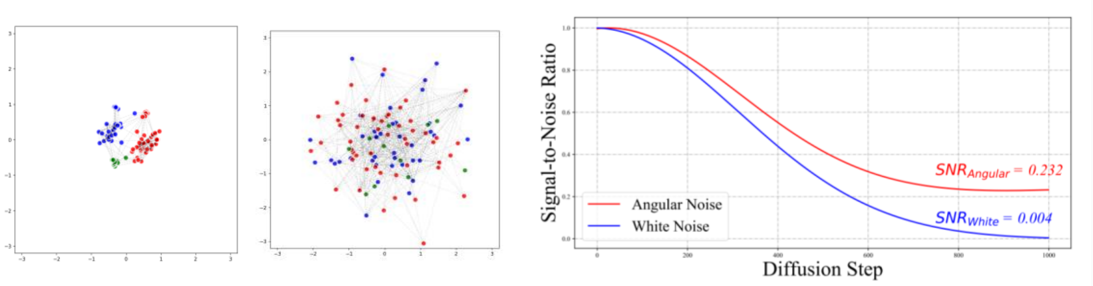


$$\boldsymbol{\eta} \not\sim \boldsymbol{\eta}_1 \oplus_c \boldsymbol{\eta}_2,$$
$$\boldsymbol{\eta} \sim \mathcal{N}_{\mathbb{H}}^c\left(0, (\sigma_1^2 + \sigma_2^2)I\right),$$
$$\boldsymbol{\eta}_1 \sim \mathcal{N}_{\mathbb{H}}^c\left(0, \sigma_1^2 I\right), \boldsymbol{\eta}_2 \sim \mathcal{N}_{\mathbb{H}}^c\left(0, \sigma_2^2 I\right).$$

The additivity issue in hyperbolic space

Challenge 2

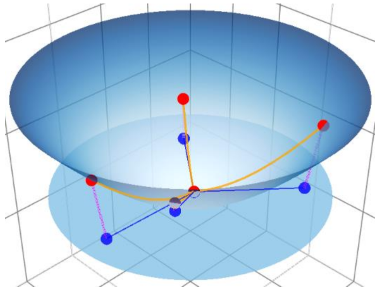
An effective anisotropic diffusion process for non-Euclidean structures.



SNR decreases rapidly with isotropic noise

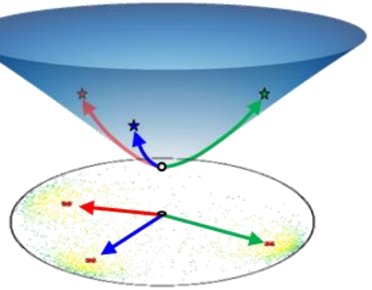
Hyperbolic Differential Approximation for Diffusion

Differential Approximation of Continuous Gaussian Processes



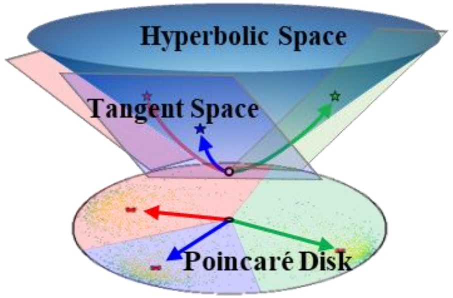
Hyperbolic Embeddings
(HGCN Encoder)

→

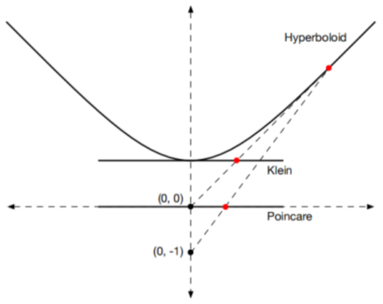


Approximate Tangent Plane Selection
(Hyperbolic K-Means Clustering)

→



Approximate Tangent Space Diffusion
(Continuous Gaussian Processes)



The hyperparameter k is allowed to control the approximation accuracy:

Error
- Upper bound: $k = 1$ → Klein model
- Lower bound: $k = N_{max}$ → Hyperboloid model

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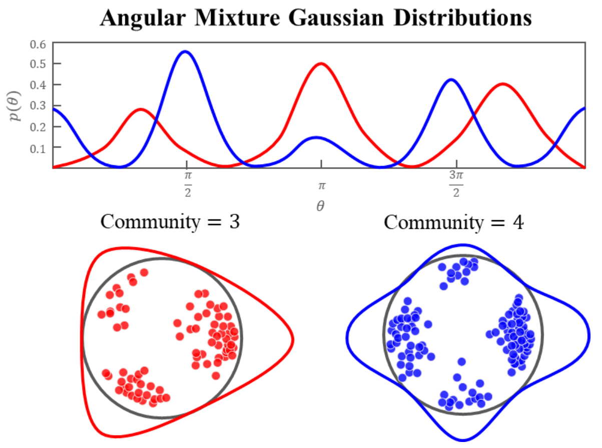
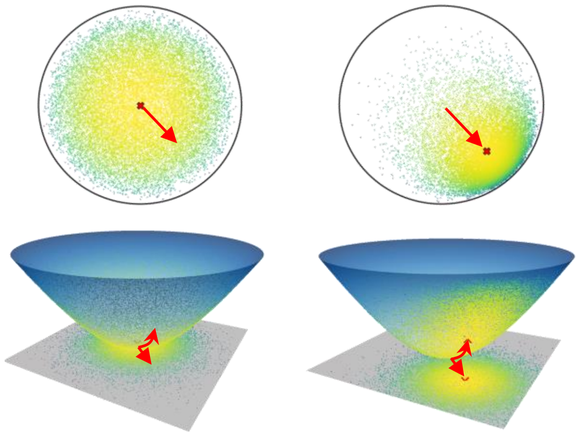
Geometrically directional constraint

Radial & Angular Constraints：





Angle constraints controls the noise direction:

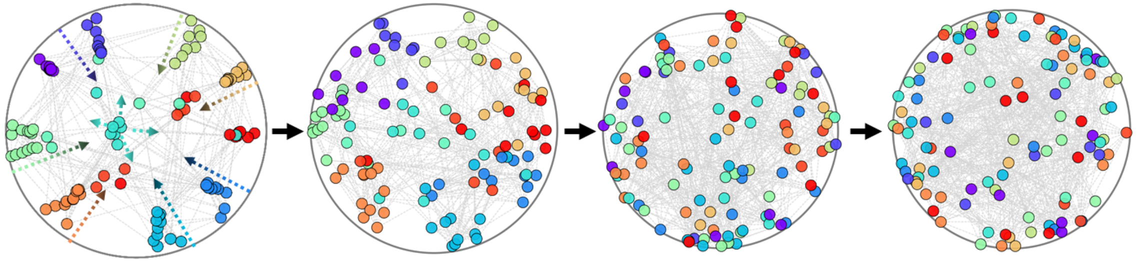
$$\mathrm{sgn}(\mathrm{logmap}_o^c(h_\mu))\varepsilon$$

Radial constraints preserve the geometric prior:

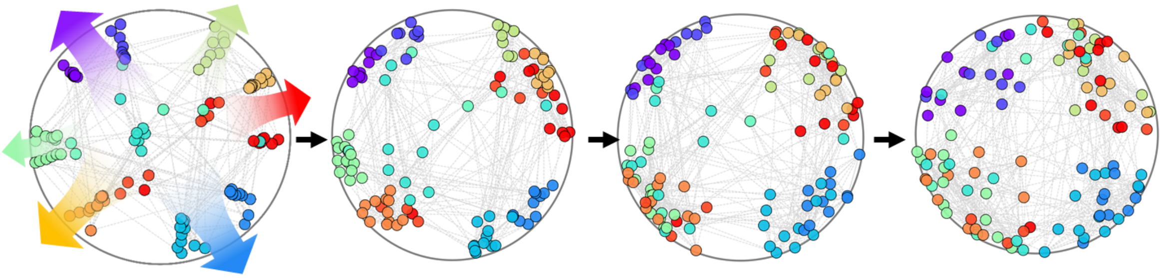
$$\delta \tanh\left(\frac{\sqrt{c}\lambda_0}{T_0}\right)x_0$$

$$x_t = \sqrt{\overline{\alpha}_t}x_0 + \sqrt{1-\overline{\alpha}_t}\mathbf{z} + \delta \tanh[\sqrt{c}\lambda_o^c t/T_0]x_0$$

Hyperbolic Latent Diffusion Process：



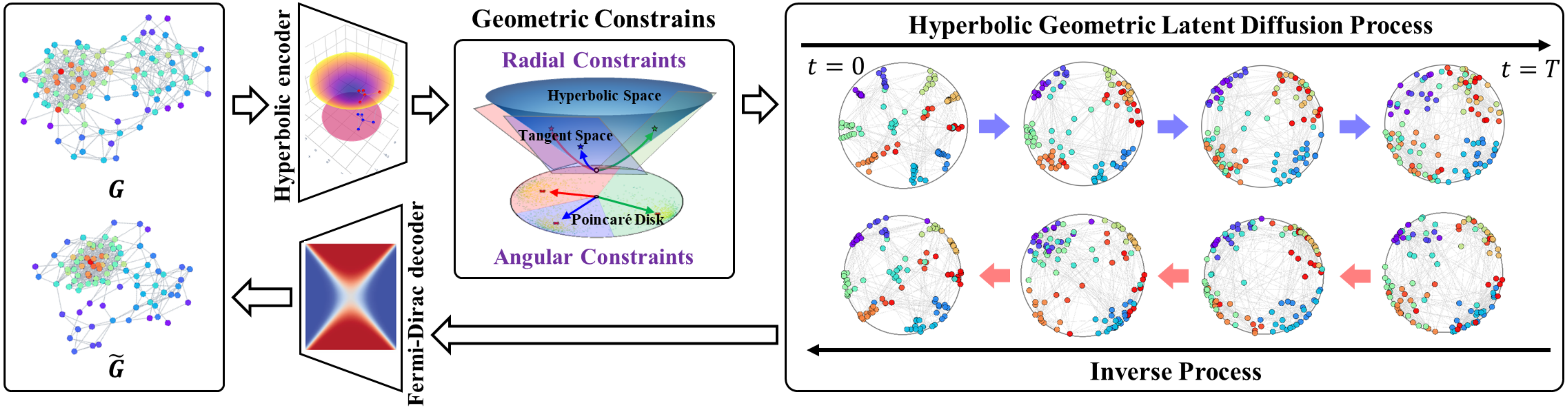
Hyperbolic Latent Diffusion Process without Geometric Constraints



Hyperbolic Latent Diffusion Process with Geometric Constraints

Our Architecture

Hyperbolic latent diffusion model consists of two main components, the hyperbolic differential approximation of the continuous diffusion process and the geometrically directional constraint.



HyperDiff Architecture

Experiments

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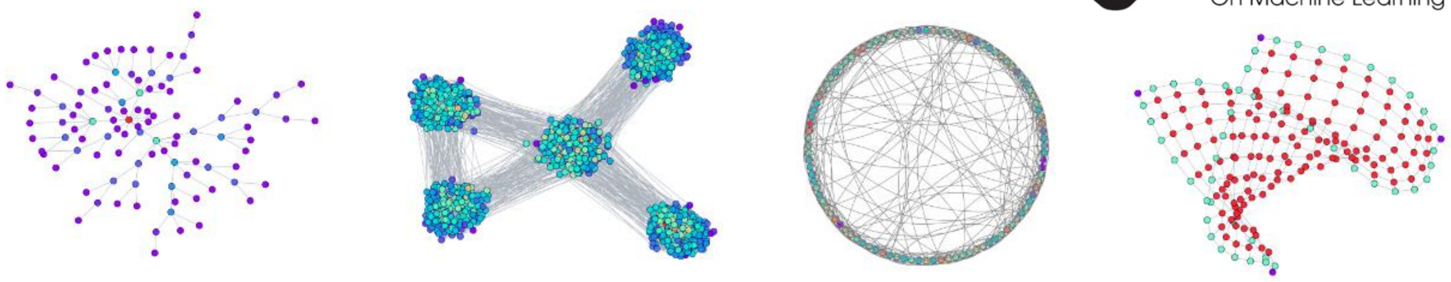
- Evaluation Settings
  - Node classification: F1 scores
  - Graph generation: MMD
- Datasets
  - Synthetic Datasets: BA, SBM, WS, Grid …
  - Real-world datasets
- Baselines
  - Euclidean graph representation methods: GraphGAN, ANE
  - Hyperbolic graph representation learning: $\mathcal{P}$-VAE, HyperANE
  - Deep graph generative models: VGAE, GraphRNN
  - Graph diffusion generative models: GDSS, DiGress, GraphGDP, EDGE



	Dataset	#Nodes	#Edges	#Features	#Avg. Degree	#Class
Link P.	Cora	2,708	5,429	1,433	3.90	7
	Citeseer	3,312	4,732	3,703	2.79	6
	Polblogs	1,490	19,025	500	25.54	3
	Dataset	**#Graphs**	**#Avg. Node**	**#Avg. Edge**	**#Max Num Node**	**#Class**
Graph G.	MUTAG	188	17.9	39.6	28	2
	IMDB-B	1,000	19.8	193.1	136	2
	PROTEINS	1,113	39.1	145.6	620	2
	COLLAB	5,000	74.5	4914.4	492	3

Experimental Results

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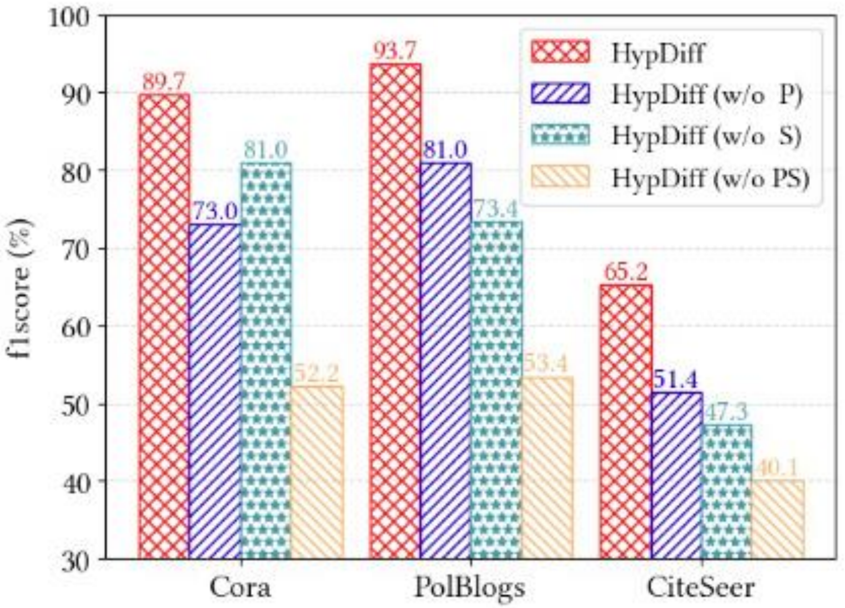
Node classification F1 score

Method	Synthetic Datasets				Real-world Datasets						Avg. R.
	SBM		BA		Cora		Citeseer		Polblogs		
	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	Mi-F1	Ma-F1	
VGAE	20.5±2.1	15.4±1.1	37.4±1.7	15.9±2.3	79.7±0.4	78.1±0.2	63.8±1.4	55.5±1.3	79.4±0.8	79.4±0.8	4.6
ANE	39.9±1.1	33.9±1.8	46.0±3.0	19.3±2.7	69.3±0.1	66.4±0.1	50.2±0.1	49.5±0.6	80.8±0.1	80.7±0.1	4.3
GraphGAN	38.6±0.5	38.9±0.3	43.6±0.6	24.6±0.5	71.7±0.1	69.8±0.1	49.8±1.0	45.7±0.1	77.5±0.6	76.9±0.4	4.8
$\mathcal{P}$-VAE	57.9±1.3	53.0±1.5	38.4±1.4	20.0±0.3	79.6±2.2	77.5±2.5	**67.9±1.7**	60.2±1.9	79.4±0.1	79.4±0.1	3.2
Hype-ANE	18.8±0.3	11.9±0.1	56.9±2.4	31.6±1.2	80.7±0.1	79.2±0.3	64.4±0.3	58.7±0.0	83.6±0.4	83.6±0.4	3.0
HypDiff	**70.5±0.1**	**69.4±0.1**	**58.3±0.1**	**40.0±0.1**	**82.4±0.1**	**81.2±0.1**	67.8±0.2	**60.4±0.3**	**85.7±0.1**	**85.4±0.1**	**1.1**

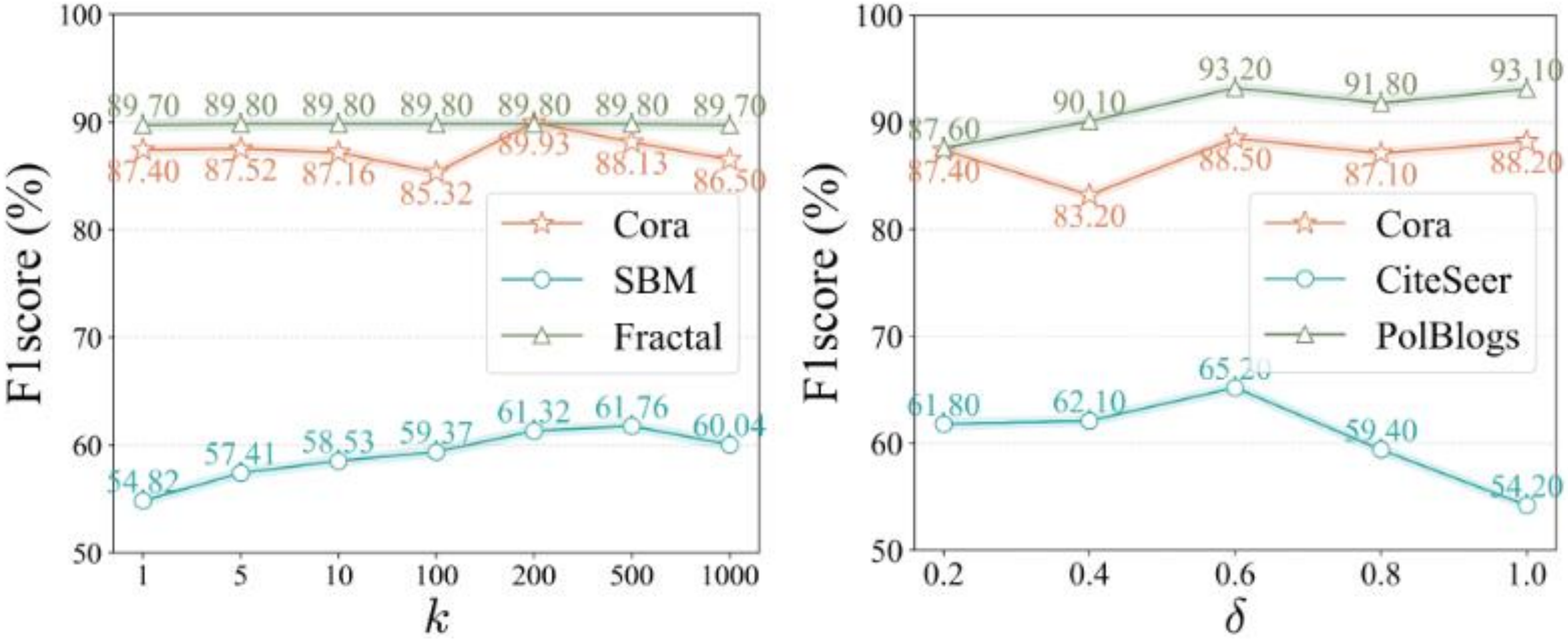
Graph generation MMD score

Method	Synthetic Datasets						Real-world Datasets					
	Community			BA-G			MUTAG			PROTRINS		
	Degree	Cluster	Spectre	Degree	Cluster	Spectre	Degree	Cluster	Spectre	Degree	Cluster	Spectre
VGAE	0.365	0.025	0.507	0.775	1.214	0.398	0.255	2.000	0.744	0.705	0.979	0.700
GraphRNN	**0.002**	0.027	**0.004**	**0.122**	0.262	0.007	0.537	0.013	0.476	**0.009**	0.071	0.017
GDSS	0.094	0.031	0.052	0.978	0.468	0.917	0.074	0.021	**0.003**	1.463	0.168	0.013
DiGress	0.226	0.158	0.194	0.654	1.171	0.268	0.100	0.351	0.082	0.108	0.062	0.079
GraphGDP	0.046	0.016	0.042	0.698	0.188	0.053	0.127	0.057	0.050	0.103	0.240	0.088
EDGE	0.021	0.013	0.040	0.282	**0.010**	0.090	**0.024**	0.597	0.468	0.033	0.523	0.024
HypDiff	**0.002**	**0.010**	0.028	0.216	0.021	**0.004**	0.048	**0.001**	0.040	0.133	**0.004**	**0.012**

Analysis of HypDiff



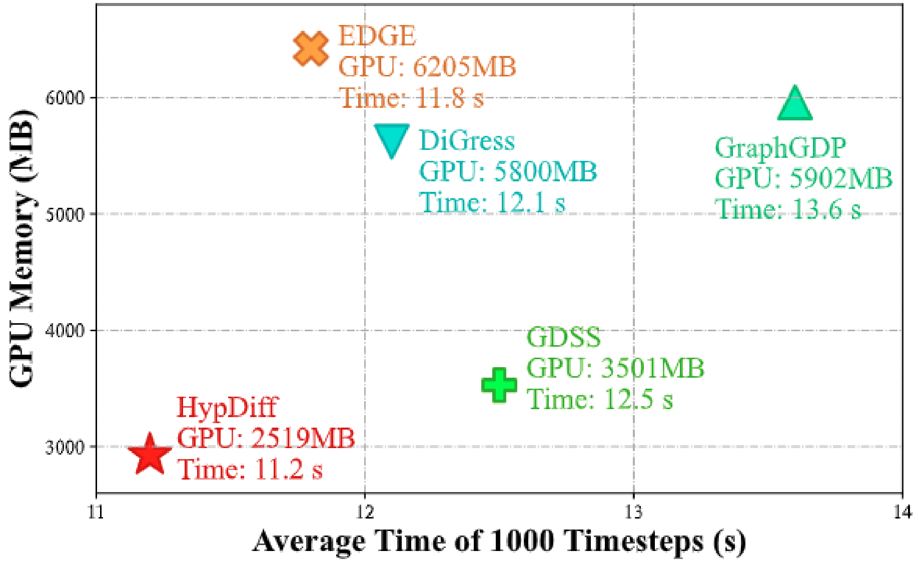
(a) Ablation Study



(b)Sensitivity Analysis of Geometric Constraints

Hyperbolic geometric prior plays a crucial role in capturing non-Euclidean structures.

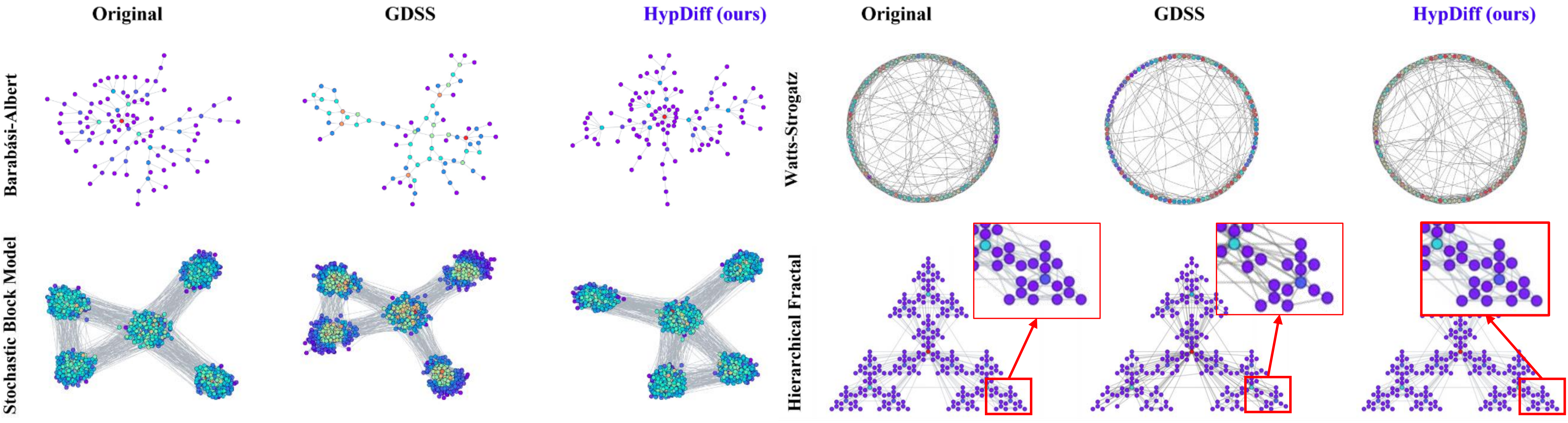
Diffusion Efficiency Analysis



HypDiff comprehensively outperforms other baselines in diffusion time and GPU memory cost.

Method	Synthetic Datasets						Real-world Datasets					
	Community		BA-G		Ego		MUTAG		PROTEINS		IMDB-B	
	Time(s)	GPU(MB)	Time(s)	GPU(MB)	Time(s)	GPU(MB)	Time(s)	GPU(MB)	Time(s)	GPU(MB)	Time(s)	GPU(MB)
GDSS	10.14	3475	11.80	7750	9.71	3883	10.79	3907	12.04	6305	12.5	3501
DiGress	9.62	3936	11.42	9012	12.28	4174	9.84	4125	11.74	6975	12.1	5800
GraphGDP	12.58	3802	14.36	13164	12.47	3848	12.85	3956	12.18	44708	13.6	5902
EDGE	9.87	2825	11.83	25236	10.24	2657	9.73	27603	10.95	26188	11.8	6205
HypDiff	10.03	2246	12.04	5697	10.15	2570	9.92	2720	10.72	4735	11.20	2519

Visualization



HypDiff exhibits significantly enhanced proficiency in reproducing the original graph structure, while consistently achieving a coherent distribution of node colors.

Highlights of HyperDiff

Geometric Prior: Hyperbolic geometry provides better priors for topological properties of graphs with non-Euclidean structure.

Graph Anisotropic Diffusion: Anisotropic diffusion provides better and more fine-grained structure details for graph structure generation.

Efficiency: HyperDiff can directly perform diffusion process in continuous hyperbolic space, and has low computational complexity and GPU occupancy.

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