Dataset Info.	QM9 $\delta = 0.7$				ZINC250k $\delta = 1$			
Method	Val. w/o corr. (%) ↑	NSPDK MMD ↓	FCD ↓	time (s) ↓	Val. w/o corr. (%)↑	NSPDK MMD ↓	FCD ↓	time (s) ↓
GraphAF	67	0.020	5.268	$2.52e^3$	68	0.044	**16.289**	$5.80e^3$
GraphDF	82.67	0.063	10.816	$5.35e^4$	89.03	0.176	34.202	$6.02e^3$
MoFlow	91.36	0.017	4.467	**4.60**	63.11	0.046	20.931	$\mathbf{2.45e^1}$
EDP-GNN	47.52	0.005	2.680	$4.40e^3$	82.97	0.049	16.737	$9.09e^3$
GraphEBM	8.22	0.030	6.143	$\underline{3.71e^1}$	5.29	0.212	35.471	$\underline{5.46e^1}$
GDSS*	<u>95.79</u>	<u>0.003</u>	<u>2.813</u>	$1.14e^2$	**95.90**	<u>0.019</u>	<u>16.621</u>	$2.02e^3$
HGDM (ours)	**98.04**	**0.002**	**2.131**	$1.23e^2$	<u>93.51</u>	**0.016**	17.69	$2.23e^3$

Table 2: Generation results on the QM9 and ZINC250k dataset. Results of the baselines are taken from (**?**). The method with $*$ denotes that results are obtained by running open-source codes. The best results are highlighted in bold and the underline denotes the second best. We report the mean graph hyperbolicity values δ of the two datasets. Due to the space limitation, we show the results of validity, uniqueness, and novelty in the Appendix.

Method	Val. w/o corr. (%)↑	NSPDK MMD ↓	FCD ↓	time (s) ↓
GDSS	95.79	0.003	2.813	$\mathbf{1.14e^2}$
GDSS+AE	95.95	0.003	2.615	$1.17e^2$
HGDM+hgcn(ours)	96.64	**0.002**	2.331	$1.48e^2$
HGDM (ours)	**98.04**	**0.002**	**2.131**	$1.23e^2$

Table 3: Generation results of the variants of GDSS and HGDM on the QM9 dataset.

distribution of the graph structure from the hyperbolic latent space and benefit from it, but the generated molecules are also close to the data distribution in the chemical space. We also report the generation results of ZINC250k in Table 2. As we observed in the generic graph datasets, the performance of HGDM in FCD and validity is slightly degraded due to the fact that the ZINC250k dataset deviates more from the hyperbolic structure and has more complex chemical properties compared to QM9. However, HGDM still maintains the advantage of generation from a geometric structure perspective that outperforms all the baselines in NSPDK MMD. Overall HGDM achieves similar performance for GDSS on the ZINC250k dataset and outperforms all other baselines. The superior performance of HGDM on the molecule generation task validates the ability of our method to efficiently learn the underlying distribution of molecular graphs with multiple nodes and edge types.

Ablation Study

We implement a variant of GDSS called GDSS+AE. It incorporates an autoencoder to generate the Euclidean embedding of nodes and uses GDSS to estimate the score function in Euclidean latent space. We use GDSS+AE to compare the effect of Euclidean and hyperbolic hidden spaces on graph diffusion. In addition, we tested HGDM using the HGCN layer as a building block, called HGDM+hgcn. The results of the above-mentioned variants in QM9 are provided in Table 3

Necessity of Hyperbolic Hidden Space We find that GDSS+AE is slightly improved in metrics compared to GDSS. It can be considered that the dense embedding generated by the auto-encoder helps to learn the distribution of the graph, but it is not comparable to our hyperbolic approach due to the restricted capacity growth of Euclidean space.

Necessity of HGAT Layers HGDM+hgcn is comparable to our model in most metrics, but the increase in time cost is higher compared to GDSS, whereas our method has only a slight increase in time, making it more suitable for scaling up to the task of generating large graphs. This demonstrates the importance of using our proposed HGAT layer.

Conclusion

In this work, we proposed a two-stage Hyperbolic Graph Diffusion Model (HGDM) to learn better the distribution of graph data and a simple hyperbolic graph attention layer that reduces the extra time spent associated with hyperbolic methods. HGDM overcomes the limitations of previous graph generation methods and is closer to the nature of graphs. We have found experimentally that learning the distribution in the hyperbolic space is beneficial for the quality of generated graph with the power-law distribution. Experimental results in generic graph and molecule generation show that HGDM outperforms existing graph generation methods in most metrics, demonstrating the importance of learning the underlying manifold for graph generation tasks. Code is available at https://github.com/LF-WEN/HGDM

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