Dataset	Ego-small				Community-small				Enzymes				Grid			
Info.	Real, $4 \leq \|V\| \leq 18$, $\delta = 0.25$				Synthetic, $12 \leq \|V\| \leq 20$, $\delta = 1$				Real, $10 \leq \|V\| \leq 125$, $\delta = 1.26$				Synthetic, $100 \leq \|V\| \leq 400$, $\delta = 9.76$			
Method	Deg.	Clus.	Orbit	Avg.	Deg.	Clus.	Orbit	Avg.	Deg.	Clus.	Orbit	Avg.	Deg.	Clus.	Orbit	Avg.
DeepGMG	0.040	0.100	0.020	0.053	0.220	0.950	0.400	0.523	-	-	-	-	-	-	-	-
GraphRNN	0.090	0.220	0.003	0.104	0.080	0.120	0.040	0.080	**0.017**	0.062	0.046	0.042	**0.064**	0.043	**0.021**	**0.043**
GraphAF	0.03	0.11	**0.001**	0.047	0.18	0.20	0.02	0.133	1.669	1.283	0.266	1.073	-	-	-	-
GraphDF	0.04	0.13	0.01	0.060	0.06	0.12	0.03	0.070	1.503	1.061	0.202	0.922	-	-	-	-
GraphVAE	0.130	0.170	0.050	0.117	0.350	0.980	0.540	0.623	1.369	0.629	0.191	0.730	1.619	**0.0**	0.919	0.846
GNF	0.030	0.100	**0.001**	0.044	0.200	0.200	0.110	0.170	-	-	-	-	-	-	-	-
EDP-GNN	0.052	0.093	0.007	0.051	0.053	0.144	0.026	0.074	0.023	0.268	0.082	0.124	0.455	0.238	0.328	0.340
GDSS	0.021	0.024	0.007	0.017	0.045	0.086	0.007	0.046	0.026	0.061	0.009	**0.032**	0.111	0.005	0.070	0.062
HGDM (ours)	**0.015**	**0.023**	0.003	**0.014**	**0.017**	**0.050**	**0.005**	**0.024**	0.045	**0.049**	**0.003**	**0.032**	0.137	0.004	0.048	0.063
Improve. over GDSS	28.6%	4.2%	57.1%	17.6%	62.2%	41.9%	28.6%	47.8%	-73.1%	19.7%	66.7%	0.0%	-23.4%	20.0%	31.4%	-1.6%

Table 1: Generation results on the generic graph datasets. Results of the baselines are taken from published papers (**???**). Hyphen (-) denotes that the results are not provided in the original paper. The best results are highlighted in bold and the underline denotes the second best. (lower is better). We report the mean graph hyperbolicity values δ of all datasets. Due to the space limitation, we provide the standard deviations in Appendix.

We also report mean graph hyperbolicity values δ (lower is more hyperbolic) of the datasets by computing Gromovs δ-hyperbolicity (**?**), a notion from group theory that measures how tree-like a graph is. The lower δ, the more hyperbolic the graph dataset, and $\delta = 0$ for trees.

Baselines We compare our proposed method against the following generative models. **GraphVAE** (**?**) is a VAE-based model. **DeepGMG** (**?**) and **GraphRNN** (**?**) are autoregressive RNN-based models. **GNF** (**?**) is a one-shot flow-based model. **GraphAF** (**?**) is an autoregressive flow-based model. **EDP-GNN** (**?**) and **GDSS** (**?**) are score-based models. **GraphDF** (**?**) is an autoregressive flow-based model that utilizes discrete latent variables.

Results Table 1 shows that HGDM significantly outperforms all baselines including GDSS, achieving optimal results in most metrics. In particular, HGDM outperforms GDSS with a 37.1% decrease of MMD on average in Ego-small and Community-small, indicating that it has unique advantages in generating graphs with low hyperbolicity ($\delta \leq 1$). Although the graphs in Enzymes deviate from a power-law distribution, HGDM still maintains the same results as GDSS in terms of average statistics. The graphs in Grid deviate more from the hierarchical structure ($\delta = 9.76$) and are closer to the Euclidean topology with 0 curvature, in which case the autoregressive model GraphRNN has an advantage over the score-based models such as GDSS. HGDM still manages to achieve comparable results to GDSS on average statistics and outperforms the other baselines except GraphRNN. This demonstrates the scalability of HGDM, which still has good modeling capability for graphs with high hyperbolicity. In general, we find that our model performs better in generating graphs with small δ-hyperbolicity.

Molecule Generation

Datasets Following the GDSS (**?**), we tested our model on the **QM9** (**?**) and **ZINC250k** (**?**) datasets to assess its ability to learn molecular distributions. QM9 dataset contains 134k stable small molecules with up to 9 heavy atoms (CONF). ZINC250k datasets encompass a total of 250k chemical compounds with drug-like properties. On average, these molecules are characterized by a larger size (with an average of 23 heavy atoms) and possess greater structural complexity when compared to the molecules in QM9. Following previous works (**??**), the molecules are kekulized by the RDKit library (**?**) with hydrogen atoms removed. We also report the mean graph hyperbolicity values δ.

Metrics We sample $10,000$ molecules using our model and evaluate their quality with the following metrics. **Frchet ChemNet Distance (FCD)** (**?**) evaluates the distance between the training sets and generated sets by analyzing the activations of the penultimate layer of the ChemNet. **Neighborhood Subgraph Pairwise Distance Kernel (NSPDK) MMD** (**?**) computes MMD between the generated molecules and test molecules while considering both node and edge features for evaluation. It is important to note that FCD and NSPDK MMD are crucial metrics that evaluate the ability to learn the distribution of the training molecules by measuring the proximity of the generated molecules to the distribution. Specifically, FCD assesses the ability in the context of chemical space, whereas NSPDK MMD measures the ability in terms of the graph structure. **Validity w/o correction**, used for fair comparing with (**?**), is the proportion of valid molecules without valency correction or edge resampling. **Time** measures the time for generating $10,000$ molecules in the form of RDKit molecules.

Baselines We use **GDSS** (**?**) as our main baseline. We also compare the performance of HGDM against **GraphAF** (**?**), **GraphDF** (**?**), MoFlow (**?**), **EDP-GNN** (**?**) and **GraphEBM** (**?**).

Results Table 2 shows that our method also exhibits excellent performance on molecular generation tasks. In particular, on the QM9 dataset, our method is optimal in all metrics and significantly outperforms our main comparator, GDSS. HGDM achieves the highest validity without the use of post-hoc valency correction. It shows that HGDM can effectively learn the valency rules of the molecules. HGDM also outperforms all baselines in NSPDK MMD and FCD, which indicates that not only does the HGDM efficiently learn the

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

Acknowledgments

This work is supported by the National Natural Science Foundation of China (42130112,62272170). This work is also supported by the "Digital Silk Road" Shanghai International Joint Lab of Trustworthy Intelligent Software (22510750100), the General Program of Shanghai Natural Science Foundation (23ZR1419300) and KartoBit Research Network(KRN2201CA).

Ex dolorum quae, est ipsam ratione porro blanditiis totam quibusdam?Inventore nostrum veritatis asperiores deleniti alias architecto voluptatibus fugit, rem tenetur adipisci quam assumenda ipsa obcaecati iure nostrum distinctio eligendi, odio quis reprehenderit ratione architecto fuga odit, dignissimos quod tempore quasi ex?Quas commodi temporibus atque fugiat rerum pariatur tempore quia odit dolorum a, in quaerat eaque quam incidunt facere quae quisquam placeat, recusandae deserunt natus?Vero maiores deleniti nisi iure incidunt unde et temporibus quos veritatis,