Advancing Graph Generation through Beta Diffusion

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[*]Equation contribution

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Motivation

Graph

Node features

- ✓ Types: Degree, Eigenvalue, Centrality, Atoms type…
- ✓ Distribution: Continuous and Discrete
- ✓ Properties: Sparse, Normal, Skew…

Edge attributes

- ✓ Types: Binary, Bonds type…
- ✓ Distribution: Discrete (binary and category)
- ✓ Properties: Sparse…

Motivation

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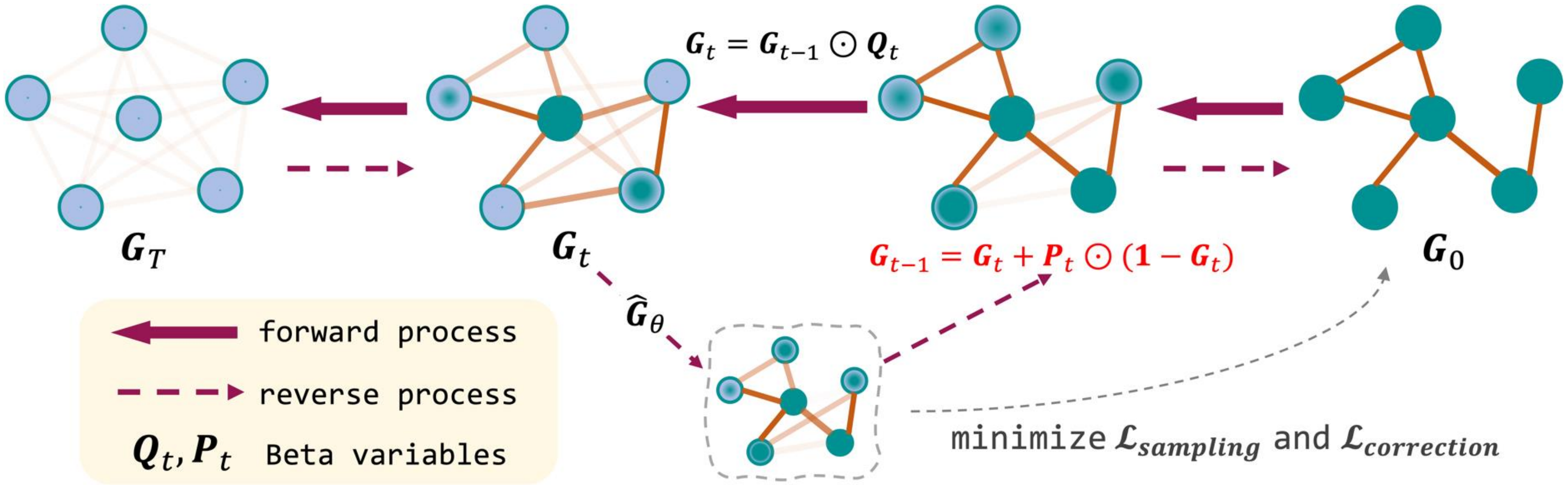
Methods \ Graph Elements	Continuous	Discrete	Both
Gaussian Diffusion Models	✅	😥	😥
Discrete Diffusion Models	🙅	✅	🙅
Beta Diffusion Model	✅	✅	✅

Bonus for Sparsity!

Graph Beta Diffusion (GBD)



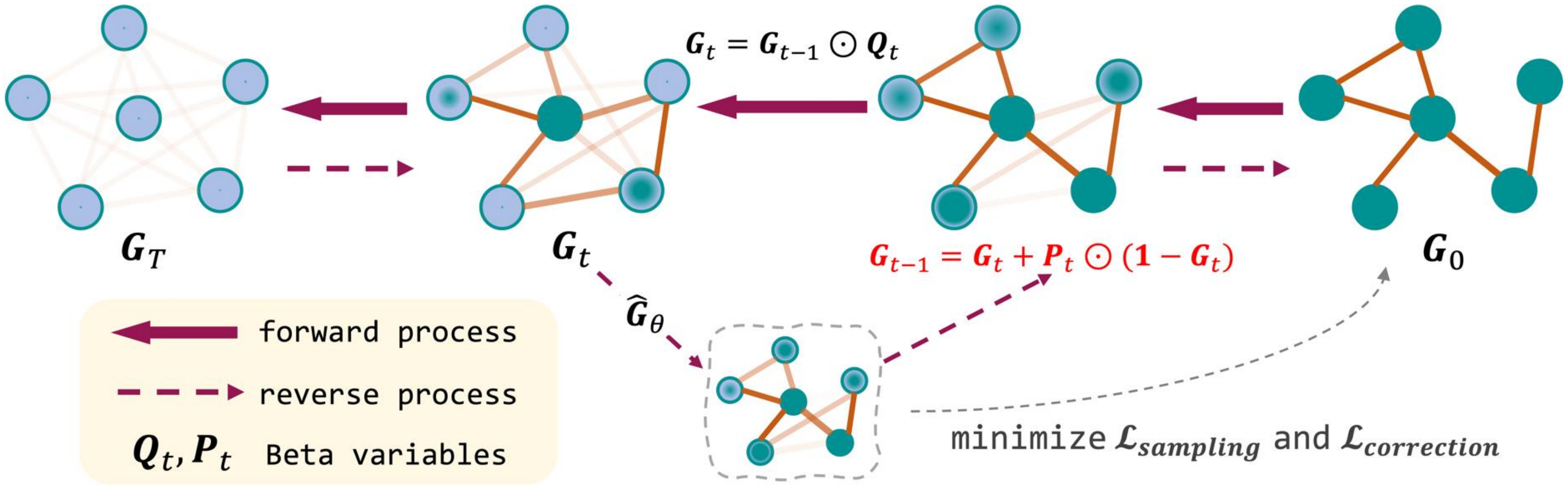
Overview of the forward and reverse diffusion processes of GBD

Forward multiplicative beta diffusion process

$$\boldsymbol{G}_t = \boldsymbol{G}_{t-1} \odot \mathbf{Q}_t, \qquad \mathbf{Q}_t \sim \mathrm{Beta}(\eta \alpha_t \boldsymbol{G}_0, \eta(\alpha_{t-1} - \alpha_t)\boldsymbol{G}_0)$$

$$q(\boldsymbol{G}_t | \boldsymbol{G}_0) = \mathrm{Beta}(\eta \alpha_t \boldsymbol{G}_0, \eta(1 - \alpha_t \boldsymbol{G}_0))$$

Graph Beta Diffusion (GBD)



Overview of the forward and reverse diffusion processes of GBD

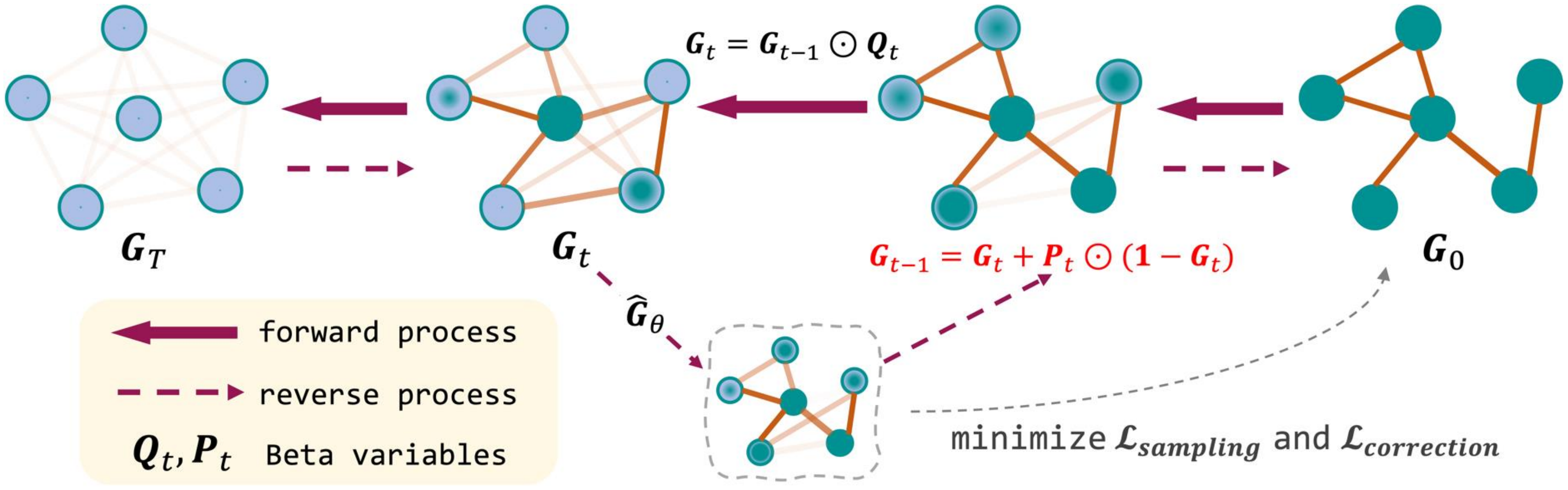
Reverse multiplicative beta diffusion process

$$G_{t-1} = G_t + \mathbf{P}_t \odot (1 - G_t), \qquad \mathbf{P}_t \sim \mathrm{Beta}(\eta(\alpha_{t-1} - \alpha_t)G_0, \eta(1 - \alpha_{t-1}G_0))$$

$$q(G_{t-1}|G_t, G_0) = \frac{1}{1 - G_t}\mathrm{Beta}\left(\frac{G_{t-1} - G_t}{1 - G_t}|\eta(\alpha_{t-1} - \alpha_t)G_0, \eta(1 - \alpha_{t-1}G_0)\right)$$

$$p_\theta(G_{t-1}|G_0) \coloneqq q\big(G_{t-1}\big|G_t, \hat{G}_\theta(G_t, t)\big)$$

Graph Beta Diffusion (GBD)



Overview of the forward and reverse diffusion processes of GBD

Training GBD following beta diffusion[1] :

$$\mathcal{L}_t = (1-\omega)\mathcal{L}_{sampling}(t, \boldsymbol{G}_0) + \omega\mathcal{L}_{correction}(t, \boldsymbol{G}_t), \omega \in [0,1]$$

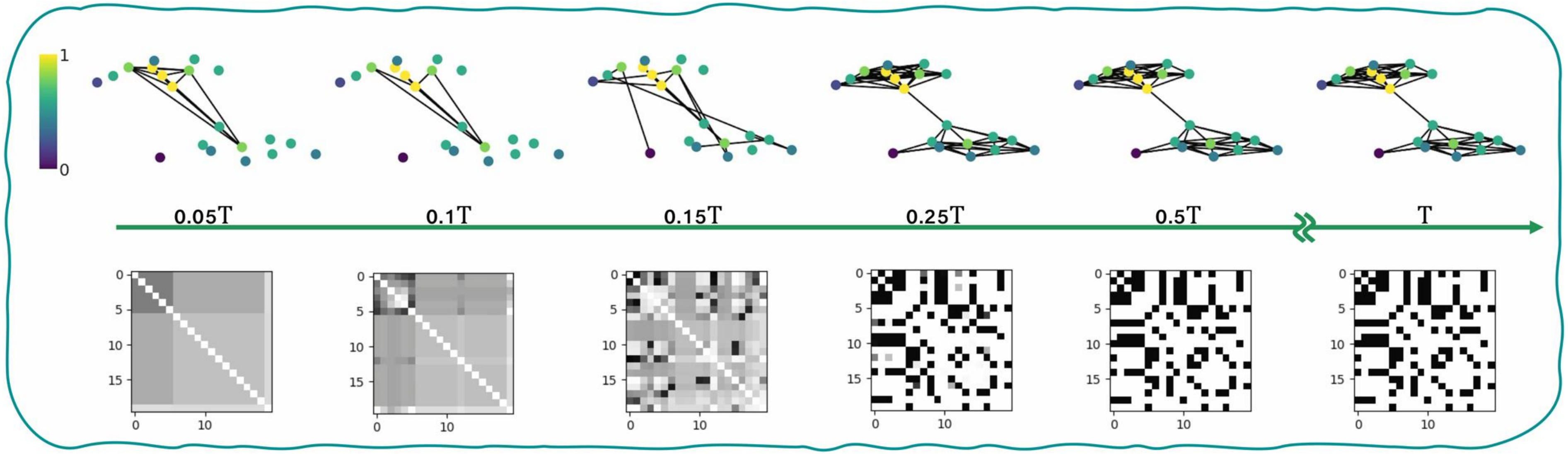
$$\mathcal{L}_{sampling}(t, \boldsymbol{G}_0) \triangleq \mathbb{E}_{q(G_t, G_0)}\mathrm{KL}(p_\theta(\boldsymbol{G}_{t-1}|\boldsymbol{G}_t) \parallel q(\boldsymbol{G}_{t-1}|\boldsymbol{G}_t; \boldsymbol{G}_0))$$

$$L_{correction}(t, \boldsymbol{G}_0) \triangleq \mathbb{E}_{q(G_t, G_0)}\mathrm{KL}(q(\boldsymbol{G}_\tau|\hat{G}_\theta(\boldsymbol{G}_t, t))||q(\boldsymbol{G}_\tau|\boldsymbol{G}_0))$$

[1] Mingyuan Zhou et al., Beta diffusion, *NeurIPS 2023*

Design Space in GBD

➢ Concentration Modulation



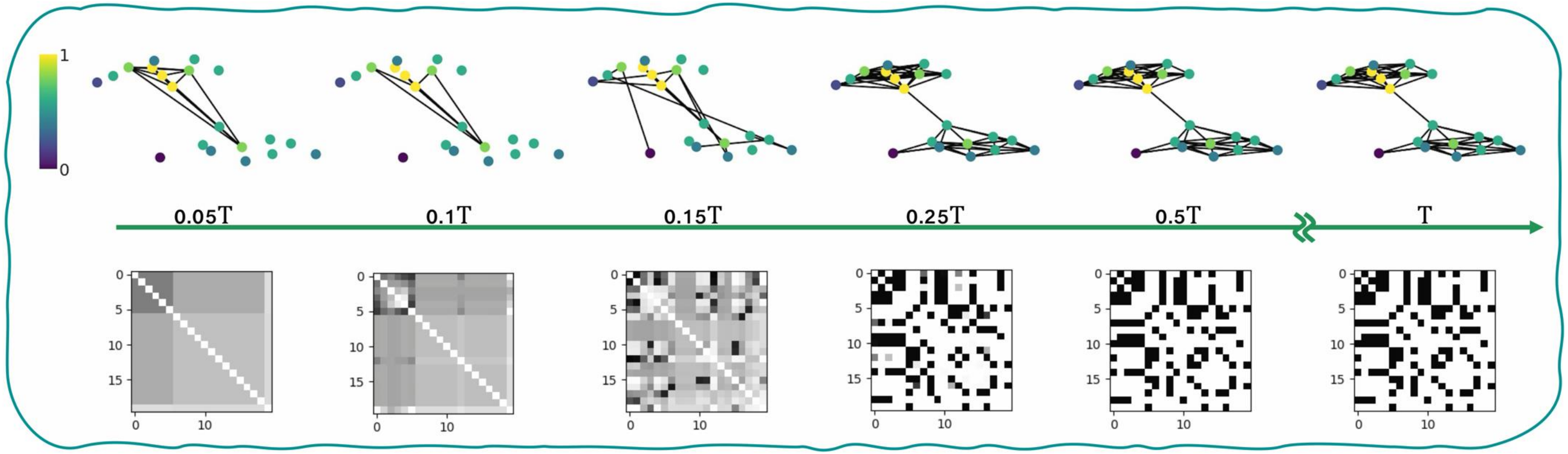
Edge generation process

"Important structures" can emerge firstly

Subgraph contains nodes of **higher degree**
Substructure contains atom & edge of **Carbon**

Design Space in GBD

- Concentration Modulation



Edge generation process

$$q(\boldsymbol{G}_t|\boldsymbol{G}_0) = \mathrm{Beta}(\boxed{\eta}\alpha_t\boldsymbol{G}_0, \boxed{\eta}(1-\alpha_t\boldsymbol{G}_0))$$

concentrate parameter

$\boldsymbol{\eta} \uparrow \Longrightarrow$ diffusion & mixing process $\downarrow$ (slower)

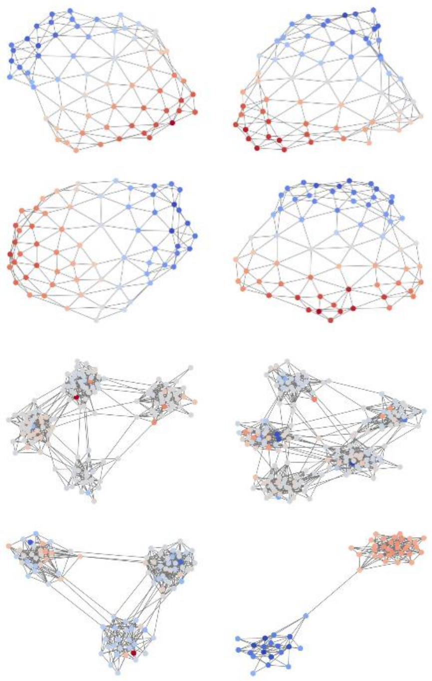
Experiments

➢ Generation Quality ➢ Topology Convergence

MMD results for complex generic graph generation

	Planar					SBM				
Method	Deg.	Clus.	Orbit.	Spec.	V.U.N.	Deg.	Clus.	Orbit.	Spec.	V.U.N.
Training set	0.0002	0.0310	0.0005	0.0052	100.0	0.0008	0.0332	0.0255	0.0063	100.0
GraphRNN	0.0049	0.2779	1.2543	0.0459	0.0	0.0055	0.0584	0.0785	0.0065	5.0
GRAN	0.0007	0.0426	0.0009	0.0075	0.0	0.0113	0.0553	0.0540	0.0054	25.0
SPECTRE	0.0005	0.0785	0.0012	0.0112	25.0	0.0015	0.0521	**0.0412**	0.0056	52.5
EDP-GNN	0.0044	0.3187	1.4986	0.0813	0.0	0.0011	0.0552	0.0520	0.0070	35.0
GDSS	0.0041	0.2676	0.1720	0.0370	0.0	0.0212	0.0646	0.0894	0.0128	5.0
GDSS+TF	0.0036	0.1206	0.0525	0.0137	5.0	0.0411	0.0565	0.0706	0.0074	27.5
ConGress	0.0048	0.2728	1.2950	0.0418	0.0	0.0273	0.1029	0.1148	-	0.0
DiGress	**0.0003**	0.0372	**0.0009**	0.0106	75.	0.0013	0.0498	0.0434	0.0400	74.0
GruM	0.0005	**0.0353**	**0.0009**	0.0062	90.0	**0.0007**	**0.0492**	0.0448	0.0050	**85.0**
GBD	**0.0003**	**0.0353**	0.0135	**0.0059**	**92.5**	0.0013	0.0493	0.0446	**0.0047**	75.0

Samples



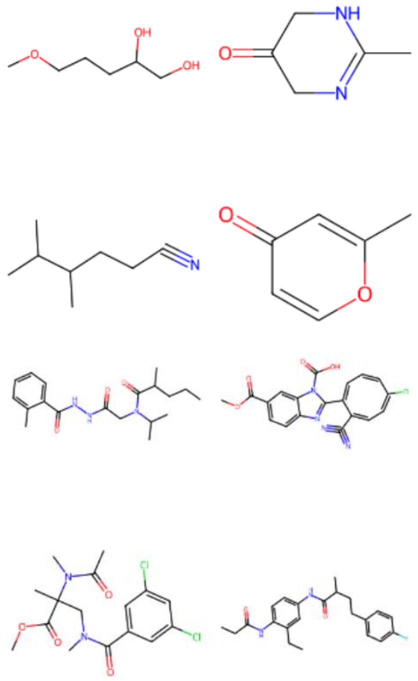
Experiments

➤ Generation Quality ➤ Topology Convergence

2D molecule generation results

Method	QM9 (|N| ≤ 9)				ZINC250K (|N| ≤ 38)			
	Valid (%) ↑	FCD ↓	NSPDK ↓	Scaf. ↑	Valid(%) ↑	FCD ↓	NSPDK ↓	Scaf. ↑
MoFlow	91.36	4.467	0.0169	0.1447	63.11	20.931	0.0455	0.0133
GraphAF	74.43	5.625	0.0207	0.3046	68.47	16.023	0.0442	0.0672
GraphDF	93.88	10.928	0.0636	0.0978	90.61	33.546	0.1770	0.0000
EDP-GNN	47.52	2.680	0.0046	0.3270	82.97	16.737	0.0485	0.0000
GDSS	95.72	2.900	0.0033	0.6983	97.01	14.656	0.0195	0.0467
GDSS+TF	99.68	0.737	0.0024	0.9129	96.04	5.556	0.0326	0.3205
DiGress	98.19	0.095	0.0003	0.9353	94.99	3.482	0.0021	0.4163
SwinGNN	99.71	0.125	0.0003	-	81.72	5.920	0.006	-
GraphARM	90.25	1.22	0.0020	-	88.23	16.26	0.055	-
EDGE	99.10	0.458	-	0.763	-	-	-	-
GruM	99.69	0.108	**0.0002**	0.9449	**98.65**	2.257	**0.0015**	**0.5299**
GBD	**99.88**	**0.093**	**0.0002**	**0.9510**	97.87	**2.248**	0.0018	0.5042

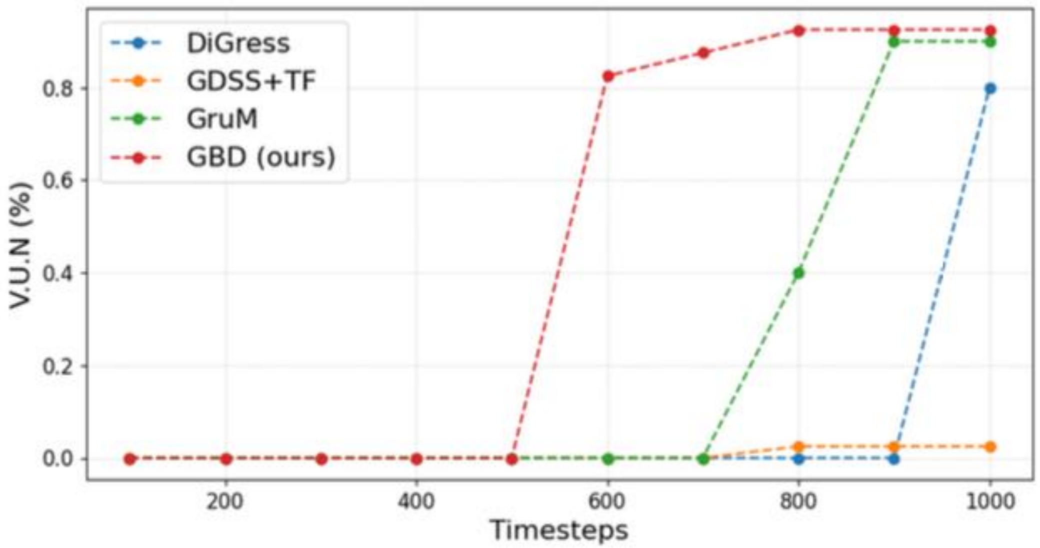
Samples

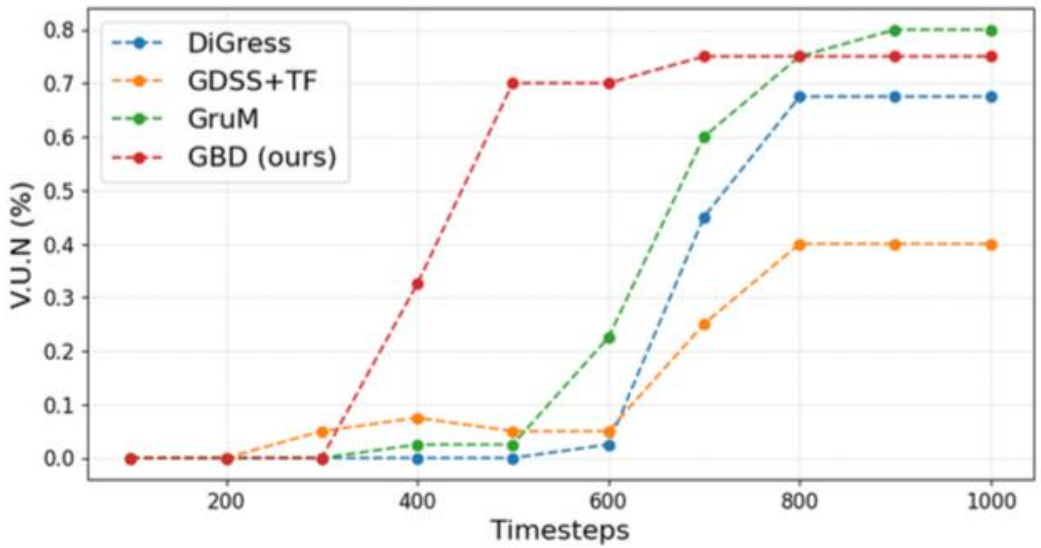


Experiments

➢ Generation Quality ➢ Topology Convergence

V.U.N. results for intermediate graph samples in the reverse chain on **Planar (left)** and **SBM (right)** datasets

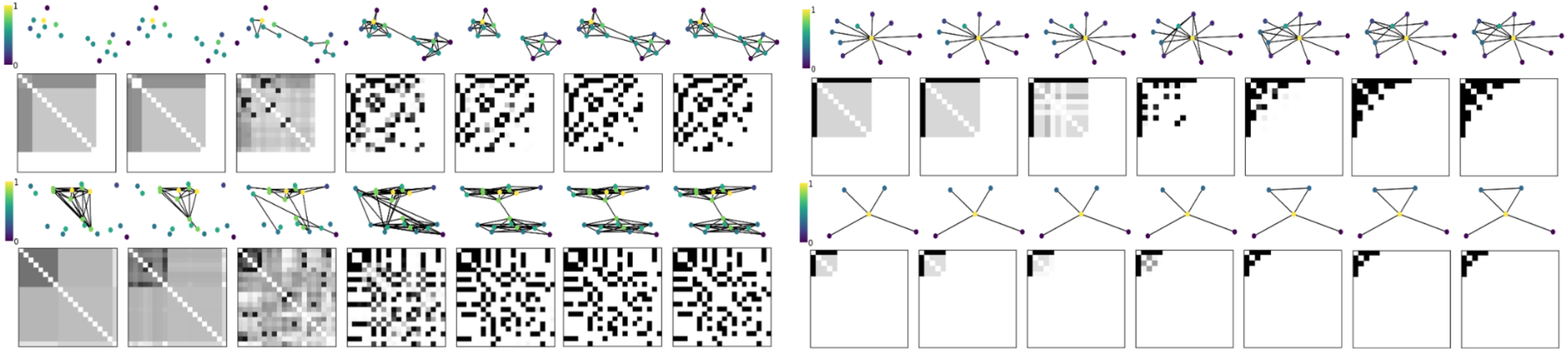




Visualization

➢ Generative Process

Edge generation process of GBD on
Community-small (left) and **Ego-small (right)** datasets



Thank you

- Paper: https://arxiv.org/abs/2406.09357
- Code: https://github.com/xinyangATK/GraphBetaDiffusion
- Xinyang's website: xinyangatk.github.io
- Email: xinyangatk@gmail.com