Efficient and Scalable Graph Generation

through Iterative Local Expansion

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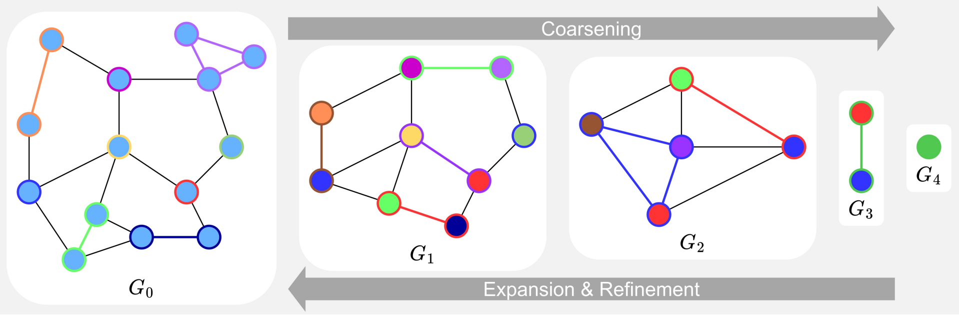
1 Excising Challenges

- **current graph generation methods**
  - model **joint distribution over all $\mathcal{O}(n^2)$ node pairs**
- **recent works to improve scalability**
  - make **simplifying assumptions** (community structure, edge independence, restricted bandwidth), sacrificing generality or sample fidelity

2 Our Idea

- model a **progressive expansion process** rather than the final graph directly
- equivalent to **inverting graph coarsening**
- achieve efficiency by only **locally modifying graphs**
- **no restrictive assumptions on the graph's structure**

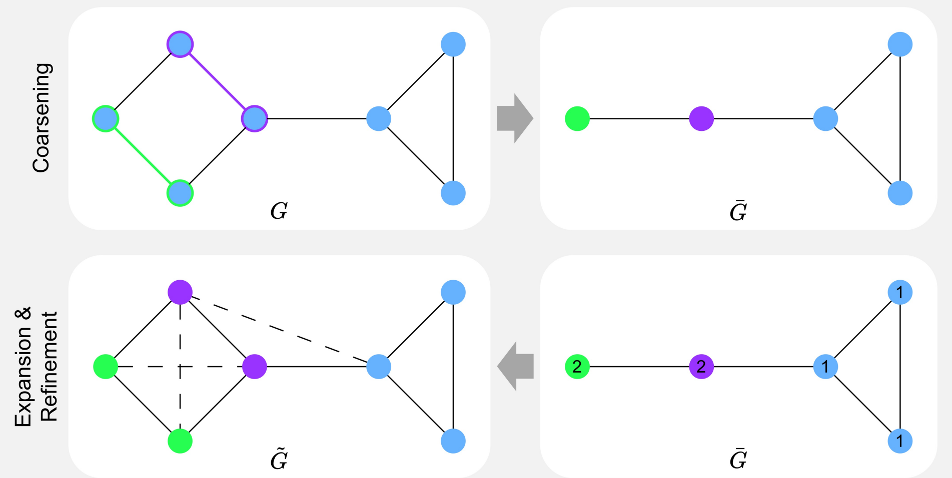


4 Local PPGN

- **novel** architecture to parameterize the diffusion model
- **efficient** on sparse graphs
- more **expressive** than message-passing GNNs
- $(\boldsymbol{h}')^{(i,j)} = \gamma\left(\boldsymbol{h}^{(i,j)}, \sum_{k \in N^-(i) \cap N^+(j)} \phi\left(\boldsymbol{h}^{(i,k)}, \boldsymbol{h}^{(k,j)}\right)\right)$

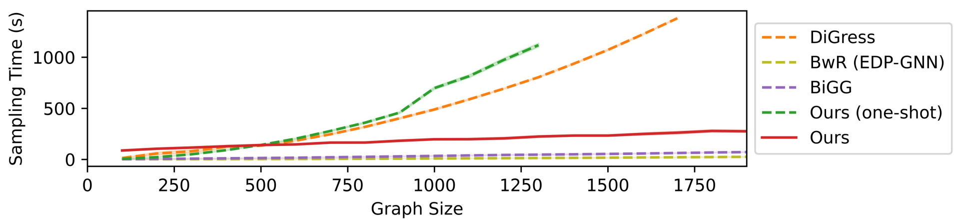
3 Details

- two-phase **inversion** of a single **graph coarsening** step
  1. **expansion** of the coarsened graph
  2. **refinement** of the resultant expanded graph
- **probabilistic inversion**
  - use **denoising diffusion** to model a distribution over
    - **node features**: size of expansion cluster
    - **edge features:** edge existence



5 Scalability

- theoretical **asymptotic complexity**: $\mathcal{O}(m \log n)$
- **scaling behaviour empirically validated on planar graphs**



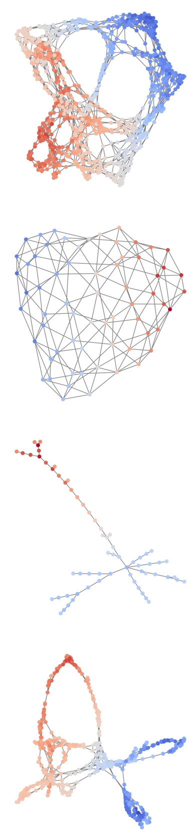
6 Generative Performance

Planar Graphs ($n_{max} = 64$, $n_{avg} = 64$)										
Model	Deg.↓	Clus.↓	Orbit ↓	Spec.↓	Wavelet ↓	Ratio↓	Valid↑	Unique ↑	Novel↑	V.U.N. ↑
Training set	0.0002	0.0310	0.0005	0.0038	0.0012	1.0	100	100	—	—
GraphRNN	0.0049	0.2779	1.2543	0.0459	0.1034	490.2	0.0	100	100	0.0
GRAN	0.0007	0.0426	0.0009	0.0075	0.0019	2.0	97.5	85.0	2.5	0.0
SPECTRE	0.0005	0.0785	0.0012	0.0112	0.0059	3.0	25.0	100	100	25.0
DiGress	0.0007	0.0780	0.0079	0.0098	0.0031	5.1	77.5	100	100	77.5
EDGE	0.0761	0.3229	0.7737	0.0957	0.3627	431.4	0.0	100	100	0.0
BwR (EDP-GNN)	0.0231	0.2596	0.5473	0.0444	0.1314	251.9	0.0	100	100	0.0
BiGG	0.0007	0.0570	0.0367	0.0105	0.0052	16.0	62.5	85.0	42.5	5.0
GraphGen	0.0328	0.2106	0.4236	0.0430	0.0989	210.3	7.5	100	100	100
Ours (one-shot)	0.0003	0.0245	0.0006	0.0104	0.0030	**1.7**	67.5	100	100	67.5
Ours	0.0005	0.0626	0.0017	0.0075	0.0013	2.1	95.0	100	100	**95.0**

Stochastic Block Model ($n_{max} = 187$, $n_{avg} = 104$)										
Model	Deg.↓	Clus.↓	Orbit ↓	Spec.↓	Wavelet ↓	Ratio↓	Valid↑	Unique ↑	Novel↑	V.U.N. ↑
Training set	0.0008	0.0332	0.0255	0.0027	0.0007	1.0	100	100	—	—
GraphRNN	0.0055	0.0584	0.0785	0.0065	0.0431	14.7	5.0	100	100	5.0
GRAN	0.0113	0.0553	0.0540	0.0054	0.0212	9.7	25.0	100	100	25.0
SPECTRE	0.0015	0.0521	0.0412	0.0056	0.0028	2.2	52.5	100	100	52.5
DiGress	0.0018	0.0485	0.0415	0.0045	0.0014	**1.7**	60.0	100	100	60.0
EDGE	0.0279	0.1113	0.0854	0.0251	0.1500	51.4	0.0	100	100	0.0
BwR (EDP-GNN)	0.0478	0.0638	0.1139	0.0169	0.0894	38.6	7.5	100	100	7.5
BiGG	0.0012	0.0604	0.0667	0.0059	0.0370	11.9	10.0	100	100	10.0
GraphGen	0.0550	0.0623	0.1189	0.0182	0.1193	48.8	5.0	100	100	5.0
Ours (one-shot)	0.0141	0.0528	0.0809	0.0071	0.0205	10.5	75.0	100	100	**75.0**
Ours	0.0119	0.0517	0.0669	0.0067	0.0219	10.2	45.0	100	100	45.0

Tree Graphs ($n_{max} = 64$, $n_{avg} = 64$)										
Model	Deg.↓	Clus.↓	Orbit ↓	Spec.↓	Wavelet ↓	Ratio↓	Valid↑	Unique ↑	Novel↑	V.U.N. ↑
Training set	0.0001	0.0000	0.0000	0.0075	0.0030	1.0	100	100	—	—
GRAN	0.1884	0.0080	0.0199	0.2751	0.3274	607.0	0.0	100	100	0.0
DiGress	0.0002	0.0000	0.0000	0.0113	0.0043	**1.6**	90.0	100	100	90.0
EDGE	0.2678	0.0000	0.7357	0.2247	0.4230	850.7	0.0	7.5	100	0.0
BwR (EDP-GNN)	0.0016	0.1239	0.0003	0.0480	0.0388	11.4	0.0	100	100	0.0
BiGG	0.0014	0.0000	0.0000	0.0119	0.0058	5.2	100	87.5	50.0	75.0
GraphGen	0.0105	0.0000	0.0000	0.0153	0.0122	33.2	95.0	100	100	95.0
Ours (one-shot)	0.0004	0.0000	0.0000	0.0080	0.0055	2.1	82.5	100	100	82.5
Ours	0.0001	0.0000	0.0000	0.0117	0.0047	4.0	100	100	100	**100**

	Proteins ($n_{max} = 500$, $n_{avg} = 258$)						Point Clouds ($n_{max} = 5037$, $n_{avg} = 1332$)					
Model	Deg.↓	Clus.↓	Orbit ↓	Spec.↓	Wavelet ↓	Ratio↓	Deg.↓	Clus.↓	Orbit ↓	Spec.↓	Wavelet ↓	Ratio↓
Training set	0.0003	0.0068	0.0032	0.0005	0.0003	1.0	0.0000	0.1768	0.0049	0.0043	0.0024	1.0
GraphRNN	0.004	0.1475	0.5851	0.0152	0.0530	91.3	OOM	OOM	OOM	OOM	OOM	OOM
GRAN	0.0479	0.1234	0.3458	0.0125	0.0341	87.5	0.0201	0.4330	0.2625	0.0051	0.0436	18.8
SPECTRE	0.0056	0.0843	0.0267	0.0052	0.0118	19.0	OOM	OOM	OOM	OOM	OOM	OOM
DiGress	0.0041	0.0489	0.1286	0.0018	0.0065	18.0	OOM	OOM	OOM	OOM	OOM	OOM
EDGE	0.1863	0.3406	0.6786	0.1075	0.2371	399.1	0.4441	0.3298	1.0730	0.4006	0.6310	143.4
BwR (EDP-GNN)	0.1262	0.4202	0.4939	0.0702	0.1199	245.4	0.4927	0.4690	1.0730	0.2912	0.5916	133.2
BiGG	0.0070	0.1150	0.4696	0.0067	0.0222	57.5	0.0994	0.6035	0.3633	0.1589	0.0994	38.8
GraphGen	0.0159	0.1677	0.3789	0.0181	0.0477	83.5	OOT	OOT	OOT	OOT	OOT	OOT
Ours (one-shot)	0.0015	0.0711	0.0396	0.0026	0.0086	13.3	OOM	OOM	OOM	OOM	OOM	OOM
Ours	0.0030	0.0309	0.0047	0.0013	0.0030	**5.9**	0.0139	0.5775	0.0780	0.0055	0.0186	**7.0**



7 Size Extrapolation

- **generalizes to larger graphs** than seen during training