Diffusing to the Top: Boost Graph Neural Networks with Minimal Hyperparameter Tuning

THE UNIVERSITY OF SYDNEY

Lequan Lin*, Dai Shi*, Andi Han, Zhiyong Wang, Junbin Gao

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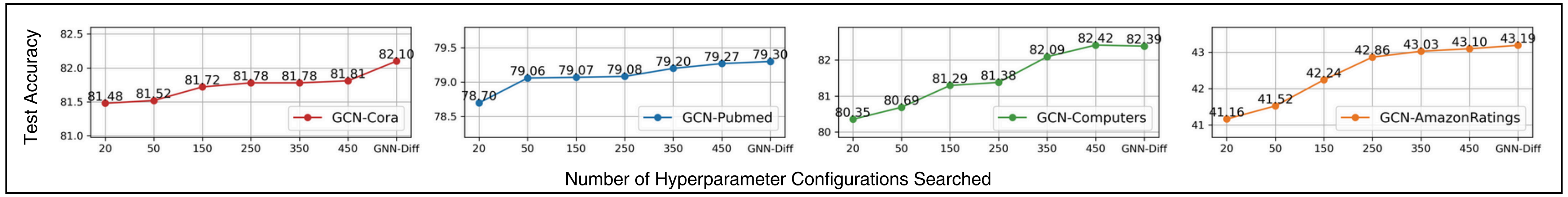
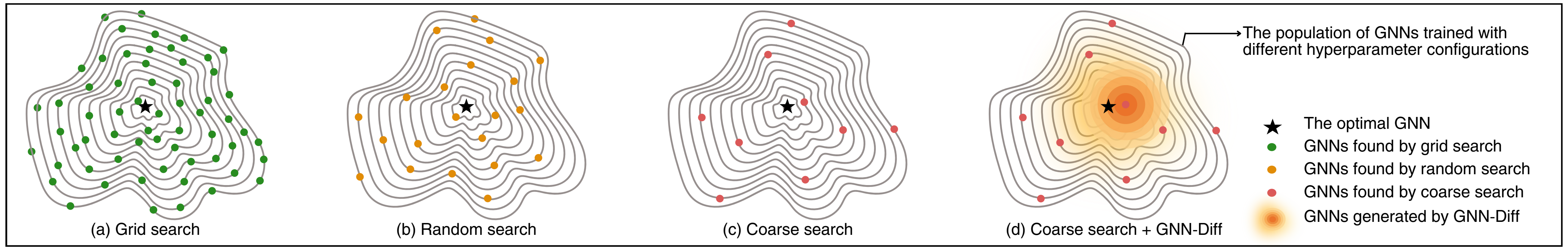
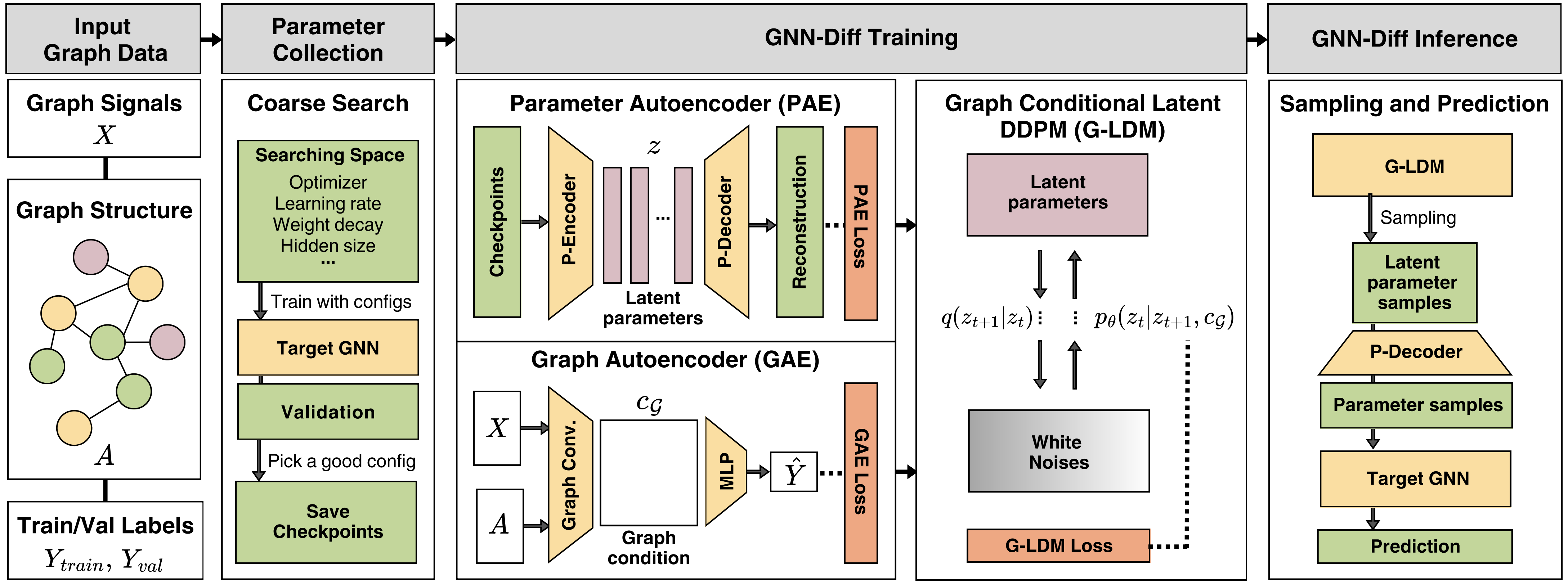
Motivation We observe that GNN's predictive accuracvy typically increases with the size of search space in hyperparameter tuning, but with a cost of very long tuning time.



The Proposed Method Collect samples from a coarse search with minimal search space (around 10% of the grid search), and then train a generative diffusion model to estimate the population of GNN parameters. Lastly, we generate high quality GNN parameters directly.



Overview of The Generative Pipeline This is a visualized process of our method (GNN-Diff) for GNN node classification. We adopt a latent conditional diffusion architecture. Parameters are converted to low-dimensional representations before learned by the diffusion process. A graph-based condition is included to guide the generation.

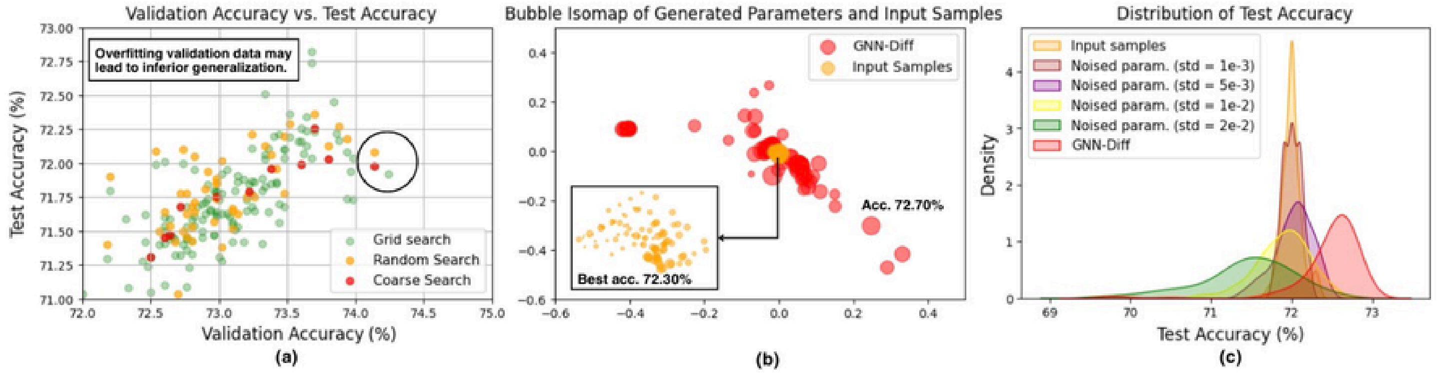


Key Results (1) Comparison with other search methods on node classification (partial results); (2) Visualization analysis; (3) Time advantage; (4) Is graph condition useful?

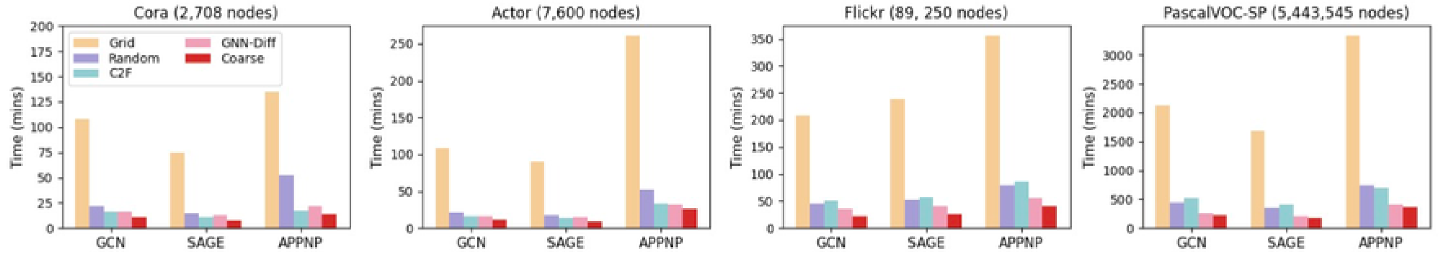
(1) GNNs with parameters generated by GNN-Diff generally perform better than those found by other search methods. We also show results for other 18 datasets and 3 tasks in the paper.

Datasets	Cora (Homophily)					Citeseer (Homophily)				
Models	Grid	Random	Coarse	C2F	GNN-Diff	Grid	Random	Coarse	C2F	GNN-Diff
MLP	59.41 ± 0.94	58.32 ± 1.21	58.28 ± 0.68	57.83 ± 1.58	$\mathbf{59.47 \pm 0.43}$	58.26 ± 1.04	57.63 ± 1.45	57.51 ± 1.30	57.63 ± 1.44	$\mathbf{58.72 \pm 0.84}$
GCN	82.04 ± 0.96	81.52 ± 0.71	81.89 ± 0.48	81.99 ± 0.95	$\mathbf{82.33 \pm 0.17}$	71.92 ± 1.10	72.04 ± 0.56	71.97 ± 0.67	72.13 ± 0.23	$\mathbf{72.37 \pm 0.29}$
SAGE	80.58 ± 1.04	80.49 ± 0.77	80.43 ± 0.78	80.43 ± 0.78	$\mathbf{80.60 \pm 0.15}$	$\mathbf{70.56 \pm 0.58}$	69.50 ± 0.61	68.81 ± 0.86	70.39 ± 0.91	70.45 ± 0.14
APPNP	81.91 ± 0.90	81.69 ± 0.62	81.47 ± 0.51	81.91 ± 0.90	$\mathbf{82.51 \pm 0.29}$	70.82 ± 1.40	69.87 ± 0.45	69.68 ± 0.63	69.60 ± 1.32	$\mathbf{71.44 \pm 0.17}$
GAT	81.10 ± 0.52	81.05 ± 0.82	80.13 ± 1.18	80.52 ± 1.29	$\mathbf{81.69 \pm 0.10}$	70.83 ± 0.58	70.81 ± 0.69	70.45 ± 1.13	69.82 ± 1.10	$\mathbf{71.50 \pm 0.09}$
ChebNet	81.83 ± 0.46	81.51 ± 0.85	81.30 ± 0.88	81.73 ± 1.09	$\mathbf{82.05 \pm 0.55}$	71.14 ± 0.13	71.24 ± 0.75	71.02 ± 1.12	71.14 ± 0.13	$\mathbf{71.65 \pm 0.27}$
H2GCN	82.05 ± 0.81	81.67 ± 0.71	81.63 ± 0.88	82.11 ± 0.72	$\mathbf{82.17 \pm 0.12}$	71.49 ± 0.89	71.30 ± 1.31	71.39 ± 0.19	71.12 ± 0.98	$\mathbf{71.78 \pm 0.25}$
SGC	81.89 ± 0.94	82.09 ± 0.55	81.60 ± 0.80	82.09 ± 0.55	$\mathbf{82.10 \pm 0.24}$	71.94 ± 0.56	71.82 ± 0.26	71.77 ± 0.23	71.70 ± 0.43	$\mathbf{72.10 \pm 0.18}$
GPRGNN	81.03 ± 0.65	81.34 ± 0.63	81.21 ± 0.64	81.41 ± 0.84	$\mathbf{81.79 \pm 0.20}$	70.93 ± 1.19	70.44 ± 0.71	70.05 ± 0.94	70.93 ± 1.19	$\mathbf{71.86 \pm 0.19}$
MixHop	80.08 ± 1.43	79.39 ± 0.77	78.81 ± 0.66	79.50 ± 0.73	$\mathbf{80.32 \pm 0.71}$	70.88 ± 0.94	70.54 ± 1.27	70.15 ± 0.68	70.81 ± 1.16	$\mathbf{71.50 \pm 0.49}$

(2) We notice via visualization that: i) grid search may lead to overfitting on validation; ii) GNN-Diff indeed generates parameters by looking into the potential population; iii) Parameters generaterd by GNN-Diff are of better quality than simply adding random noises.



(3) Time costs of GNN-Diff (pink). Clear time advantage compared to grid search. Generate better parameters in much shorter time. Almost free lunch!



(4) p-Diff is the unconditional version of GNN-Diff, where graph condition is not included. We obseve that parameters generated by GNN-Diff show better accuracy & stability.

Models	GCN		SAGE	
Methods	GNN-Diff	p-diff	GNN-Diff	p-diff
Cora	$\mathbf{82.33 \pm 0.17}$	81.96 ± 0.31	$\mathbf{80.60 \pm 0.05}$	80.19 ± 0.60
Actor	$\mathbf{31.24 \pm 0.26}$	30.96 ± 0.30	36.11 ± 0.09	$\mathbf{36.25 \pm 0.31}$
Flickr	$\mathbf{52.84 \pm 0.04}$	52.70 ± 0.11	$\mathbf{53.70 \pm 0.02}$	53.55 ± 0.23
PascalVOC-SP	$\mathbf{23.52 \pm 0.08}$	23.49 ± 0.09	$\mathbf{28.24 \pm 0.06}$	28.12 ± 0.02

More experiment results & analyses can be found in the paper. For any questions, please contact:

lequan.lin@sydney.edu.au

*Equal contributions. In memory of MeiMei , whose love and companionship will always be remembered.