GNN2GNN: Graph Neural Networks to Generate Neural Networks

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Introduction

Motivations

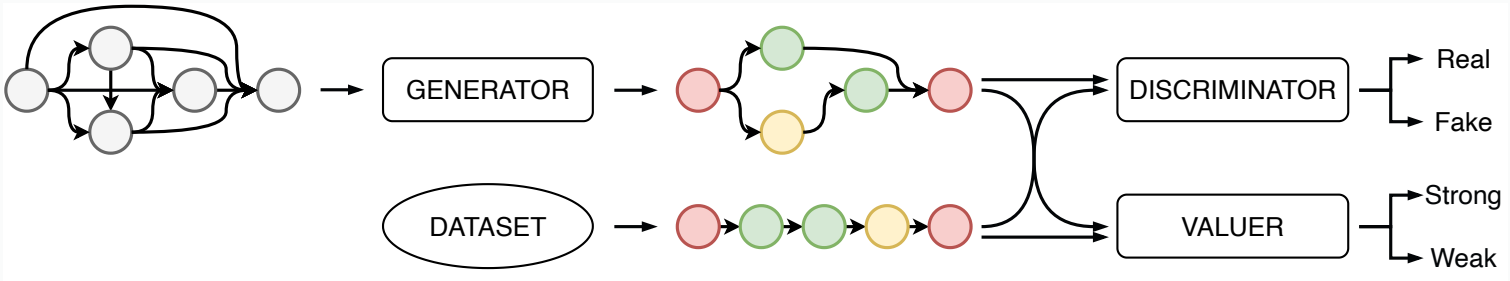
- NNs performance vastly depends on their architecture
- NAS automatically search optimal NN structures
- NAS learn *to search* rather than *to build*
- NAS lack in flexibility and generality

Contributions

- GNN2GNN, the first GNN-based framework to generate powerful NN architectures, without inefficient search
- Show GNN2GNN's effectiveness over two state-of-the-art datasets, highlighting flexibility and generalization capability

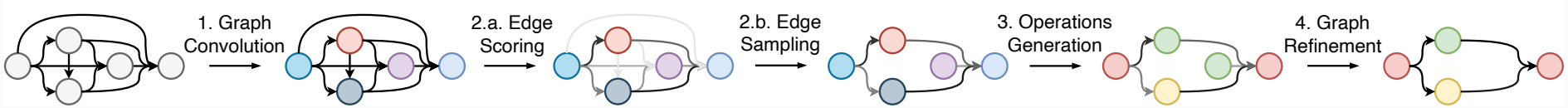
GNN2GNN Framework

Three-way generative adversarial framework



$$\mathcal{L}_G = \lambda \cdot \underbrace{\log(1 - D(G(z)))}_{\text{standard GAN loss}} + (1 - \lambda) \cdot \underbrace{\mathcal{L}_R(V(G(z)))}_{\text{reward loss}}$$

Generator framework



Experiments & Results

GNN2GNN vs GANs

Dataset	Model	Novelty	Top-5	Top-10	Top-50	Acc_{90}	|Acc|
NAS101	GNN2GNN	82.60%	45.91%	52.21%	57.37%	81.79%	92.04%
	MOLGAN	65.41%	22.63%	27.29%	45.20%	59.71%	89.39%
	RNN	96.34%	1.69%	2.32%	4.81%	53.04%	89.32%
	Random	51.81%	11.17%	13.74%	28.43%	43.18%	88.54%

Quality Degradation

Dataset	N	Novelty	Top-5	Top-10	Top-50	Acc_{90}	|Acc|
NAS101	10%	82.60%	45.91%	52.21%	57.37%	81.79%	92.04%
	20%	83.01%	45.54%	52.32%	58.48%	82.05%	91.98%
	30%	83.67%	46.10%	51.07%	57.04%	80.14%	91.68%
	40%	84.89%	45.80%	51.03%	58.71%	81.03%	91.55%
	50%	85.00%	44.01%	48.81%	56.30%	79.24%	91.33%
	60%	84.58%	44.40%	49.12%	57.72%	80.30%	91.30%
	70%	84.20%	44.66%	49.38%	56.71%	79.52%	91.37%
	80%	84.33%	43.90%	48.27%	55.51%	78.16%	91.27%
	90%	85.71%	42.77%	46.70%	55.72%	78.24%	91.22%

Generalisation

Dataset Train	Dataset Test	Novelty	Top-5	Top-10	Top-50	|Acc|
$NATS_{C10}$	$NATS_{C10}$	76.73%	1.65%	3.39%	15.61%	68.91%
NAS101	$NATS_{C10}$	73.67%	2.64%	5.08%	16.55%	70.25%
$NATS_{C100}$	$NATS_{C100}$	71.71%	1.30%	3.28%	13.10%	33.03%
NAS101	$NATS_{C100}$	72.03%	2.64%	4.82%	16.90%	35.40%
$NATS_{I}$	$NATS_{I}$	81.03%	0.91%	2.17%	8.42%	16.75%
NAS101	$NATS_{I}$	82.30%	1.93%	3.64%	11.49%	18.84%

GNN2GNN vs NAS

Model	|Acc|	Best Acc	Best Rank
DARTS [1]	92.21%	93.02%	57079
NAO [2]	92.59%	93.33%	19552
ENAS [3]	91.83%	92.54%	96939
$GNN2GNN_{90}$	92.04%	94.32%	5372
$GNN2GNN_{60}$	91.68%	94.18%	7843
$GNN2GNN_{30}$	91.30%	94.01%	9371
$GNN2GNN_{10}$	91.22%	93.69%	12570

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