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SGAS: Sequential Greedy Architecture Search

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Overview

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Background

- NAS
- Existing Problems

SGAS: Sequential Greedy Architecture Search

- Greedy Decision
- Selection Criteria

Search architectures for CNN and GCN

- CNN (CIFAR-10 & ImagNet)
- GCN (ModelNet & PPI)

NAS - Motivation

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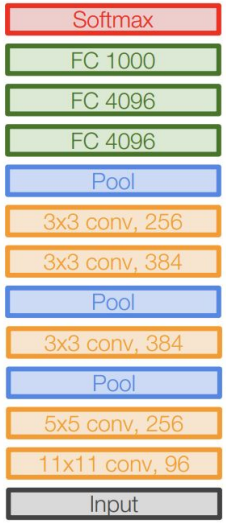
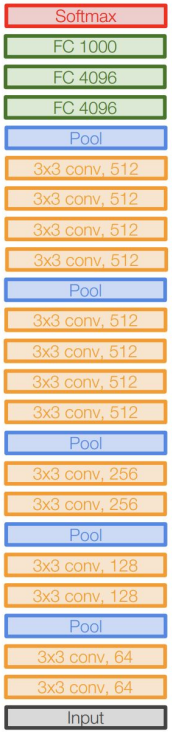
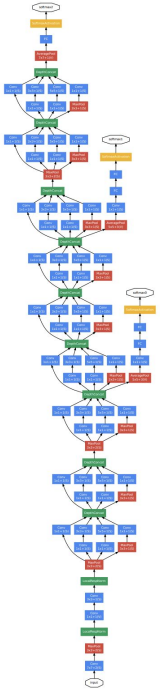


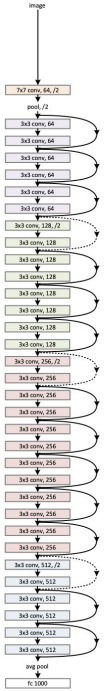
AlexNet



VGG19



GoogleNet

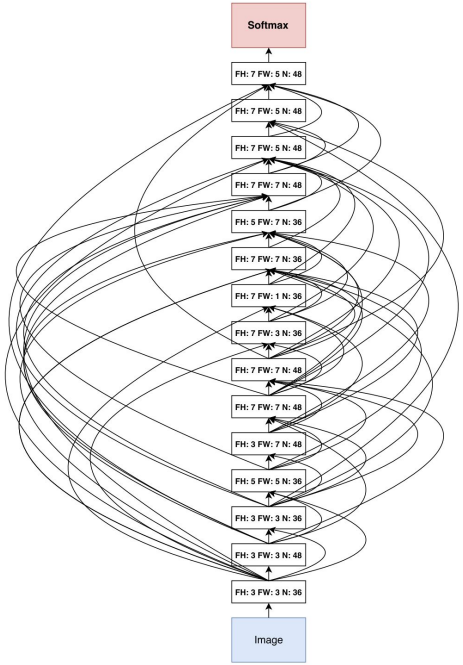


ResNet

…

Designing Arch. is Painful!

A Smarter Way?



NAS with RL

NAS - Problem Definition

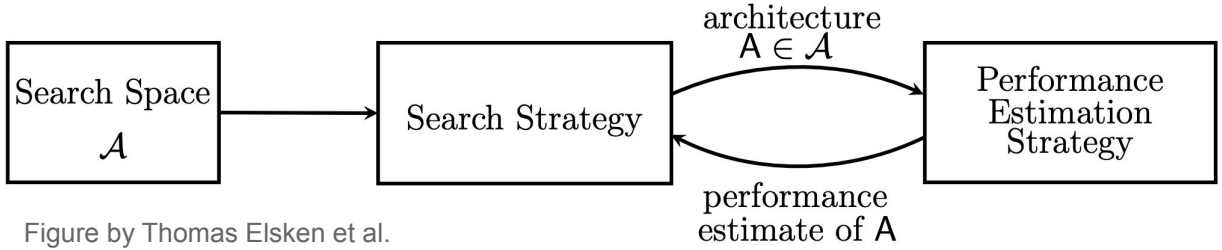
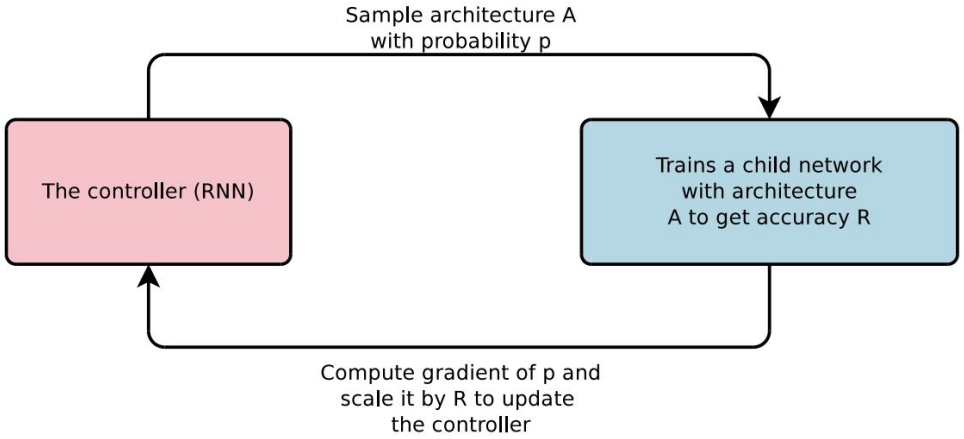


Figure by Thomas Elsken et al.

- **Given:** A Search Space
- **Goal:** Find The Best Arch.
- **Approach:** Design A Good Search Strategy

Design a search strategy instead of an instance of architecture

NAS - RL Based



Search Space:

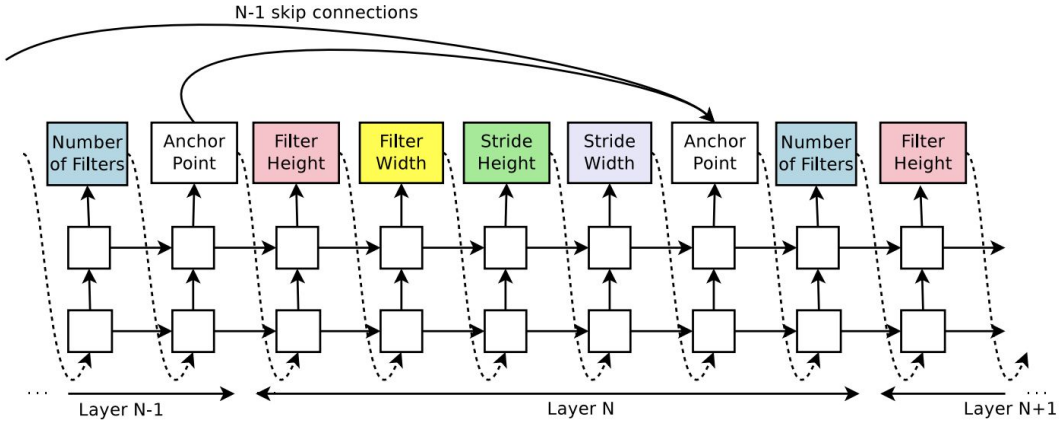
Filter Height [1, 3, 5, 7]
Filter Width [1, 3, 5, 7]
# of Filters [24, 36, 48, 64]

Search Strategy:

A RNN Controller
Learn to Generate Model Descriptions
Trained by REINFORCE

Zoph B, Le Q. Neural Architecture Search with Reinforcement Learning (ICLR'2017)

NAS - RL Based



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Trained by REINFORCE

800 GPUs, 21-28 Days

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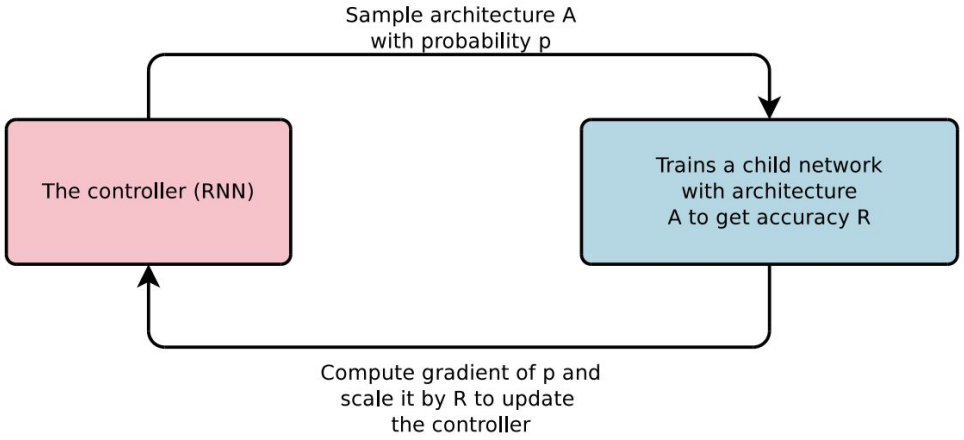
NAS - RL Based



NASNet: Cell Based, 450 GPUs, 3-4 Days

ENAS: Weight Sharing, 1 GPU, 0.45 (4*) Days

MnasNet: Platform-Aware, 64 TPUs, 4.5 Days

MobileNetV3, EfficientNet, NAS-FPN, ...

Zoph B, Le Q. Neural Architecture Search with Reinforcement Learning (ICLR'2017)

NAS - Evolution Based

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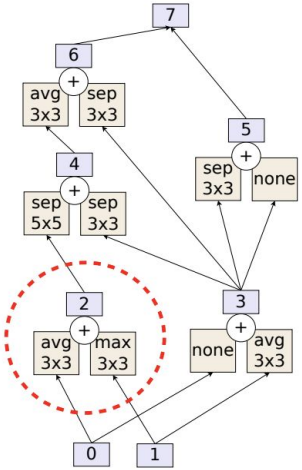
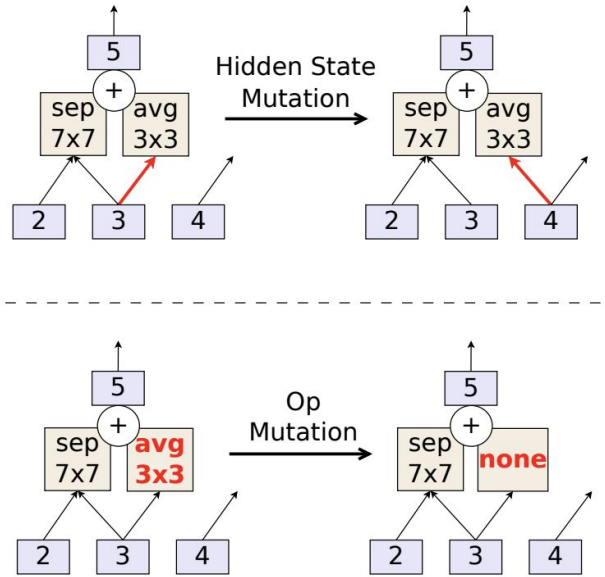
AmoebaNet





Search Space:

Cell Based

Pairwise Combinations of ops

Candidate ops:

none (identity);

3x3, 5x5 and 7x7 sep. conv.;

3x3 average pool; 3x3 max pool;

3x3 dilated sep. conv.;

1x7 then 7x1 conv.

Search Strategy:

Aging Evolution:

Population, Mutation, Aging

2000 GPU Days

Real, E., Aggarwal, A., Huang, Y. and Le, Q.V., Regularized Evolution for Image Classifier Architecture Search (AAAI'2019)

SMASH, Hier. Evo., SPOS, FairNAS, AutoML-Zero...

NAS - Gradient Based

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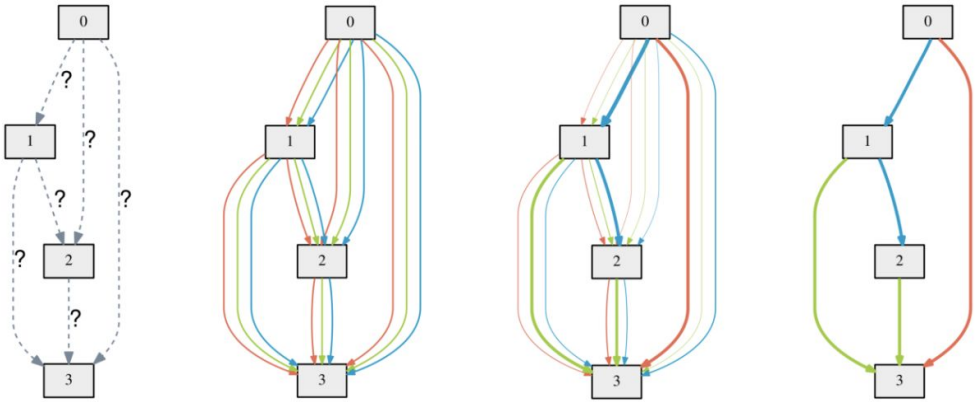
DARTS



Search Space:

- Cell Based
- DAG
- Candidate ops:
  - identity, and zero;
  - 3 × 3, 5 × 5 sep. conv.;
  - 3 × 3, 5 × 5 dilated sep. conv.;
  - 3 × 3 max pool, 3 × 3 average pool.

Search Strategy:

- Super-net
- Softmax Over All Possible ops (like attention)
- Weight Sharing
- Trained by Gradient Descent

Liu H, Simonyan K, Yang Y. DARTS: Differentiable Architecture Search (ICLR'2019)

NAS - Gradient Based

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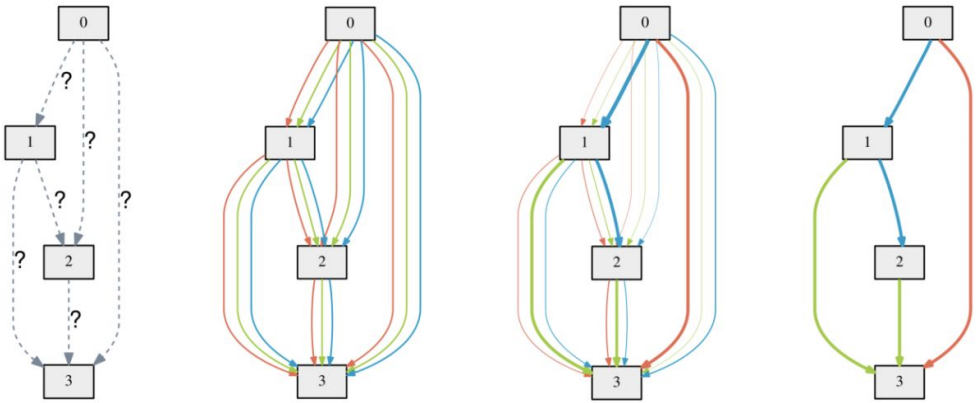
DARTS



Liu H, Simonyan K, Yang Y. DARTS: Differentiable Architecture Search (ICLR'2019)

Softmax Over All Possible ops:

$$\bar{o}^{(i,j)}(x) = \sum_{o \in \mathcal{O}} \frac{\exp(\alpha_o^{(i,j)})}{\sum_{o' \in \mathcal{O}} \exp(\alpha_{o'}^{(i,j)})} o(x)$$

Select The Most Likely op:

$$o^{(i,j)} = \text{argmax}_{o \in \mathcal{O}} \ \alpha_o^{(i,j)}$$

Only 1 GPU Day!

SNAS, FBNet, ProxylessNAS, P-DARTS, GDAS, MdeNAS, PC-DARTS, FairDARTS, ...

Existing Problems

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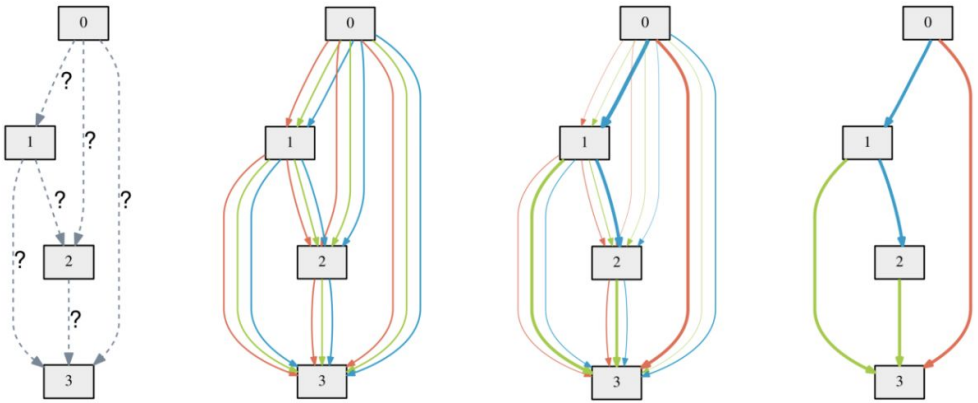
DARTS



Devils in Softmax and Weight Sharing:

(1) Softmax is too soft
(2) Soft model cannot reflect the true accuracy
(3) Discrete model w/o weight sharing never gets evaluated during the search

An Extreme Case:

skip-connect (0.34), 3x3Conv (0.33), 5x5 Conv (0.33)
&
skip-connect (0.33), 3x3Conv (0.34), 5x5 Conv (0.33)

Liu H, Simonyan K, Yang Y. DARTS: Differentiable Architecture Search (ICLR'2019)

Existing Problems

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Search Ranking	Evaluation Ranking: DARTS (1st Order)	DARTS (2nd Order)	SGAS (Criterion 1)	SGAS (Criterion 2)
1	4	8	2	4
2	2	5	3	6
3	7	9	1	1
4	8	6	6	2
5	1	4	8	3
6	5	3	7	10
7	10	7	4	5
8	9	1	5	8
9	6	10	10	9
10	3	2	9	7
Kendall τ	0.16	-0.29	0.56	0.42
Avg. Acc.	97.15	97.18	97.34	97.33

Figure 1. Comparison of search-evaluation Kendall coefficients.

Architectures with a higher validation accuracy during the search phase may perform worse in the evaluation (see Figure 1).

Degenerate Search-Evaluation Correlation Problem

SGAS

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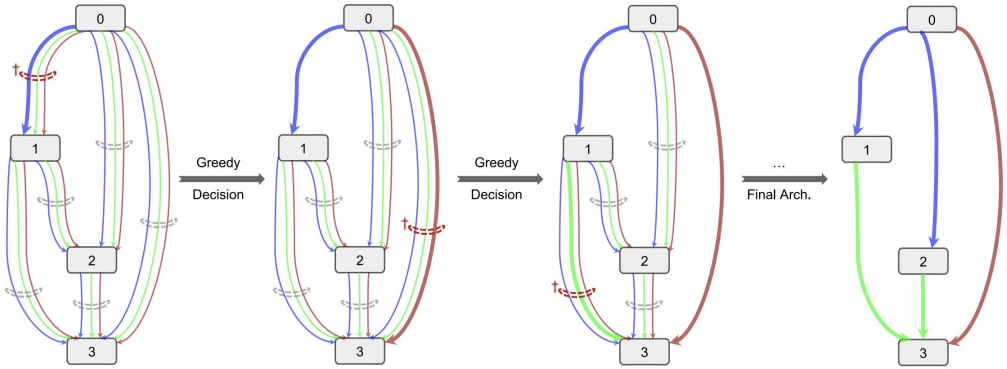

SGAS: Sequential Greedy Architecture Search (CVPR'2020, Guohao Li et.al)

https://www.deepgcns.org/auto/sgas

SGAS

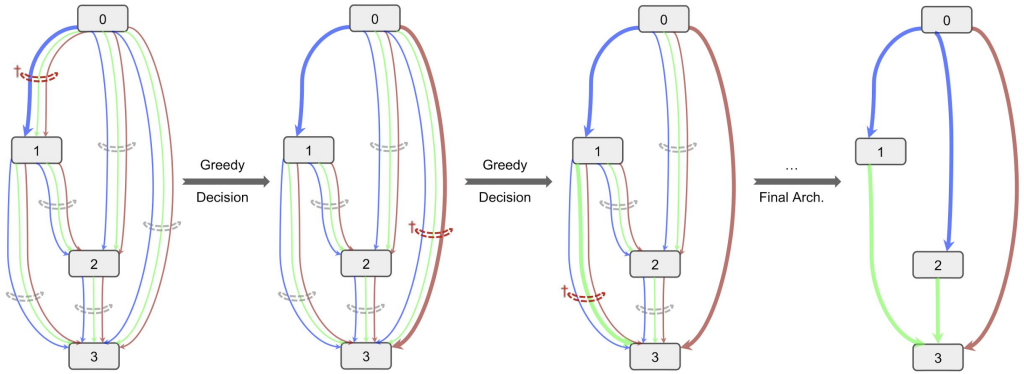

Figure 2. Illustration of Sequential Greedy Architecture Search.

Aiming to alleviate this common issue, we introduce sequential greedy architecture search (SGAS), an efficient method for neural architecture search.

By dividing the search procedure into sub-problems, SGAS chooses and prunes candidate operations in a greedy fashion.

SGAS - Greedy Decision

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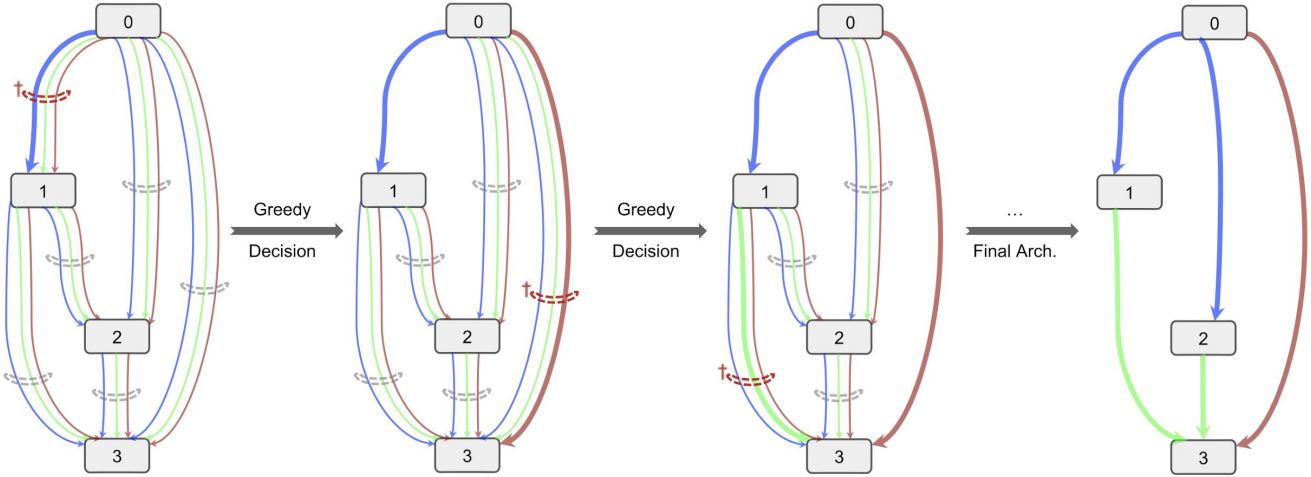

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SGAS - Greedy Decision

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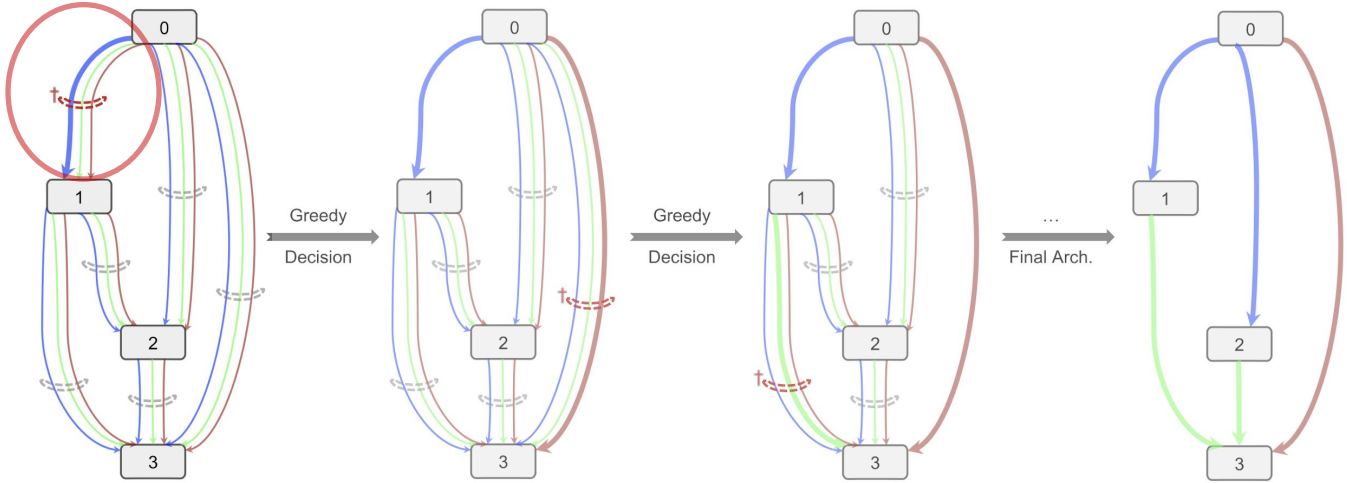

Figure 2. Illustration of Sequential Greedy Architecture Search.

1 If a decision epoch, select an edge $(i^\dagger, j^\dagger)$ based on the greedy *Selection Criterion*

SGAS - Greedy Decision

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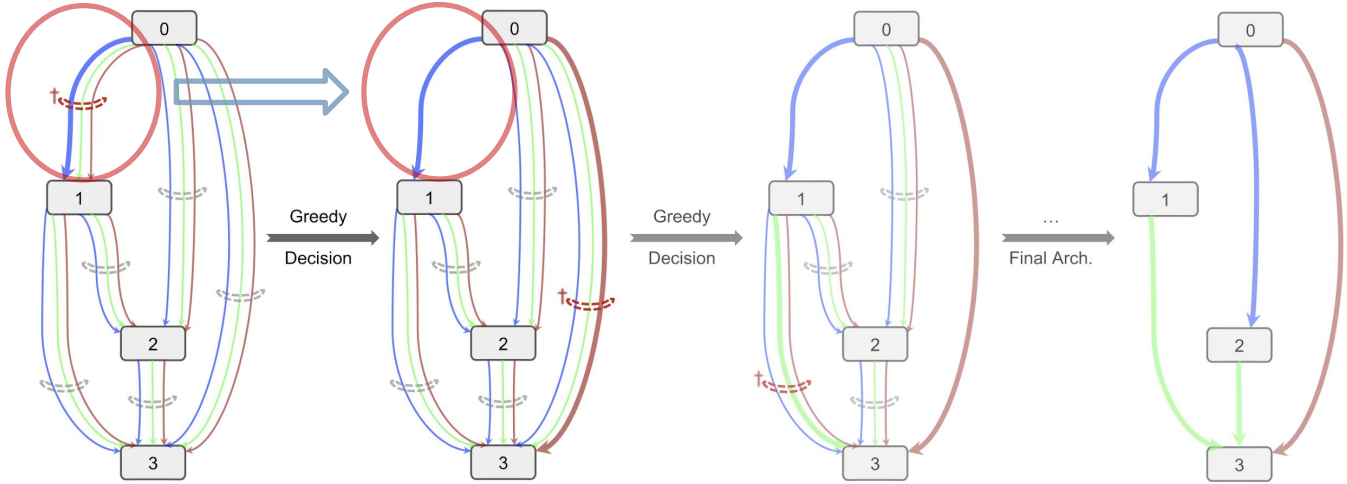
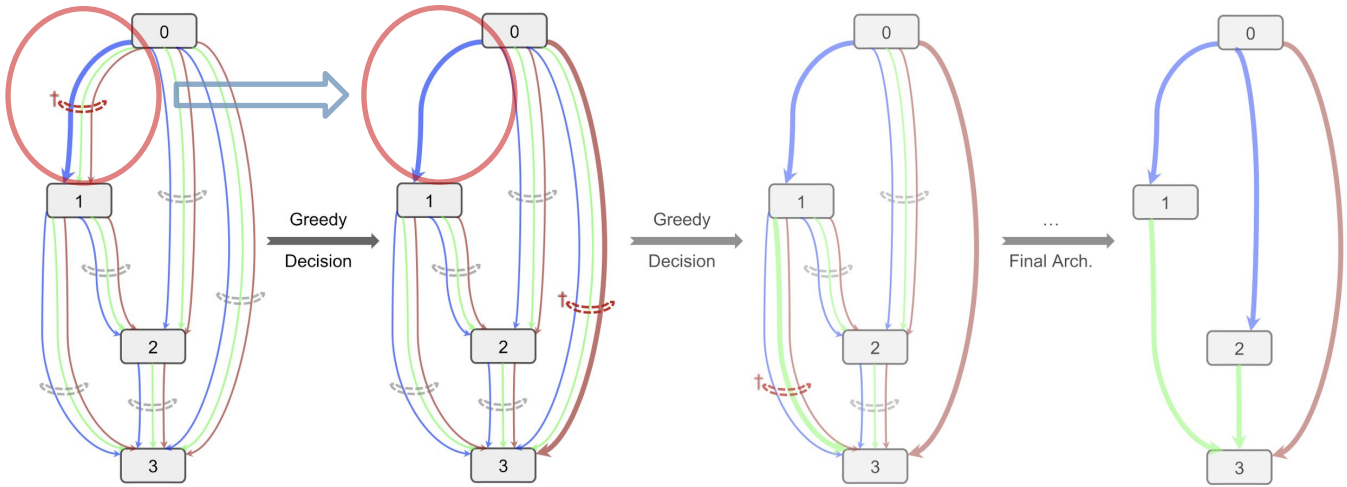


Figure 2. Illustration of Sequential Greedy Architecture Search.

1. If a decision epoch, select an edge $(i^\dagger, j^\dagger)$ based on the greedy *Selection Criterion*
2. Determine the operation by replacing $\bar{o}^{(i^\dagger,j^\dagger)}$ with $o^{(i^\dagger,j^\dagger)} = \text{argmax}_{o\in\mathcal{O}} \ \alpha_o^{(i^\dagger,j^\dagger)}$

SGAS - Greedy Decision

DeepGCNs.org



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3. Prune unchosen weights from $\mathcal{W}$, Remove $\alpha^{(i^\dagger,j^\dagger)}$ from $\mathcal{A}$

SGAS - Greedy Decision

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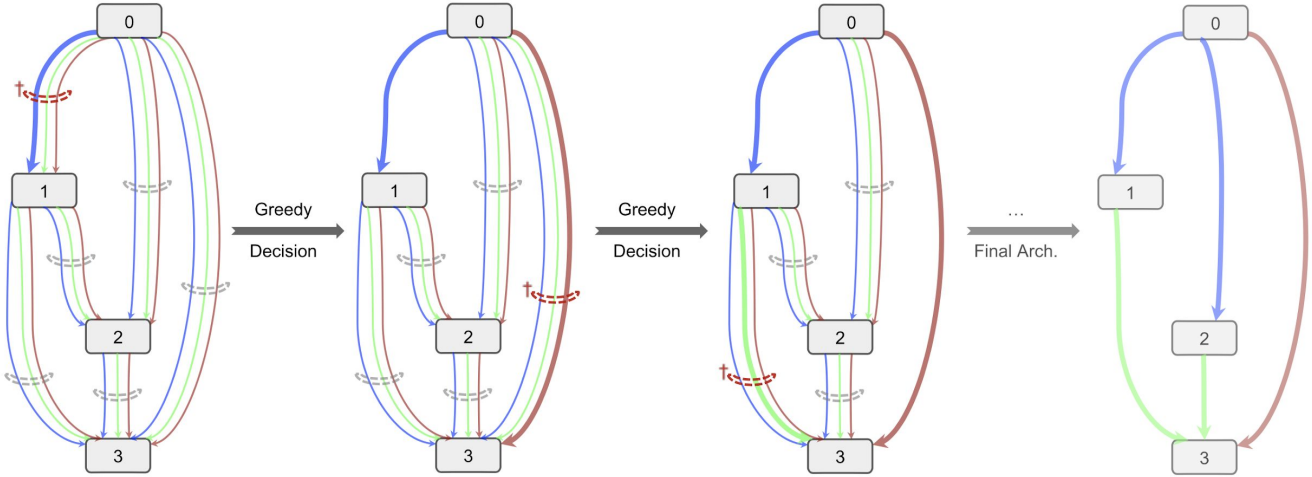
Repeat…



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SGAS - Greedy Decision

DeepGCNs.org

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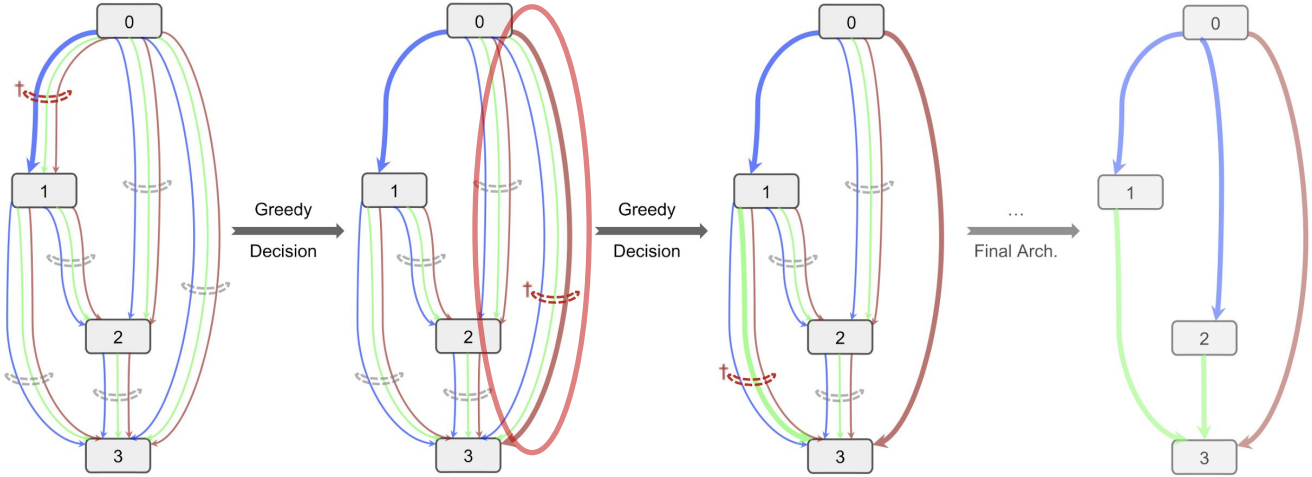

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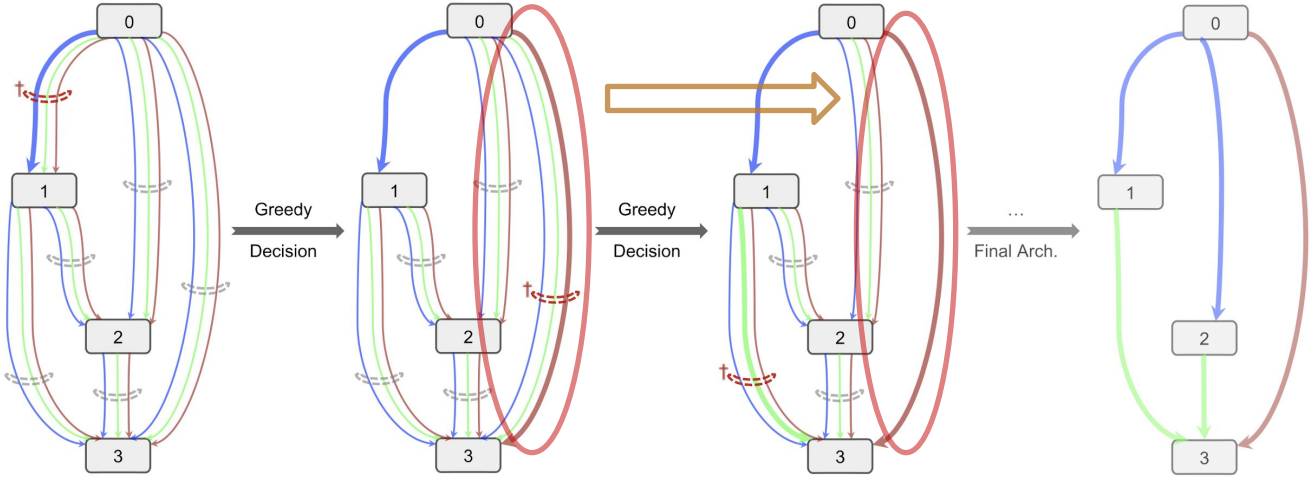

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SGAS - Greedy Decision

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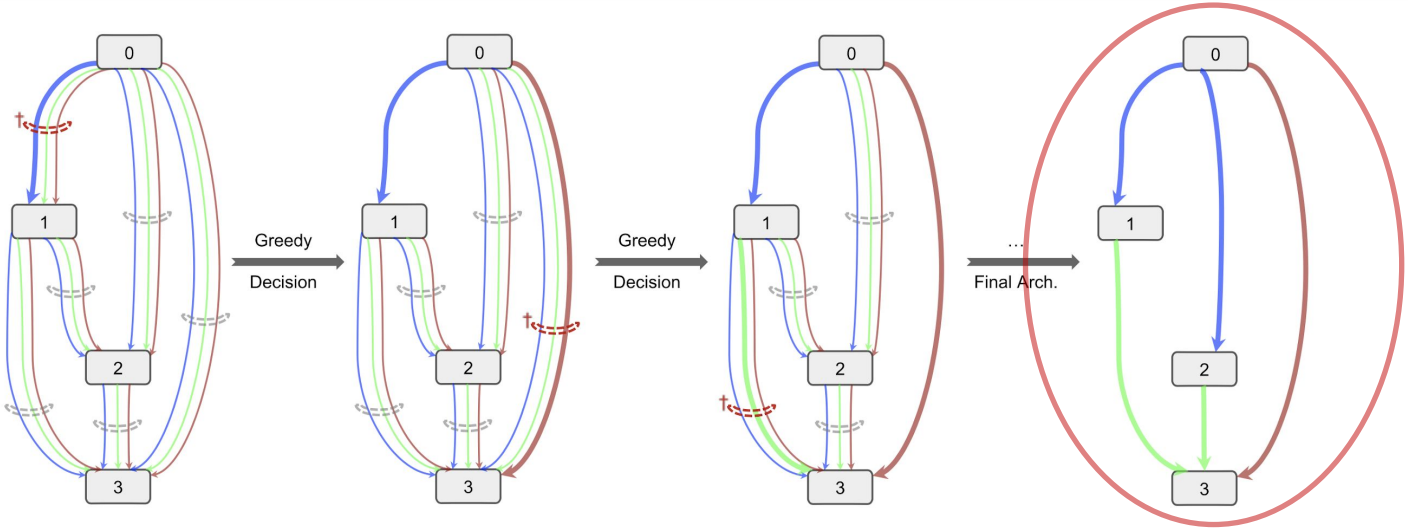
Until…



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3. Prune unchosen weights from $\mathcal{W}$, Remove $\alpha^{(i^\dagger,j^\dagger)}$ from $\mathcal{A}$

SGAS - Selection Criteria

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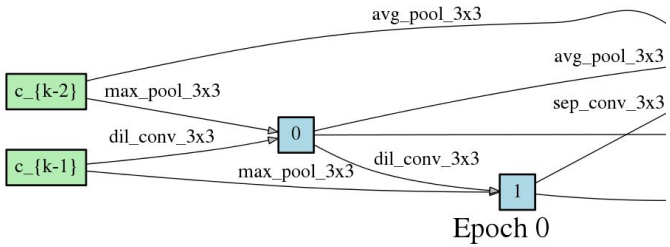
To maintain the optimality, the design of the selection criterion is crucial.



Edge Importance:

$$S_{EI}^{(i,j)} = \sum_{o \in \mathcal{O}, o \neq zero} \frac{\exp(\alpha_o^{(i,j)})}{\sum_{o' \in \mathcal{O}} \exp(\alpha_{o'}^{(i,j)})}$$

Selection Certainty:

$$p_o^{(i,j)} = \frac{\exp(\alpha_o^{(i,j)})}{S_{EI}^{(i,j)} \sum_{o' \in \mathcal{O}} \exp(\alpha_{o'}^{(i,j)})}, o \in \mathcal{O}, o \neq zero$$

$$S_{SC}^{(i,j)} = 1 - \frac{-\sum_{o \in \mathcal{O}, o \neq zero} p_o^{(i,j)} \log(p_o^{(i,j)})}{\log(|\mathcal{O}| - 1)}$$

Selection Stability:

$$S_{SS}^{(i,j)} = \frac{1}{K} \sum_{t=T-K}^{T-1} \sum_{o_t \in \mathcal{O} o_t, \neq zero} \min(p_{o_t}^{(i,j)}, p_{o_T}^{(i,j)})$$

SGAS - Selection Criteria

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Criterion 1:

$$S_1^{(i,j)} = \text{normalize}(S_{EI}^{(i,j)}) * \text{normalize}(S_{SC}^{(i,j)})$$

Criterion 2:

$$S_2^{(i,j)} = S_1^{(i,j)} * \text{normalize}(S_{SS}^{(i,j)})$$

$normalize(\cdot)$: a standard Min-Max scaling normalization

Edge Importance:

$$S_{EI}^{(i,j)} = \sum_{o \in \mathcal{O}, o \neq zero} \frac{\exp(\alpha_o^{(i,j)})}{\sum_{o' \in \mathcal{O}} \exp(\alpha_{o'}^{(i,j)})}$$

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SGAS for CNN on CIFAR-10

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Architecture	Test Err. (%)	Params (M)	Search Cost (GPU-days)	Search Method
DenseNet-BC [18]	3.46	25.6	-	manual
NASNet-A [55]	2.65	3.3	1800	RL
AmoebaNet-A [36]	3.34±0.06	3.2	3150	evolution
AmoebaNet-B [36]	2.55±0.05	2.8	3150	evolution
Hier-Evolution [28]	3.75±0.12	15.7	300	evolution
PNAS [27]	3.41±0.09	3.2	225	SMBO
ENAS [34]	2.89	4.6	0.5	RL
NAONet-WS [31]	3.53	3.1	0.4	NAO
DARTS (1st order) [29]	3.00±0.14	3.3	0.4	gradient
DARTS (2nd order) [29]	2.76±0.09	3.3	1	gradient
SNAS (mild) [49]	2.98	2.9	1.5	gradient
ProxylessNAS [7]	2.08	-	4	gradient
P-DARTS [8]	2.5	3.4	0.3	gradient
BayesNAS [52]	2.81±0.04	3.4	0.2	gradient
PC-DARTS [50]	2.57±0.07	3.6	0.1	gradient
SGAS (Cri.1 avg.)	2.66±0.24*	3.7	0.25	gradient
SGAS (Cri.1 best)	2.39	3.8	0.25	gradient
SGAS (Cri.2 avg.)	2.67±0.21*	3.9	0.25	gradient
SGAS (Cri.2 best)	2.44	4.1	0.25	gradient

Table 3. Performance comparison with state-of-the-art image classifiers on CIFAR-10.

SGAS for CNN on CIFAR-10

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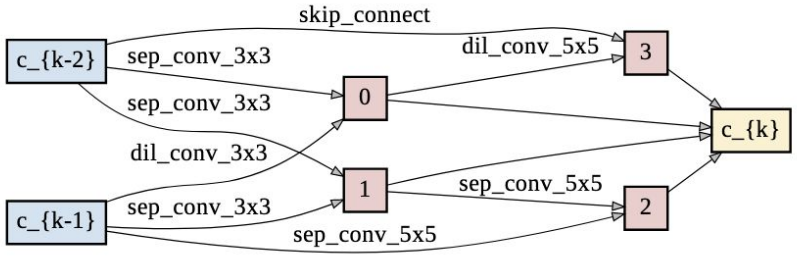
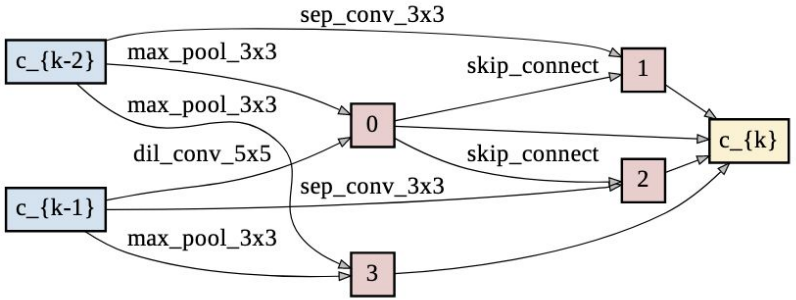
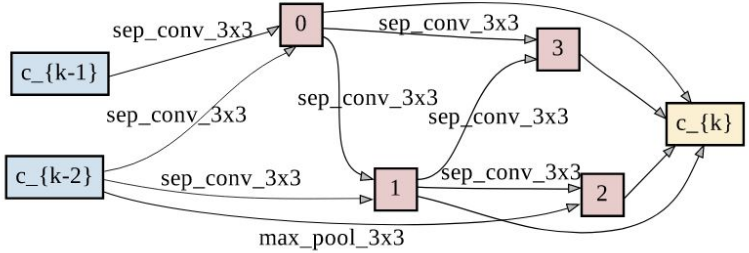


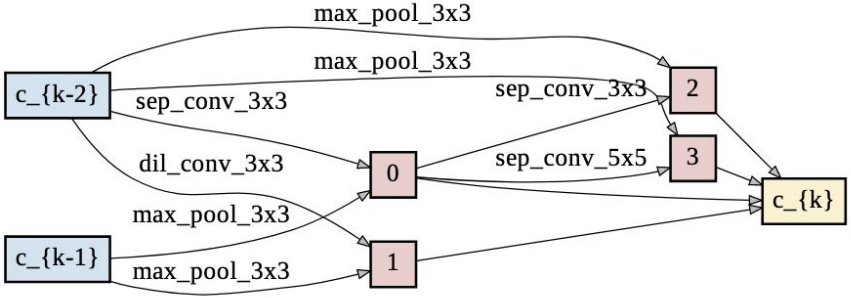
(a) Normal cell of the best model with SGAS (Cri. 1) on CIFAR-10



(b) Reduction cell of the best model with SGAS (Cri. 1) on CIFAR-10



(c) Normal cell of the best model with SGAS (Cri. 2) on CIFAR-10



(d) Reduction cell of the best model with SGAS (Cri. 2) on CIFAR-10

SGAS for CNN on ImageNet

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Architecture	Test Err. (%) top-1	top-5	Params (M)	×+ (M)	Search Cost (GPU-days)	Search Method
Inception-v1 [41]	30.2	10.1	6.6	1448	-	manual
MobileNet [16]	29.4	10.5	4.2	569	-	manual
ShuffleNet 2x (v1) [51]	26.4	10.2	~5	524	-	manual
ShuffleNet 2x (v2) [32]	25.1	-	~5	591	-	manual
NASNet-A [55]	26	8.4	5.3	564	1800	RL
NASNet-B [55]	27.2	8.7	5.3	488	1800	RL
NASNet-C [55]	27.5	9	4.9	558	1800	RL
AmoebaNet-A [36]	25.5	8	5.1	555	3150	evolution
AmoebaNet-B [36]	26	8.5	5.3	555	3150	evolution
AmoebaNet-C [36]	24.3	7.6	6.4	570	3150	evolution
PNAS [27]	25.8	8.1	5.1	588	225	SMBO
MnasNet-92 [42]	25.2	8	4.4	388	-	RL
DARTS (2nd order) [29]	26.7	8.7	4.7	574	4.0	gradient
SNAS (mild) [49]	27.3	9.2	4.3	522	1.5	gradient
ProxylessNAS [7]	24.9	7.5	7.1	465	8.3	gradient
P-DARTS [8]	24.4	7.4	4.9	557	0.3	gradient
BayesNAS [52]	26.5	8.9	3.9	-	0.2	gradient
PC-DARTS [50]	25.1	7.8	5.3	586	0.1	gradient
SGAS (Cri.1 avg.)	24.4±0.2	7.3±0.1	5.3	579	0.25	gradient
SGAS (Cri.1 best)	24.2	7.2	5.3	585	0.25	gradient
SGAS (Cri.2 avg.)	24.4±0.2	7.4±0.1	5.4	597	0.25	gradient
SGAS (Cri.2 best)	**24.1**	7.3	5.4	598	0.25	gradient

Table 4. Performance comparison with state-of-the-art image classifiers on ImageNet.

SGAS for CNN on ImageNet

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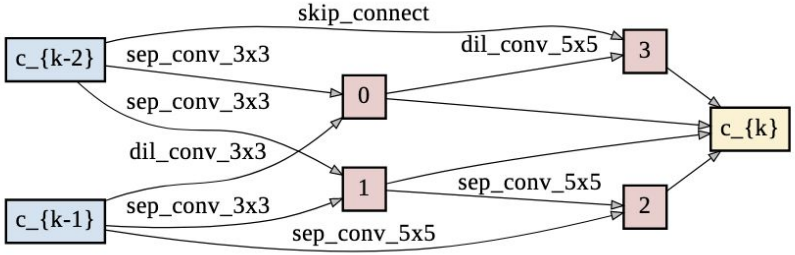
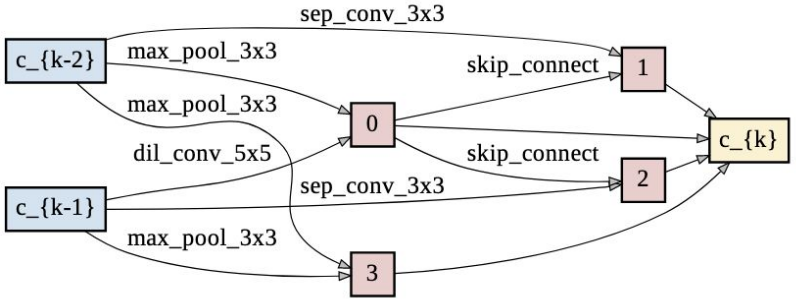
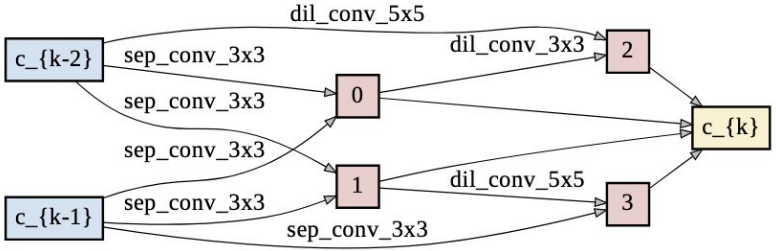


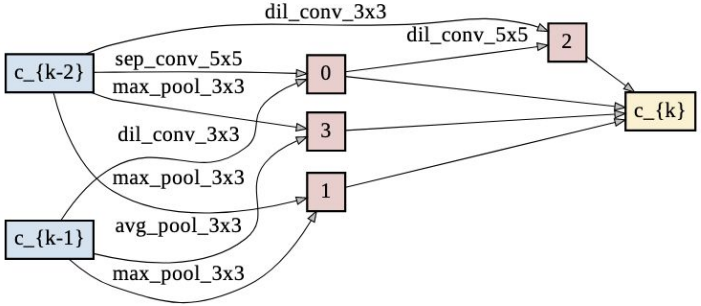
(a) Normal cell of the best model with SGAS (Cri. 1) on ImageNet



(b) Reduction cell of the best model with SGAS (Cri. 1) on ImageNet



(c) Normal cell of the best model with SGAS (Cri. 2) on ImageNet



(d) Reduction cell of the best model with SGAS (Cri. 2) on ImageNet

SGAS for GCN

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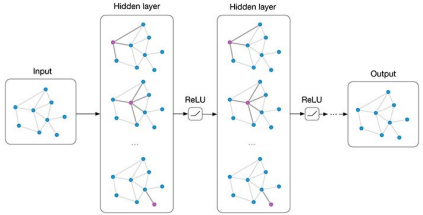
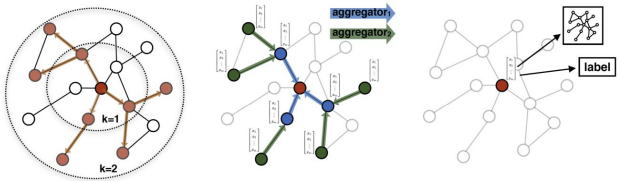
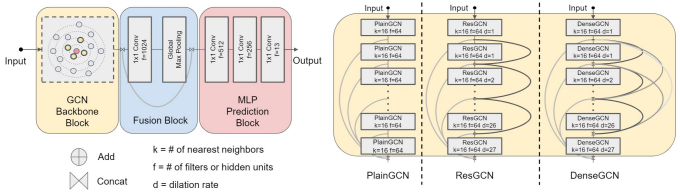


Kipf, T.N. and Welling, M., 2016. Semi-Supervised Classification with Graph Convolutional Networks.

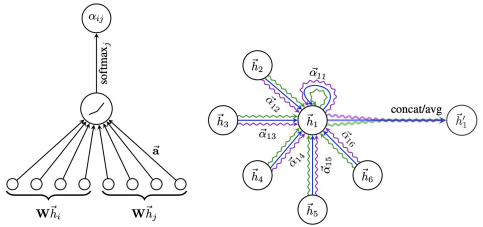


Hamilton, W.L., Ying, R. and Leskovec, J., 2017. Inductive Representation Learning on Large Graphs.

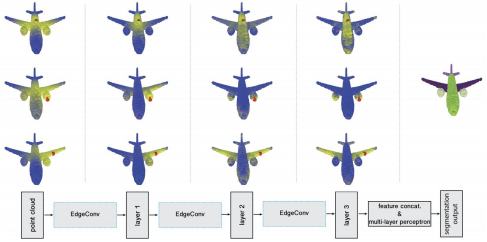


Li, G., Müller, M., Thabet, A. and Ghanem, B., 2019. DeepGCNs: Can GCNs Go as Deep as CNNs?

SemiGCN, GraphSage, GAT, EdgeConv, DeepGCNs, … are manually designed



Veličković, P., Cucurull, G., Casanova, A., Romero, A., Liò, P. and Bengio, Y., 2018. Graph Attention Networks.



Wang, Y., Sun, Y., Liu, Z., Sarma, S.E., Bronstein, M.M. and Solomon, J.M., 2018. Dynamic Graph CNN for Learning on Point Clouds.

Search Space:
skip-connect, zero operation, conv-1×1, MRConv, EdgeConv, GAT, SemiGCN, GIN, SAGE, RelSAGE,

SGAS for GCN on ModelNet

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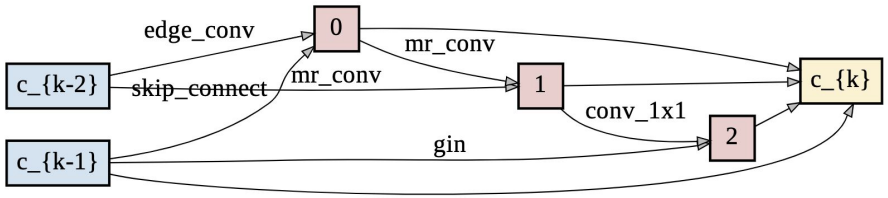
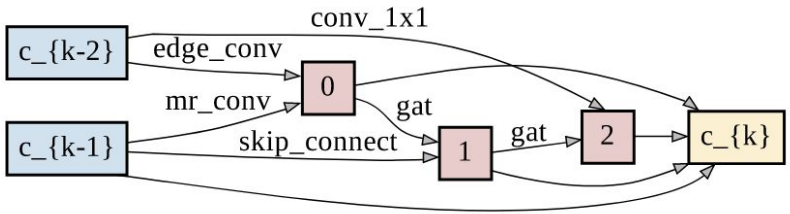
Architecture	OA (%)	Params (M)	Search Cost (GPU-days)
3DmFV-Net [3]	91.6	45.77	manual
SpecGCN [46]	91.5	2.05	manual
PointNet++ [37]	90.7	1.48	manual
PCNN [2]	92.3	8.2	manual
PointCNN [25]	92.2	0.6	manual
DGCNN [47]	92.2	1.84	manual
KPConv [44]	92.9	14.3	manual
Random Search	92.65±0.33	8.77	random
SGAS (Cri.1 avg.)	92.69±0.20	8.78	0.19
SGAS (Cri.1 best)	92.87	8.63	0.19
SGAS (Cri.2 avg.)	92.92±0.19	8.87	0.19
SGAS (Cri.2 best)	**93.23**	8.49	0.19
SGAS (Cri.2 small best)	93.07	3.86	0.19

Table 1. Comparison with state-of-the-art architectures for 3D object classification on ModelNet40.



(a) Normal cell of the best model with SGAS (Cri. 1) on ModelNet



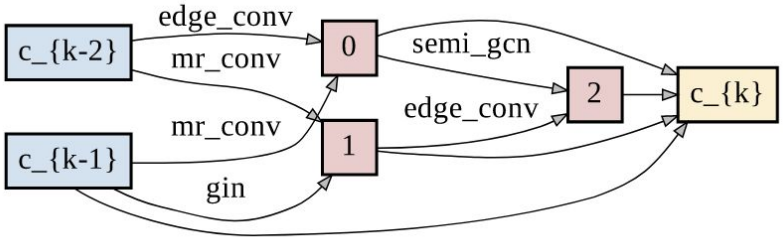
(b) Normal cell of the best model with SGAS (Cri. 2) on ModelNet

SGAS for GCN on PPI

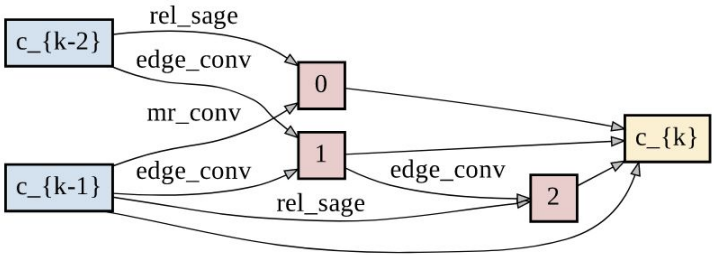
DeepGCNs.org

Architecture	micro-F1 (%)	Params (M)	Search Cost (GPU-days)
GraphSAGE (LSTM) [14]	61.2	0.26	manual
GeniePath [30]	97.9	1.81	manual
GAT [44]	97.3±0.2	3.64	manual
DenseMRGCN-14 [23]	99.43	53.42	manual
ResMRGCN-28 [23]	99.41	14.76	manual
Random Search	99.36±0.04	23.70	random
SGAS (Cri.1 avg.)	99.38±0.17	25.01	0.003
SGAS (Cri.1 best)	**99.46**	23.18	0.003
SGAS (Cri.2 avg.)	99.40±0.09	25.93	0.003
SGAS (Cri.2 best)	**99.46**	29.73	0.003
SGAS (small)	98.89	0.40	0.003

Table 2. Comparison with state-of-the-art architectures for node classification on PPI.



(a) Normal cell of the best model with SGAS (Cri. 1) on PPI



(b) Normal cell of the best model with SGAS (Cri. 2) on PPI

Conclusion

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- **Greedy Fashion:**
  - Alleviate the degenerate search-evaluation correlation problem
  - Very Fast and less GPU memory usage
  - Subproblems are easier to optimize, which leads to a better solution
- **Selection Criteria**: Maintain optimality in the search space
- **Application:**
  - Design CNN architectures (CIFAR-10 & ImageNet)
  - Design GCN architectures (ModelNet & PPI)

Team

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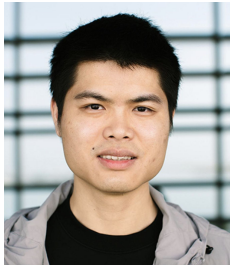

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(PI)

Project Links

DeepGCNs.org

- **Arxiv:** https://arxiv.org/abs/1912.00195
- **Project webpage:** https://www.deepgcns.org/auto/sgas
- **Code:** https://github.com/lightaime/sgas

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THANK YOU

SGAS: Sequential Greedy Architecture Search

More information see my personal website https://ghli.org

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