NAT: Neural Architecture Transformer for Accurate and Compact Architectures

Yong Guo[1*], Yin Zheng[2*], Mingkui Tan[1*†], Qi Chen[1],
Jian Chen[1†], Peilin Zhao[3], Junzhou Huang[3,4]

[1]South China University of Technology
[2]Weixin Group, Tencent [3]Tencent AI Lab
[4]University of Texas at Arlington

Published in NeurIPS 2019

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Background

Deep neural networks have achieved great success in many computer vision tasks, such as image classification, face recognition, object detection, etc.

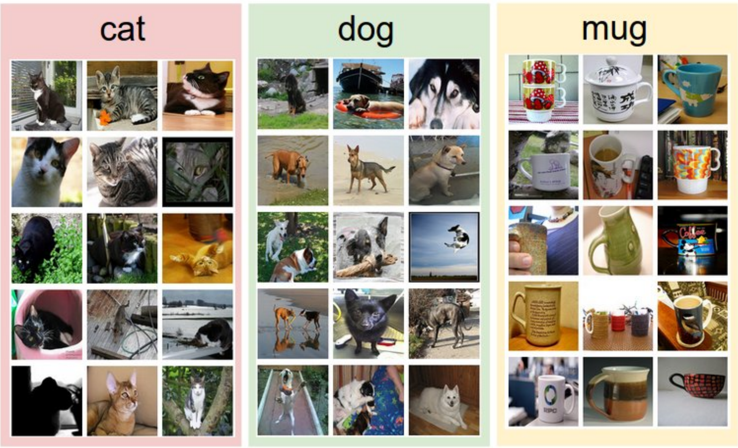
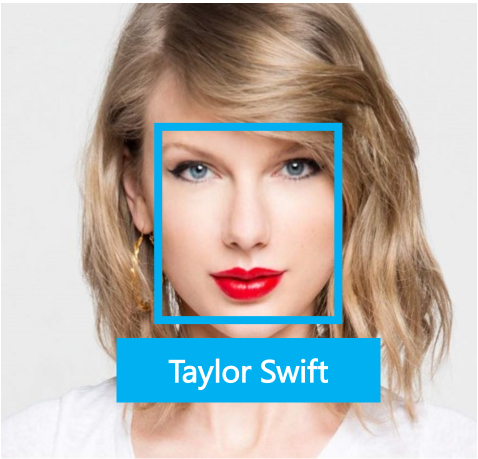
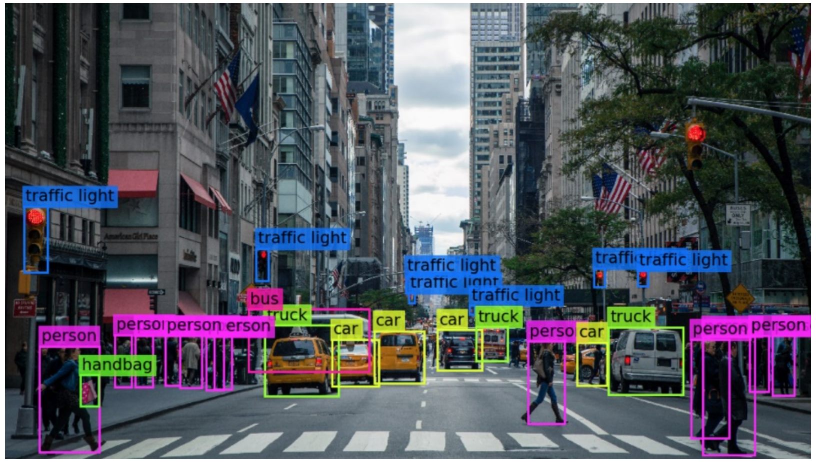


Image Classification



Face Recognition



Object Detection

Figure: Applications of deep neural networks.

Neural Architecture Design

- Neural architecture design is one of the key factors behind the success of deep neural networks.

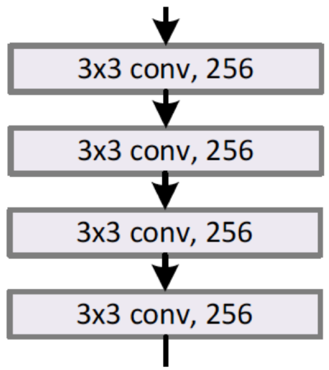
- Existing architectures can be divided into two categories:

  1. Hand-crafted architectures

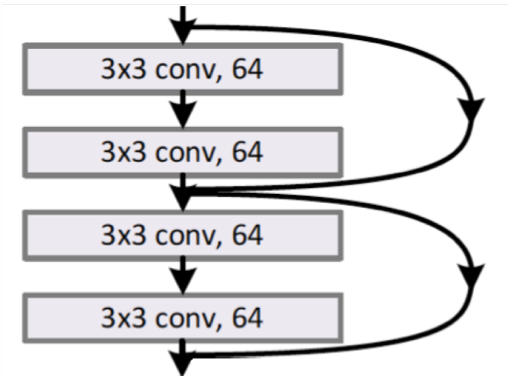
  2. Automatically searched architectures

Hand-crafted Architectures

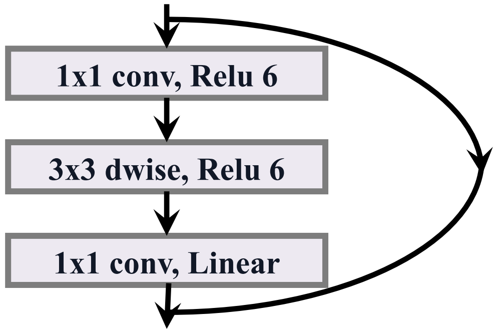
Several widely used hand-crafted architectures:



VGG



ResNet



MobileNetV2

Limitations of hand-crafted architecture design process

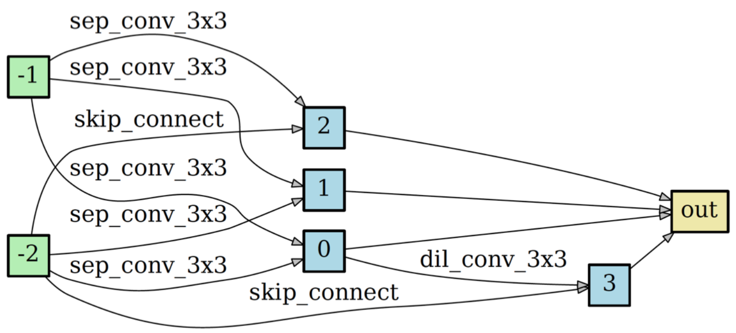
- Hand-crafted methods rely on substantial human expertise.
- Hand-crafted methods cannot fully explore the whole architecture space.

Automatically Searched Architectures

- There is a growing interest to replace the manual process of architecture design by Neural Architecture Search (NAS).

Graph Representation of Architectures: an architecture can be represented by a directed acyclic graph (DAG).

- Node: feature maps of a specific layer
- Edge: a computational operation, e.g., convolution



DARTS normal cell

Limitations of NAS methods

- Search space is extremely large, *e.g.*, billions of candidate architectures.
- NAS methods may find suboptimal architectures with limited performance.

Architecture Optimization

Since both the hand-crafted and NAS based architectures are not optimal, can we optimize architectures to obtain the better ones?

- One can design architecture optimization methods to optimize existing architectures for better performance.

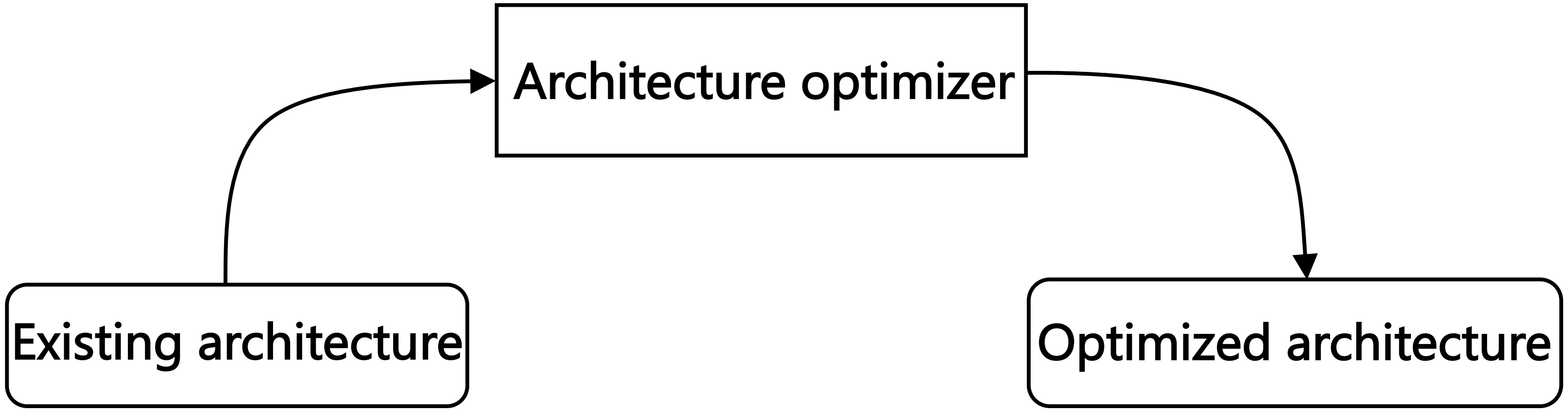
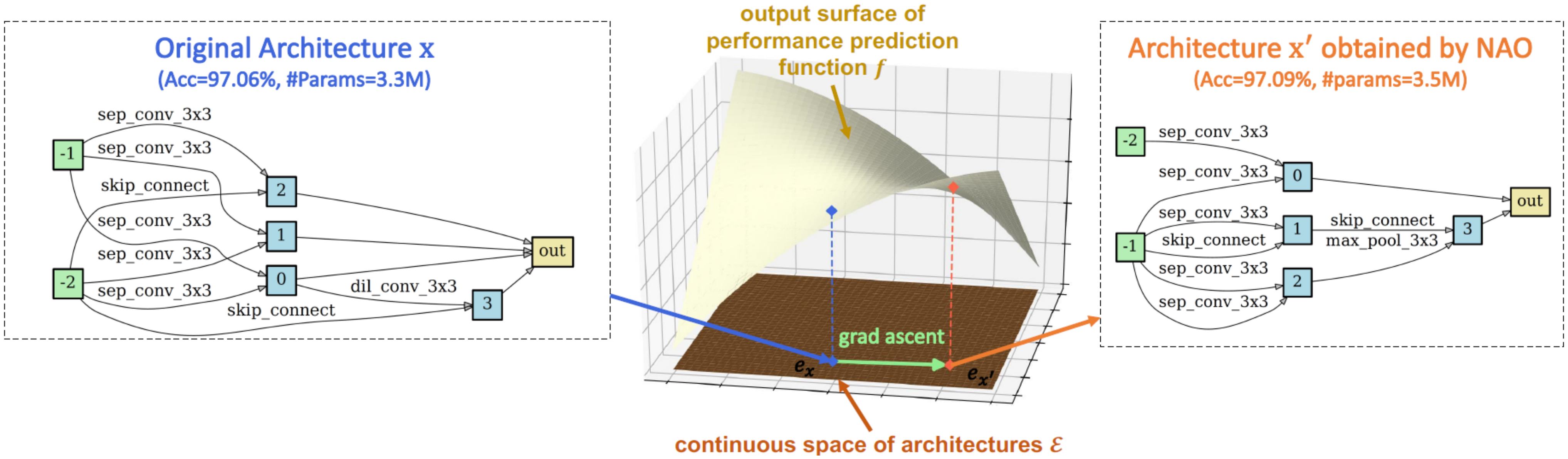


Figure: Architecture optimization scheme.

Existing Architecture Optimization Methods

- Neural Architecture Optimization (NAO)



Limitations of NAO

- NAO may introduce extra parameters or additional computational cost.
- NAO has a NAS search space that is unnecessarily huge and expensive to train.

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Motivation

- Both hand-crafted architectures and NAS based architectures may contain non-significant or redundant operations.
- Existing architecture optimization methods may introduce extra parameters or additional computational cost into the architectures.

How to transform the redundant operations in **any arbitrary architecture** to improve the performance without introducing extra computational cost?

Problem Definition

Our goal: Transforming any arbitrary architecture for **better performance and less computational cost**.

One solution: Replacing the redundant operations with the **more efficient ones**.

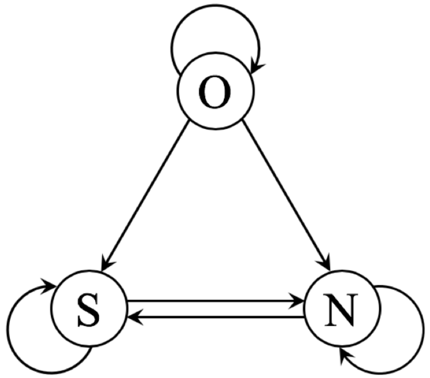


Figure: Operation transformation scheme.

- We divide the operations into three categories $\{S, N, O\}$. S denotes skip connection, N denotes null connection, O denotes the other operations.
- We have $c(O)>c(S)>c(N)$, where $c\,(\cdot)$ evaluates the computational cost.
- To reduce the computational cost, we allow the transitions: $O\rightarrow S$, $O\rightarrow N$, $S\rightarrow N$.
- Since skip connection has negligible cost but often can significantly improve the performance, we also allow $N\rightarrow S$.

Optimization for Arbitrary Architecture

Given any arbitrary architecture $\beta \sim p(\cdot)$, we seek to find the corresponding optimal architecture α . Then, the optimization problem can be formulated as

$$\max_{\theta} \mathbb{E}_{\beta \sim p(\cdot)} \left[R\left(\alpha | \beta\right) \right], \text{ s.t. } c(\alpha) \leq \kappa$$

- $R(\alpha|\beta) = R(\alpha, w_\alpha) - R(\beta, w_\beta)$ denotes the performance improvement between the optimized architectures α and the given architectures β. w_α and w_β are the parameters of α and β .
- $c(\cdot)$ is a function to measure the computation cost of architectures.
- κ is an upper bound of the computational cost.

Optimization for Arbitrary Architecture

$$\max_{\theta} \mathbb{E}_{\beta \sim p(\cdot)} \left[R\left(\alpha | \beta\right) \right], \text{ s.t. } c(\alpha) \leq \kappa$$

- It is non-trivial to directly obtain the optimal α.
- We instead sample α from the well learned policy, denoted by $\pi(\cdot \mid \beta; \theta)$, *i.e.*, $\alpha \sim \pi(\cdot \mid \beta; \theta)$.

To learn the policy, we solve the following optimization problem:

$$\max_{\theta} \mathbb{E}_{\beta \sim p(\cdot)} \left[\mathbb{E}_{\alpha \sim \pi(\cdot \mid \beta; \theta)} R(\alpha \mid \beta) \right], \text{ s.t. } c(\alpha) \leq \kappa, \alpha \sim \pi(\cdot \mid \beta; \theta)$$

where $\mathbb{E}_{\beta \sim p(\cdot)} [\mathbb{E}_{\alpha \sim \pi(\cdot \mid \beta; \theta)} R(\alpha \mid \beta)]$ denotes the expectation of $R(\alpha \mid \beta)$ over the distribution of $\beta \sim p(\cdot)$ and the distribution of $\alpha \sim \pi(\cdot \mid \beta; \theta)$.

Optimization for Arbitrary Architecture

$$\max_{\theta} \mathbb{E}_{\beta \sim p(\cdot)} [\mathbb{E}_{\alpha \sim \pi(\cdot|\beta;\theta)} R(\alpha \mid \beta)], \text{ s.t. } \underline{c(\alpha) \leq \kappa}, \alpha \sim \pi(\cdot \mid \beta; \theta)$$

Several challenges regarding the optimization problem

- It is hard to find a comprehensive measure to accurately evaluate the cost.
- The upper bound of computational cost κ is hard to determine.

Markov Decision Process for Learning NAT

Our solution

- We cast the optimization problem into an architecture transformation problem and reformulate it as a Markov decision process (MDP).
- We seek to optimize architectures by making a series of decisions to replace redundant operations with the more computationally efficient operations.

Benefits: We do not have to evaluate the cost $c(\alpha)$ or determine the upper bound κ to obtain an architecture with less computational cost.

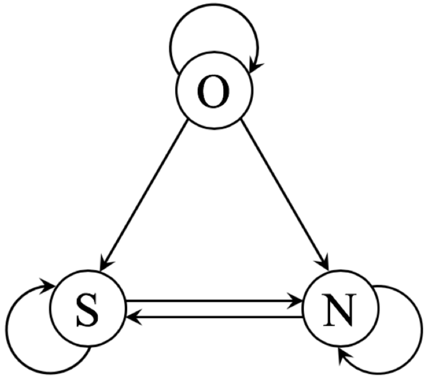


Figure: Operation transformation scheme.

Markov Decision Process for Learning NAT

Details of MDP

- An **architecture** is defined as a **state**.
- A **transformation mapping** $\beta \to \alpha$ is defined as an **action**.
- The **accuracy improvement** on validation set is regraded as **reward**.
- The **policy** $\pi(\cdot \mid \beta; \theta)$ parameterized by θ is the **probability distribution of the action**.

Based on MDP, how to build a model to learn the optimal policy π ?

Policy Learning by Graph Convolution Networks

To better exploit the adjacency information of the operations in an architecture, we use a two-layer graph convolutional network (GCN) to build the controller:

$$\mathbf{Z} = f(\mathbf{X}, \mathbf{A}) = \mathrm{Softmax}\left(\mathbf{A}\sigma\left(\mathbf{A}\mathbf{X}\mathbf{W}^{(0)}\right)\mathbf{W}^{(1)}\mathbf{W}^{\mathrm{FC}}\right)$$

Notations

- $\mathbf{A}$: adjacency matrix of the architecture graph.
- $\mathbf{X}$: attributes of the nodes in the graph.
- $\mathbf{W}^{(0)}$ and $\mathbf{W}^{(1)}$: weights of two graph convolution layers.
- $\mathbf{W}^{\mathrm{FC}}$: weight of the fully-connected layer.
- σ : non-linear activation function.
- $\mathbf{Z}$: probability distribution of different candidate operations, *i.e.*, the learned policy.

Training Method

We train the transformer parameters θ and the model parameter w in an alternative way.

- Training the model parameters w :

$$w \leftarrow w - \eta \frac{1}{m} \sum_{i=1}^{m} \nabla_w \mathcal{L}(\beta_i, w)$$

where $\mathcal{L}(\cdot)$ is the cross-entropy loss, η is the learning rate.

- Training the transformer parameters θ :

To encourage exploration, we introduce an entropy regularization term:

$$\begin{aligned} J(\theta) &= \mathbb{E}_{\beta \sim p(\cdot)} \left[\mathbb{E}_{\alpha \sim \pi(\cdot|\beta;\theta)} \left[R(\alpha, w) - R(\beta, w) \right] + \underline{\lambda H\big(\pi(\cdot|\beta;\theta)\big)} \right] \\ &= \sum_{\beta} p(\beta) \left[\sum_{\alpha} \pi(\alpha|\beta;\theta) \big(R(\alpha, w) - R(\beta, w) \big) + \underline{\lambda H\big(\pi(\cdot|\beta;\theta)\big)} \right] \end{aligned}$$

where $H(\cdot)$ evaluates the entropy of the policy, and λ controls the strength of the entropy regularization term.

Training Method

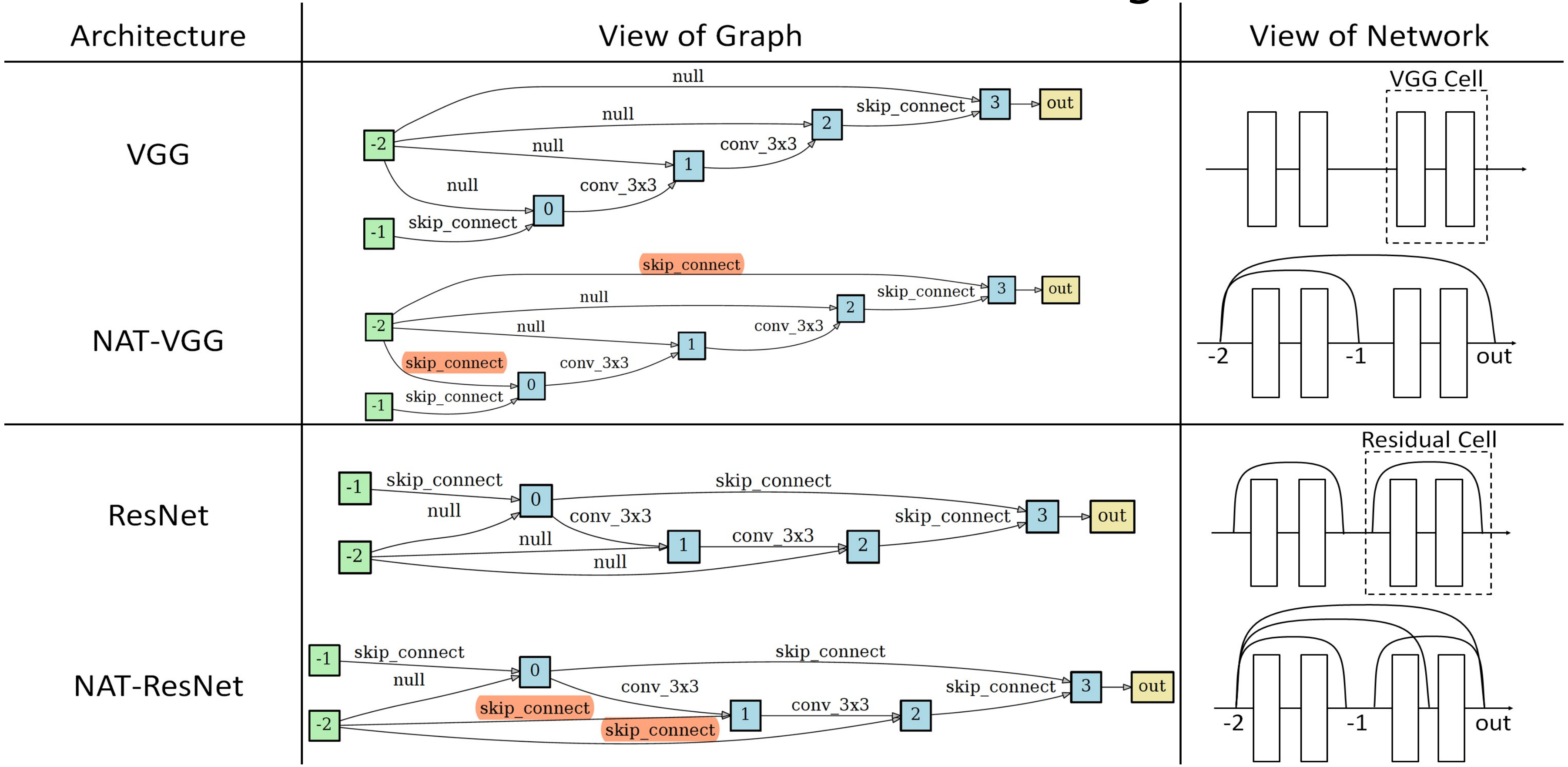
Algorithm 1 Training method for Neural Architecture Transformer (NAT).

Initiate w and θ.
while not convergent **do**
  for each iteration on training data **do**
    Sample $\beta_i \sim p(\cdot)$ to construct a batch $\{\beta_i\}_{i=1}^{m}$.
    Update the model parameters w by descending the gradient.
  end for
  for each iteration on validation data **do**
    Sample $\beta_i \sim p(\cdot)$ to construct a batch $\{\beta_i\}_{i=1}^{m}$.
    Obtain $\{\alpha_j\}_{j=1}^{n}$ according to the policy learned by GCN.
    Update the parameters θ by ascending the gradient.
  end for
end while

Contents

Visual Results of Hand-crafted Architectures

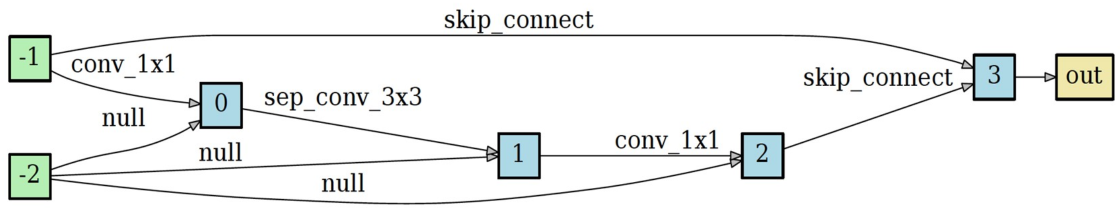
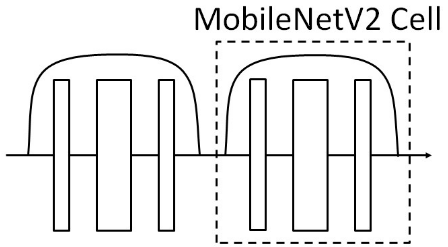
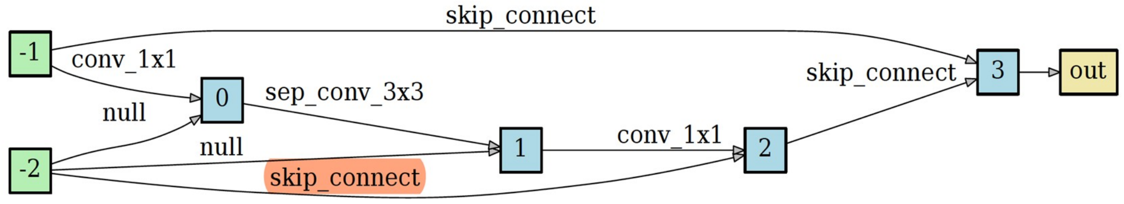
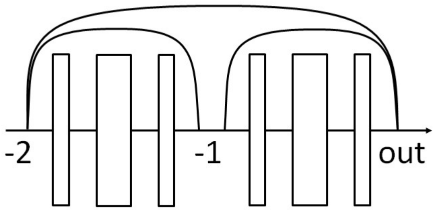
- Results on several hand-crafted architectures, including VGG, ResNet, and MobileNet.



➢ NAT introduces additional skip connections to improve the performance.

Visual Results of Hand-crafted Architectures

- Results on several hand-crafted architectures, including VGG, ResNet, and MobileNet.

Architecture	View of Graph	View of Network
MobileNetV2		
NAT-MobileNetV2		

➢ NAT introduces additional skip connections to improve the performance.

Comparison on Hand-crafted Architectures

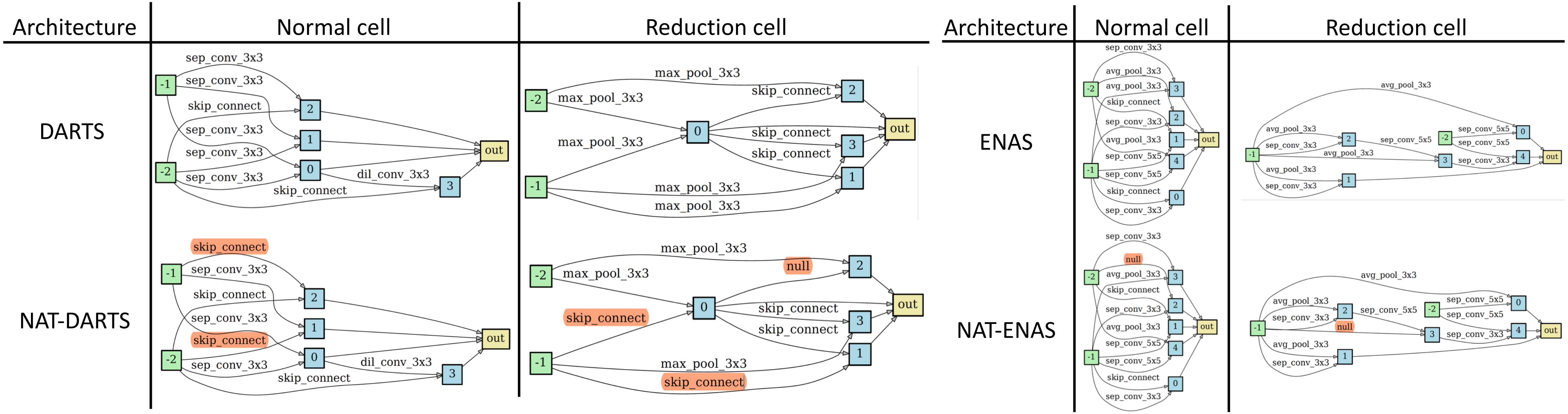
- Results on several hand-crafted architectures, including VGG, ResNet, and MobileNet.

CIFAR-10					ImageNet					
Model	Method	#Params (M)	#MAdds (M)	Acc. (%)	Model	Method	#Params (M)	#MAdds (M)	Acc. (%) Top-1	Acc. (%) Top-5
VGG16	/	15.2	313	93.56	VGG16	/	138.4	15620	71.6	90.4
	NAO[32]	19.5	548	95.72		NAO [32]	147.7	18896	72.9	91.3
	NAT	15.2	315	**96.04**		NAT	138.4	15693	**74.3**	**92.0**
ResNet20	/	0.3	41	91.37	ResNet18	/	11.7	1580	69.8	89.1
	NAO [32]	0.4	61	92.44		NAO [32]	17.9	2246	70.8	89.7
	NAT	0.3	42	**92.95**		NAT	11.7	1588	**71.1**	**90.0**
ResNet56	/	0.9	127	93.21	ResNet50	/	25.6	3530	76.2	92.9
	NAO [32]	1.3	199	95.27		NAO [32]	34.8	4505	77.4	93.2
	NAT	0.9	129	**95.40**		NAT	25.6	3547	**77.7**	**93.5**
MobileNetV2	/	2.3	91	94.47	MobileNetV2	/	3.4	300	72.0	90.3
	NAO [32]	2.9	131	94.75		NAO [32]	4.5	513	72.2	90.6
	NAT	2.3	92	**95.17**		NAT	3.4	302	**72.5**	**91.0**

- NAT based models yield significantly better performance with approximately the same computational cost as the baseline models.

Visual Results on NAS based Architectures

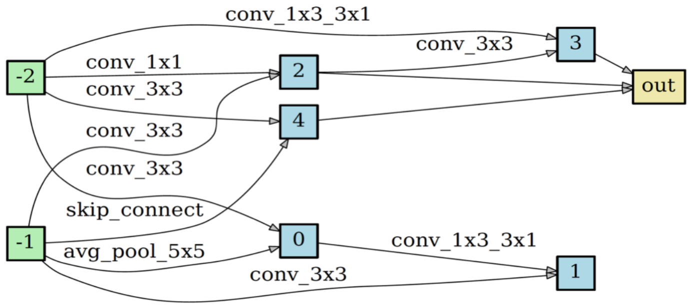
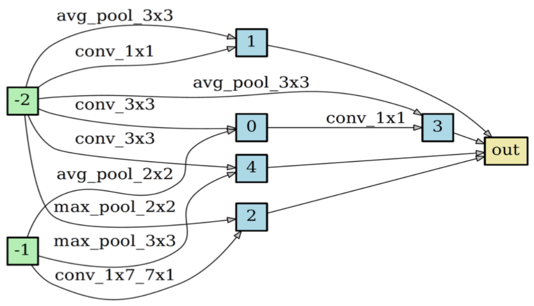
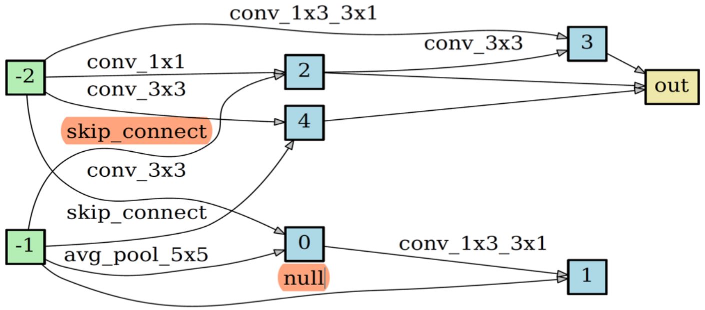
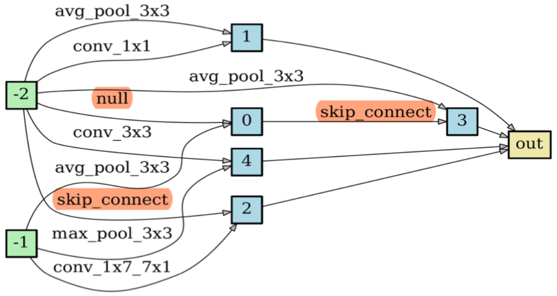
- Results on several NAS based architectures, including ENAS, DARTS, and NAONet.



➢ NAT replaces several redundant operations with the skip connections or directly removes the connections to reduce computation cost.

Visual Results on NAS based Architectures

- Results on several NAS based architectures, including ENAS, DARTS, and NAONet.

Architecture	Normal cell	Reduction cell
NAONet		
NAT-NAONet		

➢ NAT replaces several redundant operations with the skip connections or directly removes the connections to reduce computation cost.

Comparison on NAS based Architectures

- Results on several NAS based architectures, including ENAS, DARTS, and NAONet.

CIFAR-10					ImageNet					
Model	Method	#Params (M)	#MAdds (M)	Acc. (%)	Model	Method	#Params (M)	#MAdds (M)	Acc. (%) Top-1	Acc. (%) Top-5
AmoebaNet† [37]	/	3.2	-	96.73	AmoebaNet [37]	/	5.1	555	74.5	92.0
PNAS† [29]	/	3.2	-	96.67	PNAS [29]	/	5.1	588	74.2	91.9
SNAS† [50]	/	2.9	-	97.08	SNAS [50]	/	4.3	522	72.7	90.8
GHN† [54]	/	5.7	-	97.22	GHN [54]	/	6.1	569	73.0	91.3
ENAS† [36]	/	4.6	804	97.11	ENAS [36]	/	5.6	679	73.8	91.7
	NAO [32]	4.5	763	97.05		NAO [32]	5.5	656	73.7	91.7
	NAT	4.6	804	**97.24**		NAT	5.6	679	**73.9**	**91.8**
DARTS† [30]	/	3.3	533	97.06	DARTS [30]	/	5.9	595	73.1	91.0
	NAO [32]	3.5	577	97.09		NAO [32]	6.1	627	73.3	91.1
	NAT	3.0	483	**97.28**		NAT	3.9	515	**74.4**	**92.2**
NAONet† [32]	/	128	66016	97.89	NAONet [32]	/	11.35	1360	74.3	91.8
	NAO [32]	143	73705	97.91		NAO [32]	11.83	1417	74.5	92.0
	NAT	113	58326	**98.01**		NAT	8.36	1025	**74.8**	**92.3**

➢ NAT based models yield significantly better performance with less or comparable computational cost as the baseline models.

Comparison of Different Policy Learners

- We compare several policy learners, including Random Search, LSTM, and two GCN based methods.

Method	VGG16	ResNet20	MobileNetV2	ENAS†	DARTS†	NAONet†
/	93.56	91.37	94.47	97.11	97.06	97.89
Random Search	93.17	91.56	94.38	96.58	95.17	96.31
LSTM	94.45	92.19	95.01	97.05	97.05	97.93
Maximum-GCN	94.37	92.57	94.87	96.92	97.00	97.90
Sampling-GCN (Ours)	**95.93**	**92.97**	**95.13**	**97.21**	**97.26**	**97.99**

- Our Sampling-GCN method significantly outperforms the other methods.

Contents

Conclusion

- We propose a novel Neural Architecture Transformers (NAT) to optimize any arbitrary architectures for better performance without extra computational cost.
- We cast the problem into a Markov decision process (MDP) and employ graph convolutional network (GCN) to learn the optimal policy.
- Extensive experiments show the effectiveness of NAT on both hand-crafted and NAS based architectures.

Thanks!

Q & A