NAT: Neural Architecture Transformer for Accurate and Compact Architectures

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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.

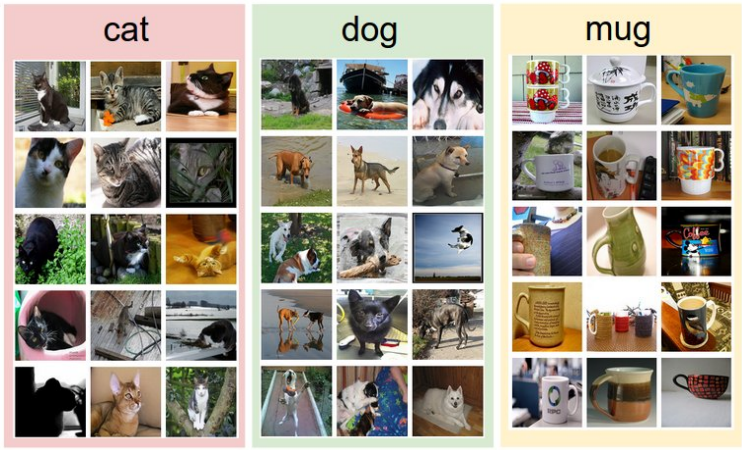
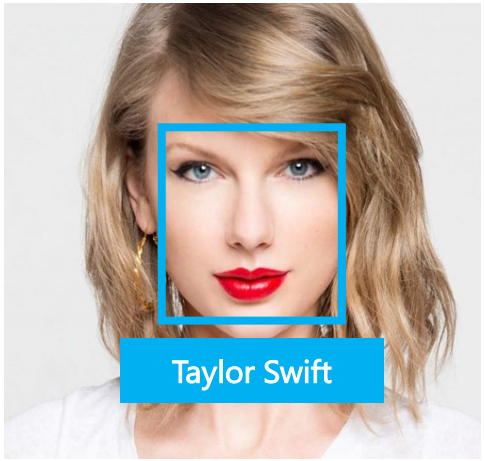
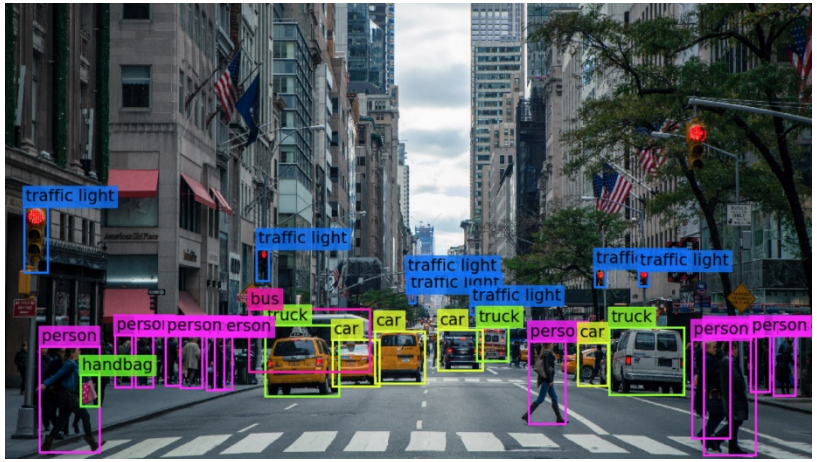


Image Classification



Face Recognition



Object Detection

Figure: Applications of deep neural networks.

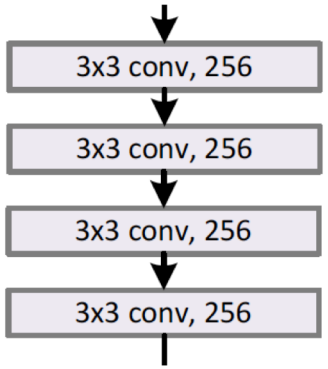
Neural Architecture Design

- Neural architecture design is one of the key factors behind the success of deep neural networks.
- Existing architectures can be divided into two categories:

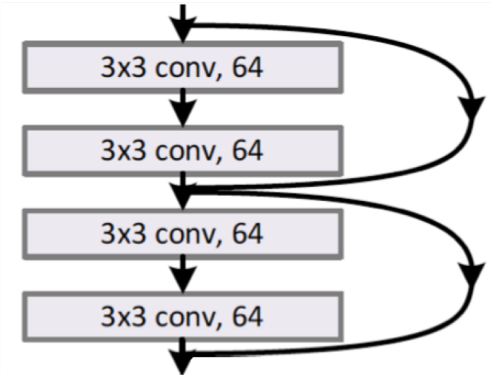
1. Hand-crafted architectures
2. Automatically searched architectures

Hand-crafted Architectures

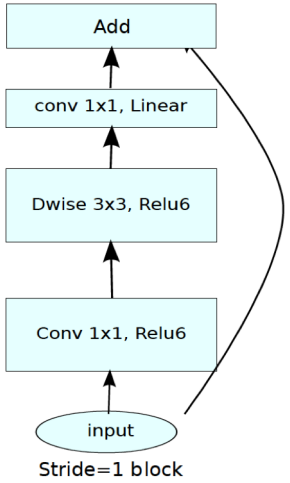
Several widely used hand-crafted architectures:



VGG



ResNet



MobileNetV2

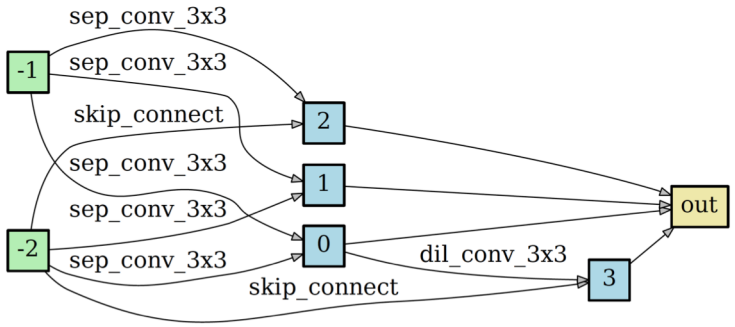
Figure: Examples of hand-crafted architectures.

Limitations of hand-crafted architecture design process

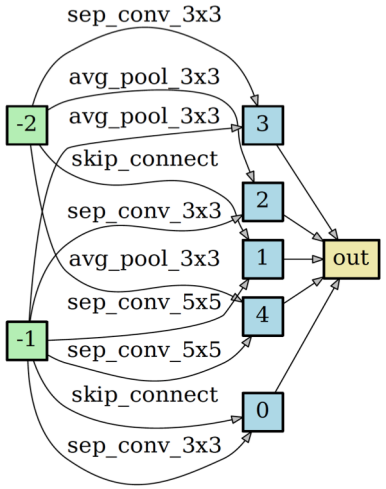
- Hand-crafted methods rely on substantial human expertise.
- Hand-crafted methods cannot fully explore the whole architecture space.

Automatically Searched Architectures

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



DARTS normal cell



ENAS normal cell

Figure: Examples of NAS based architectures.

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.

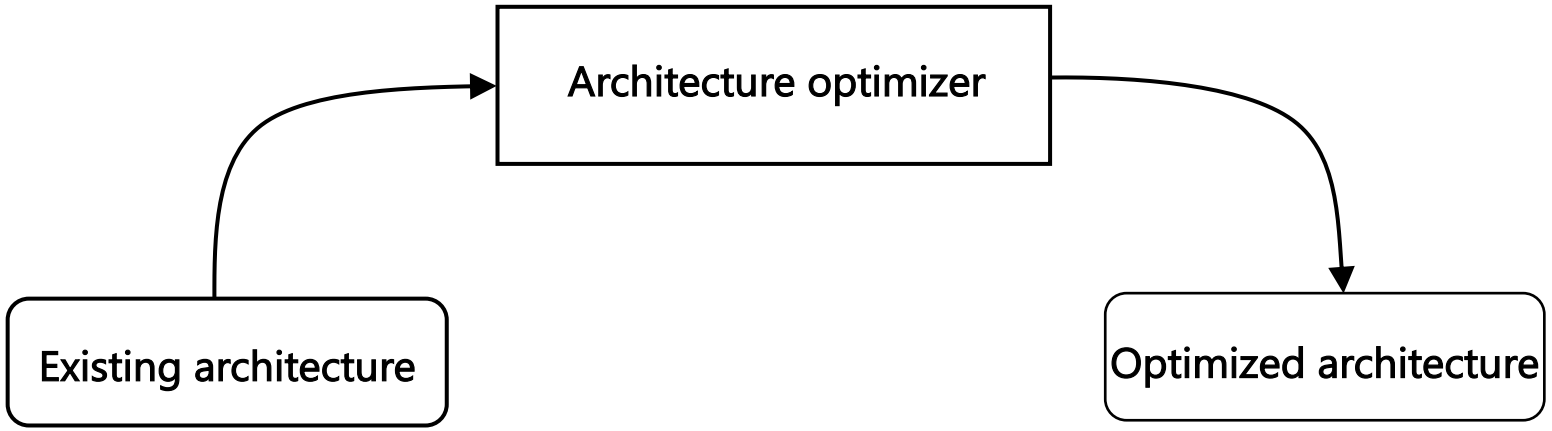


Figure: Architecture optimization scheme.

Existing Architecture Optimization Methods

- Neural Architecture Optimization (NAO)

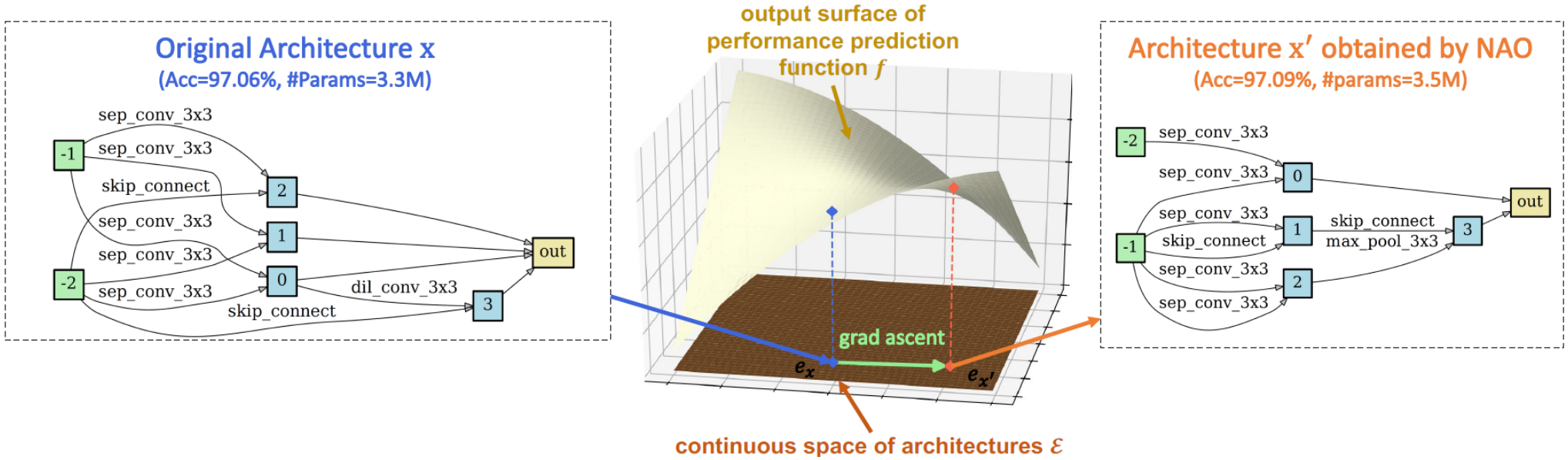


Figure: Framework of Neural Architecture Optimization (NAO).

Limitations of NAO

- NAO often produces a totally different architecture from the input one.
- NAO may introduce extra parameters or additional computational cost.

Contents

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**.

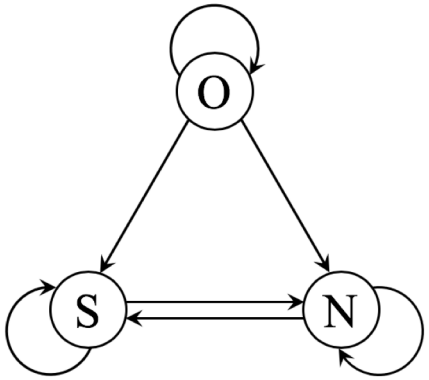


Figure: Operation transformation scheme.

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 $c(\cdot)$ is a function to evaluate 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 Single Architecture

Given a specific architecture $\hat{\beta}$, we seek to find the optimal architecture α. Then, the optimization problem can be formulated as

$$\max_{\alpha} R(\alpha \mid \hat{\beta}), \text{ s.t. } c(\alpha) \leq \kappa$$

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

Optimization for Arbitrary Architecture

- The previous optimization problem is only concentrated on one specific $\hat{\beta}$.
- We hope to find a transformer to optimize any arbitrary architecture $\beta \sim p(\cdot)$.

To this end, we seek to train the transformer parameterized θ by optimizing the objective

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

where $\mathbb{E}_{\beta \sim p(\cdot)}[\mathbb{E}_{\alpha \sim \pi(\cdot|\beta;\theta)} R(\alpha \mid \beta)]$ 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

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

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.
- How to compute $\mathbb{E}_{\beta \sim p(\cdot)}[\mathbb{E}_{\alpha \sim \pi(\cdot|\beta;\theta)} R(\alpha \mid \beta)]$ still remains a question.

Markov Decision Process for Learning NAT

Our solution

- We cast the optimization problem into a Markov decision process (MDP).
- We seek to make 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.

Markov Decision Process for Learning NAT

Details of MDP

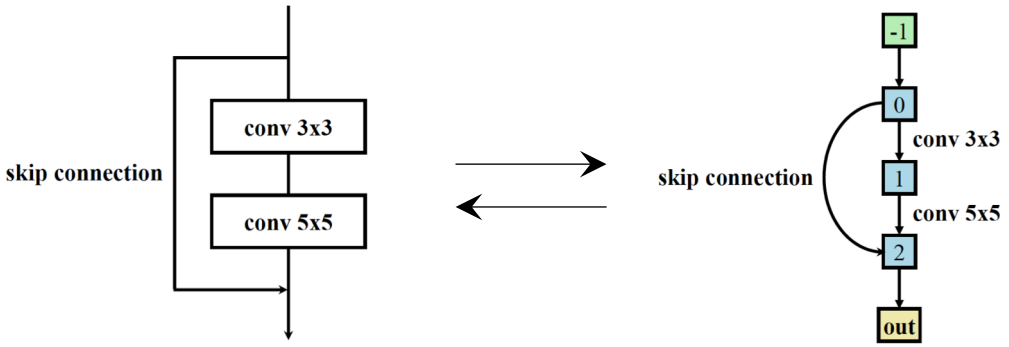
- An **architecture** is defined as a **state**.
- A **transformation mapping** $\beta \rightarrow \alpha$ is defined as an **action**.
- The **accuracy improvement** on validation set is regraded as **reward**.
- The policy $\pi(\cdot \mid \beta;\theta)$ parameterized by θ is the **probability distribution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

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

Policy Learning by Graph Convolution Networks

Graph Representation of Architectures: We use the directed acyclic graph (DAG) to represent both hand-crafted architectures and NAS based architectures.

- Node: feature maps of a specific layer in deep networks
- Edge: a computational module or operation, e.g., convolution or max pooling



(a) network view (b) graph view

Figure: Graph representation examples of hand-crafted architectures.

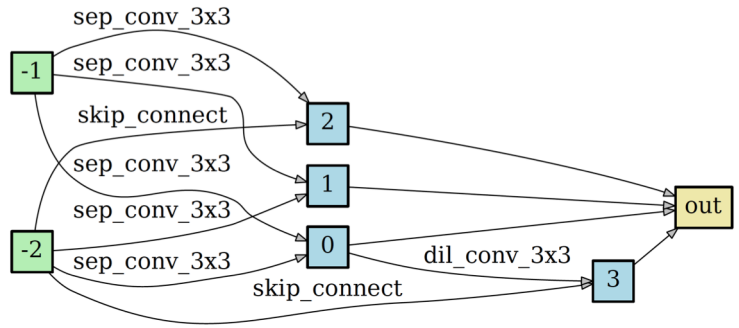


Figure: Graph representation examples of NAS based architectures.

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

- $\mathbf{A}$: the adjacency matrix of the architecture graph.
- $\mathbf{X}$: the attributes of the nodes together with their two input edges in the graph.
- $\mathbf{W}^{(0)}$ and $\mathbf{W}^{(1)}$: the weights of two graph convolution layers.
- $\mathbf{W}^{\mathrm{FC}}$: the weight of the fully-connected layer, σ is a non-linear activation function.
- $\mathbf{Z}$: the 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:

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

$$= \sum_{\beta} p(\beta) \left[\sum_{\alpha} \pi(\alpha|\beta;\theta) \left(R(\alpha, w) - R(\beta, w) \right) + \lambda H\left(\pi(\cdot|\beta;\theta)\right) \right]$$

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).

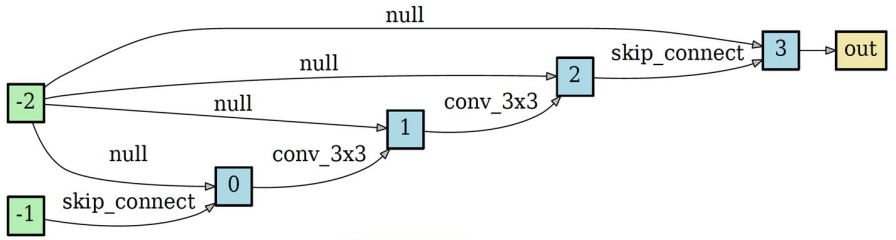
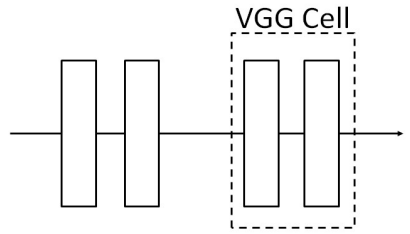
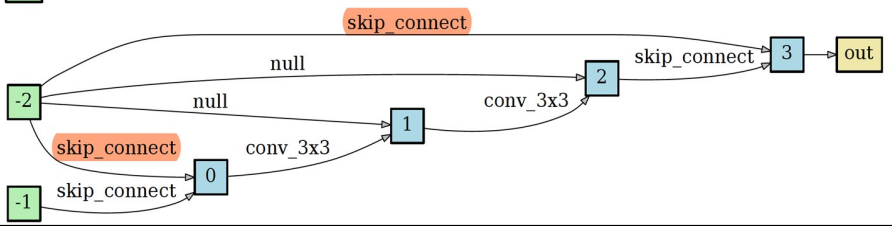
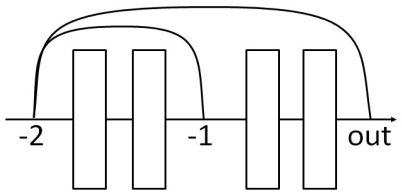
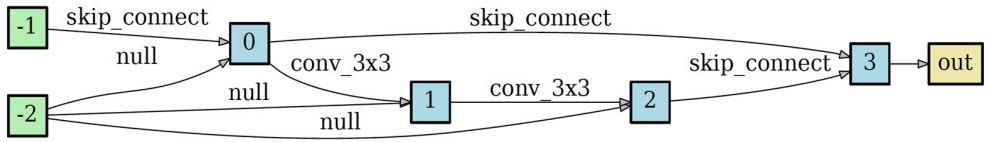
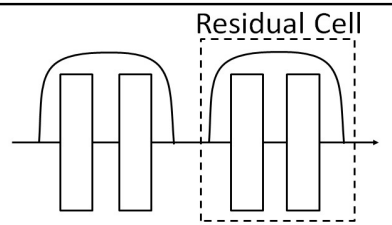
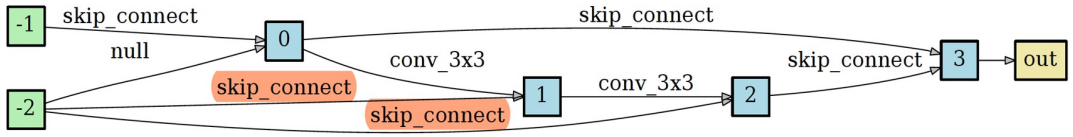
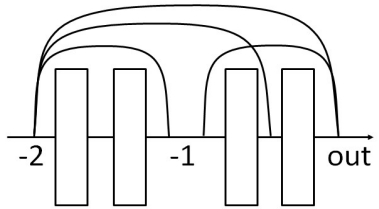
Require: The number of sampled input architectures in an iteration m, the number of sampled optimized architectures for each input architecture n, learning rate η, regularizer parameter λ, input architecture distribution $p(\cdot)$, shared model parameters w, transformer parameters θ.

Initiate w and θ.
while not convergent **do**
  for each iteration on training data **do**
    // Fix θ and update w.
    Sample $\beta_i \sim p(\cdot)$ to construct a batch $\{\beta_i\}_{i=1}^m$.
    Update the model parameters w by descending the gradient:
      $w \leftarrow w - \eta \frac{1}{m} \sum_{i=1}^m \nabla_w \mathcal{L}(\beta_i, w)$.
  end for
  for each iteration on validation data **do**
    // Fix w and update θ.
    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 descending the gradient:
      $\theta \leftarrow \theta - \eta \frac{1}{mn} \sum_{i=1}^m \sum_{j=1}^n \left[\nabla_\theta \log \pi(\alpha_j|\beta_i;\theta)\big(R(\alpha_j, w) - R(\beta_i, w)\big) + \lambda \nabla_\theta H\big(\pi(\cdot|\beta_i;\theta)\big)\right]$.
  end for
end while

Contents

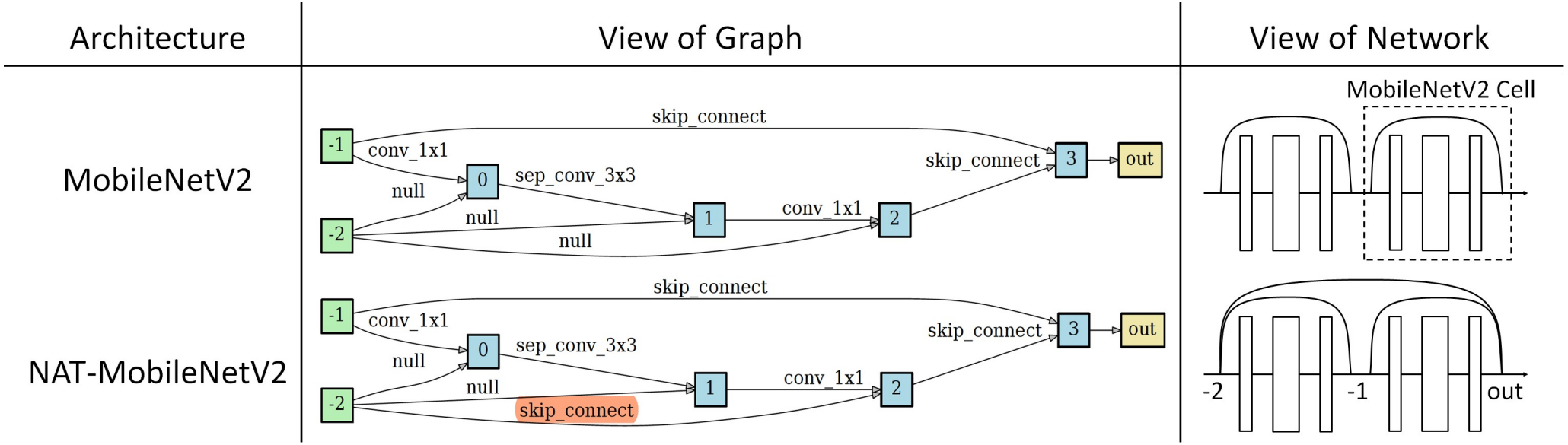
Visual Results of Hand-crafted Architectures

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

Architecture	View of Graph	View of Network
VGG		
NAT-VGG		
ResNet		
NAT-ResNet		

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.

Comparison on Hand-crafted Architectures

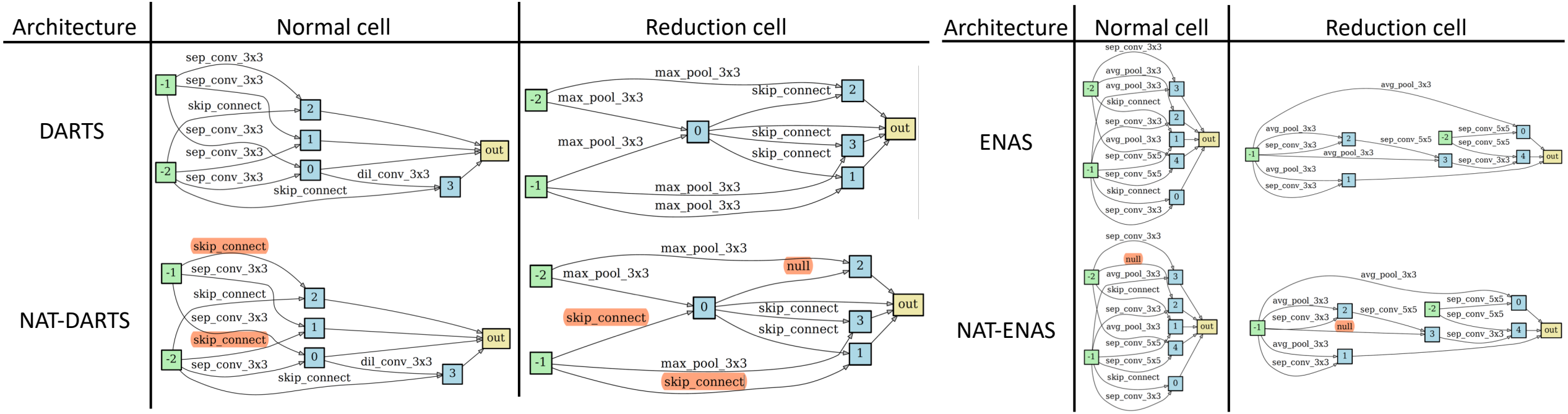
- Results on several hand-crafted architectures, including VGG, ResNet, and MobileNet.

CIFAR-10					ImageNet					
Model	Method	#Params (M)	#MAdds (M)	Acc. (%)	Model	Method	#Params (M)	#MAdds (M)	Acc. (%)	
									Top-1	Top-5
VGG16	/	15.2	313	93.56	VGG16	/	138.4	15620	71.6	90.4
	NAO[31]	19.5	548	95.72		NAO [31]	147.7	18896	72.9	91.3
	NAT	15.2	313	**96.04**		NAT	138.4	15620	**74.3**	**92.0**
ResNet20	/	0.3	41	91.37	ResNet18	/	11.7	1580	69.8	89.1
	NAO [31]	0.4	61	92.44		NAO [31]	17.9	2246	70.8	89.7
	NAT	0.3	41	**92.95**		NAT	11.7	1580	**71.1**	**90.0**
ResNet56	/	0.9	127	93.21	ResNet50	/	25.6	3530	76.2	92.9
	NAO [31]	1.3	199	95.27		NAO [31]	34.8	4505	77.4	93.2
	NAT	0.9	127	**95.40**		NAT	25.6	3530	**77.7**	**93.5**
MobileNetV2	/	2.3	91	94.47	MobileNetV2	/	3.4	300	72.0	90.3
	NAO [31]	2.9	131	94.75		NAO [31]	4.5	513	72.2	90.6
	NAT	2.3	91	**95.17**		NAT	3.4	300	**72.5**	**91.0**

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

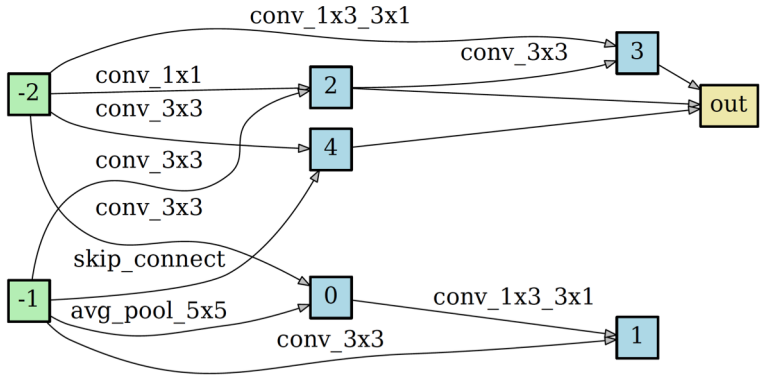
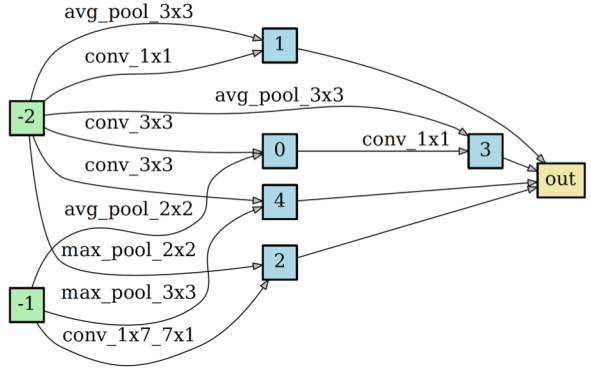
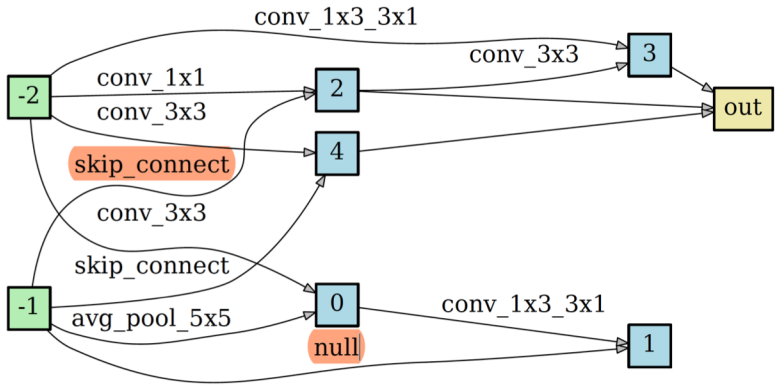
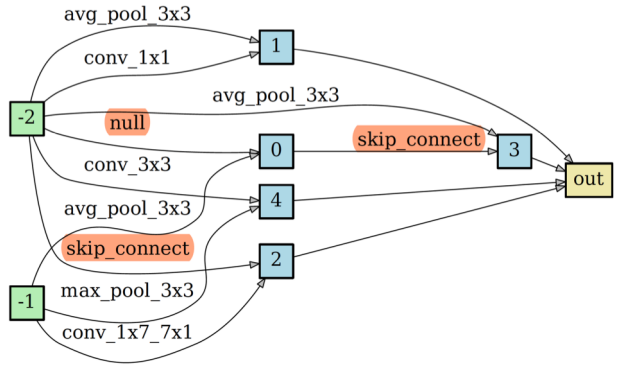
Visual Results on NAS based Architectures

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



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		

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† [34]	/	3.2	-	96.73	AmoebaNet [34]	/	5.1	555	74.5	92.0
PNAS† [28]		3.2	-	96.67	PNAS [28]		5.1	588	74.2	91.9
SNAS† [48]		2.9	-	97.08	SNAS [48]		4.3	522	72.7	90.8
GHN† [52]		5.7	-	97.22	GHN [52]		6.1	569	73.0	91.3
ENAS† [33]	/	4.6	804	97.11	ENAS [33]	/	5.6	679	73.8	91.7
	NAO [31]	4.5	763	97.05		NAO [31]	5.5	656	73.7	91.7
	NAT	4.6	804	**97.24**		NAT	5.6	679	**73.9**	**91.8**
DARTS† [29]	/	3.3	533	97.06	DARTS [29]	/	5.9	595	73.1	91.0
	NAO [31]	3.5	577	97.09		NAO [31]	6.1	627	73.3	91.1
	NAT	3.0	483	**97.28**		NAT	3.9	515	**74.4**	**92.2**
NAONet† [31]	/	128	66016	97.89	NAONet [31]	/	11.35	1360	74.3	91.8
	NAO [31]	143	73705	97.91		NAO [31]	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