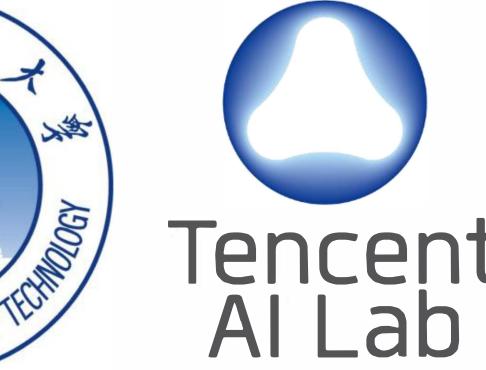


NAT: Neural Architecture Transformer for Accurate and Compact Architectures

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BACKGROUND AND MOTIVATION

Neural architectures can be divided into two categories, namely hand-crafted and NAS based architectures.

Limitations of existing architecture design methods:

- Hand-crafted architecture design methods rely on substantial human expertise and cannot fully explore the whole architecture design space.
- Neural architecture search (NAS) methods: often produce subopimal architectures with limited performance due to the extremely large search space.

Both hand-crafted architectures and NAS based architectures may contain non-significant or redundant modules or operations.

CONTRIBUTIONS

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

PROBLEM DEFINITION

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

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

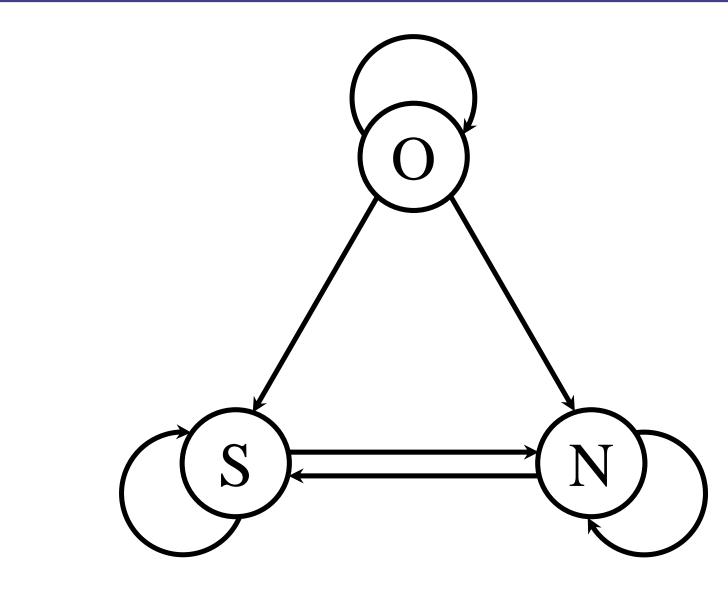


Figure 1: Operation transformation.

- We divide the operations into **three categories** $\{S, N, O\}$. S denotes skip connection, N denotes null connection, O denotes the operations other than skip or null connection.
- We have c(O) > c(S) > c(N), where $c(\cdot)$ is a function to evaluate the **computational cost**.
- We constrain the possible transitions among S, N, and O in Figure 1 to reduce the computational cost.

MARKOV DECISION PROCESS FOR NAT

Let $R(\alpha, w)$ be the **performance measure** for architecture α with parameters w, e.g., the validation accuracy on validation data set. Then the **architure optimization problem** can be formulated as:

$$\max_{\theta} \mathbb{E}_{\beta \sim p(\cdot)} \left[\mathbb{E}_{\alpha \sim \pi(\cdot|\beta;\theta)} R(\alpha|\beta) \right], \text{ s.t. } c(\alpha) \leq \kappa, \ \alpha \sim \pi(\cdot|\beta;\theta), \quad (1)$$

- $R(\alpha|\beta) = R(\alpha, w_{\alpha}) R(\beta, w_{\beta})$ denote the **performance difference** between the optimized architectures α and the given architectures β . w_{α} and w_{β} are the parameters of α and β , respectively.
- $\mathbb{E}_{\beta \sim p(\cdot)} \left[\mathbb{E}_{\alpha \sim \pi(\cdot|\beta;\theta)} R(\alpha|\beta) \right]$ indicates the **expectation** of $R(\alpha|\beta)$ over the distribution of the given architectures $\beta \sim p(\cdot)$ and the distribution of the optimized architectures $\alpha \sim \pi(\cdot|\beta;\theta)$.
- $c(\cdot)$ is a function to measure the computation cost of architectures and κ is an upper bound of the cost.

To solve problem (1), we reformulate the constrained optimization problem into a Markov decision process (MDP), where

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

POLICY LEARNING BY GCN

To better exploit the adjacency information of architecture graph, we use a two-layer GCN and build the controller:

$$\mathbf{Z} = f(\mathbf{X}, \mathbf{A}) = \text{Softmax}\left(\mathbf{A}\sigma\left(\mathbf{A}\mathbf{X}\mathbf{W}^{(0)}\right)\mathbf{W}^{(1)}\mathbf{W}^{\text{FC}}\right).$$
 (2)

- A denotes the adjacency matrix of the architecture graph.
- X denotes the attributes of the nodes together with their two input edges in the graph.
- $W^{(0)}$ and $W^{(1)}$ denote the weights of graph convolution layers.
- W^{FC} denotes the weight of the fully-connected layer, σ is a non-linear activation function.
- **Z** refers to probability distribution of different operations, *i.e.*, the learned policy $\pi(\cdot|\beta;\theta)$.

TRAINING AND INFERENCE METHOD

Training method for NAT

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 .

- 1: Initiate w and θ . 2: **while** not convergent **do**
- : for each iteration on training data do
- // Fix θ and update w.
- 5: 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
- 9: **for** each iteration on validation data **do** 10: // Fix w and update θ .
- 11: Sample $\beta_i \sim p(\cdot)$ to construct a batch $\{\beta_i\}_{i=1}^m$.
- 12: Obtain $\{\alpha_j\}_{j=1}^n$ according to the policy learned by GCN.
- Update the parameters θ by descending the gradient: $\theta \leftarrow \theta \eta \frac{1}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} \left[\nabla_{\theta} \log \pi(\alpha_{j} | \beta_{i}; \theta) \left(R(\alpha_{j}, w) R(\beta_{i}, w) \right) + \lambda \nabla_{\theta} H(\pi(\cdot | \beta_{i}; \theta)) \right].$
- 15: end for
- Inferring the optimized architectures
- 1. Sample candidate architectures from the learned policy $\pi(\cdot|\beta;\theta)$.
- 2. Select the architectures with the highest validation accuracy.

RESULTS ON DIFFERENT ARCHITECTURES

• Results on hand-crafted architectures (comparisons on ImageNet)

Model	Method	#Params (M)	#MAdds (M)	Acc. (%)	
WIOUCI	Michiod	$\pi 1$ afailis (1V1)		Top-1	Top-5
VGG16	/	138.4	15620	71.6	90.4
	NAO	147.7	18896	72.9	91.3
	NAT	138.4	15620	74.3	92.0
ResNet18	/	11.7	1580	69.8	89.1
	NAO	17.9	2246	70.8	89.7
	NAT	11.7	1580	71.1	90.0
ResNet50	/	25.6	3530	76.2	92.9
	NAO	34.8	4505	77.4	93.2
	NAT	25.6	3530	77.7	93.5
MobileNetV2	/	3.4	300	72.0	90.3
	NAO	4.5	513	72.2	90.6
	NAT	3.4	300	72.5	91.0

Results on NAS based architectures (comparisons on ImageNet)

Model	Method	#Params (M)	#MAdds (M)	Acc. (%)	
				Top-1	Top-5
AmoebaNet [34]		5.1	555	74.5	92.0
PNAS [28]		5.1	588	74.2	91.9
SNAS [48]		4.3	522	72.7	90.8
GHN [52]		6.1	569	73.0	91.3
ENAS [33]	/	5.6	679	73.8	91.7
	NAO	5.5	656	73.7	91.7
	NAT	5.6	679	73.9	91.8
DARTS [29]	/	5.9	595	73.1	91.0
	NAO	6.1	627	73.3	91.1
	NAT	3.9	515	74.4	92.2
NAONet [31]	/	11.35	1360	74.3	91.8
	NAO	11.83	1417	74.5	92.0
	NAT	8.36	1025	74.8	92.3

VISUALIZATION OF ARCHITECTURES

• Architecture optimization results on hand-crafted architectures

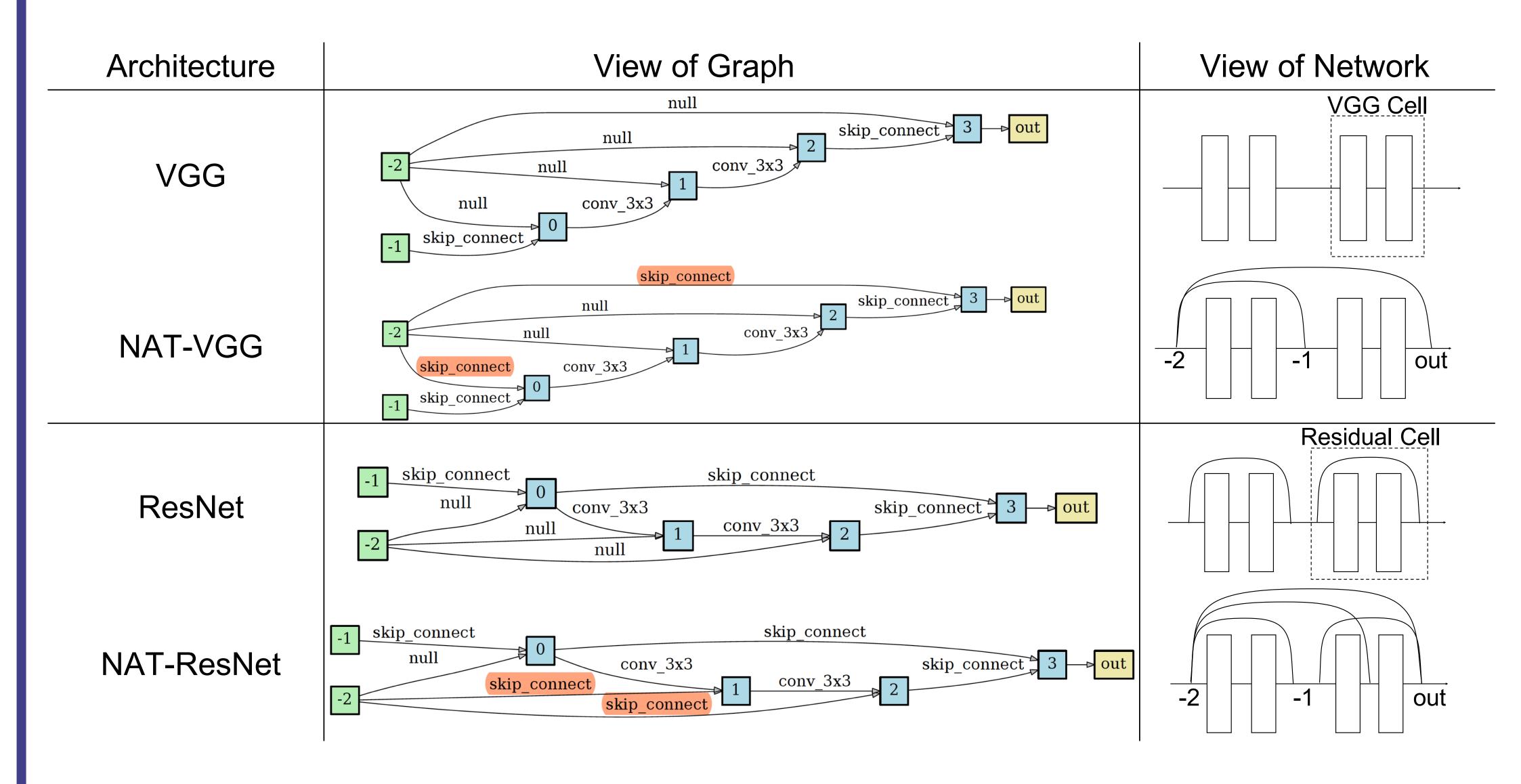


Figure 2: Visualization of some optimized hand-crafted architectures

• Architecture optimization results on NAS based architectures

Architecture	Normal cell	Reduction cell
DARTS	sep_conv_3x3 skip_connect sep_conv_3x3 sep_conv_3x3 sep_conv_3x3 sep_conv_3x3 out -2 sep_conv_3x3 skip_connect 3 skip_connect 3	max_pool_3x3 -2 max_pool_3x3 skip_connect 2 max_pool_3x3 out skip_connect 3 skip_connect 3 max_pool_3x3 max_pool_3x3
NAT-DARTS	skip_connect sep_conv_3x3 skip_connect sep_conv_3x3 skip_connect -2 sep_conv_3x3 skip_connect 3 skip_connect 3	max_pool_3x3 -2 max_pool_3x3 skip_connect max_pool_3x3 -1 max_pool_3x3 skip_connect skip_connect skip_connect
ENAS	sep_conv_3x3 avg_pool_3x3 -2 avg_pool_3x3 sep_conv_3x3 2 avg_pool_3x3 1 out skip_conv_5x5 skip_conv_5x5 4	avg_pool_3x3 sep_conv_5x5 sep_conv_5x5 -1 avg_pool_3x3 sep_conv_5x5 avg_pool_3x3 sep_conv_3x3 avg_pool_3x3 sep_conv_3x3 sep_conv_3x3 4 out
NAT-ENAS	sep_conv_3x3 -2 avg_pool_3x3 sep_conv_3x3 3 sep_conv_5x5 4 -1 sep_conv_5x5 4 sep_conv_5x5 4 out skip_connect 0	avg_pool_3x3 avg_pool_3x3 sep_conv_5x5 -2 sep_conv_5x5 avg_pool_3x3 sep_conv_3x3 avg_pool_3x3 sep_conv_3x3 1 sep_conv_3x3 1

Figure 3: Visualization of some optimized NAS-based architectures

CONTACT INFORMATION AND CODE

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- Code: https://github.com/guoyongcs/NAT

