Revisiting Neural Architecture Search

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Abstract

Neural Architecture Search (NAS) is a collection of methods to craft the way neural networks are built. Current NAS methods are far from ab initio and automatic, as they use manual backbone architectures or micro building blocks (cells), which have had minor breakthroughs in performance compared to random baselines. They also involve a significant manual expert effort in various components of the NAS pipeline. This raises a natural question - Are the current NAS methods still heavily dependent on manual effort in the search space design and wiring like it was done when building models before the advent of NAS? In this paper, instead of merely chasing slight improvements over state-of-the-art (SOTA) performance, we revisit the fundamental approach to NAS and propose a novel approach called ReNAS that can search for the complete neural network without much human effort and is a step closer towards AutoML-nirvana. Our method starts from a complete graph mapped to a neural network and searches for the connections and operations by balancing the exploration and exploitation of the search space. The results are on-par with the SOTA performance with methods that leverage handcrafted blocks. We believe that this approach may lead to newer NAS strategies for a variety of network types.

1 Introduction

Deep Learning has proven to be successful in many application areas such as image classification, object detection, semantic segmentation, NLP etc. Much of the current success is through large datasets and powerful, often handcrafted, neural network models. It is hard to construct or search for new models ab initio. Neural Architecture Search (NAS) refers to finding the neural network for a given task automatically, instead of handcrafting the building blocks or layers of the model. It has a great potential to simplify the trial-and-error approach of manually designing neural networks, can be adapted to work with different compute backends and for a varied number of tasks. NAS methods have used Reinforcement Learning ([Zoph & Le (2017); Baker et al. (2016)]), Evolutionary algorithms ([Real et al. (2017a)]), Graph Hypernetworks ([Zhang et al. (2019)]) while requiring enormous computation resources. More recent NAS methods like ENAS ([Pham et al. (2018)]) and differentiated architecture search methods ([Liu et al. (2019); Cai et al. (2019)]) have reduced the search time to a few GPU days on many different tasks like image classification and language modelling. However, current NAS methods still do not achieve full automation and have the following limitations -

1. The search space is based on human-made state-of-the-art networks and thus is already optimal. Hence, a prior is introduced in the architecture resulting in similar performance as the random search baselines. The standard deviation in accuracy of architectures in such a search space is very low.

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2. In most existing NAS methods, the search is done on a micro search space to find the most optimal building block or cell, using a much smaller network. The best cell is then stacked according to the size of the dataset to form a larger network. The improvements this approach bring are due to the cell engineering rather than the search method itself. That is, the architecture of the cell itself is designed such that any network formed will be good. This also leads to another manual step and additional hyperparameters, thus making such methods far from a generic full-fledged architecture search.

The above mentioned shortcomings do not take full advantage of the resources and find the structures or patterns which are not known in the literature. Also, too much effort is spent in improving the SOTA performance instead of decreasing the human insight of the network (e.g. starting cell structures etc). In this paper, we take a different view and propose a new approach towards Neural Architecture Search, a differentiated architecture search method that searches for the optimal connections as well as the operations of the neural network by varying the exploration vs exploitation trade-off. Our goal is slightly different than merely pure SOTA performance.

Several recent works have shown the inefficiency of the DARTS (Liu et al. (2019)) based search space. Yang et al. (2020) showed that the hand-designed cell structure is more important than the micro structure (operations) and these cell architectures have a very narrow accuracy range. By sampling many random architectures (including the connections sampling as well), the accuracy of all the architectures were similar and doesn’t degrade much when the search space is reduced with inefficient operations. Similarly, Xie et al. (2019a) showed that optimal wiring can beat many NAS based architectures without searching for the operations. Yu et al. (2020) observed that the search policies of different NAS algorithms perform similarly if not worse with random search due to a constrained search space. Shu et al. (2020) also discover that with the same connection topologies as the popular NAS cells but different operations, all random variants achieve nearly the same convergence as the popular NAS architectures. This highlights the importance of connections in the architecture search as opposed to the current NAS methods, which are inhibited by the fact that the underlying cell has a strong prior (e.g., every node has exactly two input nodes). This makes the network space restrictive and explains why random policy has been as effective as sophisticated NAS algorithms. Hence, it is not clear whether the advantage one NAS method show over another is due to the search itself or because of lucky initialization (Frankle & Carbin (2019)) or the training protocol. In this paper, we argue that a more principled approach for NAS is required to move the space.

Our method, named ReNAS, searches for a complete neural network with no predefined backbone, wiring pattern and operations. We start with a complete graph, mapping it to a neural network: a node representing a transformation like convolution or pooling and edges representing information flow. Every node’s channels are clustered in blocks. Instead of forming layer-wise connection pattern, we connect block of channels for each node in our network to every other node block. This makes our method search on a much larger space than layer-wise connections, previously unexplored by human experts. It also increases the search speed unlike DNW (Wortsman et al. (2019)) where every channel is connected to another one making the search computationally very expensive. Our proposed ReNAS method is based on the weight sharing differentiable architecture search.

Our work can be seen as an application of differentiable search. Previous work in discovering neural wiring (Wortsman et al. (2019)) worked on a MobileNet backbone based on a static structure as the dynamic case is too expensive to optimize. Xie et al. (2019a) explore different wiring patterns through a random graph generator but their wiring is also fixed and is not prior free. To the best of our knowledge, our work is the first step towards full automation of the architecture construction without a predefined backbone or cell. It removes the manual expert effort in designing various components of the NAS pipeline.

2 Related Work

Here we discuss prior work and their shortcomings and specify how our work overcomes them.

Neural network wiring and topology: Different types of wiring neural networks have been studied extensively. Inception nets (Szegedy et al. (2015)) uses modules having parallel paths with different filters and concatenates them. ResNet (He et al. (2016)) uses shortcut or skip connections to learn the residual function \( F(x) + x \), while DenseNet (Huang et al. (2017)) uses connections between
every pair of layers in a block. MaskConnect \cite{ahmed2018learning} learns the connection between modules in a residual network by assigning each connection a real valued weight. They chose K (hyperparameter) input connections for each module and learn the connection weights along with network parameters. \cite{xie2019stochastic} uses stochastic network generator to generate a graph which is mapped to a neural network (RandWire). The wiring in RandWire is fixed by the network generator’s prior (WS, ER, BA) and the seed. \cite{yuan2019designing} uses complete graphs in stages and learns the connection weights in a stage by continuous relaxation as in DARTS. However, the learned architecture is never discretized at the end of training, resulting in a DenseNet style architecture with weighted incoming connections instead of a concatenation of all connections. Our work does not search for layer-wise connections, instead finds connections between channel partitions. \cite{wortsman2019structured} relaxes the notion of layers and learn the wiring between channels. However, due to their expensive optimization, it is constrained to generating smaller networks in low computation regime. Our work is motivated by finer connections than layer or node, but instead of allowing all channel wise connections, which is more computationally and memory expensive, uses blocks of channel connections.

**Neural Architecture Search:** \cite{zoph2017neural} used a controller RNN and trained it with reinforcement learning to search for architectures. Since then, numerous NAS methods have been studied. Based on major search strategy, NAS methods can be classified into Reinforcement Learning (Baker et al. (2016); Cai et al. (2018); Zhong et al. (2018); Zoph et al. (2018); Pham et al. (2018); Neuro-Evolution (Real et al. (2017b); Suganuma et al. (2018); Liu et al. (2018b); Keal et al. (2019); Elsken et al. (2019)) and gradient-based (Liu et al. (2019); Cai et al. (2019); Xie et al. (2019b); Nayman et al. (2019); Xu et al. (2020); Chen et al. (2019a)). Other methods include Random Search (Li & Talwalkar (2019)), Bayesian Optimization (Jin et al. (2019); Kandasamy et al. (2018) and some custom methods (Chen et al. (2019b); Kamath et al. (2018); Carlucci et al. (2019); Liu et al. (2018a)). In this work, we search for the connection as well as the operations. Unlike previous NAS methods, which uses a backbone or pre-designed cell, and then search on them, we visualize the neural network as a graph having groups of channel-wise connections. Our method prunes the redundant connections and search for the operations at the same time.

3 Method

In this section, we describe our method for learning the structure as well as the operations of a neural network at the same time. We first describe the construction of the over-parameterized neural network, then the search space, and finally the method.

3.1 Constructing the Parent Network

The searchable parent network consists of multiple directed acyclic graphs (DAG) $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ where every node $v \in \mathcal{V}$ is assigned an index. There is an edge $e_{ij} \in \mathcal{E}$ for every node $v_i$ to $v_j$, $i < j$. Nodes represent some transformation of the input data (e.g., pooling, convolution) and edges represent data flow. A node $v_i$ having $C$ channels can be partitioned into $K$ channel blocks. Every channel block $H_i$, for pair of nodes $v_i$ and node $v_j$, there are $K^2$ connections. Each edge $e_{ij}$ has weight $\gamma_{ij}$. Each DAG $G_n$’s input is the output of the previous DAG $G_m$, $m < n$. The input feature map’s size of every DAG is reduced by half and the channels are increased to twice by the first node of every DAG. Figure 1 depicts the node level connections in the one-shot network.

3.2 Search Space

We search for the complete architecture on target task and dataset, without any proxy, similar to \cite{cai2019proxylessnas, hu2020searching}. Our approach doesn’t require any predefined backbone architecture though, as with previous approaches. For a complete DAG with $N$ nodes, there are $2^{N(N-1)/2}$ possible connections. For every node in a DAG, there is an operation (e.g. convolution, pooling) associated with it, thus for $O$ operations, there are total $O^N \times 2^{N(N-1)/2}$ networks, since every choice is independent. For $M$ such DAG’s, there are $M \times O^N \times 2^{N(N-1)/2}$ networks in our search space. This is significantly larger than earlier methods, which use either building blocks in a backbone architecture or expert engineered cells which have a restricted search space.
3.3 Architecture Search

The architecture search is based upon the differentiable architecture search \cite{Liu2019, Cai2019}. In this method, we start with an over-parameterized (parent) network having all operations in the search space (e.g., convolution, pooling, etc.). Every operation and edge is assigned a weight parameter which is trainable like the weights of the neural network. Every iteration is composed of two steps - 1) The weights $w$ of the neural network are trained by gradient descent algorithms on a training set keeping the architecture parameters fixed and 2) The architecture parameters $\alpha$ are trained on a separate validation set according to gradient based methods (SGD or exponential) keeping the weights fixed. The parameters $\gamma$ of the connections are trained along with the weight parameters of the parent network. Algorithm 1 details the steps of our method.

**Algorithm 1** ReNAS

Construct the over-parameterized network $G(w, \alpha, \gamma)$ by initializing every DAG in the network

while not converged do
  for each $G$ in $G(w, \alpha, \gamma)$ do
    for each node $v$ in $G$ do
      1. Partition the node into $K$ channel blocks
      2. Calculate $x^k$ for $k = 1, ..., K$ according to Eq. 1
      3. Sample an operation from the Operation Search Space
      4. Calculate the resulting featuremap $X$ for node by concatenating $X^k \forall k$ according to Eq. 2
      5. Update the weights $w$ and $\gamma$ using SGD
      6. Fix $\gamma$, $w$ and update $\alpha$ based on Eq. 3
    end
  end
end

For each node, retain the operations with highest $\alpha$ and half channel block connections with highest $\gamma$. Prune all other connections

\begin{align}
x^k &= \sum_{l=1}^{K} \gamma_{ijl} * X^k_i \quad \text{for } k = 1, ..., K \quad \forall \quad j > i \quad (1) \\
X^k &= o_j(x^k) \quad \text{for } k = 1, ..., K \quad (2)
\end{align}
Here $x^k$ is the intermediate variable, $X_i$ is the featuremap of node $i$ and $o_j$ is the sampled operation for node $j$ from the operation search space.

The procedure starts by constructing the parent network by wiring $M$ DAG’s $G$ as described in section 5.1. Every node’s channels in $G$ are partitioned into $K$ channel blocks. Here $K$ is a hyperparameter which controls the granularity of our search; $K = 1$ means there is no partition. If $K$ is the number of channel in node $v_i$ it means that every channel is connected to every other channel and the wiring of the over-parameterized network is similar to Wortsman et al. (2019). Each partition of node $v_i$ can be visualized as a separate entity or node. Each channel block of node $v_i$ is connected to every other channel block of node $v_j$, thus forming $K^2$ connections. After that, each such connection is weighted through the connection parameter $\gamma_{ij}$ according to Eq. (1). Then, one of the operations is sampled from the operation search space and its parameter $\alpha$ is updated. Figure 2 depicts the node level expansion. The operation sampling is based on the path sampling heuristic of Cai et al. (2019), in which two candidate paths (operations) are sampled from a multinomial distribution over all operations. We update these parameters $\alpha$ of the over-parameterized network using the loss gradient equation as described in Cai et al. (2019). Here, $\delta_{mn}$ is equal to 0 when $m$ is not equal to $n$ and 1 when $m = n$, $p_m$ and $p_n$ are the probabilities of choosing the operation $m$ and $n$ respectively using the multinomial probability distribution on parameters $\alpha$ of operations.

$$\frac{\partial L}{\partial \alpha_m} = \sum_{n=1}^{2} \frac{\partial L}{\partial y_n} p_n (\delta_{mn} - p_m)$$ (3)

The selected operation $o$ is then applied to the input $x$ to obtain the featuremap of node $v_j$. This process is repeated for every node of every DAG in the over-parameterized network until convergence. We prune half of the connection parameters $\gamma$ after training the over-parameterized network. For every node, the operation with highest alpha are retained.

Our method allows us to search for more diverse architectures than previous NAS and hand-crafted architectures. It is more fine-grained than those methods yet efficient than searching via all channel level connections. Also, the exploration and exploitation of the search space can be controlled by changing the value of $K$, which allows our method to be useful in various environments ranging from 1 to hundreds of GPUs.

4 Experiments

We take the target task as image classification in our experiments, hence we search for a convolutional neural network directly without cells or building blocks. Our experiments are run on NVIDIA Tesla V100 GPUs. Our operations search space consists of $3 \times 3$, $5 \times 5$ and $7 \times 7$ depthwise separable convolutions and $3 \times 3$, $5 \times 5$ and $7 \times 7$ convolutions.

We demonstrate the efficacy of our method on the CIFAR-10 (Krizhevsky et al. (2009)) image classification benchmark dataset. CIFAR-10 dataset consists of 60000 coloured images of size 32X32 split in 50000 training and 10000 test images equally in 10 classes. We sample 5000 images randomly from the training data for the training of the operation parameters $\alpha$. The weights $w$ and $\gamma$ are updated via SGD optimizer with a momentum of 0.9 and a cosine learning rate scheduler with initial learning rate of 0.1. For updating $\alpha$, we use the Adam optimizer with an initial learning rate of 0.006. Table 1 compares our results with previous NAS methods. The value of the hyperparameter $K$ is equal to 4 in the experiments.

The search time of our method ReNAS with other details is specified in the last row. We note that like other methods, ReNAS is a two-stage approach, having a search and retrain stage. The table shows that ENAS (Pham et al. (2018)) has a slightly lower search time but has higher error rate (lower accuracy) in spite of having more parameters. Similarly, ProxylessNAS (Cai et al. (2019)) has a slightly better accuracy but uses considerably higher search time to come up with higher number of parameters.

We note that while PCDARTS (Xu et al. (2020)) has the least search time with slightly greater accuracy, it is a more complex technique well designed for the already optimal DARTS search space. As discussed in Section 4, this is a restricted search space with a very narrow accuracy range. For example, Yang et al. (2020) found out that from 214 sampled architecture from this search space,
Table 1: Comparison of different NAS methods

| Method                        | Params (M) | Test error (%) | Search time (GPU Days) |
|-------------------------------|------------|----------------|------------------------|
| NASNet-v3 (Zoph & Le (2017))  | 37.4       | 3.65           | 1800                   |
| Block-QNN (Baker et al. (2016)) | 39.8       | 3.54           | 96                     |
| AmoebaNet-B (Real et al. (2017a)) | 34.9       | 2.13           | 3150                   |
| PNAS (Liu et al. (2018a))     | 3.2        | 3.41           | 225                    |
| ENAS (Pham et al. (2018))     | 4.6        | 3.54           | 0.45                   |
| DARTS (Liu et al. (2019))     | 4.6        | 2.76           | 4                      |
| ProxylessNAS (Cai et al. (2019)) | 5.7        | 2.08           | 8.3                    |
| SNAS (Xie et al. (2019b))     | 2.85       | 2.8            | 1.5                    |
| PCDARTS (Xu et al. (2020))    | 3.6        | 2.57           | 0.1                    |
| DNW-MobileNetV1               | 12.11      | 9.8            | 0.2                    |
| ReNAS                         | 4.2        | 2.72           | 0.5                    |

all perform similarly with a mean accuracy of 97.03 ± 0.23. The main purpose of this paper is not to introduce another expert designed method for a niche space and the goal is not to beat the state-of-the-art, but to design a principled approach to finding interesting structures and patterns through automation.

We also compare ReNAS with DNW (Wortsman et al. (2019)), as it unifies core parts of the sparse neural network literature with the neural architecture search problem. Strictly speaking, DNW is not a NAS method and takes a backbone architecture like MobileNet and discovers the edge connections, but it has a constraint that the total number of edges at every round is limited by a hyperparameter $k$. In our method, we do not have such a restriction on the number of edges and explore all block level connections without any backbone architecture and simultaneously search for the operations. Even though the proposed method has a significantly large search space, its performance is on-par with other NAS methods.

5 Discussion

Our method is able to control the granularity of the architecture search. We have observed that the current deep learning frameworks are able to optimize the computation in a layer wise neural network. Our method is not based on layer-wise architecture and instead has node level connections. Hence, the weight computations between nodes in such an architecture does not take advantage of the many tensor optimizations in current frameworks. This is one of the reason why our method is not able to beat the current SOTA methods though it is on par with those methods. Our method should be able to learn complex connections and patterns which are not prevalent in the current literature. We expect it to perform better on unseen and unconventional datasets, thus making this approach applicable to a wider set of problems.

6 Conclusions

In this paper, we take a fresh look at NAS, beyond chasing SOTA performance. We recognize various problems in the current NAS methods, e.g., the problem of searching within a limited space with hand crafted cells and manual backbones and present a novel solution using a gradient-based approach. We use a finer-grained search by having channel-wise block connections, which is better than searching all channel-to-channel connections. Searching channel level connections instead of the block-of-channel connections is expected to provide a more fine grained result, which is a part of our future work. The preliminary results, shown in this paper, are promisingly close to SOTA, and we believe that this pattern will apply to other NAS problems.

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