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TASK-AWARE NEURAL ARCHITECTURE SEARCH

Cat P. Le Mohammadreza Soltani Robert Ravier

Vahid Tarokh

Department of Electrical and Computer Engineering, Duke University

ABSTRACT

The design of handcrafted neural networks requires a lot of time and resources. Recent techniques in Neural Architecture Search (NAS) have proven to be competitive or better than traditional handcrafted design, although they require domain knowledge and have generally used limited search spaces. In this paper, we propose a novel framework for neural architecture search, utilizing a dictionary of models of *base* tasks and the similarity between the *target* task and the atoms of the dictionary; hence, generating an adaptive search space based on the base models of the dictionary. By introducing a gradient-based search algorithm, we can evaluate and discover the best architecture in the search space without fully training the networks. The experimental results show the efficacy of our proposed task-aware approach.

Index Terms— Neural Architecture Search, AutoML, Task Taxonomy

1. INTRODUCTION

Neural Architecture Search (NAS) has been a major focal point for work on automated machine learning (AutoML). Initially studied through the lens of reinforcement learning [1], a modern development of NAS algorithms largely focuses on minimizing both search time and prior knowledge. Though NAS techniques have greatly improved, many recently proposed methods require significant prior knowledge, e.g. the explicit architecture search domain, or the specific task at hand, as input. This requirement restricts their ability to adapt to situations in which future tasks are potentially unknown.

In this work, we propose a novel, flexible NAS framework, which we call Task-Aware Neural Architecture Search (TA-NAS). The ultimate goal of TA-NAS is to develop an algorithm that dynamically learns an appropriate architecture for a given task at hand, making decisions based on prior history and any information input by the user. Our pipeline is composed of three key components. First, we start with a dictionary of base tasks, the atoms of which consist of architectures that accurately perform said tasks. The dictionary serves as a base on which we dynamically build architectures for new tasks not in the dictionary. Based on the idea that similar tasks should require similar architectures, an oftenused assumption in both transfer and lifelong learning, we propose a novel similarity measure for tasks to find the closest base tasks to the new task. Then, we construct a dynamic search space, based on the combined knowledge from the related tasks, without the need for prior domain knowledge. Finally, we present a gradient-based search algorithm, called *Fusion Search* (FUSE). The FUSE algorithm is designed to evaluate the performance of network candidates without fully train any of them. Our experimental evaluation will show the efficacy of our proposed approach.

2. RELATED WORK

Many recently proposed NAS techniques have resulted in architectures with performance comparable to those of handtuned architectures. The techniques themselves are based on a wide range of techniques, including evolutionary algorithms [2], reinforcement learning (RL) [3], and sequential model-based optimization (SMBO) [4]. All of these approaches, however, are very time-consuming and need require computational resources, e.g. potentially thousands of GPUdays. To alleviate these issues, differentiable search [5-9] and random search together with sampling sub-networks from a one-shot super-network [10-12] have been introduced in the literature. For instance, DARTS [6] smooths the architecture search space using a softmax operation. It then solves a bilevel optimization problem which can accelerate the discovery of the final architecture by orders of magnitude [1-4]. Other recent methods include random search [11, 13–15], RL based approaches via weight-sharing [16], and network transformations [17–19].

Besides, [10] has thoroughly analyzed the one-shot architecture search using weight-sharing and correlation between the super-graph and sub-networks. None of the above techniques have yet explored the role of the closeness of tasks in the search neural architecture space. Consequently, the search space used by these techniques is often biased and based on the domain knowledge from the well-performed handcrafted neural network architectures. Here, we propose an approach to encode the similarities between tasks for a more efficient search strategy.

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Algorithm 1: Task-Aware NAS

Initialization: A set of baseline task-data set pairs *B*; **Input**: Task-data set pairs $(T_1, X_1), ..., (T_K, X_K)$, Threshold τ, ϵ ; **Output**: Best architecture for the incoming tasks t; for $t = (K+1), (K+2), \dots$ do for $b \in B$ do Calculate distance $d_{b,t}$ to find the related tasks: end Define search space by combining operations, cells, skeleton from related tasks; while criteria not met do Sample C candidates from search space; Evaluate these candidates using FUSE; end Add the task t and its architecture to *B*. end

3. PROPOSED APPROACH

The pseudocode of TA-NAS is given in Algorithm 1. At time t, we assume that we have access to a dictionary consisting of both previous pairs $(T_1, X_1), ..., (T_{t-1}, X_{t-1})$, of tasks T_k and data sets X_k is a given data set, as well as a collection of such pairs that were available upon initialization. Each pair is represented in our dictionary by a trained network. Given the target pair of (T_t, X_t) , our goal is to find an architecture for achieving high performance on the target task. In summary, TA-NAS works as follows:

- 1. **Task Similarity.** Given a new task-data set pair, TA-NAS finds the most related task-data set pairs in the dictionary.
- 2. Search Space. TA-NAS defines a suitable search space for the incoming (target) task-data set pair, based on the related pairs.
- 3. Search Algorithm. TA-NAS searches to discover an optimal architecture in term of performance for the target task-data set pair on the search space.

3.1. Task Similarity

The TA-NAS pipeline heavily depends on the notion of similarity between task-data set pairs. We define the similarity between task-data set pairs in terms of a model-transformation complexity, N_t . In particular, we first construct a dictionary with the atoms given by the by trained architectures performing well in each base task-data set pairs. More precisely, let $\ell_{(T,X)}(N)$ be a function that measures the performance of a given architecture N on task T with input data X.



Fig. 1. Illustration of the procedure to compute the distance from task A to task B.

Here, $\ell_{(T,X)}(N) = 1$ denotes the highest performance, while $\ell_{(T,X)}(N) = 0$ denotes a complete failure of architecture N on task T. For a fixed $0 < \epsilon < 1$, we say that an architecture N is ϵ -representative for (T, X) if $\ell_{T,X}(N) \ge 1 - \epsilon$. In other words, an architecture N is ϵ -representative if it performs sufficiently well on the given task-data set pair. We thus restrict our attention to ϵ -representative networks.

We now define our measure of dissimilarity between two task-data set pairs using the notion of ϵ -representative architecture. Let $A = (T_A, X_A)$ and $B = (T_B, X_B)$ be two taskdata set pairs, where N_A and N_B are two trained architectures that are ϵ -representative for A and B, respectively. We can define a dissimilarity measure between A and B as follows (hence, the similarity between A and B is given by $1 - d_{A,B}^{\epsilon}$):

$$d_{A,B}^{\epsilon} = \min_{\{N_t \in S_t : \ell_B(N_t \circ N_A) \ge (1-\epsilon)\}} O(N_t), \tag{1}$$

where S_t is a given transform network search space, and O is a general measure of complexity (e.g., the number of parameters in a network). The symbol \circ denotes function (network) composition. In this setting, we assume that the first layer of N_t is the same as the *penultimate* layer of N_A . In practice, the role of N_t is to transform the features of the penultimate layer of N_A generated by elements of X_B and transform them into elements of $N_B(X_B)$. In other words, the model transformation network N_t should be such that it can transfer the $N_A(X_B)$ into $N_B(X_B)$ with minimum complexity. For instance, if N_t is the identity matrix, it means that T_A and T_B are exactly the same as $N_B(X_B) = N_A(X_B)$. In general, $d_{A,B}^{\epsilon}$ is asymmetric measure, i.e., $d_{A,B}^{\epsilon} \neq d_{B,A}^{\epsilon}$. Ideally, O should be zero for two identical tasks, implying that the architecture for A is also suitable for B. In practice, finding the least-complex transform network can be achieved by iterative pruning some super-network for which N_t is a sub-graph with the performance as good as the super-network. The dissimilarity measure is the percentage of the non-zero parameters in the pruned N_t , and it ranges between 0 and 1. This is illustrated in Figure 1.

3.2. Search Space

Defining a meaningful search space is the key to efficiently finding the best architecture for a specific task. In the NAS



Fig. 2. Illustration of the cell and the skeleton.

literature, the search space is typically defined by stacking a structure called cell, as illustrated in Figure 2. A cell is a densely connected directed-acyclic graph (DAG) of nodes, where all nodes are connected by operations. Other NAS techniques such as one-shot approaches (e.g., DARTS [6], NAS-Bench201 [20]) have also introduced another structure in the search space referred to as skeleton. A skeleton is a combination of cells with other operations, forming the complete network architecture. A skeleton is normally predefined, and the goal of NAS algorithms is to find the optimal cells. In this paper, we similarly define the search space in terms of skeletons and cells. Specifically, we focus our search on cells and their operations. As mentioned, cells consist of nodes and operations. Each node has 2 inputs and 1 output. The operations (e.g., identity, zero, convolution, pooling) are set so that the dimension of the output is the same as that of the input. If n is the number of nodes in a cell and m denotes the number of operations, the total number of possible cells is given by: $\mathbf{m} \times \exp\left(\frac{\mathbf{n}!}{2(\mathbf{n}-2)!}\right).$

Our use of a dissimilarity measure gives us knowledge about how related two tasks are. Build upon this knowledge, we can define the search space of the target task-data set pair by combining the skeletons, cells, and operations from only the most similar pairs in the dictionary. Since the search space is restricted to only related tasks, the architecture search algorithm can perform efficiently and requires few GPU hours to find the best candidate network. We have illustrated this in the experimental section.

3.3. Search Algorithm

The Fusion Search (FUSE) is a novel search algorithm that considers the network candidates as a whole and performs the optimization using gradient descent. Let C be the set of candidate networks on which we define the search space. Given $c \in C$ and training data X, denote by c(X) the output of the network candidate c. The FUSE algorithm, as illustrated in Algorithm 2, is based on the continuous relaxation of the network outputs. It is capable of searching through all networks in the relaxation space without fully training them. We use as our relaxed space C the set of all convex combinations of can-

Algorithm 2: FUSE Algorithm			
Input : search space S, X_{train} , X_{val} , I;			
Initilization : c^* , α ;			
Output: Best architecture;			
for $i = 1,, I$ do			
$C = [c^*, and candidates sampled from S];$			
while α not converge do			
Update C by descending $\nabla_w \mathcal{L}_{train}(w; \alpha, \bar{c});$			
Update α by descending $\nabla_{\alpha} \mathcal{L}_{val}(\alpha; w, \bar{c})$;			
end			
$c^* = \arg\max_{c \in C} \alpha_c;$			
end			

didate networks, which each weight in the combination given by exponential weights:

$$\bar{c}(X) = \sum_{c \in C} \frac{\exp\left(\alpha_c\right)}{\sum_{c' \in C} \exp\left(\alpha_{c'}\right)} c(X), \tag{2}$$

where \bar{c} is the weighted output of network candidate c, and α_c is a continuous variable that assigned to candidate c's output. We then conduct our search by jointly training the network candidates and optimizing their α coefficients. Let X_{train} , X_{val} be the training and validation data set. The training procedure is based on alternative minimization and can be divided into: (i) freeze α coefficients, jointly train network candidates, (ii) freeze network candidates, update α coefficients. Initially, α coefficients are set to 1/|C|. While freezing α , we update the weights in network candidates by jointly train the relaxed output \bar{c} with cross-validation loss on training data:

$$\min_{w} \mathcal{L}_{train}(w; \alpha, \bar{c}, X_{train}), \tag{3}$$

where w are weights of network candidates in C. Next, the weights in those candidates are fixed while we update the α coefficients on validation data:

$$\min_{\alpha} \mathcal{L}_{val}(\alpha; w, \bar{c}, X_{val}).$$
(4)

These steps are repeated until α converges. The most promising candidate will be selected by: $c^* = \arg \max_{c \in C} \alpha_c$. This training procedure will deliver the best candidate among candidates in C without fully training all of them. In order to go through the entire search space, this process is repeated until certain criteria, such as the number of iterations, the performance of the current most promising candidate, is met.

4. EXPERIMENTAL STUDY

We evaluate the TA-NAS algorithm on image data sets and classification tasks. For our experiment, we initialize the TA-NAS with a set of base binary classification tasks consisting of finding specific digits in MNIST [21] and specific objects in Fashion-MNIST [22]. We find ϵ -representatives for

each task by pre-training networks on the same architecture $(\operatorname{conv}(32 \times 5 \times 5) \rightarrow \operatorname{dense}(1024) \rightarrow \operatorname{dense}(2))$. Here, we pick representative architectures that achieve at least 96% accuracy on their tasks.

In order to compute the dissimilarity between architectures, we consider for A and B (two task-data set pairs) the first two layers of their trained ϵ -representative networks, which we denote by N_A and N_B , respectively. We then wish to find the least complex architecture that maps hidden features from one task to the other. We thus consider a transform network N_t with a dense(2048) \rightarrow dense(512) \rightarrow dense(1024) architecture. We train N_t with mean-square error (MSE) loss on a data set consisting of $N_A(X_B)$ and those of $N_B(X_B)$; here, the goal is to transform $N_A(X_B)$ into $N_B(X_B)$. We then iteratively prune the trained N_t as much as possible while maintaining similar performance to N_t . We take our dissimilarity measure to be the percentage of the remaining non-zero parameters in N_t after pruning. We show our results in Figure 2. Our results suggest that two tasks from the same data set (e.g., MNIST or Fashion-MNIST) are often more similar than tasks involving different data sets. It is perhaps interesting to note that the similarity from MNIST tasks to Fashion-MNIST tasks is greater than the similarity from Fashion-MNIST tasks to those in MNIST. Consequently, we can often use Fashion-MNIST knowledge on MNIST, but not vice-versa.

The task on which we perform NAS is binary classification on Quick, Draw! [23] dataset. The Quick, Draw! is a doodle drawing dataset of 345 categories. In this experiment, we select a subset of the Quick, Draw! with a similar format to MNIST and fashion-MNIST, by choosing only 10 categories (e.g., apple, baseball bat, bear, envelope, guitar, lollipop, moon, mouse, mushroom, rabbit) with each has 60,000 data points. Our task of interest is the moon indicator from this subset of Quick, Draw! data set. We pre-train this task and compute dissimilarities to other tasks in the same manner as above. To conduct our search, we choose the top three most similar tasks to the baselines discussed above: (i) digit 0, (ii) trouser, (iii) digit 3 indicators. Due to the similarity in the shape of digit 0 and the moon, the base task of digit 0 indicator is the most related task to the moon indicator.

After obtaining the related tasks, we combine the operations and cell structures to generate a suitable search space for the target task. The cell consists of 4 nodes, with 6 edges of operations. The list of operations includes identity, zero, dil-conv3x3, sep-conv3x3, maxpool2x2. Next, the search algorithm is used to find the best architecture in this search space. Initially, three network architectures are randomly generated from the search space. At each iteration, FUSE quickly evaluates these candidates and only saves the best architecture for the next iteration. The search stops only when all criteria (e.g., a prespecified maximum number of iteration or best architecture converges) are met. The results in Table 1 give the best test error of the optimal architecture found by



Fig. 3. The distance matrix of baseline tasks.

Architecture	Error (%)	Param (M)	GPU days
ResNet-18 [25]	1.42	11.44	-
ResNet-34 [25]	1.2	21.54	-
DenseNet-161 [24]	1.17	27.6	-
Random Search	1.33	2.55	4
FUSE w. standard space	1.21	2.89	2
FUSE w. task-aware space	1.18	2.72	2

 Table 1. Comparison with state-of-art image classifiers on Quick, Draw! dataset.

TA-NAS after 20 trials, in comparison with a random search algorithm and other state-of-art handcrafted networks (e.g., DenseNet [24], ResNet [25]). The architecture produced by TA-NAS is competitive with manual-designed networks while having a smaller number of parameters. When comparing with the random search method using our pre-defined search space, TA-NAS approach achieves a higher accuracy model with less search time in terms of GPU days (i.e., the number of days for a single GPU to perform the task). Hence, this framework can utilize the knowledge of related tasks to find the efficient network architecture for the target task.

5. CONCLUSION

We proposed TA-NAS, a novel task-aware framework to address the Neural Architecture Search problem. By introducing a similarity measure for given pairs of tasks and data sets, we can define a restricted, dynamic architecture search space for a new task-data set pair based on similar previously observed pairs. Additionally, we proposed the gradient-based search algorithm, FUSE, to quickly evaluate the performance of network candidates in the search space. This search algorithm can be applied to find the best way to grow or to compress the current network.

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