TASK-AWARE NEURAL ARCHITECTURE SEARCH

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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], 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 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 for 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 often-used 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 quickly 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 hand-tuned 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 GPU-days. 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], RL based approaches via weight-sharing [16], and network transformations [17,22].

In addition, [10] has thoroughly analysed 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 closeness of tasks in the search neural architecture space. Consequently, the search space used by these techniques 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 more efficient search strategy.
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 \(\tau, \epsilon\);
Output: Best architecture for the incoming tasks;
for \(t = 1,...,K\) 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
  If desired, add the trained 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 trained networks. Given the target pair of \((T_t, X_t)\), our goal is to find an architecture for achieving a 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 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 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 \(X\).

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 literature, the search space is typically defined by stacking a
structure called cell. A cell is a densely connected directedacyclic 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 [23]) 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. An 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 \( m \exp(\frac{m}{2(n-2)}) \).

Our use of a dissimilarity measure gives us the knowledge about how related two tasks are. Build upon this knowledge, we can define 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 the 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 consider the network candidates as a whole and perform the optimization using gradient descent. Let \( C \) be the set of candidates 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, and searching through all networks in the relaxed space without fully training them. We use as our relaxed space \( C \) the set of all convex combinations of candidate networks, which each weight in the combination given by exponential weights:

\[
\bar{c}(X) = \sum_{c \in C} \sum_{c' \in C} \exp(\alpha_c) c(X),
\]

where \( \bar{c} \) is the weighted output of network candidate \( c \), and \( \alpha_c \) 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 \( \alpha \) coefficients. Let \( X_{\text{train}} \), \( X_{\text{val}} \) be the training and validation data set. The training procedure is based on alternative minimization and can be divided into: (i) freeze \( \alpha \) coefficients, jointly train network candidates, (ii) freeze network candidates, update \( \alpha \) coefficients. Initially, \( \alpha \) coefficients are set to \( 1/|C| \). While freezing \( \alpha \), we update the weights in network candidates by jointly train the relaxed output \( \bar{c} \) with cross-validation loss on training data:

\[
\min_w L_{\text{train}}(w; \alpha, X_{\text{train}}),
\]

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

\[
\min_{\alpha} L_{\text{val}}(\alpha; w, X_{\text{val}}).
\]

These steps are repeated until \( \alpha \) converges. The most promising candidate will be selected by: \( c^* = \arg \max_{c \in C} \alpha_c \). This training procedure will result the best candidate among \( C \) candidates without fully training all of them.

### 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 [24] and specific objects in Fashion-MNIST [25]. We find \( \epsilon \)-representatives for each task by pre-training networks on the same architecture (conv(\(32 \times 5 \times 5\) → dense(1024) → 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 \( \epsilon \)-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) → dense(512) → 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
Fig. 2. The distance matrix of baseline tasks.

$N_i$. We take our dissimilarity measure to be the percentage of the remaining non-zero parameters in $N_i$ 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 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! [26] 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 for-
ding 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.

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

| Architecture            | Error (%) | Params (M) | GPU days |
|-------------------------|-----------|------------|----------|
| ResNet-18 [28]          | 1.42      | 11.44      | -        |
| ResNet-34 [28]          | 1.2       | 21.54      | -        |
| DenseNet-161 [27]       | 1.17      | 27.6       | -        |
| Random Search           | 1.33      | 2.55       | 4        |
| FUSE with standard space| 1.21      | 2.89       | 2        |
| FUSE with task-aware space| 1.18     | 2.72       | 2        |

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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