Neural Architecture Search Over a
Graph Search Space

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Abstract

Neural architecture search (NAS) enabled the discovery of state-of-the-art architectures in many domains. However, the success of NAS depends on the definition of the search space, i.e., the set of the possible to generate neural architectures. State-of-the-art search spaces are defined as a static sequence of decisions and a set of available actions for each decision, where each possible sequence of actions defines an architecture. We propose a more expressive formulation of NAS, using a graph search space. Our search space is defined as a graph where each decision is a vertex and each action is an edge. Thus the sequence of decisions defining an architecture is not fixed but is determined dynamically by the actions selected. The proposed approach allows to model iterative and branching aspects of the architecture design process. In this form, stronger priors about the search can be induced. We demonstrate in simulation basic iterative and branching search structures and show that using the graph representation improves sample efficiency.

1 Introduction

Deep neural networks have yielded success in many supervised learning problems [LeCun et al., 2015]. However, the design of state-of-the-art deep-learning algorithms requires many decisions, involving human time and expertise. AutoML speeds up this process by automating some of the decisions [Yao et al., 2018]. AutoML algorithms may be used to design different aspects of the downstream learning algorithm, from tuning individual hyperparameters, to building architectures, or composing parametric optimization functions. AutoML algorithms are usually based on an optimization routine, for which many strategies have been proposed: random search [Bergstra and Bengio, 2012], evolutionary algorithms [Real et al., 2018], and Bayesian optimization [Swersky et al., 2013, Hutter et al., 2011].

In this paper we focus on neural architecture search (NAS) [Zoph and Le, 2017]. This approach to AutoML relies on a neural controller to learn to explore the search space of architectures. The parameters of the controller are optimized to maximize the performance of generated networks on the downstream task. This approach has shown many recent successes, with automatic design of RNN cells [Zoph and Le, 2017], convolutional blocks [Zoph et al., 2017], activation functions [Prajit Ramachandran, 2018] and optimizers [Bello et al., 2017, Wichrowska et al., 2017].

The success of neural architecture search hinges on the search space. State-of-the-art search spaces are defined as a linear chain of decisions and a set of available actions for each decision. For example, the first decision might be “select the learning rate” and the corresponding set of actions might be: {0.1, 0.01}, and the second decision might be “choose the number of layers” and its set of available

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actions might be: \{1, 2, 3\}. Each possible sequence of actions defines a single architecture. The controller samples one architecture by sampling one action for each decision in the fixed sequence.

A limitation of the current approaches is that the sequence of available decisions is a static sequence with fixed length and order. This limits the application to problems in which the search space cannot be efficiently defined as a linear sequence of decisions. For example, consider a search space that first picks between more optimizers and then chooses the hyperparameters for the picked optimizer. Performing search over this space using a static sequence of decisions forces the controller to make decisions about hyperparameters of all optimizers, rather than only of the picked one. Or as another example, consider a search space that stacks an arbitrary number of convolutional layers and choose different parameters for every added convolution, with a linear search space this iterative component can be represented only by rolling out the loop for a fixed number of iterations.

The main goal of this paper is to lift the limitation of the linear search space for NAS methods. Inspired by other approaches to AutoML [Swersky et al. 2013], we propose to model the search space in NAS as a graph, where each decision is a vertex and each action is an edge. Thus the sequence of decisions defining an architecture is not fixed but is determined dynamically by the choice of the prior actions. With this approach the controller may branch and iterate over states, both natural processes in architecture design, resulting in more efficient optimization, as we will show in our experiments.

In summary, we propose a novel neural controller whose dynamic RNN architecture allows to select a path through the graph and condition the actions’ distributions on the prior actions. The proposed graph search space may replace static linear search spaces used by any neural optimizers, therefore this technology can be used in conjunction with other advances in neural architecture search.

2 Neural Architecture Search Over a Graph Search Space

In this section we describe the two main contributions of this paper: 1) the generalization of NAS to a graph search space; 2) the dynamic neural architecture controller, capable of learning to search over graph search spaces.

2.1 Neural architecture search as a walk in a graph

NAS aims to find the optimal architecture for a given ML task. To do this, NAS takes an iterative approach. At each iteration, a generative neural network, called the controller, proposes a new architecture. Next, this architecture is then trained and evaluated on the ML task. Finally, the task’s evaluation metric is used as a reward to update the controller, using an RL algorithm.

Zoph and Le [2017] propose to model the search space as a fixed length sequence of states \(s_1:T\), one state for each decision. This approach allows to implement the controller as a recurrent neural network. In each state \(s_t\) the controller takes one of the available actions \(a_t\). The final sequence of actions \(a_1:T\) defines the new architecture to be tested by the trainer.

Modeling the search space as a static length sequence has important limitations, as we discussed in the introduction. For example, consider a search space that first picks between more optimizers and then chooses the hyperparameters for the picked optimizer. Performing search over this space using a static sequence of decision forces the agent to make decisions about hyperparameters of all optimizers, rather than only of the picked one. In general, the linear search space formalism does not allow to efficiently model iterative and branching components of the architecture design process. Furthermore, simple combinations of such constructs are not feasibly represented with a linear search space.

To overcome these limitations, we propose to model the search space as a directed graph, \(\mathcal{G} = (V, A)\), where each state is represented by a vertex, \(v_t \in V\), and each action is represented by a directed edge, \(a_t \in A\). Note that this formalism allows for multiple edges between each pair of vertices, and the graph can be cyclic. Each path from the start state to a terminal state yields a sequence of actions defining an architecture.

When traversing the graph, paths are sampled, starting from the start state \(v_0\). Actions \(a_t\) are sampled iteratively from those available at the current state \(A_{v_t}\). Actions are sampled from the distributions inferred by the controller \(p_{v_t}(a_t)\). The next vertex, \(v_{t+1}\), is determined by following the sampled
Add a layer?  Type of layer  Which optimizer?  Learning rate  Adam β1

(a) Search space represented as a sequence

(b) Search space represented as a graph

Figure 1: Example search space defining two design choices: 1) whether to add a layer, 2) what optimization scheme to use. This is configured as a linear search space on the left (a) and as a graph search space on the right (b). In the graph instantiation, the controller does not have to make unnecessary decisions: if it chooses not to use Adam, it still has to choose a value for Adam’s β1. Also, the graph search space allows to create a distinct state for choosing the learning rate for each optimizer choice, easing the learning of eventual conditioning.

(\text{edge } a_t). The walk is terminated upon reaching any of the terminal vertices. After termination, the sampled architecture is defined by the sequence of actions \((a_1, \ldots, a_T)\). Note that \(T\) does not have to be constant, and each state can be visited multiple times. For an example see Figure 1.

2.2 Dynamic neural controller architecture

To optimize over a graph search space, we propose a modification of the RNN-based neural controller model from \cite{Zoph and Le 2017}. The proposed architecture allows the controller to sample a path from an arbitrary graph, while dynamically setting the sequence of RNN steps to match the sequence of sampled states. Such dynamic architecture is needed to explore graph search spaces, since each action distribution is inferred by a distinct portion of the controller architecture, and the action distribution to sample from at a given timestep \(t\) is determined only after the action is sampled at the prior timestep \(t-1\). Instead, for the linear search space, each RNN timestep \(t\) always correspond the same action distribution, thus allowing to work with a static controller architecture.

Figure 2 depicts the architecture for a timestep of the dynamic RNN controller. At each timestep, the controller takes as input: 1) the current state \(v_t\), 2) the previous action \(a_{t-1}\), 3) the RNN cell state. These inputs are aggregated by the timestep independent network. This is the part of the network whose parameters are the same at each timestep. This includes the action and state embedding tables. The embeddings of \(a_{t-1}\) and \(v_t\) are aggregated with a fully connected network. Then, this aggregation is the input to an LSTM RNN cell. Which has the function of conditioning on learned representation of the prior actions sequence. The following portion of the architecture is timestep dependent. It has the function of inferring the action distribution of the current state \(v_t\). Note that the shapes and parameters of this part of the architecture can be determined only after \(a_{t-1}\) is sampled at the previous timestep. Thus it is set dynamically as the actions sequence is sampled. The outputs are: 1) the action \(a_t\) sampled from the timestep dependent action distribution, 2) the next state \(v_{t+1}\) determined by \(a_t\) 3) the new RNN state.

The training is analogous to \cite{Zoph and Le 2017}. The controller learns the action distributions with the objective of maximizing the expected reward of the generated architectures using policy gradient methods.

Notice that the dynamic controller is not required to visit all the states in the search space. This brings multiple benefits that can improve the sample efficiency and stability the controller. Firstly, the controller visits less states, easing credit assignment. Secondly, gradient updates are performed only for actions that are relevant to the generated model. This reduces the variance of the policy gradient updates \cite{Greensmith et al. 2004}.
3 Experiments

We demonstrate the potential benefit of performing architecture search with a graph search space, and the ability of the dynamic controller to optimize this space, using two artificial tasks. For this, we present hand-crafted optimization problems that are representative of the branching and iterative components of architecture design. For each toy task, we compare the efficacy of modeling the search space as a sequence or a graph.

The first task models the iterative process of stacking layers. The second task models a decision that involves branching, such as picking the optimizer among few alternatives, and tuning its parameters. In both tasks we demonstrate that expressing the search space as a graph significantly improves the sample efficiency of the controller.

In all experiments we use the dynamic neural controller introduced in Section 2.2, trained with the REINFORCE algorithm [Williams, 1992]. All experiments are repeated 4 times, and the results are averaged.

3.1 Stacking layers task

The first task is based on an iterative, or cyclic, search space. This task simulates the process of constructing a neural network with a variable number of layers. In this task, a search space over a simulated “number of layers”, \( n \), is defined. The controller must choose the optimal number. The reward in this simulation is defined as \(- (n - L)^2\). The maximum reward is achieved by constructing a network with exactly \( L \) layers. Otherwise, a squared error penalty is applied. Note that extensions of this task might include setting different parameters for each layer, such as number of units or learning rate.

To compare the two approaches, we define both linear and graph instances of this search space. Both are shown in Figure 3. A linear search space describing this task is defined as a sequence of states of length \( 2L \). At each state only 2 actions are available, either to add 1 extra layer or to terminate. The graph search space is defined as a single state with 2 actions. The action to add a new layer is represented as a cyclic edge on the unique state. The second action transitions to the terminal state, after which no more layers are added.
Figure 3: “Stack layers” task of length $L$. The controller is maximally rewarded if it makes $L$ consecutive steps and is penalized for taking more or fewer steps. This is inspired by the common phenomenon in constructing architectures where using either too few, or too many layers leads to poorer performance.

Figure 4: Results for the “stack layers” task. Average reward over time is given for linear (red) and graph based search space (green). The shaded area corresponds to maximum and minimum reward attained between the trials. The task is solved by achieving reward 1.

For the following experiments, $L$ is set to 10. The reward is normalized to $[0, 1]$ range. The controller is trained with learning rate 0.001 and entropy regularization 0.1.

The results are summarized in Figure 4. The graph search space improves training speed, converging to the maximum reward much more rapidly. In fact, in this search space, linear fails to attain maximal reward in the number of trials ran, 200. In the linear case the controller is forced to output a fixed number of decisions, which, in this task, forces an arbitrary upper bound (for we chose $2L$ based on prior knowledge of the simulated task). However, the graph search space has no bound on number of iterations, thus, lifting the constraint on the maximum number of layers required by the linear version. The graph search space could be harder to optimize, because it may accept an infinite number of trajectories. Despite the added complexity, the dynamic controller is able to solve the task more effectively searching over the graph.

3.2 Select an optimizer task

The second task is based on a branching choices search space. This task simulates picking between several optimizers, then choosing optimizer specific hyper-parameters, such as learning rate or decay rate. Thus, we designed a toy task that requires the controller to first choose an optimizer $b$ among $B$ options, and then chooses 4 optimizer specific hyper-parameters: $p_1, p_2, p_3, p_4$. For the following experiments $B$ may take a value in $\{2, 4\}$, and each of the hyperparameter can be set to a value in the range $[1, 100]$.

The reward is defined as follows. The agent is maximally rewarded for setting all the 4 relevant hyperparameters to the value of 50. Let $M(b, p_1, p_2, p_3, p_4) = \arg \min_{i=1,...,4} p_i \neq 50$, i.e. $M$
denotes index of the first incorrect \( p_i \). The unnormalized reward is then given by:

\[
r(b, p_1, p_2, p_3, p_4) = -(p_M - 50)^2 - \sum_{i=M+1}^{4} 50^2
\]

We normalize the reward to \([0, 1]\) range. This specific choice of the reward function is motivated by our early experiments in which we found that random search can be a strong baseline. To highlight the potential of graph based search space we decided to use a reward which is difficult to optimize using a random search.

Figure 5 illustrates how the "pick an optimizer" task may be defined as linear and graph search space. Both search spaces have one state to choose the optimizer, and then four states for each optimizer choice. The main difference is that the graph search space allows one to build a tree structure having a branch dedicated to each optimizer specific list of hyperparameters. The linear formulation requires to flatten the tree structure into a sequence and choose also the hyperparameters of unused optimizers.

Again, the reward is normalized to \([0, 1]\), and the controller is trained with learning rate 0.001 and entropy regularization 0.1.

The maximum reward achieved by each time step is shown in Figure 4 for environment with two branches (left) and four branches (right). Similar to results on the previous toy task, the graph search space improves optimization speed. We observe a larger benefit in the environment with more branches.
4 Related Work

The complexity of model engineering in machine learning is widely recognized. Recent successes in automated model design have spurred further work in learning to learn [Thrun and Pratt, 2012]. A variety of optimization methods have been proposed to search over architectures, hyperparameters, and learning algorithms. These include random search [Bergstra and Bengio, 2012b], parameter modeling [Bergstra et al., 2013], meta-learned hyperparameter initialization [Feurer et al., 2015], deep-learning based tree searches over a predefined model-specification language [Negrinho and Gordon, 2017], learning of gradient descent optimizers [Wichrowska et al., 2017; Bello et al., 2017], and learning to generate network weights directly [Ha et al., 2016; Brock et al., 2017]. An emerging body of neuro-evolution research has adapted genetic algorithms for these complex optimization problems [Conti et al., 2017], including to set the parameters of existing deep networks [Such et al., 2017], evolve image classifiers [Real et al., 2017], and evolve generic deep neural networks [Miikkulainen et al., 2017].

Our work is most closely related to deep RL based methods for auto ML. Neural Architecture Search (NAS) [Zoph and Le, 2017] introduced the idea to use deep neural network controller, trained with RL, to generate architecture configurations. NAS was applied to construct Convolutional Neural Networks (CNNs) for the CIFAR-10 task and Recurrent Neural Networks (RNNs) for the Penn Treebank tasks. Significant efforts have been made to achieve increased sample efficiency efficient using a progressive search procedure [Liu et al., 2017], parameter sharing [Cai et al., 2017; Pham et al., 2018], or transfer learning [Wong et al., 2018].

This paper proposes a more expressive formalism for defining model architecture search space for RL based approaches, by generalizing the linear search spaces to graphs. Extension of linear search spaces to tree structures have been proposed in prior work in the domain of automatic model selection and hyperparameter tuning for approaches based on Bayesian Optimization. These include using specific kernels [Swersky et al., 2013] or random forests [Thornton et al., 2013] to model the acquisition function.

5 Conclusions

We introduce a more expressive formalism for defining neural architecture search spaces. We present a dynamic controller that is able to efficiently learn to explore this new class of search spaces. In simulation, we show significant improvements in sample efficiency in exploring common iterative or branching architecture design patterns. As next steps, we plan to apply this method to real neural architecture search tasks and design a new class of search spaces that are not feasible in the linear form.

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