Research Article

Alexandr Udeneev, Petr Babkin, and Oleg Bahteev

Surrogate assisted diversity estimation in NES

https://doi.org/10.1515/sample-YYYY-XXXX
Received Month DD, YYYY; revised Month DD, YYYY; accepted Month DD, YYYY

Abstract: The automated search for optimal neural network architectures (NAS) is a challenging computational problem, and Neural Ensemble Search (NES) is even more complex. In this work, we propose a surrogate-based approach for ensebmle creation. Neural architectures are represented as graphs, and their predictions on a dataset serve as training data for the surrogate function. Using this function, we develop an efficient NES framework that enables the selection of diverse and high-performing architectures. The resulting ensemble achieves superior predictive accuracy on CIFAR-10 compared to other one-shot NES methods, demonstrating the effectiveness of our approach.

Keywords: NES, GCN, triplet loss, surrogate function.

1 Introduction

Neural network ensembles often demonstrate better accuracy compared to single models, especially in classification and regression tasks [1, 2]. This fact gives rise to the problem of constructing an efficient ensemble of models (NES) [3]. NES, in turn, relies on Neural Architecture Search (NAS) methods, which are extensively studied and applied to search for individual neural network architectures, such as evolutionary algorithms [4, 5], reinforcement learning [6–8], and Bayesian optimization [9, 10]. Selecting an optimal architecture for even a single model is a challenging task, particularly when considering data-specific constraints and computational limitations [11].

The simplest approach for ensemble construction is the use of DeepEns [12], implemented through DARTS [13]. It involves a random search for several architectures, which are then combined into an ensemble. Despite its simplicity in implementation and hyperparameter tuning, this method is computationally expensive. More sophisticated adaptation techniques are presented in some recent works [3, 14, 15], which are designed to efficiently combine multiple networks into an ensemble.

Our research also adapts ideas from NAS for NES, specifically using a surrogate function. Some modern NAS methods widely use surrogate functions to estimate architecture quality without requiring full model training [16–18]. These functions significantly reduce computational costs, expanding the applicability of such methods. For example, in [16], evolutionary algorithms were proposed in combination with surrogate models for real-time semantic segmentation. In [18], a Surrogate-assisted Multiobjective Evolutionary-based Algorithm (SaMEA) is used for 3D medical image segmentation.

In this work, we propose a method for constructing neural network ensembles using a surrogate function that accounts for both model classification accuracy and architectural diversity. Diversity is crucial because ensembles consisting of similar models often fail to provide a significant performance gain. The surrogate function is used to encode the architecture into a latent space [19], which reflects both the diversity and predictive ability of the architectures. Since a neural network architecture is represented as a graph, using a Graph Neural Network (GNN) [20] as a surrogate function [21] seems natural. To train it to predict model diversity, we use Triplet Loss [22], similar to [19]. We validate this approach on CIFAR-10, demonstrating the effectiveness of the surrogate function for predicting diversity and constructing ensembles. We claim

that ensembles constructed in this manner achieve state-of-the-art accuracy compared to one-shot NES algorithms, such as DeepEns [12].

Main Contributions:

1) We propose a method for encoding the DARTS [13] search space into a representation suitable for training a Graph Neural Network (GNN), where graph nodes correspond to operations within the network.

2) We propose a way for training the surrogate function to predict the diversity of architectures.

3) We adapt surrogate functions for ensemble construction, taking into account both predictive performance and architectural diversity.

2 Problem statement

2.1 Neural Architecture Search

Let us consider a set of nodes $\mathcal{V} = \{x_1, \ldots, x_N\}$, representing the layers of a neural network. Additionally, let $\mathcal{O}$ denote the set of possible operations that can be applied to these nodes (e.g., convolutions or poolings). Furthermore, let $\mathcal{A}$ be the set of feasible architectures, represented as vectors.

Denote $\mathcal{L}_{train}$ and $\mathcal{L}_{val}$ as the training and validation losses, respectively. The NAS problem can then be formulated as the search for an optimal architecture α^* that minimizes $\mathcal{L}_{val}(\alpha^*, \omega^*)$, under the constraint that the weights are obtained by minimizing the training loss:

$$\omega^* = \arg\min_{\omega \in \mathcal{W}} \mathcal{L}_{train}(\alpha^*, \omega)$$

This can be expressed as the following optimization problem:

$$\begin{aligned} &\min_{\alpha \in \mathcal{A}} \mathcal{L}_{val}(\omega^*(\alpha), \alpha) \\ &\text{s.t.} \quad \omega^*(\alpha) = \arg\min_{\omega \in \mathcal{W}} \mathcal{L}_{train}(\omega, \alpha) \end{aligned} \tag{1}$$

The primary challenge in this optimization lies in the immense search space of possible architectures (e.g., in DARTS [13], it is approximately 10^{25}).

2.2 Neural Ensemble Search

The primary objective of NES is to find an optimal ensemble of neural networks whose architectures lie within the NAS search space.

As before, we denote $\alpha \in \mathcal{A}$ as a network architecture and $\omega(\alpha)$ as its corresponding weights. The action of this network on an input x is denoted by $f_\alpha(x, \omega(\alpha))$. Let $S \subset \mathcal{A}$ be a subset of architectures. Then, the NES problem can be formally described as follows:

$$\begin{aligned} &\min_{S} \mathcal{L}_{val}\left(\frac{1}{|S|}\sum_{\alpha \in S} f_\alpha(x, \omega^*(\alpha))\right) \\ &\text{s.t.} \quad \forall \alpha \in \mathcal{S}: \ \omega^*(\alpha) = \arg\min_{\omega(\alpha)} \mathcal{L}_{train}(f_\alpha(x, \omega(\alpha))) \end{aligned} \tag{2}$$

Thus, in addition to searching over a vast number of architectures, we now also need to find the optimal ensemble composition.

3 Method

Table of Notation

Symbol	Description
$\mathcal{A}$	**The space of architectures**
α	**A specific architecture**
$\omega(\alpha)$	**Network weights corresponding to architecture** α
$f_\alpha(x, \omega(\alpha))$	**The output of the model with architecture** α **on input** x
$\mathcal{V}$	**The set of nodes in a normal or reduction cell**
$\mathcal{O}$	**The set of operations on the nodes**

In this work, we consider the transformation of the architecture space proposed in DARTS [13] for application in Graph Convolutional Networks (GCN) (see Section 3.1). In Section 3.2, we analyze the trade-off between accuracy and model diversity for ensemble construction using the Hellinger distance. In Section 3.3, we present the architecture of the surrogate function and describe its working principle, while Section 3.4 provides a detailed discussion of the ensemble construction method based on this surrogate function.

3.1 The space of architectures

One of the key aspects of this work is the training of a surrogate function. The training data consist of neural network architectures, their prediction logits, and the accuracy on a validation dataset.

The models are constructed using the DARTS search space, which includes the following operations:

- separable convolutions of size 3×3 and 5×5;
- dilated separable convolutions of size 3×3 and 5×5;
- 3×3 max pooling;
- 3×3 average pooling;
- identity;
- zero.

As in the original paper, both normal and reduction cells are utilized; however, in our work these cells are generated randomly. In our approach, each cell is represented as a directed acyclic graph consisting of n nodes and m edges, where each edge corresponds to one of the aforementioned operations. The nodes are interpreted as latent states—i.e., the result of applying the operations (specifically, the average of the sum of the outputs of these operations).

Thus, the architecture space $\mathcal{A}$ is defined as the set of directed acyclic graphs constructed from sequential blocks representing normal and reduction cells.

Note that, unlike in the original DARTS, where a continuous relaxation of the operations is employed, in our approach the operations are selected discretely and their weights are not updated during optimization.

In our work, both normal cells and reduction cells consist of five nodes. From each node, two edges emerge, with each edge being assigned an operation randomly chosen from the DARTS search space.

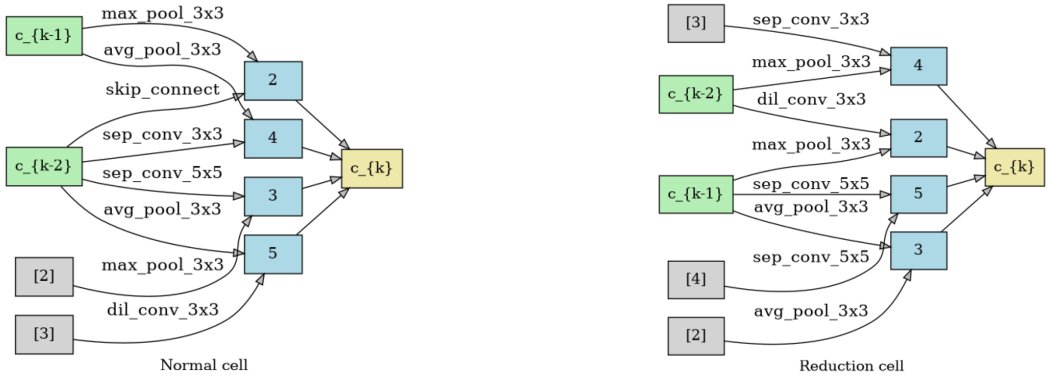

Fig. 1: Example of cells used in the generated models.

The models used for training the surrogate function are built based on two normal cells and one reduction cell. Consequently, the total number of possible architectures is estimated as

$$\left(\binom{2}{2}\cdot\binom{3}{2}\cdot\binom{4}{2}\cdot\binom{5}{2}\cdot 8^8\right)^2 \approx 10^{18},$$

which makes an exhaustive search over all architectures computationally infeasible.

3.2 Performance vs. Diversity Trade-off

3.3 Surrogate Function

3.4 Ensemble Construction

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