Surrogate-Assisted Diversity Estimation in Neural Ensemble Search

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Motivation and Approach

Objective:

To develop an effective surrogate-assisted method for Neural Ensemble Search (NES).

Motivation:

Accurate diversity estimation in ensembles is crucial for improving performance.

Proposed Approach:

Project network architectures into a latent space equipped with the Euclidean norm.

Related Work

This study builds upon the following research:

- Similarity surrogate-assisted evolutionary neural architecture search with dual encoding strategy (Xue, Zhang, Neri, 2024)
- Neural Predictor for Neural Architecture Search (Wen et al., 2019)

Problem Statement

Let $\boldsymbol{\alpha} \in \mathcal{A}$ denote a network architecture, and $\boldsymbol{\omega}(\boldsymbol{\alpha})$ its trained weights. The output of a network on input $\boldsymbol{x}$ is $f_{\boldsymbol{\alpha}}(\boldsymbol{x}, \boldsymbol{\omega}(\boldsymbol{\alpha}))$. Given a subset $S \subset \mathcal{A}$, the NES problem is formally defined as:

$$\min_{\mathcal{S}} \mathcal{L}_{val} \left(\frac{1}{|S|} \sum_{\boldsymbol{\alpha} \in S} f_{\boldsymbol{\alpha}}(\boldsymbol{x}, \boldsymbol{\omega}^*(\boldsymbol{\alpha})) \right)$$

$$\text{s.t.} \quad \forall \boldsymbol{\alpha} \in \mathcal{S}: \ \boldsymbol{\omega}^*(\boldsymbol{\alpha}) = \arg\min_{\boldsymbol{\omega}(\boldsymbol{\alpha})} \mathcal{L}_{train}(f_{\alpha}(\boldsymbol{x}, \boldsymbol{\omega}(\boldsymbol{\alpha})))$$

Challenges:

- A vast search space of possible architectures
- Exponentially many ensemble combinations

Surrogate Functions

Overview

We propose using two surrogate functions:

- $f_{\text{acc}} : \mathcal{A} \to \mathbb{R}$ — a regression model that predicts the accuracy of a network given its architecture.
- $f_{\text{div}} : \mathcal{A} \to \mathbb{R}^d$ — a function that maps architectures to a latent space. Trained using Triplet Loss based on a similarity matrix derived from model outputs.

Surrogate assisted ensemble construction.

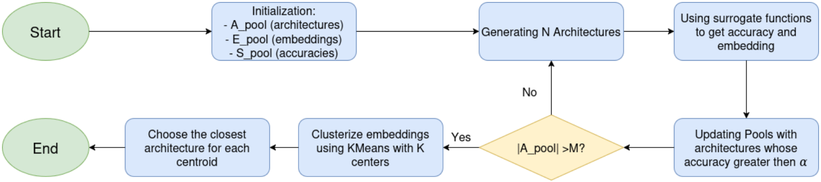


Figure: The proposed ensemble construction algorithm.

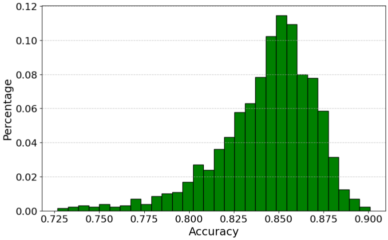
Goals of the Computational Experiment

1. Construct a training dataset of architectures and their evaluations
2. Evaluate the surrogate models' ability to predict accuracy and diversity
3. Assess the effectiveness of the ensemble construction strategy

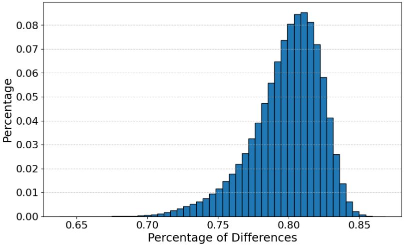
Dataset Collection from the DARTS search space

We generate architectures from the DARTS search space.

- A total of 1,000 architectures were trained to obtain ground truth accuracy and predictions for train dataset.
- For inference, we use 16192 models with predicted accuracy above 0.87. We use KMeans with K = 6 to create clusters.



Distribution of model accuracies



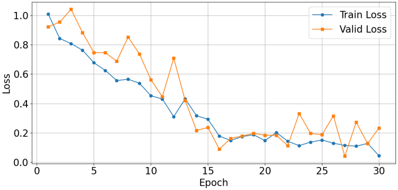
Distribution of model diversity

Surrogate Model Performance

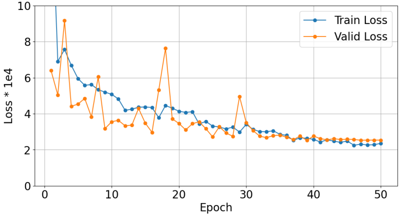
We trained:

- the accuracy surrogate using the Mean Squared Error (MSE) loss,
- the diversity surrogate using the Triplet Loss.

To evaluate the learned diversity representation, we computed the Pearson correlation between distances in the latent space and output similarity, obtaining approximately –0.4, indicating that the surrogate captures the inverse relationship.



Training process of the diversity surrogate



Training process of the accuracy surrogate

Ensemble Effectiveness

In our main experiment, we selected 16,192 candidate architectures with predicted accuracy above 87%. Among them, the top five models achieved an average test accuracy of approximately 91.43% on CIFAR-10. When combined, the ensemble of these six models reached a test accuracy of 94.2%.

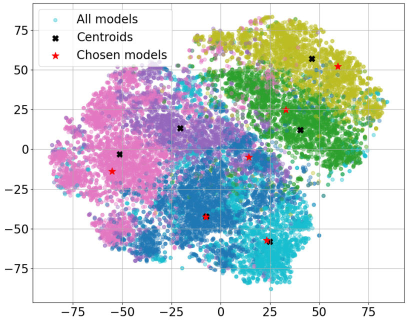


Figure: Learned architecture clusters in latent space.

Conclusion

1. Proposed a method to encode architectures from the DARTS search space for training a Graph Attention Network (GAT), with nodes representing network operations.
2. Developed a surrogate model for predicting architectural diversity based on latent representations.
3. Demonstrated the effectiveness of using surrogate models to guide ensemble construction, balancing performance and diversity.