Surrogate-Assisted Diversity Estimation in Neural Ensemble Search

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Motivation and Approach

Problem
Develop an efficient method for Neural Ensemble Search (NES)

Challenge
Neural architecture search is computationally expensive, and constructing optimal ensembles leads to a exponential explosion of candidate ensemble configurations.

Proposed Approach
Employ a surrogate-assisted method by embedding architectures into a latent space, where similar networks are close and dissimilar ones are far.

Motivation
Efficient estimation of ensemble diversity enables better ensemble selection without exhaustive training.

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:

- Exponentially growing number of architectures
- Exponentially growing number of ensemble combinations

Surrogate Functions

Overview

We propose two surrogate functions:

- $f_{\text{acc}}^{\theta} : \mathcal{A} \to \mathbb{R}$ — predicts network accuracy. Trained by minimizing mean squared error (MSE):

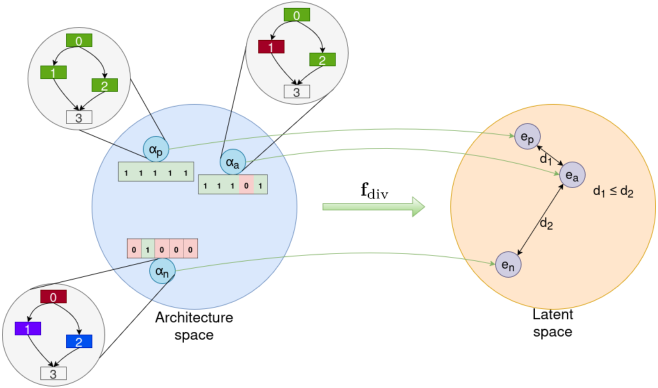
$$\theta^* = \arg\min_{\theta} \sum_i \left(f_{\text{acc}}^{\theta}(\alpha_i) - y_i \right)^2$$

- $\mathbf{f}_{\text{div}}^{\theta} : \mathcal{A} \to \mathbb{R}^d$ — maps architectures to a latent space. Trained with triplet loss to preserve diversity:

$$\theta^* = \arg\min_{\theta} \sum_{(\alpha_a, \alpha_p, \alpha_n)} \max \Big(\|\mathbf{f}_{\text{div}}^{\theta}(\alpha_a) - \mathbf{f}_{\text{div}}^{\theta}(\alpha_p)\|_2^2 - \|\mathbf{f}_{\text{div}}^{\theta}(\alpha_a) - \mathbf{f}_{\text{div}}^{\theta}(\alpha_n)\|_2^2 + m, 0 \Big)$$

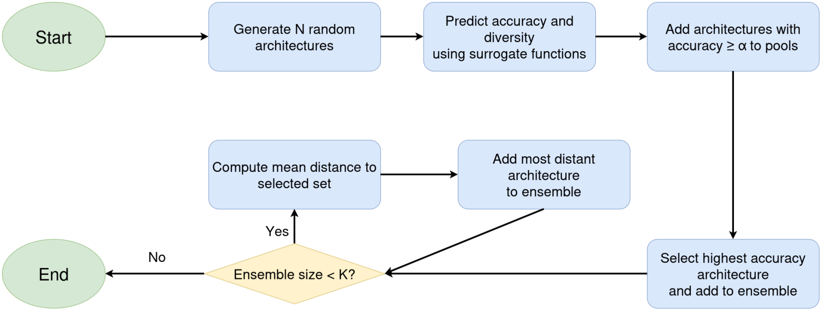
where $(\alpha_a, \alpha_p, \alpha_n)$ denote anchor, positive, and negative architectures, m $\in \mathbb{R}$ denote margin.

Surrogate Diversity Function



- Surrogate function maps discrete architectures into a continuous latent space.
- Similar architectures are embedded close together, while dissimilar ones are mapped farther apart (e.g., $\mathbf{e}_a$ vs $\mathbf{e}_p$ and $\mathbf{e}_a$ vs $\mathbf{e}_n$).
- Latent-space geometry allows efficient diversity evaluation without pre-training all architectures.

Surrogate assisted ensemble construction



The proposed ensemble construction algorithm.

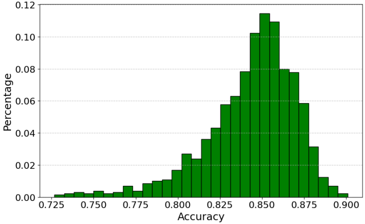
Goals of the Computational Experiment

On datasets FashionMNIST, CIFAR10, CIFAR100:

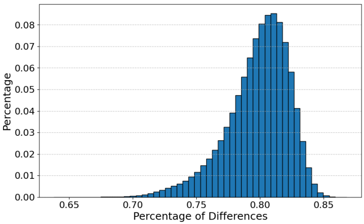
- Construct a training dataset of architectures and their evaluations
- Evaluate the surrogate models' ability to predict accuracy and diversity
- Assess the effectiveness of the ensemble construction strategy
- Compare surrogate-assisted method with DeepEns and RandomSearch

Dataset of Architectures

For each dataset, 3,000 neural architectures were partially trained.
The train/validation split was set to 0.8/0.2 for all datasets.
As an example, the resulting distributions for CIFAR10 are shown below:



Distribution of model accuracies



Distribution of model diversity

Comparison of Surrogate-Assisted NES and DeepEns

Metric	Surrogate-Assisted NES	DeepEns
FashionMNIST		
Ensemble size = 3		
Top-1 Accuracy	95.3%	**95.4**%
Average Model Accuracy	94.7%	**95.1**%
NLL	0.263	**0.256**
CIFAR10		
Ensemble size = 5		
Top-1 Accuracy	**97.80**%	97.61%
Average Model Accuracy	96.73%	96.73%
NLL	**0.208**	0.209
CIFAR100		
Ensemble size = 5		
Top-1 Accuracy	**85.17**%	84.16%
Average Model Accuracy	**80.50**%	79.54%
NLL	**0.692**	0.735

Conclusion

- We propose a surrogate function for predicting architectural diversity.
- We introduce a surrogate-assisted framework for neural ensemble construction.
- Our method matches or outperforms DeepEns and Random Search on FashionMNIST, CIFAR-10, and CIFAR-100 by explicitly accounting for architectural diversity during ensemble construction.
- The work is ready for submission to a conference or journal.