

Plan

Term Paper Plan

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1 Introduction

Today, Artificial Neural Networks (ANN) have proven to be potent Machine Learning (ML) models, capable of learning and approximating any arbitrary function, given enough learnable parameters.

However, they aren't currently without flaws. Anyone who has developed an ANN to fit a particular application dataset would undoubtedly have to toil with the frustration of searching and tuning the numerous hyperparameters of the neural network model. This is because an ANN requires an adequate combination of hyperparameters values to perform its best. Those hyperparameters are not learned by the model, leaving this arduous task of hyperparameter optimization to the developer. To make things worse, the search space for those hyperparameters is often infinite. The general list of potential hyperparameters to tune includes but is not limited to:

1. Numerical hyperparameters
 - Number of hidden layers
 - Number of hidden units within each hidden layer
 - Learning rate
 - Number of training epochs
 - Momentum rate
 - Batch size (if input batches are being used)
 - Dropout rate
 - Weight Initialization tensor
 - Weight decay rate
 - Number of folds (if K-fold cross-validation is applied)
2. Non-numerical hyperparameters
 - Activation function (possibly at each unit)
 - Optimization algorithm
 - Loss function
 - Regularization techniques
 - Network topology (given cell type modules such as fully connected, convolutions, pooling, multi-head attention, etc.)

Furthermore, some hyperparameters can even be adaptively adjusted for performance gains (e.g., adaptive learning rate to reduce training time).

Unlike other machine learning approaches such as Decision Trees, ANNs have too many hyperparameters to tune. This results in a lot of development time spent fine-tuning them and retraining each time before optimally training for the best model for the chosen application. Deep Learning (DL), the branch of machine learning dealing with ANN, is currently more art than science. Unfortunately, that slows the progress made in DL, ML, and Computer Science as a whole. It's imperative to solve the problem of hyperparameter initialization and tuning by providing an automated or learned way to reliably set all the hyperparameters to the optimal value for any given task. This problem is also called Auto-ML or meta-machine learning [6].

2 Related Work

Our problem being hyperparameters search, we are aiming at providing a better, more reliable, and efficient method for hyperparameter initialization and tuning than the simple manual search. Other attempts at hyperparameter search or optimization are random search, grid search, automated hyperparameter tuning using Bayesian optimization or Genetic Algorithm, and Artificial Neural Network tuning using deep reinforcement learning [3]. Before exploring our approach, we first look at some state-of-the-art methods.

Manual search is the most basic and time-consuming approach, taking hours to months. The following technique that comes to mind is grid search, where every hyperparameter and its values are arranged on a grid and exhaustively searched to find the best combination of hyperparameter values. Unfortunately, Grid search is only applicable at low dimensions (2-4 hyperparameters to search) and is impractical at much higher dimensions where we usually need hyperparameter tuning for practical reasons. Random search improves on that, but at the cost of guaranteed optimality. Random search applies to larger search spaces and provides better results in less iteration than Grid search. Random search

can also be run in parallel. Work done by Bergstra et al. demonstrates the superiority of Random search compared to Grid search and manual search [4]. However, like Grid Search, Random search doesn't leverage the information gained from the previous iterations; each new guess is independent of the previous one. Work done by Zoph et al. explores the application of using ANN or gradient-based methods to search optimal architectures (number of hidden layers, hidden units hyperparameters, and the type of layer units). This work leverages the information obtained at every guess and does better at providing the optimal model than just a random search [9]. However, since this work exploits a neural network to optimize the hyperparameters of another neural network, there's no significant reduction in hyperparameters to optimize. Finally, considerable strides have been made in applying evolution to hyperparameter optimization. Real et al. successfully applied genetic-based search to hyperparameter optimization with the introduction of aging evolution in the search [5]. Their work proved to systematically find more optimal models and find them quicker than Random search or ANN-based search.

Another more recent work by Li, Ang, et al. builds on it and provides a general framework for population-based training (PBT). Unlike other approaches, which first optimize the parameters then train the models, population-based training jointly optimizes hyperparameters and learnable parameters [7, 8]. In addition to the optimal models, this approach also provides hyperparameters schedules that more dynamically apply hyperparameters such as learning rate to optimally train models (not just a single hyperparameter value). Evolution-based methods have the added advantage of being able to be massively parallelized. However, PBT hasn't been developed to support deep architecture searches and doesn't cover design choices about the neural network topology. Our approach aims to augment PBT with architecture search to provide the optimal AutoML solution.

3 Approach

Our approach is building on the works by Real, Esteban, et al., Jaderberg, Max, et al., and Li, Ang et al. to devise a population-based method that not just optimize usual numeric hyperparameters such as learning rate, dropout rate, momentum, etc. But also searches for the optimal topology or architecture of the neural network given an initial set of architecture cells or modules (such as convolution, pooling, attention, fully connected, etc.) to compose from.

Our algorithm will work by providing an efficient way to encode and include the neural network topology in the population-based search, eventually coming up with the optimal model with the optimal topology and hyperparameter schedule in a single joint efficient search.

4 Evaluation

To solve AutoML, we propose an augmentation of a general framework for population-based training that searches for the optimal network architecture. To evaluate our approach against current methods, we will be attempting to find optimal hyperparameters for optimal ANN models on the following datasets:

- Iris Dataset
- Tennis Dataset
- Identity Dataset

The ANN models would be feedforward neural networks. We aim to demonstrate the superiority of our approach in providing the optimal models with the optimal set of hyperparameters in a quick, reliable, and computationally inexpensive fashion. The performance metrics we will use to evaluate our method include:

- Top Test Accuracy (the accuracy of the best model produced by the approach, higher is better).
- Experiment time (or the amount of time it took for the approach to run overall, lower is better).
- Model conciseness (or the model's overall size expressed in terms of the number of parameter weights and biases in the model, lower is better).

With these metrics, we aim to demonstrate that our method performs better consistently across the board when compared to other similar approaches such as grid search, random search, and ANN search.

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