Proposal Submission to the UMASS Computer Science Self Study Program

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The Effectiveness of Varying Search Algorithms on Hyperparameter Optimization in Machine Learning

1 Motivation

The machine learning space is vast, offering various solutions to each problem that needs to be solved. For example, a popular neural network creation tool, Keras, offers over 150 options for different layers of nodes that affect how a model is trained and performs. This creates a need to explore which hyperparameters (parameters that determine model architecture) are optimal for each use case in machine learning and data science. Over the years, this process has been automated using hyperparameter optimization frameworks such as Keras Tuner, RayTune, and Optuna. Additionally, recent developments in the AutoML space, assisted by AI, have further enhanced the hyperparameter search process.

During my time at Corning Incorporated through Magnit, I was tasked with developing a 'manual' on hyperparameter tuning to establish a general approach for achieving effective machine learning models. After exploring possible standardizations, I encountered hyperparameter optimization frameworks. During the remainder of my time there, I explored the potential of Optuna and Keras Tuner paired with a Keras-TensorFlow model, as well as several of the search algorithms they offer.

I plan for this paper to extend my previous research by focusing more deeply on algorithm selection rather than serving as an introductory resource on the frameworks. Additionally, it will leverage the PyTorch library to enable testing on various popular neural network architectures.

1.1 Research Objectives

The primary goal of this research is to establish a reference framework for selecting model structures, hyper-parameter optimization search algorithms, and optimization frameworks when developing models for various applications, addressing the lack of effective documentation in the machine learning space to guide developers in these decisions. The extensive data collected, along with relevant applications demonstrated through case studies, aims to benefit the broader community while identifying potential areas for improvement within these frameworks.

2 Research Plan

Machine learning has many potential applications, all which may benefit from hyperparameter optimization to achieve an optimal model. This proposal outlines the search space for the algorithms and presents several real-world applications to evaluate these algorithms on. Following the evaluation, the performance of each algorithm and its corresponding data will be analyzed to identify recurring themes.

2.1 Task 1: Data and Application Selection

All datasets will be chosen from Kaggle, based on the following:

1) Classification Dataset

This dataset will serve as a baseline test conducted on a simple 30-core CPU or a single GPU node without parallelization or specialized distributed training. The results will establish baseline performance and demonstrate how specialized algorithms outperform primitive methods such as Grid Search, Random Search, and Brute Force Search.

2) Forecasting Dataset

This dataset will be significantly more complex, containing over 20 features and providing predictive values that yield a percentage of error rather than a binary classification output, such as revenue prediction or a similar concept. For instance, datasets like the restaurant revenue prediction dataset. Additionally, a much larger computing cluster will be utilized to facilitate more advanced learning with GPU nodes.

3) Other Miscellaneous Dataset and Application

I also intend to use this study as an opportunity to familiarize myself with additional datasets, selecting a third dataset later if time permits, to further develop valuable skills. Potential application areas include natural language processing (NLP), image processing or segmentation, general reinforcement learning for specific use cases, transfer learning for larger datasets, and recommendation algorithms.

2.2 Task 2: Algorithm Selections

1. Optuna:

   Samplers:

   (a) RandomSampler

   (b) GridSampler

   (c) TPESampler

(d) CmaEsSampler
(e) NSGAIISampler
(f) QMCSampler
(g) GPSSampler
(h) BoTorchSampler
(i) BruteForceSampler

Pruners: Compatible with a,b,c,f,i

(a) MedianPruner
(b) PatientPruner
(c) PercentilePruner
(d) SuccessiveHalvingPruner HyperbandPruner
(e) ThresholdPruner
(f) WilcoxonPruner

2. Keras Tuner:

   (a) RandomSearch Tuner
   (b) GridSearch Tuner
   (c) BayesianOptimization Tuner
   (d) Hyperband Tuner
   (e) NSGAIISampler
   (f) QMCSampler
   (g) GPSSampler
   (h) BoTorchSampler
   (i) BruteForceSampler

3. RayTune:

   (a) AxSearch
   (b) BayesOptSearch
   (c) BOHBSearch
   (d) HEBOSearch
   (e) NevergradSearch
   (f) RepeatedEvaluations
   (g) ConcurrencyLimiter

4. Auto ML Platform

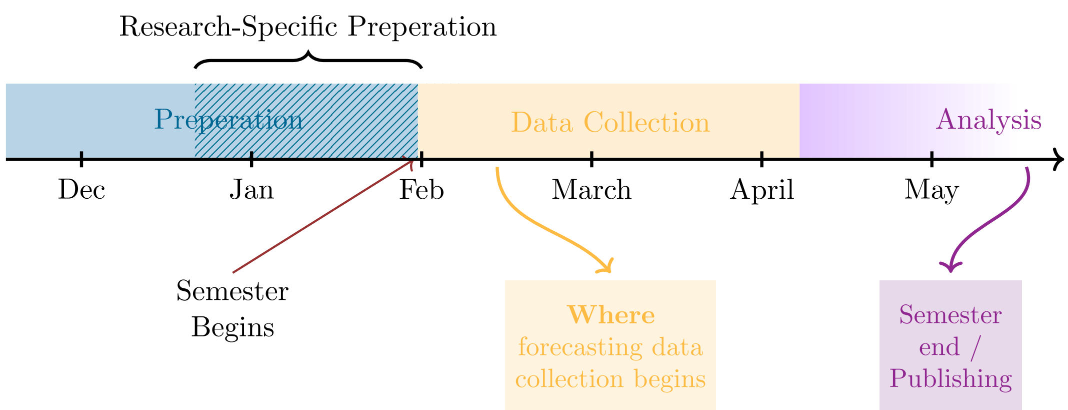
   Possibly Inquire to Auto ML platforms about experimentation with their software to compare it to other Frameworks

3 Project Management

Preparation phase: Expand on pytorch and keras skills for Neural Networks for different types of datasets. Familiarize myself with UNITY, Cuda, CudNN, and frameworks on distributed systems. Learn Raytune Skills and inquire about auto ML possibilities. Practice data collection and data presentation in different programs / python.

Data Collection: Start with standardized data collection. Ensure data is clean and datasets accurately depict the differences between algorithms.

Analysis: Python graph creation, research paper, claims for specific search algorithms and effectiveness of certain frameworks.



4 Expected Outcomes

I aim to keep this research entirely open-source and publicly accessible, allowing anyone to evaluate my work and form their own opinions based on it. The potential benefits of this approach include:

1. Lowering the barrier to knowledge about effective model development. Combined with the first part of this paper, the introduction to hyperparameter optimization and general tuning will be easily accessible, addressing a challenge I personally encountered when entering the field.

2. Increasing efficiency and improving the quality of results during the tuning process. The analysis proposed in this research could facilitate the development of a practical guide to identify the best approaches for tuning models. This is particularly valuable given the substantial lack of research on optimization frameworks and their search algorithms, a gap this work seeks to address.

3. Advancing technologies. If problems are identified during these trials, they may highlight areas for improvement that could enhance the quality of existing technologies. Furthermore, this research could provide newer technologies with a benchmark for performance evaluation, offering an alternative to unsupported claims of meeting or exceeding industry standards.

5 Resources Required

The only service I require is to the UNITY clusters, so I can effectively evaluate frameworks in an industry setting. Without access to this, my research is irrelevant.

6 Credit

I would like this to be a 496 3-4 credit class, as many of the skills I am applying to this are acquired in **CS 589**; however, since I am not yet a graduate student, a 400 level elective seems like a reasonable compromise.
The criteria for grading should be a paper that correctly encapsulates all of my findings.