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MLOps approach for application specific performance tuning for machine learning systems

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ML	Machine Learning
MLOps	Machine Learning Operations
TODO	TODO

Contents

1 Introduction

Machine learning (ML) and Artificial Intelligence (AI) have been a hot topic of discussion in the past decade. While there is a mountain of academic research on ML methods and tools, there is a lack of attention paid to practical real-world challenges encountered when developing or running ML systems. DevOps has previously addressed similar challenges in software engineering and a field of MLOps which is DevOps applied to ML has emerged. Machine learning operations (MLOps) focuses on solving challenges related to operating real world machine learning systems (Kreuzberger, Kühl, and Hirschl 2023).

Machine learning (ML) systems are widely adopted and many organizations successfully have ML models running in production. Examples of machine learning systems in different fields include recommender systems , targeted ads (Domingos October 1, 2012), drug design (Domingos October 1, 2012) or search engines (Domingos October 1, 2012).

Find ref

Find ref

Most recent breakthroughs that have generated media attention have been in the fields of computer vision in the form of latent diffusion models (LDM) (Rombach et al. April 13, 2022) such as Stable Diffusion (Stability AI August 22, 2022) for generating images from prompts and natural language processing in the form of large language models (LLM) (Touvron et al. February 27, 2023) such as ChatGPT (OpenAI November 30, 2022). There have also been great developments in tooling for machine learning such as Tensorflow, Pytorch or scikit-learn for model development, Ray, Horovod or DeepSpeed for distributed training and MLFlow or Tensorboard for machine learning monitoring.

TF, Pytorch, scikit-learn refs

Ray, Horovod and DeepSpeed refs

MLFlow, Tensorboard refs

Despite wide adoption and many successes, there are still challenges with machine learning systems in practice . The required amount of computation for machine learning has been on the rise. According to an OpenAI technical blog the trend is exponential and more compute leads to better performance (Amodei and Hernandez May 16, 2018). Increased compute requirements also mean increased costs such as financial, operational or environmental. Strubell et al. (April 3, 2020) in their extended abstract bring attention to the environmental impact of training models and in particular hyperparameter tuning, during which costs of training many relatively inexpensive models quickly adds up.

Find ref, state of MLOps?

In addition to cost there may be other requirements for machine learning systems. For example machine learning systems on the edge might encounter system requirements such as latency and energy use or have limited resources such as memory or compute (Chen and Ran August 2019). Ways of meeting these requirements include hyperparameter tuning, reducing the amount of parameters in the model or model compression such as knowledge distillation (Chen and Ran August 2019).

Early stopping has been used as a cost optimization technique to reduce training time by stopping training when performance of the model stops improving on the validation set (Prechelt June 1, 1998). More recent work on larger models shows that models might still improve later if training continues for a longer time (Hoffer, Hubara, and Soudry January 1, 2018). Using early stopping with other performance metrics such as system metrics has not been as thoroughly studied.

The aim of this thesis is to investigate whether using early stopping with system metrics leads to more efficient hyperparameter tuning when there are resource constraints. Investigation is limited to a small set of widely available machine learning algorithms and datasets that do not require a lot of computation. While more complex and effective hyperparameter optimization methods exist only the simplest are used to simplify the experiments for clarity.

The theoretical significance of the thesis is to show that traditional hyperparameter optimization techniques can not only be used on machine learning performance metrics but also alternative metrics such as system metrics. The practical outcomes are reducing costs and allowing for quickly and efficiently tailoring models to fit specific system metric constrains.

This thesis is structured in the following manner: Chapter 1 provides an introduction and context for the thesis. Chapter 2 contains background information about machine learning, DevOps and MLOps and how they relate to each other. Chapter 3 describes the performed experiments and their methods and design including research questions, datasets and algorithms used. Chapter 4 presents the results of the experiments. Chapter 5 revisits the research questions and discusses the interpretation of the results, limitations, related work and future work. Chapter 6 concludes the thesis by summarizing key findings.

2 Machine Learning Operations

Add outline of how ML, DevOps and MLOps fit together

2.1 Machine Learning

2.1.1 Overview

Intro to ML

Writing programs and developing algorithms to complete specific tasks is a labor intensive task requiring professional programming expertise. A different approach is to develop generic algorithms that can change behavior by learning. The field studying these types of algorithms is called machine learning. Machine learning algorithms learn by applying an optimization algorithm to adjust set of parameters called a model and this process is called training the model (LeCun, Bengio, and Hinton May 2015). A simplified machine learning workflow consists of splitting the data into training and test datasets, performing preprocessing separately for each dataset, training the model on the training dataset and finally evaluating the trained model on the test dataset.

ref

Machine learning is widely used in applications like search, drug design or ad placement and can be also known as data mining or predictive analytics (Domingos October 1, 2012). Developing machine learning systems, which are systems that are based on machine learning, can be a difficult task. Unlike traditional software development, experiments with both code and data as inputs are central to machine learning development (Zaharia et al. 2018) and reproducibility of the experiments is often problematic. While plenty of research focuses on machine learning methods or even datasets and data quality, the biggest bottleneck is human cycles (Domingos October 1, 2012). Faster iterations improve the machine learning developer or researcher experience. An important metric to pay attention to and optimize is the mean iteration cycle for machine learning developers.

Machine learning can be practiced with two different goals in mind. First is explanatory modeling with the purpose of scientific theory building and testing and the second is predictive

modeling mostly used outside of scientific research (Shmueli August 1, 2010). One practical difference is that unlike predictive modeling, explanatory modeling rarely uses holdout test sets or cross validation for evaluation (Shmueli August 1, 2010). Lack or presence of evaluation on a test set can be used as a heuristic to quickly determine whether a machine learning project is explanatory or predictive in nature. However, even explanatory modeling benefits from evaluating the predictive power (Shmueli August 1, 2010). Domingos (October 1, 2012) in their paper assume all machine learning is predictive in nature and state the following:

> The fundamental goal of machine learning is to generalize beyond the examples in the training set.

It is important to keep in mind the end goals of a machine learning project, because common practices in a research setting might not be applicable when creating machine learning systems.

Machine learning algorithms can be categorized as supervised learning, unsupervised learning or reinforcement learning. The main differences are related to whether the model learns ref by using "right answers" provided by labeled data in supervised learning, by finding structure in the dataset in unsupervised learning or by interacting with the world in reinforcement learning. Model evaluation is also different with supervised learning mostly relying on universal cross-validation on previously unseen data and unsupervised or reinforcement learning relying on internal evaluation metrics tied to the specific algorithm. Unsupervised learning ref has the advantage of not requiring labeled data which is an advantage for problems where labels are uncommon (Le et al. July 12, 2012). ref

2.1.2 Machine learning performance metrics

Intro

Training vs Validation metrics

Domain specific metrics

2.2 DevOps

2.2.1 Overview

A common interpretation of DevOps is a focus on software quality, collaboration between development and operations, process speed and rapid feedback (Mishra and Otaiwi November 1, 2020; Waller, Ehmke, and Hasselbring April 3, 2015; Perera, Silva, and Perera September 2017). Defining DevOps is difficult as there is no consensus on the exact definition (Smeds, Nybom, and Porres 2015; Mishra and Otaiwi November 1, 2020). DevOps can be viewed from different points of view such as culture, collaboration, automation, measurements and monitoring (Mishra and Otaiwi November 1, 2020; Waller, Ehmke, and Hasselbring April 3, 2015). In DevOps there is a focus on speed and quality with incremental changes that are recurrent and continuous (Mishra and Otaiwi November 1, 2020). The goal is to bridge the gap between development and operations (Smeds, Nybom, and Porres 2015). This is done through sharing tasks and responsibilities from development to deployment and support (Mishra and Otaiwi November 1, 2020).

Continuous integration, continuous deployment and continuous monitoring are well known practices in DevOps (Waller, Ehmke, and Hasselbring April 3, 2015) describing the automatic nature of integrating, deploying and monitoring code changes. Feedback includes performance metrics data which is then fed as an input during planning and development (Smeds, Nybom, and Porres 2015). Performance profiling and monitoring are similar activities and the main difference is whether it's done during the development process or during operations respectively (Waller, Ehmke, and Hasselbring April 3, 2015) with DevOps bridging the gap between them (Brunnert et al. August 18, 2015). Continuous benchmarking allows for detecting performance regressions during continuous integration (Waller, Ehmke, and Hasselbring April 3, 2015) and infrastructure monitoring with a feedback loop allows for performance optimization in production (Smeds, Nybom, and Porres 2015). Resource demands might change depending on the inputs (Brunnert et al. August 18, 2015) making it important to systematically measure performance not only based on code changes but also on configuration changes or even data changes.

Performance evaluation is a useful tool for optimizing the overall system design and tailoring

for a specific production environment in addition to correctly sizing resources (Brunnert et al. August 18, 2015; Waller, Ehmke, and Hasselbring April 3, 2015).

2.2.2 Software performance metrics

Performance metrics are fundamental to all activities involving performance evaluation such as profiling or monitoring (Brunnert et al. August 18, 2015). Common metrics involve measuring the CPU, but other metrics such as memory usage, network traffic or I/O usage do not have clear definitions (Brunnert et al. August 18, 2015). Collecting metrics happens through hardware based monitors or software monitors instrumented into software through code modification or indirectly for example through middleware interception (Brunnert et al. August 18, 2015). Metrics can be event driven in which a monitor is triggered with every occurrence or based on sampling at fixed time intervals (Brunnert et al. August 18, 2015). The types of metrics collected and what information is expected depends on the performance goals and the life cycle of the software (Brunnert et al. August 18, 2015).

Metrics can be divided into application metrics such as response time or throughput and resource utilization metrics such as CPU utilization or available memory (Brunnert et al. August 18, 2015). There is little peer reviewed research available with specifics on which metrics are to be collected or how they are defined.

Measurement based performance evaluation requires a system to test while model based performance evaluation allows to predict the performance of the future system (Brunnert et al. August 18, 2015). This type of performance prediction allows for better planning and comparing use cases especially when an existing legacy system exists with measured performance metrics (Brunnert et al. August 18, 2015).

2.3 MLOps

2.3.1 Overview

While the focus of machine learning research has been on improving models, it is essential for the industry to be able to design production-ready machine learning pipelines (Posol-

dova November 2020). The data often used for research is of higher quality than real-world data that is often messy, unstructured and unlabeled (Posoldova November 2020). Continuous integration, continuous deployment and automated testing are also relevant to machine learning systems (Posoldova November 2020) which are familiar concepts from DevOps. A new concept of MLOps addresses this issue of designing and maintaining machine learning systems just like DevOps addressed it for traditional software (Kreuzberger, Kühl, and Hirschl 2023).

Add ML specific practical problems

Performance measuring software is not new, but ML brings additional challenges in the form of models and data which requires a modified approach (Breck et al. 2017). It is also important to note, that not every data scientist or machine learning engineer working on machine learning systems has a software engineering background (Finzer 2013) and might lack the necessary knowledge to apply software engineering best practices to machine learning systems.

Requirements for a machine learning system are different depending on the task. For example speech and object recognition might have no particular performance requirements during training but has strict latency and computational resource restrictions when deployed to serve large amounts users (Hinton, Vinyals, and Dean March 9, 2015). MLOps has to take into account both machine learning performance metrics familiar from machine learning and software performance metrics familiar from DevOps and software engineering. Feedback from metrics collected during development and from monitoring of production systems are core MLOps principles (Kreuzberger, Kühl, and Hirschl 2023).

2.3.2 Hyperparameter optimization

Parameters given as part of a configuration to the machine learning model are called hyperparameters (Yang and Shami November 2020).

Find simple examples

Automatic tuning of hyperparameters can help achieve state-of-the-art performance in machine learning systems (Maclaurin, Duvenaud, and Adams April 2, 2015). Hyperparameter optimization techniques include grid search, random search, gradient based optimization

and Bayesian optimization and they have different benefits and limitations (Yang and Shami November 2020).

Similar concepts to hyperparameter optimization are neural architecture optimization and meta modeling where model structure or modeling algorithm is treated as a tunable parameter (Baker et al. November 8, 2017). For example a machine learning system can automate the choosing of the number of neural network layers, the type of layers or even the type of machine learning algorithm. Tuning hyperparameters is generally a difficult task (Maclaurin, Duvenaud, and Adams April 2, 2015).

Traditional hyperparameter tuning methods such as Bayesian optimization are unfeasible for more than 10-20 hyperparameters (Maclaurin, Duvenaud, and Adams April 2, 2015). More advanced techniques are required if a larger amount of tunable hyperparameters is desired. Performance prediction is an important step to reduce the amount of computation required for neural architecture search and hyperparameter optimization (Baker et al. November 8, 2017).

2.3.3 Performance prediction and early stopping

Early stopping is a technique in which model training is halted before completion to avoid wasting computational resources (Prechelt June 1, 1998).

Machine learning systems in addition to machine learning performance metrics and system performance metrics will have their performance metrics tied to product or organization metrics such as user churn rate or click-through rate (Shankar et al. September 16, 2022). Choosing the right metrics to evaluate a machine learning system is important and the metrics will be different for different machine learning systems (Shankar et al. September 16, 2022).

3 Methods

3.1 Research setup

3.1.1 Scope

The scope of the study is limited to 5 performance metrics of 3 different ML models trained and tested on 3 different datasets using a distributed computing framework Ray Tune (Liaw et al. July 13, 2018).

TODO different models, different datasets

TODO Vertailukriteeristö: tapana ohjelmistopuolella + tapana koneoppimispuolella

TODO different resources (memory, time, accuracy)

3.1.2 Research Questions

This master's thesis asks the following research questions:

- *RQ1*: How early stopping on resource usage metrics affects required computation during hyperparameter optimization?
- *RQ2*: How early stopping on application performance metrics affects required computation during hyperparameter optimization?
- *RQ3*: Can resource usage metrics from early stopped models be used to predict resource usage metrics of fully trained models?
- *RQ4*: Can resource usage metrics from models trained on reduced training datasets be used to predict resource usage metrics of models trained on full training datasets?
- *RQ5*: Can application performance metrics from early stopped models be used to predict application performance metrics of fully trained models?
- *RQ6*: Can application performance metrics from models trained on reduced training datasets be used to predict application performance metrics of models trained on full training datasets?

3.1.3 Methodology

Methodology used is expanded from an existing methodology for machine learning experiment design (Fernandez-Lozano et al. December 1, 2016) to include AutoML and

3.2 Experiments

3.2.1 Datasets

MNIST (Deng November 2012)

Penn Machine Learning Benchmarks (Olson et al. December 11, 2017)

3.2.2 Machine Learning algorithms

3.2.3 Metrics

3.2.4 Training and validation

3.2.5 Inference

4 Results

TODO This is a results chapter

5 Discussion

5.1 Research Questions revisited

5.1.1 Research question RQ1

5.1.2 Research question RQ2

5.1.3 Research question RQ3

5.2 Interpretation

5.2.1 Implications for research

5.2.2 Implications for practice

5.3 Limitations

5.3.1 Datasets

5.3.2 Machine Learning algorithms

5.3.3 Metrics

5.3.4 Training and validation

5.3.5 Inference

5.4 Related Work

To find relevant related work both reverse snowballing and forward snowballing is used on a set of MLOps papers previously known to the author.

Benchmarking ML systems (Cardoso Silva et al. December 2020)

5.5 Future Work

TODO This is a discussion chapter

6 Conclusions

Summary

TODO This is a conclusions chapter

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