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MLOps approach for application specific performance tuning for machine learning systems

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Glossary

ML	Machine Learning
MLOps	Machine Learning Operations
TODO	TODO

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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 2012), drug design (Domingos 2012) or search engines (Domingos 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. 2022) such as Stable Diffusion (Stability AI 2022) for generating images from prompts and natural language processing in the form of large language models (LLM) (Touvron et al. 2023) such as ChatGPT (OpenAI 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

TODO computational budgets, cost, efficiency

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 2018). Increased compute requirements also mean increased costs such as financial, operational or environmental. Strubell et al. (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

Find ref, state of MLOps?

relatively inexpensive models quickly adds up.

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 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 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 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 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

Software involving machine learning adds additional complexity to the overall system. Developing, deploying and monitoring machine learning systems involves both traditional software system concepts and some new machine learning specific concepts. Section 2.1 introduces machine learning and evaluating model performance from a practical perspective. Section 2.2 introduces DevOps and performance evaluation. Section 2.3 combines machine learning and DevOps for production machine learning systems and introduces hyperparameter optimization and performance prediction.

2.1 Machine Learning

Real world applications of machine learning are often messy with a large number of decisions for the developer that can result in different behavior of the machine learning model. This section introduces machine learning from a practical standpoint including necessary performance metrics for model training and empirical performance evaluation.

2.1.1 Practical machine learning

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 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 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 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 2010). One practical difference is that unlike predictive modeling, explanatory modeling rarely uses holdout test sets or cross validation for evaluation (Shmueli 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 2010). Domingos (2012) in their paper assume all machine learning is predictive in nature and state that machine learning should generalize beyond 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. Unsupervised learning has the advantage of not requiring labeled data which is an ref advantage for problems where labels are uncommon (Le et al. 2012).

2.1.2 Model evaluation

Performance evaluation of machine learning models is usually done empirically using cross-validation (Forman and Scholz, no date; Sokolova and Lapalme 2009). Cross-validation

involves splitting the data into k-folds and using all but one of the folds for training and the last one for validating the performance of the model after which the procedure is repeated k times with each fold being used for validation (Cawley and Talbot, no date). For example 3-fold validation would use a third of the data for validation and two thirds for training repeated three times. The performance metrics collected during the computationally expensive cross validation are typically averaged (Cawley and Talbot, no date). These types of global averages might not be desirable and instead of random folds the data can be sliced according to some criterion such as by country and allow detecting performance differences between slices (Breck et al. 2017).

Machine learning training involves minimizing an optimization criterion such as log loss, squared hinge loss or Cauchy-Schwarz Divergence (Janocha and Czarnecki 2017). Different loss metrics are chosen depending on the application such as resistance to noisy data or labels (Janocha and Czarnecki 2017). The loss metric is sometimes not informative of model performance such as in classification tasks. In these cases performance metrics such as accuracy, precision, recall, specificity, error-rate , AUC and F-score are used (Sokolova and Lapalme 2009; Forman and Scholz, no date). Metrics such as accuracy are well defined, but the final F-score from cross-validation may be computed in several ways resulting in different results (Forman and Scholz, no date).

Even more informative metrics can be created for specific applications. For example Torrabla and Efros (2011) developed performance metrics to compare different datasets and determine a "market value" for the data by using the generalization performance of machine learning models on the datasets. Defining correctness of the prediction is an important part when defining performance metrics (Lin et al. 2014)

TODO: Define batch, training step, epoch TODO: Loss math formulas TODO: Algorithm example of a training loop

2.2 DevOps

DevOps is a well known topic in the field of software engineering that brings together development and operations. This section briefly introduces DevOps and provides and overview

to the main benefits related to continuous integration, continuous deployment and continuous performance evaluation. Later it describes the importance of performance metrics with examples and wraps up the section by introducing performance prediction.

2.2.1 Benefits of DevOps

A common interpretation of DevOps is a focus on software quality, collaboration between development and operations, process speed and rapid feedback (Mishra and Otaiwi 2020; Waller, Ehmke, and Hasselbring 2015; Perera, Silva, and Perera 2017). Defining DevOps is difficult as there is no consensus on the exact definition (Smeds, Nybom, and Porres 2015; Mishra and Otaiwi 2020). DevOps can be viewed from different points of view such as culture, collaboration, automation, measurements and monitoring (Mishra and Otaiwi 2020; Waller, Ehmke, and Hasselbring 2015). In DevOps there is a focus on speed and quality with incremental changes that are recurrent and continuous (Mishra and Otaiwi 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 2020).

Add definition

Continuous integration, continuous deployment and continuous monitoring are well known practices in DevOps (Waller, Ehmke, and Hasselbring 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 2015) with DevOps bridging the gap between them (Brunnert et al. 2015). Continuous benchmarking allows for detecting performance regressions during continuous integration (Waller, Ehmke, and Hasselbring 2015) and infrastructure monitoring with a feedback loop allows for performance optimization in production (Smeds, Nybom, and Porres 2015).

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. 2015; Waller, Ehmke, and Hasselbring 2015). Resource demands might change depending on the inputs (Brunnert et al. 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 directly tied to defining and collecting performance metrics and monitoring.

2.2.2 Performance evaluation

Performance metrics are fundamental to all activities involving performance evaluation such as profiling or monitoring (Brunnert et al. 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. 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. 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. 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. 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. 2015). There is little peer reviewed research available with specifics on which metrics are to be collected or how they are defined. Kounev et al. (2020) in their textbook on systems benchmarking bring up the following quality attributes for benchmark metrics: easy to measure, repeatable, reliable, linear, consistent and independent. Most metrics will not satisfy all of the above quality attributes and aggregated higher level composite metrics are requires (Kounev, Lange, and Von Kistowski 2020).

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. 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. 2015).

TODO: measuring CPU, memory, times (real, wall etc.)

2.3 MLOps

Machine learning operations or MLOps is a fairly new concept related to building and running real-world machine learning systems. This section introduces the concept of MLOps and provides context for the types of problems it aims to solve. Later in the section the concepts of hyperparameter optimization, performance prediction and early stopping are introduced. The section finishes with performance metrics related to machine learning systems and their business objectives and the performance of the overall system.

2.3.1 Production machine learning systems

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 (Posoldova 2020). The data often used for research is of higher quality than real-world data that is often messy, unstructured and unlabeled (Posoldova 2020). Continuous integration, continuous deployment and automated testing are also relevant to machine learning systems (Posoldova 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).

Bring DevOps to MLOps

Managing technical debt is even more important in machine learning systems, because of machine learning specific issues that cannot be solved with traditional methods (Sculley et al. 2015). Main culprit for the challenges with machine learning systems is that data changes the behavior of the system and cannot be expressed with code alone (Sculley et al. 2015). Challenges like entanglement, correction cascades or feedback loops are common with machine learning systems and are difficult to diagnose with common tools (Sculley et al. 2015).

Requirements for a machine learning system are different depending on the task. For exam-

ple 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 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). For example possible meta-level requirements include users requesting data deletion, prohibitions on specific features like age or deperecated sources (Breck et al. 2017).

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. Monitoring for machine learning systems has to be carefully designed (Sculley et al. 2015). Hyperparameter optimization is a kind of performance optimization, where the goal is to improve machine learning metrics. It is not always necessary to train the model to completion to verify that training code is correct and training loss is decreasing (Breck et al. 2017).

2.3.2 Hyperparameter optimization

Parameters given as part of a configuration to the machine learning model are called hyperparameters (Yang and Shami 2020). Examples of hyperparameters include learning rate, number of layers in a neural network, regularization coefficients, batch size, step size or initialization conditions (Maclaurin, Duvenaud, and Adams 2015; Baker et al. 2017; Breck et al. 2017). Hyperparameter tuning or hyperparameter optimization can be defined as finding the optimal hyperparameter values by searching through possible hyperparameter values (Baker et al. 2017). This hyperparameter search can also demonstrate whether the training is stable and reliable (Breck et al. 2017).

The main goal of hyperparameter optimization is to reduce the amount of expert labor required for creating high-performance machine learning models (Baker et al. 2017). Another benefit of finding optimal hyperparameters is that it can help achieve state-of-the-art performance in machine learning systems (Maclaurin, Duvenaud, and Adams 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 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. 2017). This allows for automating the creation of neural networks from scratch (Baker et al. 2017). The amount of potential neural network architecture configurations is large and checking them is computationally expensive (Baker et al. 2017).

Tuning hyperparameters is generally a difficult task (Maclaurin, Duvenaud, and Adams 2015). Traditional hyperparameter tuning methods such as Bayesian optimization are unfeasible for more than 10-20 hyperparameters (Maclaurin, Duvenaud, and Adams 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. 2017).

TODO: add things from (Shallue et al. 2019) TODO: Computational budget, steps,

2.3.3 Performance prediction and early stopping

Data gathered at the beginning of model training can be used to predict performance of the trained model given the chosen hyperparameters (Baker et al. 2017). A small sample of hyperparameter configurations can be used for training a performance prediction model which then can be used to predict the performance for the rest of hyperparameter configurations with only a small amount of training (Baker et al. 2017).

Early stopping is a technique in which model training is halted before completion to avoid wasting computational resources (Prechelt 1998). Early stopping can be based on a threshold value decided upon ahead of time or based on a performance prediction model (Baker et

al. 2017). Low thresholds for rejection of suboptimal solutions will radically reduce the amount of computation required, but run the risk of rejecting an optimal solution as well (Baker et al. 2017).

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. 2022). Important metrics from a machine learning system performance perspective include CPU usage, GPU usage, task completion time, inference time and latency (Cardoso Silva et al. 2020). 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. 2022).

3 Methods

3.1 Research setup

3.1.1 Scope

In this thesis the choice of machine learning algorithms is limited to implementations with iterative training and a possibility for metric collection between training steps.

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. 2018).

TODO different models, different datasets

TODO Vertailukriteeristö: tapana ohjelmistopuolella + tapana koneoppimispuolella

TODO different resources (memory, time, accuracy) TODO Methodology used is expanded from an existing methodology for machine learning experiment design (Fernandez-Lozano et al. 2016) to include AutoML and

3.1.2 Research Questions

This master's thesis asks the following research questions:

- *RQ1*: How do changes in hyperparameters affect system performance during model training?
- *RQ2*: How does early stopping on system performance criteria affect computational budgets during model training?

3.2 Experimental setup

Kannattaako tässä osiossa perustella valintoja?

Onko parempi, jos tulokset olisivat tässä mukana eikä erillisenä lukuna?

3.2.1 Software and Hardware

Experiments were performed using Ray Tune (2.7.1) (Liaw et al. 2018). MLFlow (2.7.1) (Chen et al. 2020) was used for recording metrics and tracking experiments. Scikit-learn (1.3.2) (Pedregosa et al. 2011) for training, collecting machine learning performance metrics and evaluating machine learning models. Psutil (Rodola 2023) was used for collecting system performance metrics from the operating system. Hardware used to perform the experiments consisted of Intel Core i7-9700 @ 3.00GHz CPU and Nvidia 3060 GPU.

3.2.2 Datasets

Penn benchmark dataseteilla on viite, mutta ei sen kummempaa tietoa lähteestä. Kannattaako vaihtaa ja valita itse 5-6 datasettia ja kertoa niistä enemmän?

Datasets used were chosen from Penn Machine Learning Benchmarks (Olson et al. 2017). Mnist dataset was chosen because of popularity and familiarity in the machine learning community. The rest of the datasets were chosen by hand instead of randomly sampled to represent small and large datasets in both classification and regression tasks, because the repository is unbalanced and contains a lot of very similar datasets. Table 1 summarizes the machine learning task and dimensionality of the datasets. The datasets are loaded using the Penn Machine Learning Benchmark (Olson et al. 2017) python package and consist of input features and a target variable.

Dataset	Type	Task	Examples	Features
mnist	image	classification	70000	784
kddcup	tabular	classification	494020	41
diabetes	tabular	classification	768	8
1191_BNG_pbc	tabular	regression	1000000	19
529_pollen	tabular	regression	3848	5

Table 1. Summary of the datasets used.

3.2.3 Metrics and evaluation

Kannattaako olla kaavat jokaiselle metriikalle?

Metrics to be evaluated can be divided into machine learning metrics and system performance metrics and are summarized in Table 2. Training loss was computed with each training step and the rest of the metrics were computed every 100 training steps. Machine learning metrics were computed using scikit-learn (Pedregosa et al. 2011) and system performance metrics were collected from the operating system using psutil (Rodola 2023).

In accordance with Ray documentation (The Ray Team 2023) to avoid double counting memory used by the object store the memory usage of the worker was computed in the following way:

$$\text{memory} = \text{resident set size (RSS)} - \text{shared memory usage (SHR)}$$

Machine learning models were validated by splitting the dataset into a 70% training set and a 30% test set. To make sure that measurements are not sensitive to chosen data five-fold cross validation using the training set was performed when tuning hyperparameters.

Metric	Type
training loss	machine learning
validation loss	machine learning
accuracy	machine learning
root mean square error	machine learning
average training step time	system performance
total training time	system performance
cpu (%)	system performance
memory (MB)	system performance

Table 2. Summary of the metrics

3.2.4 Algorithms

Algorithms were chosen to support training in batches without being computationally heavy. Linear regression, logistic regression and support vector machine (SVM) are based on stochastic gradient descent (SGD) implementation found in Scikit-learn (Pedregosa et al. 2011). Al-

gorithms and hyperparameters are summarized in Table 3. Model training, evaluation and hyperparameter optimization was performed in parallel with each worker process using one CPU core each.

Hyperparameters such as batch size, learning rate and regularization alpha are selected using grid search with the search space determined with preliminary experiments so that the optimal solution is not too close to the boundaries. Batch size search space was 2^i for all i from 1 until 2^i was equal to the number of samples in the dataset. Learning rate search space was 10^i for all i between -1 and -4 .

Parempi tapa esittää, että batch size oli 2. potenssi välillä 2-n ja learning rate oli 10. potenssi välillä 0.1 - 0.0001

For practical

Algorithm	Loss	Hyperparameters
Linear regression	squared	batch size, learning rate, alpha
Logistic regression	log	batch size, learning rate, alpha
Support Vector Machine	hinge	batch size, learning rate, alpha

Table 3. Summary of the algorithms

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. 2020)

5.5 Future Work

TODO This is a discussion chapter

6 Conclusions

Summary

TODO This is a conclusions chapter

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