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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 October 1, 2012), drug design (Domingos October 1, 2012) or search engines (Domingos October 1, 2012).

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.

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

Find ref

TF, Py-torch, scikit-learn refs

Ray, Horovod and DeepSpeed refs

MLFlow, Tensorboard refs

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 constraints.

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.

Types of ML



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 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 has the advantage of not requiring labeled data which is an advantage for problems where labels are uncommon (Le et al. July 12, 2012).

Practical problems

### 2.1.2 Machine learning performance metrics

Intro

### 2.1.3 Hyperparameter optimization

Parameters given as part of a configuration to the machine learning model are called hyperparameters (Yang and Shami November 2020). For example learning rate, batch size or a classification threshold are hyperparameters set before the model is trained. Most common hyperparameter selection technique in practice is manually adjusting the hyperparameters and is humorously called graduate student descent.

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).

Optimizing hyperparameter search

Early stopping

Early stopping is a technique in which model training is halted before completion. This is done to save on computational resources and the main reason for early stopping is predicting that the model will have poor performance. Performance prediction usually relies on predicting a machine learning performance metric such as RMSE or F1 score given the current model is performing during training compared to other models.

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## 2.2 DevOps

### 2.2.1 Overview

Intro to DevOps

Most 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). The exact definition is problematic as there is no consensus (Smeds, Nybom, and Porres 2015). 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).

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. 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). DevOps bridges the gap between evaluating performance during the development process and during operations (Brunnert et al. August 18, 2015).

TODO Devops lifecycle steps

TODO resource allocation/resource consumption, small memory software, benchmarking

### 2.2.2 System 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 are not as well defined as a CPU metric (Brunnert et al. August 18, 2015).

- Task Completion time
- Throughput
- Latency
- CPU usage
- GPU usage
- RAM usage
- VRAM usage
- I/O usage
- Network traffic

### 2.2.3 Continuous monitoring and benchmarking

Preprocessing

Training

Serving Latency

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.

## 2.3 MLOps

### 2.3.1 Overview

TODO (Kreuzberger, Kühl, and Hirschl 2023) data scientists doing manual work issue from conclusions, definition of MLOps, limit to technical stuff and tooling

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). One of the key areas of MLOps is using machine learning in production systems in addition to data processing and machine learning model training.

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.

Projects involving machine learning often make common methodological mistakes that threaten the validity of the models, but are easily avoided.

ref

TODO MLOps lifecycle steps

### 2.3.2 Machine learning development workflow

siirretään  
MLOps  
osioon

Projects involving machine learning often make common methodological mistakes that threaten the validity of the models, but are easily avoided. [Several workflows for developing machine learning systems have emerged attempting to standardize the overall development process including CRISP-DM and KDD. These workflows will overall have similar steps. Using CRISP-DM as an example we have the following steps in the workflow:](#)

1. Business and Data Understanding
2. Data Preparation
3. Modeling
4. Evaluation
5. Deployment

Business and Data understanding refers to understanding the problem and the datasets.

Preprocessing, feature engineering

TODO what DevOps brings to ML

TODO Continuous Training

### 2.3.3 AutoML

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).

Automated Machine Learning (AutoML) aims to minimize human intervention in completing data analytics tasks using machine learning algorithms (Yang and Shami November 2022).

### 2.3.4 Performance prediction and early stopping

## 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 affects performance metrics during hyperparameter optimization?
- *RQ2*: How early stopping affects performance metrics during neural architecture optimization?

#### 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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