UKRAINIAN CATHOLIC UNIVERSITY

MASTER THESIS

Neural architecture search: a probabilistic approach

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Declaration of Authorship

I, Volodymyr LUT, declare that this thesis titled, “Neural architecture search: a probabilistic approach” and the work presented in it are my own. I confirm that:

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- Where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated.
- Where I have consulted the published work of others, this is always clearly attributed.
- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.
- I have acknowledged all main sources of help.
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Signed: ______________________________

Date: ______________________________

"It's inspiring to see how AI is starting to bear fruit that people can actually taste. There is still a long way to go before we are truly an AI-first world, but the more we can work to democratize access to the technology—both in terms of the tools people can use and the way we apply it—the sooner everyone will benefit."

Sundar Pichai, CEO Alphabet Inc., May 17, 2017

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Abstract

In this paper we review different approaches to use probabilistic methods in existing AutoML solutions using Reinforcement Learning. We focus on providing additional knowledge about probability distribution provided to Reinforcement Learning agents solving Neural Architecture Search tasks. Based on the results of the research we come with an agent designed to model Neural Architectures for image classification tasks.

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List of Abbreviations

ML	**M**achine **L**earning
AutoML	**Auto**mated **M**achine **L**earning
NAS	**N**eural **A**rchitecture **S**earch
RL	**R**einforcement **L**earning
MDP	**M**arkov **D**ecission **P**rocess
CNN	**C**onvolutional **N**eural **N**etwork
RNN	**R**ecurrent **N**eural **N**etwork

Physical Constants

Speed of Light $c_0 = 2.997\,924\,58 \times 10^{8}\,\mathrm{m\,s^{-1}}$ (exact)

List of Symbols

a	distance	m
P	power	W ($\mathrm{J\,s^{-1}}$)
ω	angular frequency	rad

For all the brave people who make it possible for millions of young Ukrainians to hold books in their hands instead of rifles and grenades.

Chapter 1

Introduction

As machine learning provides a huge variety of automation possibilities for different industries the problem of automation of ML industry itself seems natural. For decades ML engineers were pioneers in the new era of computer science research. As a result, the new industry was shaped and this industry requires automation.

AutoML is a general name of automation in routine work of ML engineers including but not limited to data preparation, feature engineering, feature extraction, neural architecture search, hyperparameters selection, etc.

ML is reshaping businesses and other aspects of everyday life worldwide. We believe that everyone would benefit from the democratization of these new tools. Having the ability to run models on portable devices, IoT chips, and other mass-market hardware we treat AutoML as a big move towards in terms of a variety of different applications created.

In recent years AutoML becomes a natural product for almost all big technological companies. Google, Amazon, Salesforce, and others are offering AutoML products that allow non-experts to create their ML solutions.

Still, existing AutoML techniques require lots of computational resources and most of the research in the field is covered by tech giants nowadays.

We are focusing on neural architecture search problems, especially on hyperparameter optimization tasks because historically this problem is solved mainly using exhaustive search techniques, such as grid search. Engineers often follow their empirical knowledge and try to guess optimal parameters to tune models.

We are using the reinforcement learning paradigm since it is performing well in solving NAS problems. RL agents can design better architectures than related hand-designed models in terms of error-rate and efficiency - see Zoph and Le, 2016.

Moreover, we believe that RL could benefit from probabilistic approaches. We are deeply inspired by DeepAR Salinas, Flunkert, and Gasthaus, 2017 used by Amazon to build forecasting models. We show that Gaussian probability distribution could be used to effectively balance the exploration and exploitation of RL agents solving NAS tasks.

Chapter 2

Background overview

2.1 History

The idea of using RL agents to build neural networks is not new, however, there are not so many research projects nowadays. Mostly the reason for this is that most of the research is held by business, and business usually is not optimistic about RL in production.

However, some good progress was made in recent years. In 2015, ResNet becomes a winner of ILSVRC 2015 in image classification, detection, and localization and winner of MS COCO 2015 detection and segmentation. This enormous network contained 152 layers optimized by a lot of professional engineers manually. This process is expensive in terms of time and resources. Image classification contests are constantly showing a growing amount of layers for best-performing networks (AlexNet, 2012 - 8 layers, GoogleNet, 2014 - 22 layers). Resnet has 1.7 million parameters. Each competition is turning researchers more and more towards automation of this work - and this is a place where NAS becomes a new trend.

Barret Zoph and Quoc Le. in Zoph and Le, 2016 used a recurrent network to generate the model descriptions of neural networks and train this RNN via RL agent to maximize the expected accuracy of the generated architectures on a validation set. This paper is one the most cited in this field and our research is heavily based on it.

In 2019, Google researchers developed a family of models, called EfficientNets, which surpass state-of-the-art accuracy with up to 10x better efficiency (smaller and faster) using AutoML - see Tan and Le, 2019.

Amazon has two AutoML products to offer - Amazon SageMaker Autopilot for the creation of the classification and regression machine learning models and Amazon DeepAR for forecasting scalar (one-dimensional) time series using RNN. This paper is also heavily based on the probabilistic approach used in DeepAR because of it's spectacular results.

This section would not be full without the paper which shares a lot in common with this project. RL agent (Q-Learning, epsilon-greedy exploration rate control, finite state space) described in the paper outperformed meta-modeling approaches for network design on image classification tasks Baker et al., 2016.

The interest to the topic becomes even hotter when the NAS benchmark and dataset was introduced by Google Research team Ying et al., 2019

A variety of methods have been proposed to perform NAS, including reinforcement learning, Bayesian optimization with a Gaussian process model, sequential model-based optimization (SMAC), evolutionary search, and gradient descent over the past few years. We see a lot of research potential in this field and we share a big passion for RL paradigm - and that's why this project exists.

2.2 Reinforcement Learning

RL is an machine learning paradigm often used when the exact mathematical model is unknown and data is unlabeled. In this project we would mainly concentrate on the Q Learning approach. We require having observable environment where software agent would be able to take actions which would lead to reward. Agent is designed in the way it should maximize reward by utilizing existing knowledge (exploitation) or exploring random actions (exploration). Algorithm needs to learn a policy which determines which action should be taken next given current state (or set of recent states). The environment agent is operating with is typically a Markov Decision Process.

2.2.1 Markov Decision Process

MDB is a generalization of mathematical framework which allows performing a sequence of actions in an environment where future states would depend on current states and yield a partly random outcomes.

2.2.2 Q Learning

2.2.3 Exploration and Exploitation problem

2.2.4 Epsilon-greedy approach

2.2.5 Upper-confidence bound

2.3 Image classification problem

2.4 Convolutional Neural Networks

2.5 Gaussian Distribution

Chapter 3

Proposed approach

3.1 Pipeline

3.2 RL agent

3.2.1 Reward function

3.2.2 Exploration and exploitation

3.2.3 Gaussian layer

When it comes to probabilistic approach to RL algorithms, scoring becomes very important and may have a big impact on action taken by the controller - see Gneiting, Balabdaoui, and Raftery, 2007

If master CNN in RL agent is solving a regression problem (which is exactly our case) this CNN would use backpropagation to update it's weights (as noted above) in a way that error metrics of a test set would be minimized. Originally outputs of the last layer would be simple values - in our case, values which determines the actions that would be taken by controller.

Those values obviously depends on input and weights. In order to receive a Gaussian distribution we would need to modify last layer so that it would return mean and variance of output variable, which is enough to describe a Gaussian distribution of this variable. This allows us to bring a prediction uncertainity into the outputs of CNN. As described in Salinas, Flunkert, and Gasthaus, 2017 this requires also another approach to computation of loss function.

Generally saying we are using Gaussian distribution instead of single values because we need to have a measure of uncertainity of prediction of output. Then, if we have quite big uncertainity, it would be smarter to explore a random action. Otherwise, agent should use predicted action.

3.3 Master CNN

3.4 Slave CNN

Chapter 4

Experiments

4.1 Datasets

Our RL agent is generating CNN architectures which are performing an image classification task on the CIFAR-10 and CIFAR-100 datasets.

CIFAR datasets are described in very deep details in Chapter 3 of Krizhevsky, 2012, especially details about it's collection.

I would not go into details, just will note that CIFAR is a set of 32×32 colour images depicting real-world objects.

After training RL algorithm on CIFAR10 it is heavily switched to use it's knowledge on CIFAR100.

Key differences between CIFAR10 and CIFAR100 is denoted in table 4.1.

Dataset	Size	Number of classes	Images in class
CIFAR10	60000	10	6000
CIFAR100	60000	100 grouped into 20 superclasses	600

TABLE 4.1: Comparison of CIFAR10 and CIFAR100 datasets

Both in CIFAR10 classes are exclusive and do not assume instances overlapping - see 4.1.

Figure 4.1 shows a boat.

We use CIFAR datasets as is, meaning that we also share same train/test dataset split for evaluating generated CNN architectures. There are 50000 training images and 10000 test images in the dataset.

4.2 Metrics

4.3 Environment and training

4.4 Results

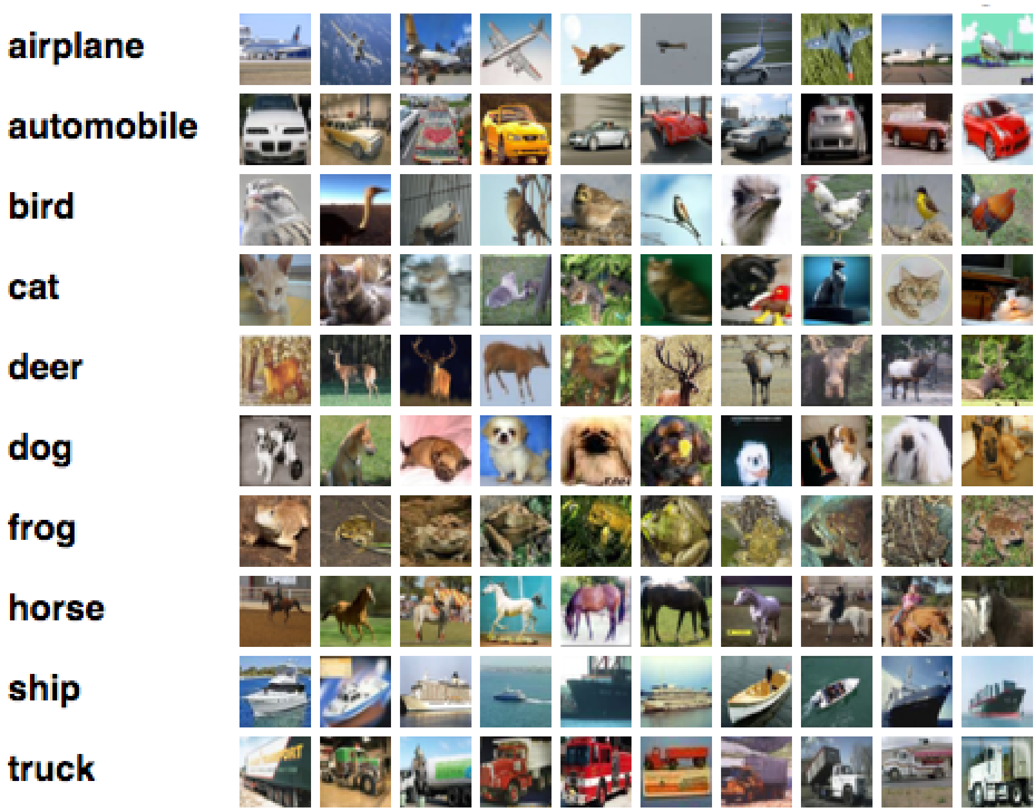

FIGURE 4.1: Classes of CIFAR10 including 10 random images from each Krizhevsky, 2012

Chapter 5

Conclusion

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