DOCTORAL THESIS

# Automated Machine Learning and Its Applications

HE, Xin

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# Abstract

Deep learning (DL), a broad family of machine learning (ML) methods based on artificial neural networks, has been widely used in various complex cognitive tasks and achieved remarkable performance. As deep neural networks continue to evolve and various models and novel modules are proposed, it is gradually realized that developing a new neural architecture is increasingly time-consuming and laborious. In addition, steps such as data augmentation and hyperparameters tuning also require much effort and expertise. These problems would inevitably hinder the application of DL in more under-explored fields due to the lack of ML specialists. Is it possible to automate all these steps? Automated machine learning (AutoML) would be a promising solution. The field of AutoML is evolving so quickly that there is still no consensus on its definition. However, AutoML is fundamentally meant to enable even beginners with limited ML expertise to build high-quality ML models tailored to their needs with minimal effort.

In this thesis, we investigate AutoML in the context of DL. We provide a comprehensive survey of AutoML from the perspective of the ML pipeline, which includes data preparation, feature engineering, model generation, and model estimation. According to current research advances, full automation of the ML pipeline may still be out of reach; therefore, the community is focusing on some sub-topics of AutoML. Neural architecture search (NAS) is one of the most popular research sub-topics of AutoML and involves two steps, model generation and model estimation, with the goal of automatically finding a superior neural architecture. We develop several NAS applications for medical image classification and

image generation tasks.

For image classification, we present two NAS applications. First, to the best of our knowledge, we were the first to apply NAS to search for 3D convolutional neural network (CNN) to classify COVID-19 3D CT scans. We propose a differentiable NAS to find promising 3D models in a well-designed weight-sharing super-network (Supernet). We discover a family of 3D models, namely *COVIDNet3D*, which outperform human-designed 3D models on three public datasets. Second, to alleviate the search instability of weight-sharing NAS, we propose an evolutionary multi-objective NAS approach, namely *EMARS*. We design a novel objective, *potential*, to estimate how promising a candidate model is. By combining potential, accuracy, and model size as objectives, the proposed methods can balance exploration and exploitation in the search process and efficiently find more competitive models.

For image generation, generative adversarial networks (GANs) are the most widely used DL models. GAN training itself suffers from instability and is prone to collapse; thus, using NAS to search GANs further exacerbates instability. To solve this problem, we propose an efficient two-stage evolutionary algorithm-based NAS framework to search GANs, namely *EAGAN*. Experiments on CIFAR-10 and STL-10 datasets demonstrate that the proposed EAGAN can find better GANs than previous NAS-GAN methods.

Last but not least, we strive to automate the three steps of data preparation, model generation, and model estimation. Specifically, we propose an end-to-end approach to jointly search data augmentation policy (DAP) and neural architecture (NA), namely *MedPipe*. Experiments on nine different medical datasets empirically validate MedPipe's effectiveness and superiority.

**Keywords:** Deep Learning, Automated Machine Learning, Neural Architecture Search, Image Classification, Image Generation, Generative Adversarial Network