摘要

近年来随着科学研究人员在机器学习领域不断地取得突破性的进展，机器学习方法已经在很多实际应用场景取得了成效，包括图像分类、人脸识别、目标检测跟踪、机器翻译等等。为了更进一步地去除机器学习过程中的人工参与，并在目标任务中取得相比于人工设计的解决方案更好的性能表现，自动机器学习的研究应运而生。然而当下绝大部分的自动机器学习研究依然存在弊端，多数提出的方法都只聚焦于机器学习流程中的单个模块。考虑到机器学习的性能由流程中的多个模块联合决定，针对单个模块的自动机器学习研究并不能对本质的问题进行解决。因此本工作提出对自动机器学习中的多模块优化问题进行探索，以网络结构、数据增强、训练超参三个模块的优化为例，提出了系列算法进行解决。

本工作的主要贡献包括：

1）提出了基于多智能体强化学习的多模块组合优化式自动机器学习方法。针对自动机器学习中的多模块优化问题，本工作将每个模块视作一个智能体，根据模块性质定义其动作，将组合得到的训练流程的性能表现视作强化学习中的奖励，以此将原问题转化为了多智能体强化学习问题。本工作将三个模块基于强化学习的优化方法组合，提出了基于多智能体强化学习的多模块组合优化算法，并在不同规模的图像分类任务集上进行了实验，实验结果说明了该多模块组合优化算法的有效性。

2）提出了基于信用分配的离策略多模块联合优化式自动机器学习方法。本工作以所提出的多模块组合优化算法为基线改进，引入了信用分配对模块间的协同性进行描述，也采用了离策略的学习方式改善优化效率，提出了多模块联合优化算法，也对该算法的理论收敛性质进行了证明。后续在分类任务数据集进行了实验，说明了所提出的多模块联合优化算法的优越性，也通过消融实验说明了信用分配的有效性和离策略学习方式对提升优化效率的显著性。

3）提出了基于计算量约束的多模块联合优化式自动机器学习方法。考虑现实应用场景往往会对机器学习计算量存在限制需求，本工作对带计算量约束的多模块优化问题进行了研究，对所提出的多模块联合优化算法进行改进，通过多目标奖励函数的方法对奖励进行了修正，引入了约束信息，提出了基于计算量约束的多模块联合优化算法。通过对比该算法的实验结果和其他先进算法系列结果的计算量和性能，印证了所提出算法的优越性。

关键词：机器学习，自动机器学习，多智能体强化学习，联合优化

Automated Machine Learning Based on Multi-Agent Reinforcement Learning

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ABSTRACT

In recent years, with the continuous breakthroughs made by scientific researchers in the field of machine learning (ML), ML methods have achieved successes in many practical applications, including image classification, face recognition, object detection and tracking, machine translation and so on. To further alleviate human involvement in ML and achieve better performance on the specific task compared with manually designed ML models, the research of automated machine learning (AutoML) emerges. However, existing work on AutoML mainly focuses on individual modules in the pipeline. Considering that the performance of ML is jointly determined by all modules in the process, AutoML methods focused on a single module cannot solve the essential problem. Therefore, our work proposes to explore the multi-module optimization problem in AutoML. Taking the optimization problem of network structure, data augmentation and training hyperparameters as an example, a series of methods are proposed.

Overall, the main contributions of our work are as follows:

1) A multi-module optimization AutoML method based on multi-agent reinforcement learning (MARL) is proposed, which is called MA2ML-Lite (Lite version of Multi-Agent Automated Machine Learning) to be a baseline method for further research. MA2ML-Lite takes each module as an agent and final performance as the reward, and transforms the multi-module optimization as an MARL problem. MA2ML-Lite combines individual RL-based modules for the optimization. Experiments on different scales of image classification datasets show the efficacy of MA2ML-Lite.

2) An off-policy multi-module optimization AutoML method based on credit assignment is proposed, which is called MA2ML (Multi-Agent Automated Machine Learning) as a modified version of MA2ML-Lite. MA2ML introduces credit assignment to describe coordination among modules, and utilizes off-policy learning pattern to enhance optimization efficiency. The theoretical guarantee of convergence of MA2ML is also provided in our work. Experi-

ments show the superiority of MA2ML. Besides, ablation study proves the efficacy of credit assignment and optimization efficiency improvement obtained by off-policy learning.

3) A multi-module joint optimization AutoML method with computational cost constraints is proposed. Considering that practical application scenarios usually have constraints of ML computational cost, our work explores the multi-module optimization problem with computational cost constraints. Our work modifies MA2ML by using multi-objective method to revise the reward function in RL, and the computational cost constraint information is added. Comparison with results achieved by other state-of-the-art methods illustrates the superiority of our proposed method.

KEY WORDS: Machine learning, Automated machine learning, Multi-agent reinforcement learning, Joint optimization