The Power of Encodings and Operators in NAS Building Blocks

Research Objective: Artificial neural networks have recently become one of the best methods of discovering patterns in data and extrapolating them especially for predictive purposes [1, 2, 3, 4, 5, 6, 7]. The structure, or architecture, of these networks contributes greatly to their success and is critical in the discovery of these patterns [8]. Historically, these neural network architectures were hand-made by human designers [5, 1, 2], which is a time consuming and costly task. More recently, an interest has started to grow in the idea of automatically generating these architectures (neural architecture search, or NAS) using various techniques [9, 10, 11, 12]. Some of these techniques have made use of building blocks to construct these neural architectures which involve searching for an inner structure for each block to maximize performance of the architecture on some task. [10, 12, 13]. These methods are still constrained by the human designers and contextualized by the encoding used to represent and the operators invoked to search the space of these inner structures. **It is hypothesized that utilizing a more flexible encoding and diversity-inducing operators will allow for evolutionary NAS to access more of the fitness landscape resulting in potentially higher performance of solutions.** This work will apply to the research direction of the student's dissertation by portraying the limiting nature of current inner cell encodings and search operators in NAS and by showing the power of more flexible, open-ended ones.

Methodology: This work will begin by observing the encodings and operators utilized in recent literature with regards to the inner cells of NAS methods. It will implement at least one of these encodings as a comparison metric and for the purpose of in-depth investigation of it. An evolutionary algorithm will then be constructed for which operators will be created that take inspiration from recent successful approaches from the field of Evolutionary NAS. This evolutionary algorithm will then be applied to a task of image recognition to observe its efficacy in producing accurate and diverse solutions. Once these tasks have been completed, another evolutionary algorithm with modified operators, aimed at diversity, will be constructed (leaving the encoding the same) and compared. Next, a new modified encoding, with the goal of flexibility, will be applied to the original evolutionary algorithm. Lastly, the modified encoding and modified evolutionary algorithm will be combined. This will ultimately yield a comparison portraying the metrics responses to the modifications of the encoding alone, the evolutionary algorithm alone, and both combined. All of these experiments will utilize the MNIST dataset and task. These results will be unique to the field of NAS, since, to the author's knowledge, this type of comparison has not been directly addressed in the literature.

Related Work: Neural networks have come to excel at extracting complex patterns from data to solve complex, nonlinear problems [1, 2, 3, 4, 5, 6, 7]. The architectural designs of these networks in many cases are derived manually by human creators [5, 1, 2]. More recently, a technique called neural architecture search, which has the goal of automating the construction of these architectures, has shown much promise [9, 10, 11, 12]. In this area of research, two main techniques for discovering these architectures extrapolate knowledge. The first method is differential neural architecture search [11, 12], and the second is evolutionary neural architecture search [9, 10]. Both of these methods are very highly constrained in their search for competitive architectures and much of the design is largely biased because it is created by a human designer [9, 11, 12]. One of the growingly popular techniques in NAS, building blocks with inner structures, has shown its capability at producing complex architectures and performing well on various tasks [10, 12, 13]. This work takes inspiration from prior research in neural architecture search and to explore the variables within the inner structures of these building block techniques and to aid in the creation of a new process of neural architecture search that will be capable of higher levels of diversity and discovery.

Rationale: Current techniques from the field of NAS have been strongly objective driven with a specific end goal in mind while also being strongly biased by recent successes of particular types of network structures. These two factors work to constrain the search space of recent research to a subset of "good" architectures. Placing this limit on search, in this author's mind, can limit the ability to find improvements and better architectures in the longer time scale. This work aims to experiment with both the encoding and evolutionary operators of evolutionary NAS to discover more exploratory versions of both. This specific work is looking particularly at the inner structures of recent "building block" approaches to NAS. The rationale for this being that if the inner structure can represent a wide diversity of architectures, then its only constraint is the outer, "building block" structure. This same type of comparison and results may apply to this structure as well.

Needs Assessment: This project will require an unknown amount of time since the modifications are not directly enumerated here. This could cause the project to be unsuccessful at satisfying the hypothesis or, if this need is ignored, to be incomplete upon its due date. It will require computational time to complete the experimentation. It will require knowledge of potential diversity-inducing modifications, which we have begun to enumerate in class. It will require a target task and dataset. MNIST will be used for the experiments here.

Proposed Timeline:
Week 1: Literature review of encodings and operators - Milestone: Decide on exact encodings / operators to implement.
Week 2: Implement these encodings and operators - Milestone: results of diversity and accuracy on MNIST
Week 3: New, modified evolutionary algorithm - Milestone: results of diversity and accuracy on MNIST
Week 4: New, modified encoding - Milestone: results of diversity and accuracy on MNIST
Week 5: Week 3 and 4 encoding and algorithm combined - Milestone: results of diversity and accuracy on MNIST

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