Enhanced Monte Carlo Tree Search for Materials Design and Discovery

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Materials design and discovery is often formulated as the selection of optimal solution from a space of candidates. Monte Carlo tree search (MCTS) has shown efficiency in solving this inverse design for several applications including but not limited to thermoelectric materials, graphene [1], [2]; however, randomization technique in MCTS can limit efficiency, particularly with very large scale problems (For example, spaces with over a million candidates for a small computational power environment). In this work, we present an enhanced Monte Carlo tree search approach using policy gradient [3].

Monte Carlo tree search is an iterative algorithm that models the search space as a shallow decision tree. Each iteration consists of 4 steps: selection, expansion, simulation, and backpropagation. In the expansion step, a child node is added randomly under the selected parent node. In this work, a neural network was applied to choose the optimal child node to be expanded using policy gradient method (Fig.1). Policy gradient (PG) is a reinforcement learning method that optimizes parametrized policies towards an expected return using gradient descent.

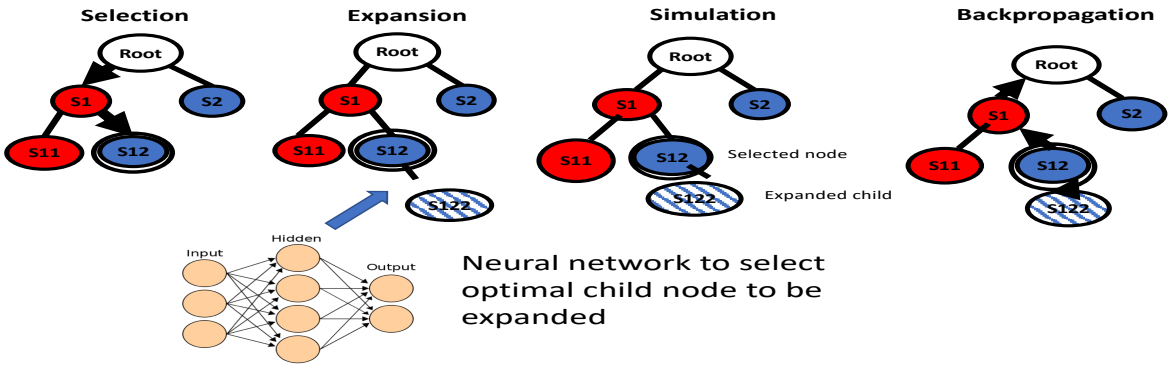

Figure 1: Enhanced Monte Carlo tree search with policy gradient

For evaluating the obtained structure, we used a Python package: *xrayutilities* [4], which is a set of algorithms to convert scattering data to reciprocal space coordinates.

This method was applied to design a depth-graded multilayer structure by determining each layer thickness from a space of candidate thickness values to maximize mean reflectivity in an angular range 0.45~0.55 ° for Cu Kα radiation in X-ray optics applications. The mean reflectivity was calculated from representative 10 points in the angular range, and the maximum mean reflectivity achieved by our proposed method was 0.8. The generality involved in this approach may provide applicability to the other problem of structure finding in material science.

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