Automatic complex materials design using Monte Carlo tree search

Keywords: Materials design, Monte Carlo tree search

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Background

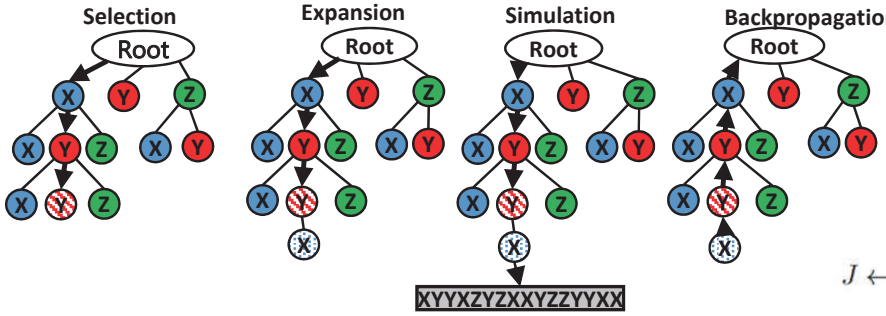
- The design of complex materials is often formulated as finding the optimal atoms configuration in the structure from a large number of potential possibilities. The importance yet exhaustive cost of this process, imposes the need for an optimal experimental design to efficiently utilize available resources.

Aim

- We propose an experimental design tool based on Monte Carlo tree search to find the optimal design with as few experiments as possible. This tool is parameter-free and works autonomously in various problems. In comparison to a Bayesian optimization package, our algorithm showed competitive search efficiency and superior scalability.

Advanced Research Topics

MDTS: Materials Design using Tree Search



Upper Confidence Bound

$$u_i = \frac{w_i}{v_i} + C\sqrt{\frac{\ln v_{parent}}{v_i}},$$

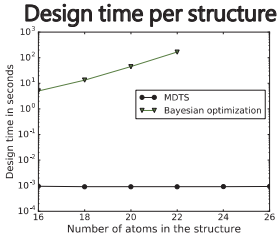
$$C = \frac{\sqrt{2}J}{4}(z_{max} - z_{min}),$$

$$J \leftarrow J + \max\{\frac{T-t}{T}, 0.1\}$$

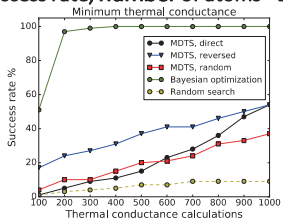
w_i:accumulated merit of the node, v_i: visit count of the node, C: constant to balance exploration vs. exploitation, z_{max} and z_{min} : maximum and minimum immediate merit observed in the downstream nodes, J : a meta-parameter used to adjust C dynamically. T is the total number of candidates to be evaluated and t is the number of candidates which already been evaluated.

Experiment Results

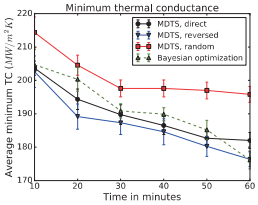
Design time per structure



Success rate, number of atoms =16



Optimal observed thermal conductance over total time, number of atoms=22



Publications

- Thaer M. Dieb, Koji Tsuda: Machine Learning-based Experimental Design in Materials Science. In: Tanaka I. (eds) Nanoinformatics. Springer, Singapore, pp65-74, (2018)
- Thaer M. Dieb, Zhufeng Hou, and Koji Tsuda: Structure Prediction of Boron Doped Graphene by Machine Learning. The Journal of Chemical Physics, 2018 148, 241716.
- Thaer M. Dieb, Shenghong Ju, Kazuki Yoshizoe, Zhufeng Hou, Junichiro Shiomi and Koji Tsuda: MDTS: Automatic Complex Materials Design using Monte Carlo Tree Search. Science and Technology of Advanced Materials , 2017, Vol 18, No.1,pp. 498-503.

Summary

- We have implemented a method to solve atom assignment problem in materials design using Monte Carlo tree search.
- MDTS is scalable with competitive performance to Bayesian optimization.

Research outcome

- MDTS works without parameter tuning in various materials design problems.
- MDTS can be applied to large scale combinatorial optimization problems.
- MDTS is available online at: https://github.com/tsudalab/MDTS