Review Paper04

1 Summary

This paper introduces Parallel and Distributed Thompson Sampling (PDTS), a new method designed for efficient large-scale exploration of chemical spaces using parallel computing. By leveraging a distributed implementation of Thompson sampling, PDTS enables the parallel evaluation of numerous molecules, significantly accelerating the identification of promising candidates for materials science and drug discovery. The research includes experiments using both Gaussian processes and Bayesian neural networks, showcasing PDTS's effectiveness in real-world high-throughput screening scenarios and highlighting its potential for substantial time and resource savings.

2 Discussion and Open Questions

- Can PDTS be used on some other tasks? For example, as far as I know, Bayesian Optimization can be used for hyperparameter tuning, so can PDTS be used on such tasks?