Report for MERIT Internship (Domestic)

Department of Chemical System Engineering, Graduate School of Engineering

Funatsu–Kotera Laboratory D1

MERIT 7th Takahiro INOUE

Host company

Preferred Networks, Inc.

Period

2019/08/07 ～ 2019/09/20

Research theme

Efficient search for compounds with desired properties using chemical structure generator

Background for research theme

A structure generator is a computer program that generates chemical structures in silico and is used as a tool to search for novel functional organic compounds in the field of drug discovery and material design.

The main use of the structure generator is virtual screening, in which we predict the properties of the generated structures with statistical models, and we adopt ones that satisfy desired physical properties as the candidate structures. In general, there are usually multiple conditions for a compound to be satisfied. Therefore, it is challenging to design a structure so that all properties are optimal. Despite this difficulty, it is necessary to search efficiently for chemical structures that satisfy all of the given conditions, if not optimal.

Contents of research

The problem of finding chemical structures that satisfy all the desired conditions can be formulated as a multi-objective optimization problem. We conducted this internship intending to obtain solutions called Pareto optimal solutions to this problem. If multiple Pareto optimal solutions were obtained, we could obtain candidate structures that satisfy all of the conditions simultaneously. In the internship program, we confirmed the usefulness of multi-objective optimization for this problem setting by implementing multi-objective optimization and conducting experiments on computers.

My impression

In my research, I am designing a structure generator. On the other hand, I conducted a case study on the use of a structure generator in this internship. I could extend my knowledge of optimization through the implementation and experiments of algorithms. Furthermore, I reconfirmed the relevance of the research field to the real world. It was an excellent opportunity to reconsider the direction of my research.

Also, I think it was useful for reviewing my research style. In this internship, there are many situations where I have discussions on my themes with those who have different backgrounds, which I felt necessary.

Acknowledgment

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