MERIT Internship (Domestic) Report

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Hayashi Group, Ph.D Student
6th Class Student of MERIT
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- Period
2019/09/02 ~ 2019/11/29

- Destination
Digital Technology Innovation Center, R&D Group, Central Research Laboratory, Hitachi Ltd.
(Supervisor: Senior Researcher, Dr. Akinori Asahara)

- Theme
Application of AI/machine learning technology to high-speed prediction of material property for development of new materials

- Purposes
The purposes of this internship are shown below:
1. To improve the understanding of Materials Informatics
2. To learn the technology of AI and machine learning and experience different researches, in order to broaden the vision of personal research
3. To experience the research environment and study life in company

- Content
The traditional methods of developing new materials with outstanding properties are: to arrange the experiment results so far as database; to propose new material according to experience and the theoretical pre-examination, e.g. first principle calculation; to examine the properties of proposed materials after synthesis. The new materials can be determined, or new better materials can be proposed based on the examining results. However, due to uncertainty of the prediction used by traditional method and the time and financial cost, more efficient method is needed. Machine learning is a technology that can recognize the pattern or value of given data by establishing the statistical model using the feature vector extracted from data. By using the model, the pattern of new data can be recognized in a much high speed. Thus, this technology is also expected to improve the efficiency of developing new materials with better properties in materials informatics. The main content of this internship is to examine and establish new feature vector generation method for specifying and realizing precise prediction of properties of organic materials by using machine learning.

The traditional method used to generate feature vector for prediction of organic materials' properties by machining learning was examined. According to the results of different machine learning methods, the traditional method was found to have bad precision in property prediction though being able to specify materials with special property. Based on this result, I established a new method to generate the feature vector for predicting organic materials' properties by machining learning, which has a better precision in specifying materials with given properties.

- Impressions

Before the internship, I have never experienced the life in company by living in school and university for more than 20 years. I have been able to experience the atmosphere in company through this internship. The theme and researching method of this time's internship were much different from what I have done in the university. Thus, I have gotten the experience of completing a program from zero base in three months. I have learned the popular technology: machine learning, which may help me in broadening my research themes. During the life in Hitachi Ltd., I also felt the free atmosphere in a research company. This experience has broadened my vision and future career decision. Finally, I have tried to solve the practical method in production based on my professional knowledge, which makes me recognize the importance of professional knowledge again.