Internship Report

Department of Applied Physics
Morimoto Lab. D2
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Overview

Institution：ZEON Corporation, R&D Center
Term：2024/10/15 ～ 2024/12/13
Form：Hybrid of online and in-office. About 2 days a week in-office at Zeon Corporation R&D Center.
Supervisor：Dr. Yuki Ono / Mr. Riku Shirota

Theme

Physical modeling of rubber production process

Background and Challenges

The rubber temperature in the production process is a critical objective variable, as it significantly affects the physical properties of the rubber. In this internship, I was involved in a machine-learning-assisted model design work for the development of simulation technology for new rubber manufacturing equipment. Since experiments using the new rubber manufacturing equipment are highly time-consuming, Computer Aided Engineering (CAE) with simulation software was considered. However, the following challenges were identified:

- **Time cost**: The simulation software cannot be automated.
- **Complexity**: The number of possible combinations of parts for the new rubber manufacturing equipment is enormous.

To address these challenges, I undertook the following two tasks during the internship:

1. Development of a surrogate model for the simulation software.
2. Exploration of efficient methods for selecting acquisition points to improve the surrogate model's accuracy.

By accomplishing these tasks, it would become possible to instantly predict the rubber temperature after experiments using the new equipment based on previously non-quantitative explanatory variables, such as combinations of parts. This, in turn, enables us to

propose new experimental conditions effectively.

Results

- **Development of a Surrogate Model for the Simulation Software**
  Initially, it was anticipated that the problem of combinatorial explosion would arise. However, through careful examination of the simulation results, the model was successfully simplified. While details cannot be disclosed due to confidentiality considerations, a high-accuracy surrogate model was developed at a realistic computational cost that avoids combinatorial explosion for data where sequence order was seemed to be critical.
  The surrogate model demonstrated high predictive accuracy, achieving an R^2 score of 0.98 on the training date of the simulation results.

- **Exploration of Efficient Acquisition Point Selection Methods to Improve Surrogate Model Accuracy**
  Given the extensive variety of patterns in the explanatory variables, it is challenging to manually identify new points to add to the training data. Bayesian optimization is often employed in such scenarios; however, due to its numerous constraints, implementing it using existing packages was difficult. As an alternative, the following acquisition point selection methods were considered:
  1. Generating random points and evaluating them based on the variance of Gaussian process regression, selecting points with maximum variance.
  2. Using a hill-climbing optimization method to maximize either the variance of Gaussian process regression or the distance from the training data.

  Both methods improved test validation accuracy compared to simply adding randomly generated points to the model. This confirmed the validity of acquisition point evaluation using the variance of Gaussian process regression. Although the hill-climbing method provided the most efficient model improvement, it also presented challenges, such as the bias of acquisition points toward specific regions. Improving the selection of initial points and refining the update algorithm remain as prospects.

Impression

Since my usual research does not involve machine learning, it was highly rewarding to apply knowledge of statistics and machine learning that I had studied only theoretically as far. Because the project was based on experiments, it was a valuable experience for me to experience firsthand the pleasure when things went well and the difficulty of detailed conditions. Additionally, I noticed a significant difference between this internship and my academic research: the tasks in this internship were part of a larger project, whereas, in university research, individuals often carry out entire projects themselves, even with some degree of role-sharing. I was surprised at the scale of the project, which is unique to corporate R&D.

Acknowledgements

I would like to express my heartfelt gratitude to everyone at ZEON Corporation for hosting me during this two-month-long internship. I am deeply thankful not only for proposing and discussing the theme but also for providing many opportunities for interaction. I also had many chances to receive valuable advice from various individuals, making this inernship an very meaningful experience. Furthermore, I am grateful to my academic supervisors Professor Takahiro Morimoto and supporting supervisor Professor Shinichiro Seki, for approving my participation in this internship. Lastly, I extend my sincere appreciation to the MP-CoMS and MERIT programs for offering such an excellent opportunity.