

Network analysis and machine learning for metabolomics of plants

Project Leader

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1. Objective

Metabolomics of plants differs from traditional targeted phytochemical analysis in various fundamental aspects. For example, non-targeted analysis is a promising methodology for identification of unknown compounds of metabolites. However, data generated from liquid chromatography/high-resolution mass spectrometry often contains thousands of detected compounds in a single sample, so development of a new metabolomics methodology that combines network analysis and machine learning would be a significant advance. This study thus aims to demonstrate the relevance of graph neural network models to heterogeneous network data on molecules, proteomes, and diseases.

2. Project Outline

To achieve the above objectives, the project will consist of the following phases:

- (a) integration of non-targeted metabolomics data and other omics data;
- (b) development of a new method combining conventional network analysis with machine learning methodology, using graph neural network models; and
- (c) extraction of meaningful knowledge from experimental data using the above new method.

3. Expected Performance

In this project, the successful candidate would be expected to:

Combine multi-omics data integration with natural language processing.

4. Required Skills and Knowledge

The successful candidate for this project will have the following knowledge and skills:

Elementary knowledge of Python programming.

References

Hiraga, Y., Ara, T., Sato, N., Akimoto, N., Sugiyama, K., Suzuki, H., & Kera, K. (2021) Metabolic analysis of unripe papaya (*Carica papaya* L.) to promote its utilization as a functional food. *Bioscience, Biotechnology, and Biochemistry*, **85**, 1194-1204.

See my webpage:

<https://www.researchgate.net/profile/Hiroshi-Frusawa>

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https://www.kochi-tech.ac.jp/english/admission/ssp_aft19oct/ssp_application_guideline.html

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