

PROPOSAL

Jesse Wood, Bing-Xue, Mengjie Zhang, Bach Hoai Nguyen, Daniel Killeen

Victoria University
Engineering and Computer Science
Kelburn, Wellington, New Zealand

ABSTRACT

Submitted in partial fulfilment of the PhD in Artificial Intelligence.

Index Terms— AI applications, Classification, Feature Selection, High-dimensional data, Multidisciplinary Mass Spectrometry, Fatty Acid

1. INTRODUCTION

- Scope - place the problem in the world.
- Specifics to New Zealand, sustainability.
- Fish processing - automation, quality control, contamination.
- Current state-of-the-art
 - GC-MS, manual, time consuming, expensive, destructive, instrumental drift.

2. LITERATURE

- Mass spectrometry [1]
- REIMS
- Classification
- Feature Selection
- Interpretable ML
- Genetic Programming
- Transfer Learning

Thanks to New Zealand Plant & Food Research for datasets, funding and expertise.

3. PRELIMINARY WORK

- Automated Fish Classification on GC-MS data.
- Genetic Programming (GP) for GC-MS data
 - Single-Tree GP
 - Multi-tree GP
- REIMS exploratory data analysis

4. CONTRIBUTIONS

- Each research question applies to the Hoki and Jack Mackerel datasets.
- For each dataset, hoki and mackerel.

These are the research questions from Plant and Food Research.

- Can REIMS data be used to classify different species tissues? What variables are responsible?
 - Classification
 - Feature Importance - Interpretable
- Can REIMS data detect mixed-species contamination in fish tissues? At what concentration? What variables are responsible?
 - Classification
 - Regression
 - Feature importance - Interpretable
- Can REIMS data detect mineral oil contamination in fish? At what concentration? What variables are responsible?
 - Classification
 - Regression
 - Feature importance - Interpretable

- Can REIMS data be used to distinguish between different fish individuals? What variables are responsible?
 - Identification
 - Feature importance - Interpretable

5. MILESTONES

- Literature Review
- EDA
- Preprocessing
- Classification
- Cross-species Contamination
- Mineral-oil Contamination
- Individual Identification
- Auto ML
- Thesis

6. THESIS OUTLINE

1. Introduction
2. Background
 - Mass Spectrometry
 - REIMS
 - Classification / Regression
 - Interpretable ML
3. Preparations
 - Exploratory Data Analysis
 - Preprocessing
4. Applications
 - Classification
 - Contamination Detection
 - Individual Identification
 - Auto ML
5. Discussion
6. Conclusion

7. RESOURCES

- Hardware
 - ECS Grid Compute
 - Rapoi
 - Niwa HPC - via Auckland University
- Software
 - Repository - Github
 - Project Management - Github Projects
 - Programming language - Python
 - Documentation - Read the Docs
- Experience
 - Field-trip to Callaghan Innovation to see REIMS
 - Field-trip to NZ Plant and Food Research (if necessary for future datasets).

8. APPENDIX

9. REFERENCES

- [1] K Eder, “Gas chromatographic analysis of fatty acid methyl esters,” *Journal of Chromatography B: Biomedical Sciences and Applications*, vol. 671, no. 1-2, pp. 113–131, 1995.