Machine Learning for NMR-based Fuel Classification

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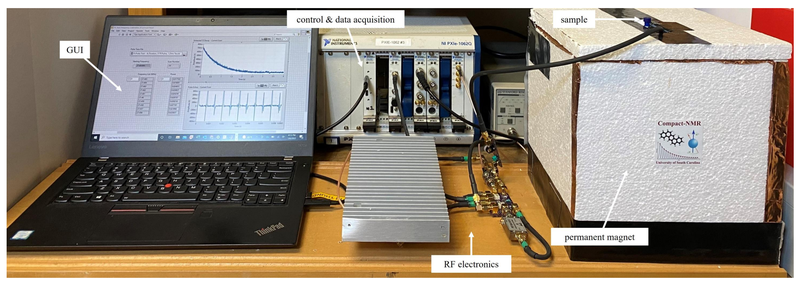
Background

- Nuclear magnetic resonance (NMR) is a form of spectroscopy used to gather information on the molecular structure of matter
- Nuclei that carry magnetic moments will precess in the presence of an applied magnetic field
- By exciting such nuclei with radio waves and measuring voltage induced in a coil as they relax, data regarding chemical composition can be collected
- NMR has applications in substance and mixture classification, quantitative analysis, chemical dynamics, and more

Objective

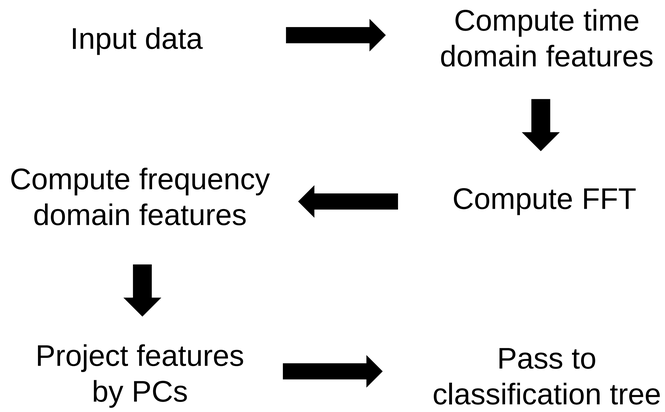
- Develop a non-neural network classifier for jet fuels that takes as input T2 decay data gathered from NMR spectroscopy
- Gain an understanding of decay data feature space



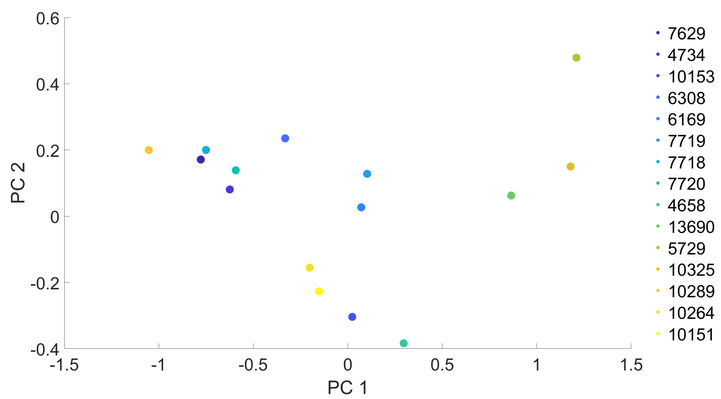
ARTS-Lab Compact NMR Setup

Methodology

- First, gather statistical metrics from decay data to use as model features
- Perform principal component analysis (PCA) on feature space
- Project new data by principal components and use classification tree for inference



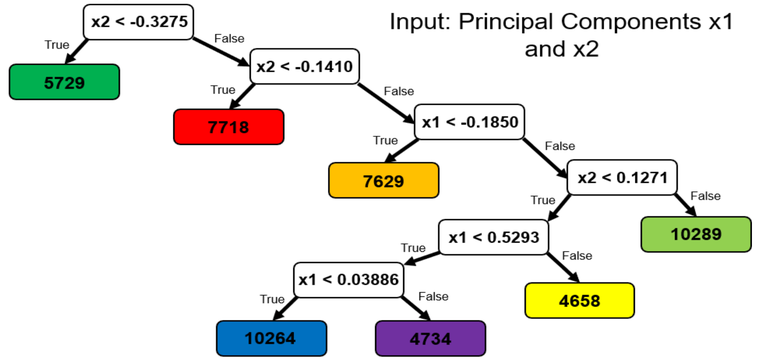
Classification Flowchart



Principal Components Across Fuel Classes

Results

- Model accuracy on test dataset of 15 fuel classes and 30 fuel instances: 67%
- Adding noise to extend training dataset yielded +40% accuracy



Base Classification Tree Architecture

Future Work

- From decay data, predict not only fuel classes, but estimate fuel properties using neural network (density, molecular weight, etc.)

References

[1] Thompson et al. Multi-modal Generative Adversarial Networks for Synthesizing Time-series Structural Impact Responses. 2022.
[2] Jeon et al. Datum Unit Optimization for Robustness of a Journal Bearing Diagnosis System. 2016.
[3] Zhu et al. Feature Selection based on Principal Component Analysis for Underwater Source Localization by Deep Learning. 2020.

Acknowledgements

This material was sponsored by the ARO under Grant Number: W911NF-21-1-0306. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of ARO or the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Government purposes notwithstanding any copyright notation herein. This work is also partly supported by the University of South Carolina under Grant No. 80004440.