UNIVERSITÄT ZU LÜBECK

TECHNISCHE HOCHSCHULE LÜBECK

Master thesis

Topic: DEVELOPMENT OF A PATTERN RECOGNITION ALGORITHM FOR CHEMICAL IDENTIFICATION IN BENCHTOP CONTINUOUS WAVE NUCLEAR MAGNETIC RESONANCE (NMR) SPECTROMETER.

Summary:

This thesis addresses the challenges faced in CW benchtop NMR spectroscopy by proposing the development of an AI-driven system to enhance chemical identification and data analysis. The primary objective was to create an artificial intelligence algorithm capable of processing and analyzing data from CW benchtop NMR spectrometers, even in noisy or incomplete conditions, to provide accurate chemical identification.

The performance of two classification models, a Convolutional Neural Network (CNN) and a Support Vector Machine (SVM), was evaluated. The CNN model achieved high training accuracy (98.04%) but struggled with overfitting, resulting in a moderate test accuracy of 67.19%. On the other hand, the SVM model demonstrated lower test accuracy (60.94%) with a significant variation in performance across different data distributions. Both models showed potential for improvement through techniques such as regularization, hyperparameter tuning, and addressing class imbalances. Future work could focus on refining these models by implementing strategies like dropout layers, data augmentation, kernel adjustments, and resampling techniques to enhance prediction accuracy and consistency.

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