Usage of deep learning in FTIR spectra analysis of functional groups

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The Fourier transform in infrared spectroscopy (FTIR) stands as a common spectroscopic technique. Spectral interpretation, while it takes a lot of time, gives crucial insights into the functional groups existing within compounds and intricate substances. Our endeavour involves the development of distinct neural network models to examine their effectiveness in classification of FTIR spectra's affiliation with individual functional groups. These ML models allow us to reduce time of functional group analysis and foster the elucidation of FTIR spectra.

In our research we used 8728 gas-phase spectra from the NIST database[1], interpreting them as one-dimensional vectors. Successfully, we train models of CNN and DNN for the most prevalent functional groups, subsequently deducing their presence in the spectra, which were not used in the training process (we are comparing our results with this publication[2]). Such models serve to broaden the scope of FTIR measurements for facile analysis of organic.

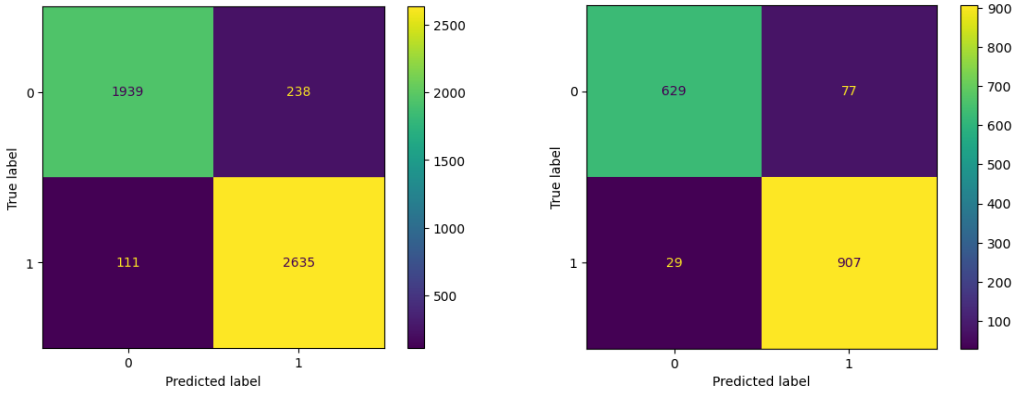

Figure 1 Accuracy of CNN model on training (left, ~96% success rate) and test (right, ~97% success rate) sets for aromatic compounds.

[1]: https://webbook.nist.gov/chemistry/
[2]: A. A. Enders et. al. Anal. Chem. 2021, 93, 28, 9711–9718

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