A Deep Learning Approach for Combining Nuclear Magnetic Resonance Spectroscopy and Mass Spectrometry based Metabolomics Data Towards Disease Prediction

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August 2024

Abstract

Nuclear magnetic resonance (NMR) and Mass spectrometry (MS) are two mainly used techniques in metabolomics that can measure abundance of hundreds of metabolites. The data generated by either techniques have already allowed a huge progress in various research fields from personalized medicine to pharmaceutical sciences. Combining measurements from both platforms through a simple concatenation also led valuable discoveries. In this work, however, we propose an alternative data fusion approach based on deep learning that aims to make use of each type of measurement and combine the derived information in a different layer for disease prediction. Rather than feeding in all data in a single vector, we create dual "pipelines", operating on the datasets separately, and then combine the outputs into a single prediction. To do this, we train the custom model on saliva data on Alzheimer's patients on which both NMR and MS data is available. We find increases in performance when creating a "dual-pipeline" architecture that initially treats NMR and MS data separately over traditional fusion methods.