

Docket #: S20-292

OmiXLearn: Machine learning analysis for metabolomics diagnostics and biomarker discovery

Scientists at Stanford have developed a machine learning program with broad potential for diagnostic applications which analyzes mass spectrometry data profiling metabolites in a patient sample ("metabolomics" data) and predicts infection status.

The researchers used metabolomic data from patients who were tested for influenza to train a machine learning program that predicts positive or negative infection status from a metabolite analysis. They were also able to determine which metabolites were the key predictors of influenza infection status, showing that this technology can also enable metabolite biomarker discovery.

While existing methods like random forests can analyze the large amount of data produced by metabolite mass spectrometry to look for patterns, this novel algorithm outperforms old methods in accuracy, reproducibility, and ease-of-use, as it takes in all available data as inputs for its analysis and requires fewer choices on the user's end. This technology also has broad potential in helping diagnose many diseases beyond influenza, especially infectious diseases. In addition to predicting a disease state from metabolomics data, this technology has exciting potential as a biomarker discovery tool, and it can enable development of novel targeted diagnostic methods that narrow clinical analyses to just a few metabolites.

Stage of Development: Prototype

Applications

- Prediction of infection status for influenza from a profile of the metabolites present in a patient sample, as determined by mass spectrometry analysis

- Assessment of individual metabolite importance as predictors or biomarkers of a disease status to enable more targeted future testing regimes
- Potentially applicable to other infectious diseases

Advantages

- Outperforms the state-of-the art in metabolomics analysis (random forests method) in model accuracy
- More streamlined, comprehensive, and reproducible than existing methods that attempt to determine disease status from metabolite analyses

Patents

- Published Application: [20220084636](#)

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