ML has been used in:

- Analyses of points or bins from the metabolomics measurements such as NMR spectra or MS spectrograms (examples of use of PCA and PLS methods are too many to reference). A recent example of an application of deep learning, as well as SVM, RF and several other machine learning algorithms was presented by Alakwaa et al. [20];
- Assignment of peaks in spectrograms or spectra for metabolite identification [12,21];
- Quantification of metabolite concentrations from high throughput data [22,23];
- Selection of a sets of the most informative attributes ("feature selection") for given sample groups [19,24];
 - ML can be used to optimise and discover metabolic pathways within the body
 - Dataset contains 29 distinct features that describe several patients' statuses with a total of 12,012 records
 - 5 nature-inspired algorithms are used to obtain relevant features
 - Variety of data points:
 - Enzyme test
 - Insulin Test
 - Age, Gender, Demographic data
 - Triglyceride levels
 - More
 - To get accuracy, true vs false pos/negs were counted
 - Very close relationship between immunity and metabolic health
 - KNN was the best model
 - Datasets were collected from variety of nomics data, lots of preprocessing was necessary for feature selection and getting rid of garbage points
 - Classification models like SVM and random forests, regression models, and Neural Nets were used
 - Neural Nets:
 - Autoencoders were used to generate compact representations of data
 - In addition to just using the models, "light grey box" methods can be used, in which certain data points are manually inputted into network and then the effects are examined
 - More hands-on approach
 - Diabetes is extremely prevalent today
 - CNN model used to analyse mouth and determine diabetes risk

Obesity

- 4 groups of metabolites were obtained with all appeared in obesity patients
- K-means and two-step were the 2 models used in the study

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