Numerical Representation of Metabolic Systems

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1. Introduction

In metabolomics we perform measurements. These measurements produce numbers which is not the same as data: data are numbers including their meaning. Data can have different properties depending on how the numbers are measured. One property is measurement scale, which ranges from ratio-scaled data to nominal-scaled data. Another property is comparability across rows and columns of our data table.

2. Approach

These different properties will be explained by simple examples from metabolomics data analysis practice. It will also be shown what the repercussions are of those properties for the type of statistical analysis to employ. We will use the example of measuring lipids using LC-MS and will distinguish different levels of measurements.

3. Discussion

The discussion will focus around the figure below which tries to synthesize all different aspects.
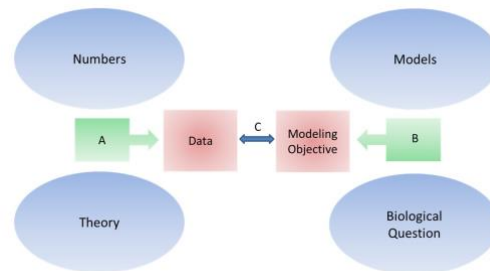
We will conclude with some recommendations and general concerns.