Interpreting Correlations in Metabolomic Networks
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Metabolomics aims at the unbiased identification and quantification of all metabolites present in a biological sample. Based on their pair-wise correlations, the data obtained from such large-scale experiments are organized into metabolic correlation networks and the key challenge is to deduce unknown pathways from the observed correlations.

However, the relationship between metabolic correlation networks and the underlying enzymatic system is largely unclear. Here, we address the interpretation of these data-generated networks in terms of the underlying biochemical pathways. We argue that cell metabolism constitutes a complex dynamical system, which is continuously subject to random fluctuations. These fluctuations induce variability in certain metabolites, propagate through the network and generate an emergent pattern of correlations.

Based on the theory of stochastic systems, it is possible to give an analytical description, which provides a ‘link’ between the observed correlation matrix and the Jacobian of the system. Thus, our results lead to a systematic relationship between the experimentally observed metabolic correlation networks and the underlying biochemical pathways. This provides a fundamental conceptual basis for the analysis of metabolomic datasets. Our approach enables to treat the observed correlations as a snapshot of the physiological state of a tissue at a given point in time. Finally, a systematic comparison of metabolic correlation networks from different tissues is shown to provide novel insights to the dynamic behaviour of metabolism.