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Abstract

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Mathematical structure of complex chemical factories

Metabolism is the set of chemical reactions that take place inside each cell of a living organism. A metabolic pathway is a sequence of such reactions that occur in successive steps to produce new material. Metabolism is a highly integrated process, with pathways connected into a complex network through shared compounds.

Understanding how this whole network works has important implications in biotechnology and medicine. It could, for example, give some indication on how the metabolism is affected by the change in activity of a single enzyme.

We present two approaches to the study the behaviour of metabolism.

The first one, based only on the topology of the network, concerns a search for sets of external compounds (called precursor sets) that produces some fundamental target metabolites. For this problem, we introduce a new model that enables to deal with the cycles in a network in a way that is biologically relevant and mathematically sound. In the second approach, we study the complexity of the problem of finding the so called "elementary modes", that is the minimal set of reaction that can be in equilibrium in terms of production and consumption of metabolites. We analyse the computational time complexity of both problems and give some initial algorithms to solve them.

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