Selected Problems about the Equilibrium States of Networks of Reversible Binding Reactions

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Presentation Abstract

We recently proposed the class of complete networks of reversible binding reactions in an effort to describe many reaction networks that are studied in pharmacology. An outcome of this effort is a positive polynomial P such that, given a vector b of total (free and bound) concentrations of the so-called elementary species, the vector x of equilibrium concentrations of these species is uniquely given by $P(x) = b$. The polynomial P is parameterized with structural and kinetic information about the network, and the equation $P(x) = b$ admits an auspicious transformation into a fixed-point equation $F(x) = x$ where the function F is positive and order-reversing. We will discuss two outstanding issues relevant to applications of this work:

1. The identifiability of kinetic and structural parameters from the complete or partial and aggregate knowledge of equilibrium state; and

2. The prospect of exploiting the fixed-point equation to calculate the equilibrium state with speed and a priori assurance of success.

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