

Positive Matrices in Systems Biology

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Abstract

Positive matrices appear naturally in systems biology. This talk will present several problems where it is necessary to either determine or to analyze positive matrices.

Many biochemical systems can be described by the following set of ordinary equations:

$$\frac{d}{dt}c(t) = Nv(c(t)) \quad (1)$$

where $c(t) \in \mathbb{R}_{\geq 0}^n$ is the vector of concentrations, $v(t, c(t)) \in \mathbb{R}^m$ the vector of fluxes and N the stoichiometric matrix. Analyzing such systems naturally leads to the analysis of positive matrices.

We first analyze the stoichiometry, thus no specific assumption on the fluxes is required. Conserved moieties are constant non-negative linear combinations of the concentrations:

$$\sum_{i=1}^n g_i c_i(t) = \text{constant}, \text{ where } g_i \geq 0 \forall i = 1, \dots, n.$$

Finding all possible conserved moieties is equivalent to finding a nonnegative matrix with N in its null space with rows that are linear independent with respect to non-negative combinations.

A similar problem is the calculation of elementary flux modes. They form a basis of the fluxes that are possible at steady-state. For irreversible fluxes, the calculation is the same as for finding conserved moieties of N^T .

The previous two problems are independent of a specific flux model. In the following we will focus on fluxes satisfying the Law of Mass Action. Linearizing Equation (1) at a steady states results in an essentially non-negative dynamics matrix (also called Metzler matrix). Also in Generalized Mass Action models does a positive matrix appear.

Open research topics are for example algorithms allowing to efficiently calculate conserved moieties for large models and model reduction taking positivity into account.