

Mathematical theory of biochemical networks

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Preliminary meeting: Friday 12th July 2024 at 10.15 room N0.008 (Endenicher Allee 60).

If you cannot come to the preliminary meeting, but are interested in the seminar, please, feel free to contact the organizers by the email given above.

During this seminar, we will study some of the main results of the theory of chemical reaction networks. We will mostly follow the book [1]. A reaction network consists of a set of molecules of certain species (reactant and products) and a set of chemical reactions. The evolution in time of the species concentrations is described by the solutions of a system of ordinary differential equations. These systems of ODEs are usually large non-linear systems, whose long-time behaviour could be difficult to study. The goal of this seminar is to study under which conditions it is possible to infer qualitative aspects of the behaviour of a chemical reaction network (for instance the existence of a unique stable steady state for the system of ODEs) analysing the topological structure of the network.

We will start by introducing the mathematical formalism necessary to model chemical reaction networks and we will introduce some basic concepts, as for instance the *stoichiometric compatibility classes*. Later, we will study the main features of chemical reaction networks that are *quasi-thermodynamics* systems, that satisfy the *detailed balance* property and that satisfy the *complex balance* property.

We will then study the Deficiency Zero theorem ([1]), that states that if a particular topological property of the network (the 'Deficiency Zero') is satisfied, if the kinetics is of mass action (the rates of the reactions are proportional to the concentrations of the reactants) and all the reactions are reversible, then there exists an asymptotically stable steady state. Depending on the number of students we will also study a generalization of the Deficiency Zero theorem, i.e. the Deficiency One theorem and we will study under which conditions it is possible to determine, via some specific type of measurements, if a linear biochemical network satisfies the detailed balance condition via some specific type of measurements, i.e. we will study [4].

Prerequisites: linear algebra, basic knowledge of ODEs.

Literature

- [1] M. Feinberg, *Foundations of Chemical Reaction Network Theory*, Springer International Publishing, 2019.
- [2] M. Feinberg. On chemical kinetics of a certain class. *Archive for Rational Mechanics and Analysis*, 46, 1972.
- [3] J. Schnakenberg. Network theory of microscopic and macroscopic behavior of master equation systems, *Reviews of Modern physics* 48(4), 1976.
- [4] E. Franco, B. Kepka, J. J. L. Velázquez, Characterizing the detailed balance property by means of measurements in chemical networks, arXiv:2402.12935.