Mathematical theory of biochemical networks: stochastic and deterministic models

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Graduate seminar on analysis (S4B1), Summer term 2026

During this seminar, we will study some of the main results in the theory of chemical reaction networks. We will study both deterministic and stochastic systems. A reaction network consists of a set of molecules (reactants and products) and a set of chemical reactions. When the concentrations of molecules are high, it is possible to model chemical networks using deterministic models. Then, the evolution in time of the concentrations of molecules is described by the solution to 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. One of the goals 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) by 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 satisfy the *detailed balance* property and of chemical reaction networks that satisfy the *complex balance* property.

We will then study the Deficiency Zero theorem ([11]), 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 a locally asymptotically stable steady state. We will also discuss the global attractor conjecture, claiming that, under the assumption of the Deficiency Zero Theorem, the steady state is not only locally stable, but also globally stable ([1, 2]).

We will then discuss stochastic chemical systems (see [4]). These stochastic models are used to study chemical systems in which the concentrations of the molecules are low. We will study the analogous of the Deficiency Zero theorem for stochastic systems ([3]) and we will study the relation between deterministic and chemical systems ([8, 9]).

Depending on the number of students we will also study some specific biological processes than can be modelled using the theory of chemical systems,

both stochastic and deterministic.

Prerequisites: linear algebra, basic knowledge in ODEs, basic knowledge of probability theory.

Preliminary meeting: Friday 6th of February 2026 at 12.15 room 2.040.

References

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[5] M. Feinberg, *Foundations of Chemical Reaction Network Theory*, Springer International Publishing, 2019.

[6] M. Feinberg. On chemical kinetics of a certain class. *Archive for Rational Mechanics and Analysis*, 46, 1972.

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