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EINLADUNG

zum

HABILITATIONSVORTRAG

Dr. Stefan Müller
(Fakultät für Mathematik, Universität Wien)

“Mathematical models of chemical and metabolic networks”

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Abstract: Many biological systems can be modeled as networks of chemical reactions, often with mass-action kinetics. Interestingly, for large classes of networks, the qualitative behavior of the resulting dynamical systems is independent of the rate constants.

We consider chemical networks with generalized mass-action kinetics, where reaction rates are power laws in the species concentrations, leading to generalized polynomial ODEs (with real exponents). We characterize uniqueness/existence of positive ''complex-balanced'' equilibria (for all rate constants and all initial conditions) in terms of sign vectors of two linear subspaces (corresponding to stoichiometric coefficients and kinetic orders, respectively). In terms of real algebraic geometry, we obtain first multivariate generalizations of Descartes' rule of signs.

As a particular cellular system, metabolism is modeled as a network of enzymatic reactions, however, often without knowledge of the kinetics. Traditionally, the analysis is based on stoichiometric information (and optimality principles), leading to linear programs.

We consider metabolic networks with kinetic information and the resulting nonlinear programs. In particular, we are interested in enzyme allocation problems where a chosen reaction rate is maximized under an enzymatic capacity constraint. Most importantly, we characterize optimal solutions in abstract terms: For arbitrary enzyme kinetics, solutions that optimize rates correspond to sign vectors with minimal support (of the kernel of the stoichiometric matrix).

Chemical and metabolic networks share common modeling paradigms (stoichiometry + kinetics) and mathematical methods (sign vectors = oriented matroids) which suggests to further exploit synergistic effects.

Mittwoch, 16. Oktober 2019,
13:00 Uhr – 13:45 Uhr,

Fakultät für Mathematik,
Ort SR 16, 3 OG.
Oskar-Morgenstern-Platz 1, 1090 Wien

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