Existence, Uniqueness and Computation of the Solution of a Polynomial System Relevant to Pharmacology

Gilles Gnacadja
Research and Development Information Systems, Amgen, Inc.
One Amgen Center Drive, Thousand Oaks, California 91320-1799, USA
gilles.gnacadja@gmail.com
http://math.GillesGnacadja.info

Presentation Abstract

We recently proposed the class of complete networks of reversible binding reactions in an effort to describe many biochemical reaction mechanisms 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. The presentation will discuss the following topics:

- How two theorems, the well known Brouwer Fixed-Point Theorem and the lesser known Global Univalence Theorem of Gale and Nikaidô, lead respectively to the surjectivity and the injectivity of the map P;
- How the fixed-point perspective enables in some cases solving the equation $P(x) = b$ with a priori assurance of success; and
- The prospect for exploiting the fixed-point perspective to solve the equation $P(x) = b$ in all cases.

Selected References

[1] D. Gale and H. Nikaidô, *The Jacobian Matrix and Global Univalence of Mappings*, Mathematische Annalen, Volume 159 (1965), Issue 2, Pages 81-93, http://dx.doi.org/10.1007/BF01360282.

[2] G. Gnacadja, *Fixed Points of Order-Reversing Maps in $\mathbb{R}^n_{>0}$ and Chemical Equilibrium*, Mathematical Methods in the Applied Sciences, Volume 30 (2007), Issue 2, Pages 201-211, http://dx.doi.org/10.1002/mma.782.

[3] G. Gnacadja, *Univalent Positive Polynomial Maps and the Equilibrium State of Chemical Networks of Reversible Binding Reactions*, Advances in Applied Mathematics, Volume 43 (2009), Issue 4, Pages 394-414, http://dx.doi.org/10.1016/j.aam.2009.05.001.