Mathematical Properties Of Stoichiometric Matrices

Susan Ghaderi¹, Hulda S. Haraldsdottir¹, Masoud Ahookhosh¹, Sylvain Arreckx¹, and **Ronan M.T. Fleming**^{1*}(ronan.mt.fleming@gmail.com)

¹ Luxembourg Centre for Systems Biomedicine, University of Luxembourg, Esch-sur-Alzette, Luxembourg

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Project Goals: Characterise the mathematical properties of stoichiometric matrices and decompose a biochemical network into a set of moiety subnetworks.

Abstract Characterising biochemical network structure in mathematical terms is a fundamental component of mathematical biology. It enables the inference of functional biochemical consequences from network structure with existing mathematical techniques and spurs the development of new mathematical techniques that exploit the peculiarities of biochemical network structure [1, 2]. The structure of a biochemical network is specified by reaction stoichiometry, that is, the relative quantities of molecular species produced and consumed in each chemical reaction of a network. The stoichiometry for the set of reactions in a network can then be compiled into a stoichiometric matrix, where every row corresponds to a molecular species and every column corresponds to a reaction. Herein, we summarise the main mathematical properties of stoichiometric matrices and emphasise those that distinguish them from arbitrary rectangular matrices.

References

- Hulda S. Haraldsdóttir and Ronan M. T. Fleming. Identification of conserved moieties in metabolic networks by graph theoretical analysis of atom transition networks. *PLOS Computational Biology*, 12(11):e1004999, November 2016.
- [2] German A. Preciat Gonzalez, Lemmer R. P. El Assal, Alberto Noronha, Ines Thiele, Hulda S. Haraldsdóttir, and Ronan M. T. Fleming. Comparative evaluation of atom mapping algorithms for balanced metabolic reactions: application to Recon3d. *Journal of Cheminformatics*, 9:39, 2017.

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