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Author: Mona Arabzadeh Morteza Saheb Zamani Mehdi Sedighi Sayed-Amir Marashi



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A Graph-Based Approach to Analyze Flux-Balanced Pathways in Metabolic Networks

Mona Arabzadeh¹, Morteza Saheb Zamani¹, Mehdi Sedighi¹, and Sayed-Amir Marashi²

¹Department of Computer Engineering and Information Technology, Amirkabir University of Technology, Tehran, Iran and ²Department of Biotechnology, College of Science, University of Tehran, Tehran, Iran. {m.arabzadeh.szamani.msedighi}@aut.ac.ir, marashi@ut.ac.ir

Abstract

An Elementary Flux Mode (EFM) is a pathway with minimum set of reactions that are functional in steady-state constrained space. Due to the high computational complexity of calculating EFMs, different approaches have been proposed to find these flux-balanced pathways. In this paper, an approach to find a subset of EFMs is proposed based on a graph data model. The given metabolic network is mapped to the graph model and decisions for reaction inclusion can be made based on metabolites and their associated reactions. This notion makes the approach more convenient to categorize the output pathways. Implications of the proposed method on metabolic networks are discussed.

Keywords: Elementary Flux Mode (EFM); Graph Data Model; Metabolic Network

1. Introduction

Metabolic network models are among the well-studied models in biotechnology. The reconstruction of these networks is possible by collecting the geneprotein-reaction information from related genomic data and literature [1]. It is important to explore biologically relevant pathways in metabolic networks. Forcing constraints to a reconstructed biochemical network results in the definition of achievable cellular functions [2]. Mathematical representation of constraints are as *flux-balance* constraints (e.g., conservation of flux) which means

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