Petri Net Recommender System to Model Metabolic Pathway of Polyhydroxyalkanoates

Sakshi Gupta, Amity University Haryana, Gurugram, India
Gajendra Pratap Singh, Jawaharlal Nehru University, New Delhi, India
Sunita Kumawat, Amity University Haryana, Gurugram, India

ABSTRACT

Due to the complexity of the metabolic pathways, their modeling has been a great challenge for the researchers. Various mathematical models have been developed and are continuing to be developed to model and study metabolic pathways. In this article, the authors have described Petri nets (PNs) as a recommender system to model one of the metabolic pathways of Polyhydroxyalkanoates. Recommender systems have become an integral part of today’s world. Their applications lie in the fields of e-commerce, bioinformatics and many more. Petri nets are one of the promising mathematical tools which can be treated as a recommender system to model and analyze the complex metabolic pathways of various organisms because of the representation of these pathways as graphs. The PN toolbox validates the obtained Petri net model. Polyhydroxyalkanoates, commonly known as PHAs, are biodegradable microbial polyesters and have properties quite similar to commonly used non-biodegradable plastics. Due to their biodegradability, biocompatibility, and eco-friendly nature, they are of biological significance and are used in various applications in wide range of sectors like medical sector, drug delivery, tissue engineering, and many more. The obtained PN model of Polyhydroxyalkanoates has been validated using PN toolbox.

KEYWORDS
Bioplastics, Metabolic Pathways, Petri net Modelling, Petri Nets, Polyhydroxyalkanoates (PHAs), Recommender System

INTRODUCTION

Petri nets are a graphical and mathematical tool used for modelling and studying concurrent, parallel, distributed and discrete event systems (Murata, 1989). Till date they have been successfully applied to various knowledge-based systems like biological networks, communication networks, industrial systems etc. due to their ability to represent any graph-based systems (Murata, 1989; Chaouiya, 2007; Marwan, Wagler & Weismantel, 2011; Reddy, Pavlovouniotis, & Liebman, 1993).

Various approaches have been applied to model the biological networks and Petri nets have been proved to be a promising and effective tool for the modelling and analysis of biological networks. In 1962, a German mathematician Carl Adam Petri first introduced the concept of Petri nets in his Doctoral Dissertation ‘Communication with Automata’ as a graphical and mathematical tool (Petri, 1966). Several theories from the authors from different backgrounds in different timeframe are available in the literature. For example, most recent proposed theory for 1-safe petri net is Boolean petri net.
(Kansal, Acharya & Singh, 2012; Kansal, Singh & Acharya, 2010, 2011, 2015; Singh, Kansal & Acharya, 2013). Apart from theory part, modelling and study of biological networks using PNs have been and are continuing to be a growing interest among the researchers due to the power of Petri nets to model complex situations. Various extensions of Petri nets such as hybrid PNs, stochastic PNs, colored PNs and hybrid functional PNs have also been used to model different types of biological networks (Chaouiyi, 2007; Hardy & Robillard, 2004).

The metabolic networks play an important part in an organism’s life since its life is dependent on its metabolism. The metabolic pathways can be regarded as subsystems of a metabolic network. A metabolic pathway is an interlinked network of biochemical reactions, catalyzed by enzymes. In these series of reactions, the output of a reaction can become the reactant for next reaction. To intuitively understand the behavior of such complex reactions, both qualitative and quantitative modelling of metabolic pathways is much needed.

For a number of metabolic networks, kinetic parameters i.e. the concentrations of the metabolites and the reaction rates, are often not known or are difficult to find. In such cases, the continuous approaches like ordinary differential equations, that need the kinetic data fails and Petri nets play its role (Koch, 2015). Also, with a rapid increase in biological database, we need a modelling tool which can be expanded upon the current state without much deviation from the already existing model. PNs have this expandability property embedded in them. Reddy et al. (1993) have first shown that the metabolic pathways can be represented and qualitatively studied using Petri nets. Since then various metabolic pathways have been represented using Petri nets. This is due to the resemblance between the concepts of Petri nets and metabolic pathways. Chaouiyi (2007) has discussed about the effectiveness of using different types of Petri nets for modelling and examining metabolic, genetic and signaling networks. Different classes of PNs; stochastic, colored and hybrid PNs have been used by the authors to model glycolysis pathway in (Hardy & Robillard, 2004). Heiner, Koch and Will (2004) have proposed an integrating method to model and examine biological pathways using PNs and their properties and it is demonstrated using an example of apoptosis. Marwan et al. (2011) has exemplified how metabolic, genetic and signal transduction pathways can be represented using Petri nets. The glycolysis pathway in Plasmodium falciparum has been modelled and then analyzed for the structural and behavioral properties using petri net theory by Oyelade, Isewon, Rotimi, and Okunoren (2016) to understand the behavior of this complex pathway. A semi-quantitative model of the complex reactions involved in the metabolism of Arabidopsis thaliana using Petri nets have been proposed by Koch, Nöthen and Schleiff (2017). The consistency of the model has been validated using the network decomposition and network reduction techniques. Since the kinetic data involved in biological systems is often vague or unknown. So, Bordon, Moškón, Zimic and Mráz (2018) have proposed Fuzzy Continuous Petri nets by combining Petri nets and fuzzy logic to model the biochemical processes for which the kinetic data is unknown by defining the firing rate functions in a fuzzy way. The approach has been described on the models of a hypothetical repressilator and Neurospora circadian rhythm. Recently, Cherdal and Mouline (2018) have considered a PN extension, called Hybrid Functional Petri Net (HFPN) to model and analyze an important metabolic pathway in humans, known as Methionine. Numerous articles have been published showing the applications and importance of Petri nets in different biological systems (Chaouiyi, 2007; Hardy & Robillard, 2004; Marwan et al., 2011; Hofestadt, 2017; Reshetova, Smilde, Westerhuis & van Kampen, 2015; Carvalho, Verbeek & Coelho, 2018).

Recommender systems are one of the vital information delivery tools in Web-Commerce. They collect information based on the preference of its users for some set of items and provide the users with recommendation of items or information needed (Bobadilla, Ortega, Hernando & Gutiérrez, 2013; Ricci, Rokach & Shapira, 2015). The term ‘item’ can refer to any book, music, online store, medicine, website, gadget etc. for which suggestions are needed by a user (Bobadilla et al., 2013). They have also been successfully applied in system biology (Fraimay et al., 2018; Alaimo, Giugno & Pulvirenti, 2016; Cheng et al., 2012). Recommender system relates users and the items for which
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