Validation and Simulation of Qualitative Models

Introduction

Qualitative models are a popular tool for the simulation of biological networks, in particular for regulatory or signaling networks. They do not require quantitative data and can even be applied to large-scale systems. In order to encode these models and to exchange them between different software tools, the community standard file format SBML has been extended by a specific package for qualitative models [1]. The Java™ library JSBML for working with SBML files provides classes and methods to read, manipulate, and write SBML-qual models [2]. The standard is also implemented in several simulation tools, such as GINsim, CellNOpt, and CellNetAnalzer, but validation of the files is still not implemented. Furthermore, it can be cumbersome to manually enter the required function terms for all transitions within these networks.

Goals

1. The Java™ library JSBML will be complemented by a validation package for qual models.
2. The program SBMLsqueezer will be extended to automatically generate function term equations within qual models that can be used for simulation.
3. In a case study the function terms within a published qual model will be replaced by newly generated terms. The validity of the resulting model will be evaluated. If passed, the altered model will be simulated in a suitable environment in order to compare results to the original outcomes.

Skills Required

Programing with Java™, particularly with JSBML; understanding of qualitative models and the qual package for SBML; ability to become acquainted with the code base of SBMLsqueezer for the implementation of suitable function terms; application and understanding of simulation software for qualitative models.

Mentors

Dr. Andreas Dräger, **[Claudine Chaouiya, Nicolas Rodriguez, others???]**

Supervisor

Prof. Dr.-Ing. Oliver Kohlbacher

References

1. Chaouiya, Claudine, Duncan Bérenguier, Sarah M. Keating, Aurélien Naldi, Martijn P van Iersel, Nicolas Rodriguez, Andreas Dräger, et al. 2013. "SBML Qualitative Models: A Model Representation Format and Infrastructure to Foster Interactions between Qualitative Modelling Formalisms and Tools." BMC Systems Biology 7: 135. doi:10.1186/1752-0509-7-135.

2. Rodriguez, Nicolas, Alex Thomas, Leandro Watanabe, Ibrahim Y Vazirabad, Victor Kofia, Harold F Gómez, Florian Mittag, et al. 2015. "JSBML 1.0: Providing a Smorgasbord of Options to Encode Systems Biology Models." Bioinformatics (Oxford, England), June, btv341-. doi:10.1093/bioinformatics/btv341.