

University of Ljubljana
Faculty of Computer and Information Science

Martin Stražar

Parallel Evolutionary Algorithm for Knowledge Discovery from a Model of a Gene Regulatory Network

ABSTRACT

Synthetic gene regulatory networks represent *state-of-the-art* achievements of synthetic biology and are promising candidates for information processing platforms in the future. Mathematical modelling plays an essential role in design and testing by enabling a theoretical insight and identification of the key system features. It is also used as a tool in predicting the gene regulatory network response under different experimental conditions or using various topologies.

Parameter estimation is one of the main problems in modelling biological systems in general. In real world modelling applications, not all parameter values are known or can be measured and are often fitted to experimental data, where optimization methods minimize some measure of error between predicted system response and actual data.

Paradigms in modeling biological systems differ in description form and precision. Intuitively, high precision of the results is proportional with computational complexity. In the present work, we present a system which merges a stochastic simulation algorithm with an evolutionary algorithm to optimize the model parameters. We made improvements of the standard simulation algorithm to optimize the execution on a parallel graphic processing unit. The results enable us to predict a precise quantitative system response, which we prove by confirming model prediction on a test experiment.

By limiting the initial guess of parameter values to valid biological estimates, the obtained parameter values reflect realistic values with high probability. These offer an insight into the machinery of a complex gene regulatory network, a bistable switch with positive feedback loop. The relative ratios between obtained parameters can be used to quantify the frequency of individual occurring reactions and explain the experimental results. By experimentally confirming obtained knowledge, we can get a step closer towards understanding complex biological systems and building structures with predictable

functions.

Key words: Gene regulatory networks, stochastic simulation algorithm (SSA), optimization, parameter estimation, parallel processing, CUDA.