

## Time series ordination for computational experiments dynamics (TSOCED) with biological models

Klimenko A.I.<sup>1, 2 \*</sup>, Vorobeva D.A.<sup>3</sup>, Lashin S.A.<sup>1, 2, 3</sup>

<sup>1</sup> Institute of Cytology and Genetics, SB RAS, Novosibirsk, Russia

<sup>2</sup> Kurchatov Genomic Center of the Institute of Cytology and Genetics, SB RAS, Novosibirsk, Russia

<sup>3</sup> Novosibirsk State University, Novosibirsk, Russia

\* [klimenko@bionet.nsc.ru](mailto:klimenko@bionet.nsc.ru)

**Key words:** dynamic regimes; parametric stability; mathematical modelling; dynamic time warping; statistical analysis of computational experiments

**Motivation and Aim:** Computational biology widely uses mathematical models of biological systems, in particular, systems of ordinary differential equations, as well as models of dynamical systems described in other formalisms, including discrete models such as finite automata, Petri nets, Boolean networks, and individual-based models. Predicting changes in the type of solution dynamics as a function of changes in model parameters is a substantial scientific problem. However, this problem does not have analytical solution for most formalisms in a general case. Widely used practice of conducting a series of computational experiments, i. e. solving a series of direct problems with different sets of parameters followed by expert analysis of solution plots, becomes arduous with a large number of parameters and decreasing step of the parametric grid. Thus, developing analytical methods that are capable of working on a set of computational experiments in an aggregated form is of eminent importance.

**Methods and Algorithms:** The mathematical package Scilab was used to calculate the set of solutions of the studied models of biological systems and to generate a set of artificial dynamics. Time series analysis using dynamic time warping (DTW) algorithm and principal coordinates analysis (PCoA) was carried out in the R system using *dtw* and *ape* packages, respectively. A modified k nearest neighbours algorithm (weighted kNN) was used to construct a solution classifier.

**Results and Conclusion:** A method of visualisation and classification of different dynamic regimes of the model was developed using a composition of dynamic time warping algorithm and principal coordinate analysis. Time series ordination for computational experiments dynamics (TSOCED) visualises the results of multiple solutions of a mathematical model in the space of reduced dimensionality. TSOCED also allows to reveal a correspondence between the parameter values and the type of dynamic modes of the model's solutions. The use of the solution classifier by type of dynamics allows to carry out an automatic evaluation of the set of solutions obtained as a result of computational experiments with models aimed at studying parametric and initial data stability. This method was tested on the Lotka-Volterra model, artificial sets of different dynamics, and applied to the gene network model.

**Funding:** The study is supported by the Budget Project FWNR-2022-0020.