Article

A New Visualisation and Analysis Method for a Convolved Representation of Mass Computational Experiments with Biological Models

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Abstract: Modern computational biology makes widespread use of mathematical models of biological systems, in particular systems of ordinary differential equations, as well as models of dynamic systems described in other formalisms, such as agent-based models. Parameters are numerical values of quantities reflecting certain properties of a modeled system and affecting model solutions. At the same time, depending on parameter values, different dynamic regimes - stationary, oscillatory, established as a result of transient modes of various types - can be implemented in the system. Predicting changes in the solution dynamics type depending on changes of model parameters is an important scientific task. Nevertheless, this problem does not have an analytical solution for all formalisms in a general case. The routinely used method of performing a series of computational experiments, i.e. solving a series of direct problems with various sets of parameters followed by expert analysis of solution plots is labor-intensive with a large number of parameters and a decreasing step of the parametric grid. In this regard, the development of methods allowing to obtain and analyze information on a set of computational experiments in an aggregate form is relevant. This work is devoted to developing a method for visualization and classification of various dynamic regimes of a model using a composition of the dynamic time warping (DTW-algorithm) and principal coordinates analysis (PCoA) methods. This method allows to obtain a qualitative visualisation of the results of the set of solutions of a mathematical model and to carry out the correspondence between the values of the model parameters and the type of dynamic regimes of its solutions. This method has been tested on the Lotka-Volterra model and artificial sets of various dynamics.

Keywords: visualization; dynamic regime; mathematical model; dynamic time warping; computational experiment

1. Introduction

Modern computational biology is using mathematical models of biological systems, in particular systems of ordinary differential equations (ODE) [1–3] and partial differential equations (PDE) [3,4], as well as models of dynamic systems described in other formalisms, such as agent-based models [5–10], Boolean networks [11,12] and cellular automata [13,14]. Parameters are numerical values of quantities reflecting certain properties of a modeled system and affecting model solutions. At the same time, depending on the parameter values, different dynamic modes - nonstationary, oscillatory,

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