

Inverse modeling of biological processes in sensitivity operator framework

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Motivation and Aim: Due to the diversity of the inverse problem statements arising in the course of sophisticated natural systems modeling, it is essential to develop a general framework that allows both solving and estimating the inverse problem solution result before its actual solution. The examples of widely used inverse problems are the coefficient identification problems of finding the unknown kinetic parameters or locating synthesis regions in bio-chemical reaction systems based on the concentration measurements for the selected set of species.

Methods and Algorithms: We work in a setting when there is a biological system model defined by a system of differential equations and measurement data on the system state provided with a measurement operator connecting measurement result with the model state function. We use an approach which consists of reducing various inverse problems to a unified quasi-linear matrix equation family with sensitivity operators constructed from an ensemble of independent solutions of adjoint problems [1]. Ensemble structure of the algorithms allows for efficient implementation on modern HPC systems. The sensitivity operator properties allow predicting the efficiency of the inverse problem solution. The projector to the orthogonal complement of the sensitivity operator matrix kernel can be used as a predictor. Parameter identification problems for biological models are often solved by various derivative-free and gradient-based algorithms. We compare the developed sensitivity operator-based algorithm results to those obtained by standard implementations of the parameter identification algorithms [2].

Results: A general sensitivity operator-based framework can be efficiently applied for solving and analyzing various inverse modeling problems arising in biological processes studies. The developed kinetic parameter identification algorithm shows high efficiency compared to the standard implementations of gradient-based and derivative-free algorithms both in accuracy and computation time.

Conclusion: The sensitivity-operator-based approach can be successfully applied to the inverse modeling of the biological processes described by the differential equation models.

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References

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