Numerical Optimization Methods for Significance Analysis of Parameters in Dynamical Systems

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Abstract: We have developed an efficient numerical method, based on sensitivity analysis for parametric optimization problems, that can be used to identify the most important parameters and variables and/or their subsets in a mathematical model that is given by a system of ordinary differential equations. In the context of metabolic pathways, our approach can be used to guide experimental biologists in their choice which proteins they should measure. Mathematically, the problem results in the question how much improvement in terms of the cost function can be achieved by adding additional terms to the underlying dynamical model, i.e., whether these are to be included or not. The cost function describes the quality of the model response in comparison to process observations. After a parameter estimation for the simplest model, we can decide fast whether additional terms should be included in the model without having to re-optimize the enlarged models. We show the capability, reliability, and efficiency of our approach using complex problems from systems biology.

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