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AUTOMATIC PARAMETER ESTIMATION OF CELLULAR PATHWAY MODELS BY USING ADJOINT SENSITIVITY ANALYSIS

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ABSTRACT

The cellular pathway models used in systems biology are usually described by ordinary differential equations (ODEs). In order to automatic parameter estimation of these models the ADFIT tool was created [1]. This tool is composed of scripts in MATLAB environment and can be used to parameters estimation of any mathematical model described by ODEs. The user only needs to provide the model in a symbolic form and the matrix of experimental data. The estimation process is based upon minimization of the quadratic objective function based on differences between the model solution and the experimental data. The gradient of the objective function with respect to the estimated parameters is calculated efficiently by using adjoint sensitivity analysis. The adjoint system is created directly from a symbolic form of the model using MATLAB Symbolic Toolbox. Additionally, to speedup the estimation process ADFIT tool generates a file that contains C code of a function that calculates the objective function and its gradient. This file can be compiled via external compiler to a special MEX file which can be called directly from MATLAB environment. As an example of using the ADFIT tool, the model of DNA repair is analysed [2].

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