

Automatic parameters estimation of mathematical models by using the ADFIT tool

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Abstract

Paper presents the ADFIT tool – a set of scripts in MATLAB environment that automates the process of parameters estimation of mathematical models. Tool is eligible for models described by system of ordinary differential equations. Estimation process is based on discrete experimental data provided by user. Additionally tool utilize the MEX files to speed-on the process and adjoint sensitivity analysis to minimize the impact of numerical errors.

1. Introduction

Numerical parameter estimation process is still a challenge in mathematical modeling. The problems that makes the process hard to complete are caused by many difficulties. First difficulties is speed. In work [1] the process takes about 4 hours to complete on computer with Pentium IV CPU. Second difficulty is numerical errors which impacts calculate the gradient of the objective function. In Fig.1a we see the errors which arises by using the variable integration step and finite difference methods to calculate the particular element of gradient. These errors can block the optimization algorithm. Another difficulty is strong dependence of the initial point of estimation. The algorithms implemented in MATLAB environment derive a very different result on different initial point..

To avoid impact of these difficulties we can use some elements of the MATLAB environment. To obtain better speed of estimation we may utilize the MEX files. These files contains a subprogram written in other language (like C or FORTRAN) and provide a faster execution speed than standard M-files. To decrease the impact of numerical errors on estimation process may uses different method for gradient calculation. For example to do this we may utilize the adjoint sensitivity analysis [1] which provide better results than standard finite difference method (see Fig. 1b) and it is relatively small computationally complex. The strong dependence on initial point of estimation may be resolved by using the randomly initial point.

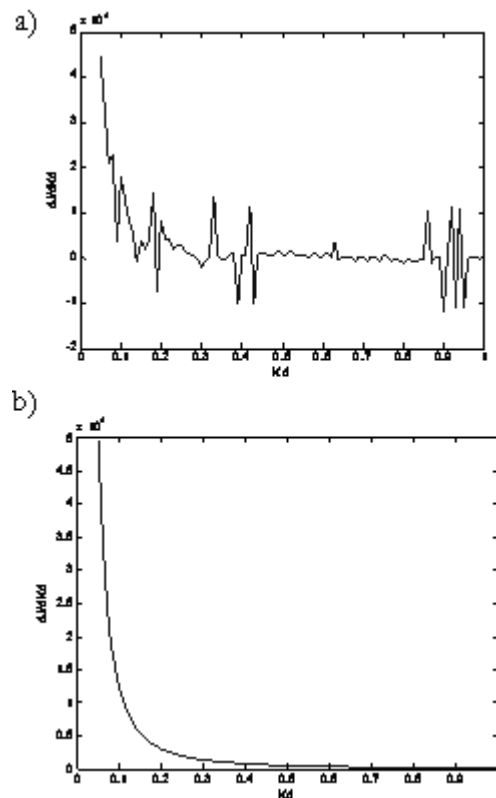


Fig.1. Charts of changes particular element of gradient of the objective function (1) used to estimate parameters of model described in work [2], a) finite difference method, b) adjoint sensitivity analysis

2. The ADFIT tool

To automatic parameters estimation for models in work [2] the ADFIT tool was created. It is a set of scripts in MATLAB environment that provide a estimations parameters based on discrete in-time experimental data of models described by system of up to 30 ordinary differential equations. It has built-in two methods for solving the ordinary differential equations: the Euler and four order Runge-Kutta methods. Tool allows user to choose from two methods to calculate the gradient of objective functions: finite difference method and adjoint sensitivity analysis (is a first tool that utilize this method). ADFIT during works create a MEX file to

provide faster execution. User only provide a symbolic form of the model and experimental data (stored in matrix *Dane*). Graphical user interface (GUI) of this tool is showed in Fig. 2 . Diagram of dataflow in the ADFIT is showed in Fig. 3. Additionally in the tool the gradient algorithm is proceed by genetic algorithm (Fig.4) to avoid the effect of dependence results of the initial point of estimation.

2.1 Features of the tool

Models if fitted to the experimental data by minimize the scalar objective function defined below:

$$J = \sum_{i=1}^n \sum_{j=1}^{N_i} (y_i(t_j) - d_i(t_j))^2 \quad (1)$$

where: n – is numbers of measured variables, N_i – is the number of measurement of variable i -th, $y_i(t_j)$ and $d_i(t_j)$ are output of the model and corresponding experimental data at time t_j .

Experimental data to the tool is provided by matrix in MATLAB environment which in first column has a discrete times of measure and next columns are values of measured variables. Currently tool is not eligible for experimental data in which different variables are obtained in different times.

Minimization is done by using the internals built in MATLAB environment algorithms: *Trust-region reflective*, *Active set* or *Interior point*. Additional informations about these algorithms it is at the MATLAB website [3]. To choose the minimization algorithm user must edit the internal script file named *jot_min.m*. Lower and upper bounds to the parameters values are also defined in this file (variables *ub* and *lb*), so user can easily edit this.

Results of estimation are saved to *mat* file in directory *Wyn* with a name equal to the final value of objective function (1).

2.2 Description of the GUI

Showed on figure 4 GUI of the ADFIT tool has many options that user can set:

- *Numbers of equations* – is a number of equations in the model
- *Y0* – columns of initial conditions of every equation in the system (if checkbox *Estimation Y0* is enabled then this column is disabled)
- d/dt – column of state variables
- $F(*)$ – right side of ordinary differential equations
- *Estimated parameters* – separated by spaces names of parameters

- *Measured state variables* – separated by spaces names of state variables(or combinations of names like: C/A B*A etc.) that are given by experimental data
- *File name* – name of file that contain the output C code for the MEX file and also name of file of the output MEX file
- *Load* – load the previously saved model from text file (name of the file is given by *File name*)
- *Save* – save the model to the text file named by *File name*
- *Y0 estimation* – checkbox that if is checked then the tool estimate all the initial conditions of the system or is unchecked that user must provide all initial condition in column *Y0*
- *Gradient* – checkbox if enabled then tool use adjoint sensitivity analysis to obtain gradient of the objective function otherwise finite difference method is used
- *Name of data file* – name of the file that contains the matrix of the experimental data
- *ODE solving method* – select the method for numerical solve the system of ordinary differential equation
- *Integration step* – select the integration step
- *Generate C code* – button that generate the output C code
- *Compile* – compiles the previously generated C code to MEX file
- *Minimize* – execute the internal script to minimize the objective function by utilizing the generated MEX file

2.3 Example

The ADFIT tool was used to estimate parameters of DNA repair models described in work [2]. Model contains system of 10 ordinary differential equations and have 15 parameters to estimate. Graphical fits of these models after estimation in the tool are showed in Fig. 5.

Single minimization time of the objective function in this model takes about 30 second by utilize the *Euler* solve method and *active-set* minimization algorithm. All estimation process takes about 2 h - to obtain fit like on fig.5 we launched the minimization process many times because genetic algorithm in the tool finds randomly every time the initial point of estimation.

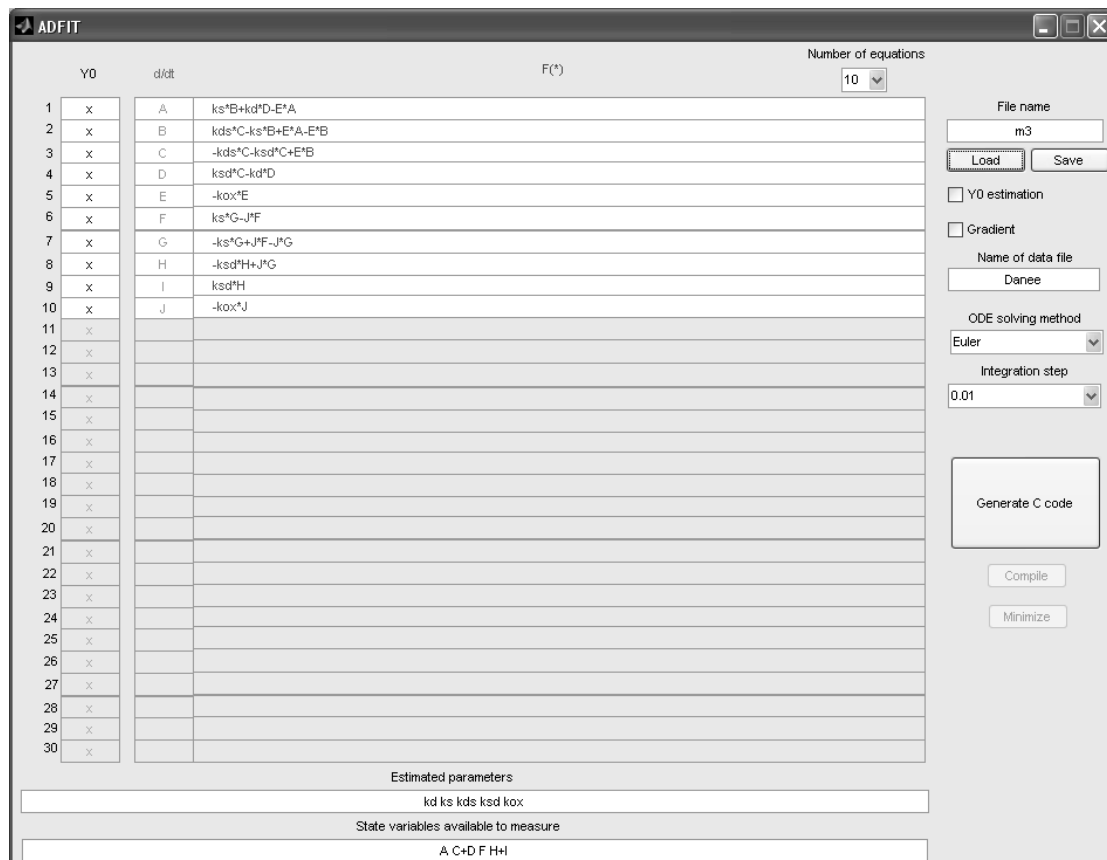


Fig.2. GUI of the ADFIT tool

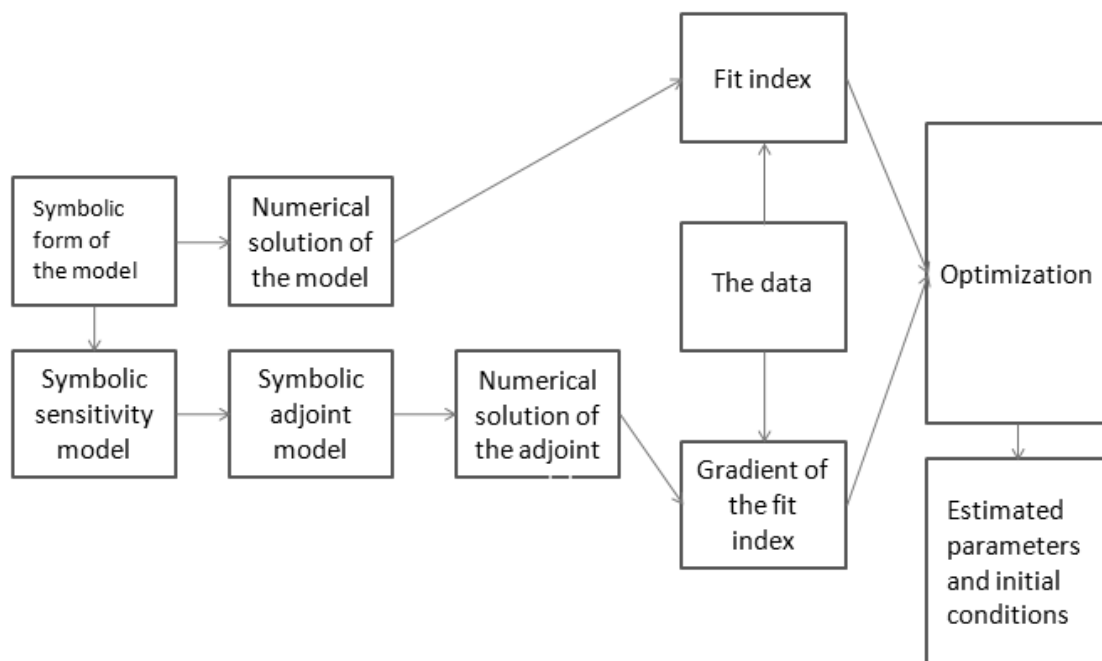


Fig.3. ADFIT dataflow

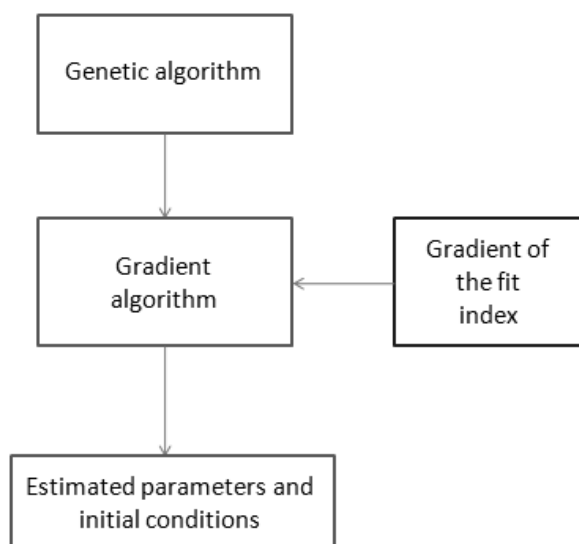


Fig.4. Two-stage optimization used in the ADFIT tool

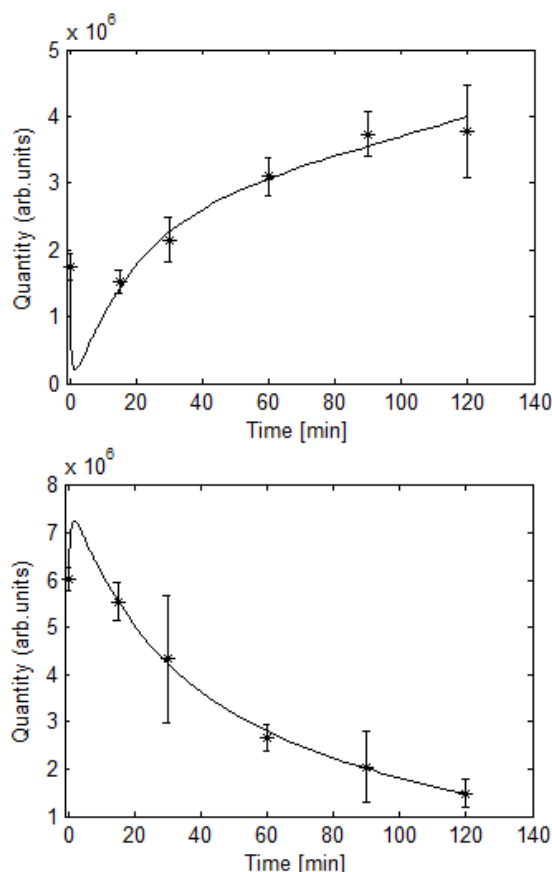


Fig.5. Fit of the mathematical model from work [2] to the experimental data after estimation parameters done in ADFIT tool. Experimental data is obtained from work [4]

3. Conclusions

MATLAB environment have many mechanism to simplify the numerical parameter estimation process. By joining the other programming language like C into MEX file we can obtain better execution speed of “bottleneck” parts of this process. With ability to provide user gradient to the minimizations algorithm we may done this process faster and more reliably by

use the alternative methods like adjoint sensitivity analysis. The ADFIT tool integrate these mechanism and provide automation the process of parameter estimation.

The tool is still developed. Future version may introduce a ability to estimate parameters of models containing delay differential equations.

Acknowledgement

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