Available online at www.sciencedirect.com

ScienceDirect

Procedia Social and Behavioral Sciences 2 (2010) 7652–7653

Procedia Social and Behavioral Sciences

Sixth International Conference on Sensitivity Analysis of Model Output

Adjoint sensitivity analysis for hybrid systems and its application to identification of biological systems

Krzysztof Fujarewicz*

Silesian University of Technology, Akademicka 16,44-100 Gliwice, Poland

Abstract

Many practical problems of identification, parameter estimation and optimization of dynamical systems have dual, continuous-discrete nature. For example the task of parameter estimation for continuous-time model when discrete-time measurements are given has such a form. The gradient-based optimization of a performance index may use the gradient obtained by both forward or adjoint sensitivity analysis. Here we present a structural approach to construction of the adjoint system for any hybrid system given as a block diagram. The method specifies a set of simple rules. In particular it explains how to handle two elements interfacing between discrete and continuous parts of the hybrid system: ideal AD and DA samplers. As an illustration we present an application of the method to estimation of parameters of models of cell signaling pathways.

Keywords: Adjoint sensitivity analysis, hybrid systems, continuaous-discrete time systems, structural methods, cell signaling pathways

1. Hybrid systems

In this paper we call a *hybrid system* any dynamical system which has dual nature, continuous and discrete in time. The continuous-time part is described by means of ordinary differential equations (ODEs) and the discrete-time part of the system is described by difference equations. Signals between these two parts are sent only in discrete time moments. An example of such a system is a digital control system of a continuous-time plant. Another example of a hybrid system (analyzed in this paper) is the problem of parameter estimation of continuous model based on discrete-time measurements. The model is continuous-time but the performance index which is minimized during gradient-based parameter estimation is discrete (sum of functions, usually quadratic, of prediction errors).

We will assume that the model is given as a block diagram. This is the form of system description frequently used for control systems. The block diagram of a hybrid system may contain elements that are listed in the first column of Table 1. Using this set of elements it is possible to model any non-linear lumped (non-distributed) parameter system.

Elements that interface between discrete- and continuous-time subsystems are: ideal analog/discrete (AD) sampler and ideal discrete/analog (DA) sampler.

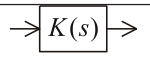
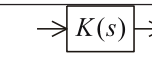
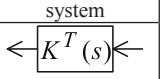
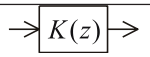
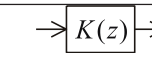
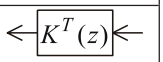
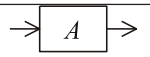
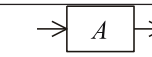
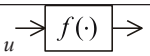
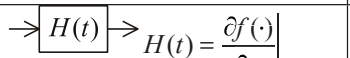
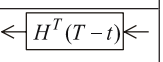
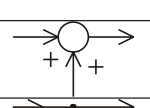
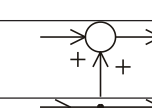
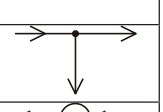
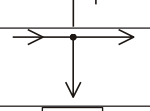
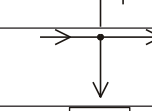
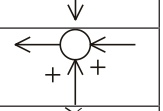
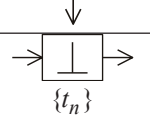
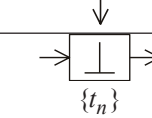
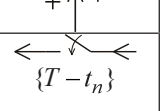
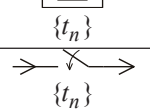
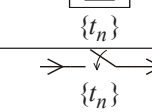
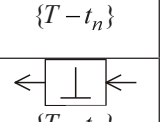
* Corresponding author. Tel.: +48-32-2372738; fax: +48-32-2372127.
E-mail address: krzysztof.fujarewicz@polsl.pl.

doi:10.1016/j.sbspro.2010.05.162

2. Rules of construction of the sensitivity and the adjoint systems

In order to build the sensitivity model (tangent-linearized) all elements should be replaced by corresponding elements from the second column of Table 1. Similarly, the so-called modified adjoint system (adjoint system "reversed" in time) can be built using elements from the third column.

Table 1. Rules for construction of the sensitivity model and the modified adjoint system

Element of the original system	Element of the sensitivity model	Element of the modified adjoint system
Linear c-t dynamical element			
Linear d-t dynamical element			
Linear static element			
Nonlinear static element			
Summing junction			
Branching node			
DA sampler			
AD sampler			

3. Applications

The rule has been first proposed in Fujarewicz et al. (2004) and the name of the full method was Generalized Back Propagation Through Time (GBPTT). It was used to learn continuous-time neural nets based on discrete measurements. In Fujarewicz (2007) the method has been used to estimate parameters of mathematical models of cell signaling pathways. Here we present further results of identification and identifiability of biological systems.

4. Acknowledgement

This work has been supported by Polish Ministry of Education and Science under grant N N514 411936.

5. References

Fujarewicz K. and Galuszka A., 2004, "Generalized Backpropagation Through Time for Continuous Time Neural Networks and Discrete Time Measurements", *LNCS*, 3070, Springer-Verlag, pp. 190–196.

Fujarewicz K., Kimmel M., Lipniacki T. and Świerniak A., 2007, "Adjoint systems for models of cell signalling pathways and their application to parameter fitting", *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, 4(3), 322-335.