89b Global Optimization for Parameter Estimation in Dynamic Systems

Youdong Lin and Mark A. Stadtherr

Parameter estimation is a key step in the development of mathematical models of physical phenomena, and is well studied [1]. In many problems, especially in chemical engineering, the systems are nonlinear in nature and described by ordinary differential equations (ODEs), or by differential-algebraic equations (DAEs). These factors lead to the important issue of multiplicity of local solutions in the parameter estimation [2,3].

In this study, we present a deterministic global optimization approach for parameter estimation in dynamic systems. The approach is based on an interval-Newton approach [4,5]. Validated solution methods [6-8] for ODEs (initial value problems) are used to produce bounds that are guaranteed to contain the true solutions of a dynamic system with uncertainty in parameters, as well as the first- and second-order sensitivities of the states with respect to parameters. Computational details and results will be presented through application to several problems involving reaction kinetics.

[1] Bard, Y. Nonlinear Parameter Estimation; Academic Press: New York, 1974.

[2] Stewart, W. E.; Caracotsios, M.; Sorensen, J. P. Parameter Estimation from Multiresponse Data. AIChE J. 1992, 38(5), 641.

[3] Esposito, W. R.; Floudas, C. A. Global Optimization for the Parameter Estimation of Differential-Algebraic Systems. Ind. Eng. Chem. Res. 2000, 39, 1291.

[4] Hanson, E.; Walster, G. W. Global Optimization Using Interval Analysis; Marcel Dekker, New York, NY, 2004.

[5] Lin, Y.; Stadtherr, M. A. LP Strategy for Interval-Newton Method in Deterministic Global Optimization. Ind. Eng. Chem. Res. 2004, 43, 3741.

[6] Moore, R. E.; Interval Analysis; Prentice-Hall, Englewood Cliffs, NJ, 1966.

[7] Berz, M.; Makino, K. Verified Integration of ODEs and Flows Using Differential Algebraic Methods on High-order Taylor Models, Reliable Computing 1998, 4, 361.

[8] Nedialkov, N. S.; Jackson, K. R. An Interval Hermite-Obreschkoff Method for Computing Rigorous Bounds on the Solution of an Initial Value Problem for an Ordinary differential Equation. Reliable Computing 1999, 5, 289.