WORKSHOP
Statistical Methods for Modeling Dynamic Systems
July 9–13, 2007

Parameter Estimation of Dynamic Systems Using Simultaneous Collocation and Large-scale Nonlinear Programming

Lorenz Biegler
Chemical Engineeering Department
Carnegie Mellon University
500 Forbes Ave.
Pittsburgh, PA 15213
USA
lb01@andrew.cmu.edu

Abstract

This talk considers the development of efficient parameter estimation strategies for systems described by differential-algebraic and partial differential equations. The approach focuses on a simultaneous approach for nonlinear programming, where both the state and control variable profiles are discretized. This approach allows a transparent handling of inequality constraints, unstable systems and even some discrete events. Here, large scale nonlinear programming strategies are essential. For this purpose, a novel barrier method, called IPOPT, is applied. This NLP algorithm incorporates a number of features for handling inequalities and improving global convergence through filter line search methods. The overall approach is Newton-based with analytic second derivatives and this leads to fast convergence rates even for problems with millions of variables.

To demonstrate the simultaneous formulation for parameter estimation, we consider a number of case studies including polymerization and contaminant detection in municipal water networks. These results illustrate the capabilities of IPOPT for very large systems. In addition they deal with advanced formulations including locally and globally distributed parameters, as well as EVM formulations. Finally, a recent object oriented implementation of IPOPT allows very flexible exploitation of large-scale structures. For instance, multi-scenario problems that arise in parameter estimation problems can be handled very efficiently with this approach.