Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
Computers and Chemical Engineering 28 (2004) 2695–2707
Computers & Chemical Engineering
www.elsevier.com/locate/compchemeng

An ESDIRK method with sensitivity analysis capabilities

Morten Rode Kristensen[a,c], John Bagterp Jørgensen[a,*], Per Grove Thomsen[b], Sten Bay Jørgensen[c]

[a] 2-Control ApS, Høffdingsvej 34, DK-2500 Valby, Denmark
[b] Informatics and Mathematical Modelling, Technical University of Denmark, Building 305, DK-2800 Lyngby, Denmark
[c] Department of Chemical Engineering, Technical University of Denmark, Building 229, DK-2800 Lyngby, Denmark

Received 21 January 2004; received in revised form 23 July 2004; accepted 9 August 2004
Available online 23 September 2004

Abstract

A new algorithm for numerical sensitivity analysis of ordinary differential equations (ODEs) is presented. The underlying ODE solver belongs to the Runge–Kutta family. The algorithm calculates sensitivities with respect to problem parameters and initial conditions, exploiting the special structure of the sensitivity equations. A key feature is the reuse of information already computed for the state integration, hereby minimizing the extra effort required for sensitivity integration. Through case studies the new algorithm is compared to an extrapolation method and to the more established BDF based approaches. Several advantages of the new approach are demonstrated, especially when frequent discontinuities are present, which renders the new algorithm particularly suitable for dynamic optimization purposes.

Keywords: Runge–Kutta methods; Sensitivity analysis; Dynamic optimization; Nonlinear model predictive control

1. Introduction

Systematic parameter estimation, design and control of systems modelled by ordinary differential equations often require knowledge of sensitivities (Russel, Henriksen, Jørgensen, & Gani, 2000). In addition sensitivity analysis is used for experimental design and model reduction as well as in bifurcation analysis (Jørgensen & Jørgensen, 1998). Enabling efficient and robust sensitivity calculations thus constitutes an important prerequisite for most systematic process and product engineering disciplines (Braatz et al., 2004). The present paper addresses the development of a methodology to achieve a fast, efficient and reliable sensitivity calculation.

Nonlinear moving horizon estimation and control also requires efficient and robust algorithms for integration and sensitivity calculations (Bauer, 2000; Grötschel, Krumke, & Rambau, 2001; Jørgensen, Rawlings, & Jørgensen, 2003). The dual requirement of both efficiency and robustness stems from the online, real-time and unsupervised implementation of nonlinear moving horizon estimation and control in nonlinear model predictive control applications. The sensitivities are needed in the evaluation of gradients required by sequential quadratic programming algorithms.

The key contributions of this paper are:

- presentation of an ESDIRK numerical integration method that can be applied to ODE as well as index-1 DAE systems. The method can be applied to stiff as well as nonstiff systems. The method is particularly efficient for methods with frequent discontinuities,
- construction of a continuous extension which means that the method can be applied to hybrid systems and discrete event systems,
- derivation of an efficient method for computation of the state and parameter sensitivities,
- description of an implementation (ESDIRK34) of the method that efficiently integrates a system of ODEs along with computation of the sensitivities.

* Corresponding author. Tel.: +45 70 222 404.
E-mail addresses: mrk@kt.dtu.dk (M.R. Kristensen), jbj@2-control.com (J.B. Jørgensen), pgt@imm.dtu.dk (P.G. Thomsen), sbj@kt.dtu.dk (S.B. Jøgensen).

0098-1354/$ – see front matter
doi:10.1016/j.compchemeng.2004.08.004

In this paper a Runge–Kutta based algorithm for the numerical computation of sensitivities in systems of ODEs is presented. The algorithm has been implemented in the code ESDIRK34 and a number of tests have been conducted comparing the performance of the code with other codes for sensitivity analysis. This comparative study is the topic of Section 4. Section 2 concerns the mathematical basis, while Section 3 covers some important implementation issues including error and convergence control.

The considered initial value problem is

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(t, \boldsymbol{x}, \boldsymbol{u}), \qquad \boldsymbol{x}(t_0) = \boldsymbol{x}_0(\boldsymbol{u}) \tag{1}$$

in which $\boldsymbol{x} \in \mathbb{R}^{n_s}$ is the n_s-dimensional state vector and $\boldsymbol{u} \in \mathbb{R}^{n_p}$ is an n_p-dimensional vector of parameters. In addition to integrating the state equations, ESDIRK34 also computes first order derivative information of the solution with respect to both state variables and parameters. The *state sensitivity* of the states $\boldsymbol{x}$ with respect to the initial state x_{0i} is defined as

$$\boldsymbol{s}_{s,i} = \frac{\partial \boldsymbol{x}(t, \boldsymbol{u})}{\partial x_{0i}}, \quad i = 1, \ldots, n_s \tag{2}$$

$\boldsymbol{s}_{s,i}$ satisfies the following sensitivity equations

$$\dot{\boldsymbol{s}}_{s,i} = \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} \boldsymbol{s}_{s,i}, \qquad \boldsymbol{s}_{s,i}(t_0) = \boldsymbol{e}_i \tag{3}$$

where $\boldsymbol{e}_i$ is the ith column of the n_s-dimensional identity matrix. Furthermore we define the *parameter sensitivity* of the states $\boldsymbol{x}$ with respect to the parameter u_i as

$$\boldsymbol{s}_{p,i} = \frac{\partial \boldsymbol{x}(t, \boldsymbol{u})}{\partial u_i}, \quad i = 1, \ldots, n_p \tag{4}$$

$\boldsymbol{s}_{p,i}$ satisfies the following sensitivity equations

$$\dot{\boldsymbol{s}}_{p,i} = \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} \boldsymbol{s}_{p,i} + \frac{\partial \boldsymbol{f}}{\partial u_i}, \qquad \boldsymbol{s}_{p,i}(t_0) = \frac{\partial \boldsymbol{x}_0}{\partial u_i} \tag{5}$$

The existence of the sensitivities is given by Gronwall's theorem, which states that provided the partial derivatives $\partial \boldsymbol{f}/\partial \boldsymbol{x}$ and $\partial \boldsymbol{f}/\partial \boldsymbol{u}$ exist and are continuous in a neighbourhood of the solution $\boldsymbol{x}(t)$, then state and parameter sensitivities exist, are continuous, and satisfy (3) and (5), respectively (Hairer, Nørsett, & Wanner, 1991).

The desire to obtain first order derivative information has extended the original problem of n_s equations to a combined system of n_s state equations and $n_s n_s + n_p n_s$ sensitivity equations. Solving this system directly would be highly inefficient. Instead, we show in this paper how the sensitivity information can be obtained with little extra effort.

Solution of (1) in the interval $[t_k, t_{k+1}] = [t_k, t_k + T_s]$ with the initial condition, $\boldsymbol{x}_k$, and the parameter, $\boldsymbol{u}_k$, may be regarded as a discrete map

$$\boldsymbol{x}_{k+1} = \boldsymbol{H}_k(\boldsymbol{x}_k, \boldsymbol{u}_k) \tag{6}$$

The sensitivities obtained by (3) with respect to the state vectors, $\boldsymbol{x}_k$, and (5) with respect to the parameters, $\boldsymbol{u}_k$, may in this difference equation interpretation be denoted as

$$\boldsymbol{A}_k = \nabla_{\boldsymbol{x}_k} \boldsymbol{H}_k(\boldsymbol{x}_k, \boldsymbol{u}_k) \tag{7a}$$

$$\boldsymbol{B}_k = \nabla_{\boldsymbol{u}_k} \boldsymbol{H}_k(\boldsymbol{x}_k, \boldsymbol{u}_k) \tag{7b}$$

Optimization algorithms for nonlinear model predictive control are developed using this discrete time view of the integration method and the sensitivities (Allgöwer, Badgwell, Qin, Rawlings, & Wright, 1999; Allgöwer & Zheng, 2000; Jørgensen et al., 2003). Hence, ESDIRK34 is a method for integration and computation of the sensitivities needed in nonlinear model predictive control applications.

1.1. Literature review

Several approaches to sensitivity analysis have been suggested. One approach is to approximate the sensitivities by finite differences, once the solution is known. Due to the adaptive nature of modern integration algorithms, direct application of finite differences should be avoided as such an *external differentiation* strategy implies inherent discontinuities with respect to the initial state and parameters (Diehl, 2001). To avoid this discontinuity problem, a finite difference approach for computation of the sensitivities should adopt an *internal differentiation* strategy in which the exact same step lengths are used for computation of the nominal and perturbed trajectories (Bock, 1981). The sensitivities may also be computed analytically utilizing the linearity of the sensitivity equations (Kristensen, 2003; Morshedi, 1986). However, it is even more efficient to solve the state equations (1) and the sensitivity equations (3)and (5) simultaneously by one of the methods discussed below. We distinguish between *forward sensitivity analysis* and *adjoint sensitivity analysis*. Here, we will not discuss the adjoint method but refer the reader to the relevant literature, e.g., Cao, Li, Petzold, and Serban (2003). The approaches used for forward sensitivity analysis may roughly be categorized into three groups.

Staggered direct method. This method is described in Caracotsios and Stewart (1985). The method first solves the state equations (1), and once an acceptable solution has been obtained in the iterations, the sensitivity equations are solved directly using the same integration method. As indicated, if the integrator for the state equations is implicit, which is almost always the case, an iterative solution is required. In subsequent sections the nature of implicit integrators are detailed, and it is explained why Newton-type iterations are needed. Because of the direct solution of the sensitivity equations, the staggered direct method requires frequent update of the Jacobian and factorization of the iteration matrix. Despite the drawback of frequent Jacobian updates (Li, Petzold, & Zhu, 2000) have found this method to be efficient for problems with a computationally complicated function evaluation and a large number of sensitivity parameters.

Simultaneous corrector method. The simultaneous corrector method, as presented by Maly and Petzold (1996),