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Efficient High-Order Methods for ODEs and DAEs

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ABSTRACT We present methods for the high-order differentiation through ordinary differential equations (ODEs), and more importantly, differential algebraic equations (DAEs). First, methods are developed that assert that the requested derivatives are really those of the solution of the ODE, and not those of the algorithm used to solve the ODE. Next, high-order solvers for DAEs are developed that in a fully automatic way turn an n-th order solution step of the DAEs into a corresponding step for an ODE initial value problem. In particular, this requires the automatic high-order solution of implicit relations, which is achieved using an iterative algorithm that converges to the exact result in at most $n+1$ steps. We give examples of the performance of the method.

41.1 Introduction

Under certain conditions, the solutions of ordinary differential equations (ODEs) and differential algebraic equations (DAEs) can be expanded in Taylor series. In these cases, we can obtain good approximations of the solutions by computing the respective Taylor series [8, 9]. Here we show how high-order methods of AD can be used to obtain these expansions in an automated way and how these methods allow differentiation through the solutions. The method can be applied to explicit and implicit ODEs. Together with a structural analysis of Pryce [14, 15, 16], it can be extended to obtain Taylor series expansions of the solutions of DAEs.

To use methods of integrating explicit ODEs to solve DAEs, we perform a structural analysis of the DAE system to convert it into an equivalent set of implicit ODEs, which is converted into an explicit system by using differential algebraic methods for the high-order inversion of functional relations. For n-th order computations, these methods are guaranteed to converge to the exact result in at most $n+1$ steps and return explicit ODEs that are order n equivalent to the original DAE problem. The resulting system of ODEs is then integrated to obtain the one-step solution of the DAE system. The method can be extended to multiple time steps by projecting the final coordinates of a particular time-step onto the constraint manifold and using the projections as consistent initial conditions for the next iteration.

This chapter is divided in three parts: differential algebraic AD tools used to solve explicit ODEs and convert implicit ODEs into explicit ones are presented in §41.2. §41.3 summarizes the structural analysis method suggested by Pryce that allows the automatic conversion of DAEs into implicit ODEs, and §41.4 presents an example that has been computed with the high-order code COSY Infinity [7]; it demonstrates how the combined method can successfully handle high-index DAE problems.

41.2 Efficient Differential Algebra Methods

For purposes of notation, we consider the set $\mathcal{C}^{n+1}(U, \mathbb{R}^w)$ (where $U \subset \mathbb{R}^v$ is an open set containing the origin) and equip it with the following relation: for $f, g \in \mathcal{C}^{n+1}(U, \mathbb{R}^w)$ we say $f =_n g$ (f equals g up to order n) if $f(0) = g(0)$, and all partial derivatives of orders up to n agree at the origin. This gives an equivalence relation on $\mathcal{C}^{n+1}(U, \mathbb{R}^w)$. The resulting equivalence classes are called DA vectors, and the class containing $f \in \mathcal{C}^{n+1}(U, \mathbb{R}^w)$ is denoted by $[f]_n$. For functions expressible via finitely many intrinsics, the class $[f]_n$ corresponds to the evaluation of f with any n-th order AD tool (see e.g. [17]). Our goal here is to determine $[f]_n$ when f is the solution of a DAE. The collection of these equivalence classes is called ${}_nD_v$ [2, 4]. When equipped with appropriate definitions of the elementary operations, the set ${}_nD_v$ becomes a differential algebra [4]. We have implemented efficient methods of using DA vectors in the arbitrary order code COSY Infinity [7].

Definition 1 *For $[f]_n \in {}_nD_v$, the depth $\lambda([f]_n)$ is defined to be the order of first non-vanishing derivative of f if $[f]_n \neq 0$, and $n+1$ otherwise.*

Definition 2 *Let $\mathcal{O}$ be an operator on $M \subset {}_nD_v$. $\mathcal{O}$ is contracting on M, if any $[f]_n, [g]_n \in M$ satisfy $\lambda(\mathcal{O}([f]_n) - \mathcal{O}([g]_n)) \geq \lambda([f]_n - [g]_n)$ with equality iff $[f]_n = [g]_n$.*

This definition has a striking similarity to the corresponding definitions on regular function spaces. A theorem that resembles the Banach Fixed Point Theorem can be established on ${}_nD_v$. However, unlike in the case of the Banach Fixed Point theorem, in ${}_nD_v$ the sequence of iterates is guaranteed to converge in at most $n+1$ steps.

Theorem 1 (DA Fixed Point Theorem) *Let $\mathcal{O}$ be a contracting operator and self-map on $M \subset {}_nD_v$. Then $\mathcal{O}$ has a unique fixed point $a \in M$. Moreover, for any $a_0 \in M$ the sequence $a_k = \mathcal{O}(a_{k-1})$ converges in at most $n+1$ steps to a.*

An extensive proof is given in [4]. In the following sections we demonstrate how this theorem can be used for high-order integration of ODEs and DAEs.

41.2.1 Integration of ODEs

Within ${}_nD_v$, high-order integration of ODEs can be accomplished by using the antiderivation operator and the DA Fixed Point Theorem.

Proposition 1 (Antiderivation is Contracting) *For $k \in \{1, \dots, v\}$, the antiderivation $\partial_k^{-1} : {}_nD_v \to {}_nD_v$ is a contracting operator on ${}_nD_v$.*

The proof of this assertion is based on the fact that if $a, b \in {}_nD_v$ agree up to order l, the first non-vanishing derivative of $\partial_k^{-1}(a-b)$ is of order $l+1$. Using antiderivation, we rewrite the ODE initial value problem $\dot{x}(t) = f(x,t), x(t_0) = x_0$ in its fixed-point form

$$\mathcal{O}(x(t)) = x_0 + \int_{t_0}^{t} f(x, \tau) d\tau.$$

According to Proposition 1, this defines a contracting operator $\mathcal{O}$ on ${}_nD_{v+1}$. Thus, ODEs can be integrated very efficiently by iterating a relatively simple operator. The iteration is guaranteed to converge to the n-th order Taylor expansion of the solution in at most $n+1$ steps.

Moreover, in the framework of DA, it is possible to replace the fixed initial value x_0 and additional parameters by additional DA variables. Thus, one not only obtains the solution of a particular initial value problem, but the method finds a Taylor expansion of the flow of the ODE as a function of the dependent variable t and all initial conditions and parameters.

41.2.2 Inversion of functional relations

In this section we show how the Implicit Function Theorem can be used in the DA framework to convert an implicit ODE to an explicit system. The following theorem shows that it is possible to compute a representative of the equivalence class $[f^{-1}]_n$ from a representative $\mathcal{M}$ of the class $[f]_n$.

Theorem 2 (Inversion by Iteration) *Assume that $f \in \mathcal{C}^{n+1}(U, \mathbb{R}^v)$ is an origin-preserving map, and let $\mathcal{M}$ be a representative of the equivalence class $[f]_n$. Write $\mathcal{M} = M + \mathcal{N}_{\mathcal{M}}$, where $\mathcal{N}_{\mathcal{M}}$ denotes the purely nonlinear part of $\mathcal{M}$. Assume furthermore that $M = \mathbf{D}f(0)$ is regular. Then*

$$\mathcal{O}(a) = M^{-1} \circ (\mathcal{I} - \mathcal{N}_{\mathcal{M}} \circ a)$$

is a well defined contracting operator on ${}_nD_v$. Moreover, for any $a_0 \in {}_nD_v$, the sequence of iterates converges in at most $n+1$ steps to a representative of the class $[f^{-1}]_n$.

The proof of this theorem uses the fact that if a and $b \in {}_nD_v$ agree up to order l, the compositions with $\mathcal{N}_{\mathcal{M}}$ agree to order $l+1$, since $\lambda(\mathcal{N}_{\mathcal{M}}) > 1$. See [4] for a full proof of this theorem.

Together with the Implicit Function Theorem, the Inversion by Iteration Theorem allows the efficient computation of explicit expressions of an implicitly described function g. Given $f \in \mathcal{C}^{n+1}(U \times V, \mathbb{R}^w)$ $(U \subset \mathbb{R}^v$

and $V \subset \mathbb{R}^w$) and $x \in \mathbb{R}^v$ and $y \in \mathbb{R}^w$, we write $f(x, y)$. Suppose that $f(0,0) = 0$ and that $f_y(0,0)$ has rank w. Then, by the Implicit Function Theorem, there exists a unique $\mathcal{C}^{n+1}(U, V)$ such that $g(0) = 0$, and in a neighborhood of $0 \in \mathbb{R}^v$, $f(x, g(x)) = 0$. Define $\Phi : \mathbb{R}^{v+w} \to \mathbb{R}^{v+w}$ by

$$\Phi \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ f(x,y) \end{pmatrix} = \begin{pmatrix} x \\ 0 \end{pmatrix}$$

and obtain an explicit expression for $g(x)$ from the last w components of $\Phi^{-1}(x, 0)$, because $(x, y) = (x, g(x)) = \Phi^{-1}(x, 0)$.

The technique of augmenting implicit systems has been used extensively to first order in bifurcation theory [12] and to high order for symplectic integration [3]. Other combinations of the Implicit Function Theorem and first order AD in the field of control theory are discussed by Evtushenko [10].

Finally, for a general function f with $f(x_0) = y_0$, one can extend the methods presented here using the fact that an origin-preserving function can be obtained via $\tilde{f}(x) = f(x + x_0) - y_0$.

41.3 Structural Analysis of DAEs

The structural analysis of DAEs is based on methods developed by Pryce [15, 16]. The signature method (Σ-method) is used to decide whether a given DAE possesses a unique solution and to transform it into an equivalent system of implicit ODEs.

We consider the DAE problem $f_1(\ldots) = \ldots = f_k(\ldots) = 0$ with the scalar independent variable t, the k dependent variables $x_j = x_j(t)$, and sufficiently smooth functions

$$f_i\left(x_1, \ldots, x_1^{(\xi_{i1})}, \ldots, x_k, \ldots, x_k^{(\xi_{ik})}, t\right) = 0.$$

For a given j, the i-th equation of this system does not necessarily depend on x_j, the derivatives $x_j^{(\eta)}$ for $\eta < \xi_{ij}$, or even any of its derivatives. However, if there is a dependence on at least one of the derivatives (including the 0-th derivative $x_j^{(0)} = x_j$), we denote the order of that highest derivative by ξ_{ij}. Using this notation, we define the $k \times k$ matrix $\Sigma = (\sigma_{ij})$ by

$$\sigma_{ij} = \begin{cases} -\infty \text{ if the } j\text{-th variable doesn't occur in } f_i \\ \xi_{ij} \text{ otherwise.} \end{cases}$$

Let P_k be the set of permutations of length k, and consider the assignment problem (AP) [1] of finding a maximal transversal $T \in P_k$ as defined by

$$\text{Maximize } \|T\| = \textstyle\sum_{i=1}^k \sigma_{i,T(i)} \text{ with } \sigma_{i,T(i)} \geq 0.$$

The DAE is ill-posed if the AP is not regular. On the other hand, if such a maximal transversal exists, it is possible to compute the (uniquely determined [16]) smallest offsets $(c_i), (d_j) \in \mathbb{Z}^k$ that satisfy the requirements

$$\text{Minimize } \bar{z} = \textstyle\sum d_j - \sum c_i \text{ with } d_j - c_i \geq \sigma_{ij} > -\infty \text{ and } c_i \geq 0\ .$$

By differentiation it is possible to derive a k-dimensional system of ODEs from the original DAEs:

$$f_1^{(c_1)} = \ldots = f_k^{(c_k)} = 0.$$

Moreover, if an initial condition (x_0, t_0) satisfies the system of intermediate equations

$$f_1^{(0)} = \ldots = f_1^{(c_1-1)} = \ldots = f_k^{(0)} = \ldots = f_k^{(c_k-1)} = 0,$$

and the system Jacobian

$$\mathbf{J} = J_{ij} = \partial f_i / \partial \left(x_j^{(d_j - c_i)} \right)$$

(with $J_{ij} = 0$ if the derivative is not present or if $d_j < c_i$) is non-singular at that point, the original DAE system has a unique solution in a neighborhood of t_0. The solution can be obtained as the unique solution of the derived ODE, and in a neighborhood of (x_0, t_0), the system has $\bar{z}$ degrees of freedom. Finally, the differentiation index ν_d of the system satisfies

$$\nu_d \leq \max c_i + \begin{cases} 0 & \text{if all } d_j > 0 \\ 1 & \text{otherwise.} \end{cases} \tag{41.1}$$

While it has been suggested that the index ν_d might equal the given expression, [18] shows that (41.1) is only an upper bound for it.

41.4 Example

Consider a pair of coupled pendulums in a frictionless environment and assume that the pendulums are massless and inextensible, with point masses on the ends (Figure 41.1). Denote the tensions in the strings by λ_1 and λ_2, respectively. Then the equations of motion expressed in Cartesian coordinates x_1, y_1, x_2, y_2 are

$$\begin{aligned}
m_1 \ddot{x}_1 + \lambda_1 x_1 / l_1 - \lambda_2 (x_2 - x_1)/l_2 &= 0 \\
m_2 \ddot{y}_1 + \lambda_1 y_1 / l_1 - \lambda_2 (y_2 - y_1)/l_2 - m_1 g &= 0 \\
m_2 \ddot{x}_2 + \lambda_2 (x_2 - x_1)/l_2 &= 0 \\
m_2 \ddot{y}_2 + \lambda_2 (y_2 - y_1)/l_2 - m_2 g &= 0 \\
x_1^2 + y_1^2 - l_1^2 &= 0 \\
(x_2 - x_1)^2 + (y_2 - y_1)^2 - l_2^2 &= 0.
\end{aligned}$$

The corresponding Σ matrix of this DAE is shown below, with the entries forming a maximal transversal in bold face.

$$\Sigma = \begin{pmatrix}
2 & -1 & 0 & -1 & \mathbf{0} & 0 \\
-1 & \mathbf{2} & -1 & 0 & 0 & 0 \\
0 & -1 & 2 & -1 & -1 & \mathbf{0} \\
-1 & 0 & -1 & \mathbf{2} & -1 & 0 \\
\mathbf{0} & 0 & -1 & -1 & -1 & -1 \\
0 & 0 & \mathbf{0} & 0 & -1 & -1
\end{pmatrix}$$

Further analysis gives the offsets $c = (0, 0, 0, 0, 2, 2)$ and $d = (2, 2, 2, 2, 0, 0)$ and reveals that the system has four degrees of freedom and a differentiation index ν_d of at most three.

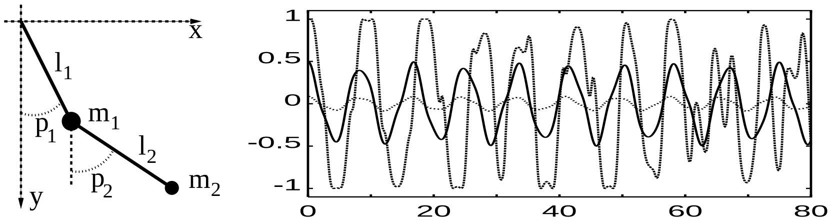

FIGURE 41.1. Coupled pendulum and x_1 as function of time.

The second plot in Figure 41.1 shows the time evolution of x_1 for the special case $g = 1, l_1 = l_2 = 1, m_1 = m_2 = 1$ and $p_1 = p_2 = 5°, 30°$ and $90°$ (Integrated to order 6, $0 \leq t \leq 80$, and $\Delta t = 0.1$), obtained with the DAE solver discussed above. The results were checked by studying energy conservation.

41.5 Conclusion

By combining existing AD methods, the Σ-method for the structural analysis of DAE systems and DA operations, we derived and demonstrated a high-order scheme for the efficient integration of high-index DAE problems. The method involves an automated structural analysis, the inversion of functional dependencies, and the high-order integration of an ODE system derived from the original DAE problem. Using techniques for the verified inversion of functional relations modeled by Taylor models [11, 6] and techniques for the verified integration of ODEs [13], the methods presented can readily be extended to verified high-order integration of DAEs.

The method presented of integrating DAEs can be simplified by realizing that in the framework of DA and Taylor models, the antiderivation is not fundamentally different from other elementary operations. Thus, the solution of ODEs and DAEs can be obtained by an inversion process. This could lead to a unified integration scheme for ODEs and DAEs that would also allow for high-order verification via Taylor models.

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