Numerical solutions for implicit differential equations with singularities

Soluções numéricas para equações diferenciais implícitas com singularidades

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Abstract

In this paper we introduce a technique to deal with implicit differential equations exhibiting singularities. Our approach is a geometrical one, we use the concept of contact structure on a manifold associated with the differential equation. In this setting we prove an existence and uniqueness theorem. We also show how it relates to known geometric results for this kind of equation. We also indicate how the method can be implemented by using continuation methods techniques and the BDF (Backward Differentiation Formula).

Keywords: Implicit differential equations; singularities; differential algebraic equations.

Resumo

Neste artigo apresentamos uma técnica para tratar com equações diferenciais implícitas exibindo singularidades. Nossa abordagem é geométrica e usamos o conceito de estrutura de contato em uma variedade associada à equação diferencial. Neste contexto provamos um teorema de existência e unicidade. Também mostramos como estas equações se relacionam com resultados geométricos conhecidos. Também indicamos como o método pode ser implementado usando técnicas de métodos de continuação e métodos BDF (Fórmula de Diferenciação Atrasada).

Palavras-chave: Equações diferenciais implícitas; singularidades; equações algébrico-diferenciais.

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Introduction

In this paper we consider the *k*-order implicit differential equation

$$F(X, Y(X), Y'(X), \ldots, Y^{(k)}(X)) = 0, \qquad (1)$$

where $F : \Omega \to I\!\!R^n$ is a sufficiently differentiable map from the open set $\Omega \subset I\!\!R^{(k+1)n+1}$.

Implicit Differential Equations (IDE), also called Differential-Algebraic Equations (DAE), have been the subject of an increasing number of papers ranging from numerical methods to theoretical aspects as well, applications. For general references on the subject see Brenan, Campbell and Petzold (1989) for BDF based methods, and Hairer and Wannes (1989) for Runge-Kutta methods. They have been the most successful ones in dealing with fixed index DAEs. Studies of boundary value problems using collocations methods can be found in Ascher and Petzold (1992).

From a geometric viewpoint (RHEINBOLDT, 1984), devised an approach to locally reduce IDEs to ordinary differential equations on manifolds. This approach was explored later in Rabier and Rheinboldt (1991).

Concerning implicit ordinary differential equations with singularities, Wasow (1965) presented asymptotic expansions to study linear differential equations in the complex domain, which are IDEs with singularities. For a single equation, Jepson and Spence (1984), have combined geometric information with continuation method techniques to understand singular points. The general equation for the case of simple folds has been treated in Rabier (1989) and bifurcation problems for singular IDEs in semi-explicit form can be seen in Sosen (1994).

Under the heading of contact structures the subject has been pionereed by Darboux (1873) and revived by Thom (1971). This approach has been further explored for the case of a single equation by Davydov (1985) and Dara (1975), by providing several normal forms to the equation. For a general reference see Arnold (1988) and references therein. In Freitas and Tavares (1991) and Feitas (1991) a simplicial approach has been introduced to solve IDEs in a contact structure environment.

Mainly in the 1990s, there was a lot of effort to develop numerical methods and codes based on these numerical methods to solve initial value problems for DAEs.

The main theories and numerical techniques can be seen in books dedicated to solving initial value problems of DAEs, as well as in more recent surveys. Among them, we can highlight the books: Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations (ASCHER; PETZOLD, 1998), Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations (BRENAN; CAMPBELL; PETZOLD, 1996), Numerical Solving Ordinary Differential Equations. II. Stiff and Differential-Algebraic Problems (HAIRER; WANNER, 1996), Theoretical and Numerical Analysis of Differential-Algebraic Equations (RABIER; RHEINBOLDT, 2002), Differential-Algebraic Equations Analysis and Numerical Solution (KUNKEL; MEHRMANN, 2006) and Differential-Algebraic Systems: Analytical Aspects and Circuit Applications (RIAZA, 2008).

The purpose of this paper is to present a new class of solutions to initial value problems for DAEs that can be more stable near some types of singularities and to present a code, called GSDAE, that is efficient to solve DAEs close to singularities.

The sections in this paper are as follows. In section **Basic Concepts** we introduce the basic definitions, while in section **Existence and Uniqueness Theorems** are the main results of the paper: an existence and uniqueness theorem for a generic class of fully implicit differential equations. In section **Singularities** we identify the solutions singularities. In section **Numerical Method** we indicate an algorithm to solve the equation numerically; in section **Results** we show the solution for a family of implicit differential equations. Finally the section **Conclusion** we present the contributions of the paper and conclusions.

Basic concepts

Definition 1. *A map $Y : \mathscr{I} \to I\!\!R^n$, $\mathscr{I}$ open interval, is said to be a classical solution of equation (1) if $Y \in C^k(\mathscr{I})$ and satisfies the equation (1).*

Definition 2. *The image of a map $c : I \to I\!\!R^{(k+1)n+1}$ is said to be the general solution of equation (1) if $c \in C^1(I)$ and satisfies*

$$\begin{cases} F(c(s)) & = & 0 \\ y_1(s)x'(s) - y_0'(s) & = & 0 \\ y_2(s)x'(s) - y_1'(s) & = & 0 \\ & \vdots & \\ y_k(s)x'(s) - y_{k-1}'(s) & = & 0 \end{cases} \qquad (2)$$

for all $s \in I$, where $c(s) = (x(s), y_0(s), y_1(s), \ldots, y_k(s))$.

Observe that if $\alpha : J \to I$ is a C^1-diffeomorfism and $c : I \to I\!R^{(k+1)n+1}$ is of class C^1 and satisfies (2) ($c(I)$ is a general solution of the equation (1)), then $c \circ \alpha : J \to I\!R^{(k+1)n+1}$ is also of class C^1 and satisfies the equation (2) (($c \circ \alpha)(J)$ is a general solution of the equation (1)), but c and $c \circ \alpha$ have the same trace, that is $c(I) = (c \circ \alpha)(J)$.

Lemma 1. *Let be given a general solution of the equation (1) by the map $c : I \to I\!R^{(k+1)n+1}$. If $x'(s) \neq 0$ in an interval $\mathscr{I} \subset I$, then $y_0(s) = Y_0(x(s)), y_1(s) = \frac{d}{dx}Y_0(x(s)), \ldots, y_k(s) = \frac{d^k}{dx^k}Y_0(x(s))$ on $\mathscr{I}$ and Y_0 defined in $x(\mathscr{I})$ is a classical solution of the equation (1).*

Proof.

As $x'(s) \neq 0$ in $\mathscr{I} \subset I$, $x(\mathscr{I})$ is an interval and x is a diffeomorphism from $\mathscr{I}$ into $x(\mathscr{I})$. Hence, $Y_i : x(\mathscr{I}) \to I\!R^n$ with $Y_i(x(s)) = y_i(s)$, $i = 0, 1, \ldots, k$ are C^1 maps.

Then :

$$y_i(s)x'(s) = y'_{i-1}(s) = \frac{d^i}{dx^i}Y_0(x(s))x'(s) \Rightarrow$$

$$y_i(s) = \frac{d^i}{dx^i}Y_0(x(s)) = Y_i(x(s)), i = 1, \ldots, k.$$

Thus, $Y_i : x(\mathscr{I}) \to I\!R^n$ are C^{k-i}, $i = 0, 1, \ldots, k$ maps and

$$F(x(s), Y_0(x(s)), \frac{d}{dx}Y_0(x(s)), \frac{d^2}{dx^2}Y_0(x(s)), \ldots$$

$$\ldots, \frac{d^k}{dx^k}Y_0(x(s))) =$$

$$= F(x(s), Y_0(x(s)), Y_1(x(s)), Y_2(x(s)), \ldots, Y_k(x(s))) =$$

$$= F(x(s), y_0(s), y_1(s), y_2(s), \ldots, y_k(s)) = 0.$$

Hence, Y_0 is a classical solution of the equation (1) in the set $x(\mathscr{I})$. ∎

Definition 3. *The initial value problem for equation (1) is defined as:*

$$\begin{cases} F(X, Y(X), Y'(X), \ldots, Y^{(k)}(X)) = 0 \\ \quad Y^{(i)}(x_0) = a_i, i = 0, 1, \ldots, k, \end{cases} \quad (3)$$

where $F(x_0, a_0, a_1, \ldots, a_k) = 0$.

Definition 4. *An ω-structure for the implicit differential equation (1) is a function $\omega : \Omega \to I\!R^{kn((k+1)n+1)}$ defined by*

$$\omega(x, y_0, y_1, \ldots, y_k) = \begin{pmatrix} \omega_k(x, y_0, y_1, \ldots, y_k) \\ \omega_{k-1}(x, y_0, y_1, \ldots, y_k) \\ \vdots \\ \omega_2(x, y_0, y_1, \ldots, y_k) \\ \omega_1(x, y_0, y_1, \ldots, y_k) \end{pmatrix} =$$

$$= \begin{pmatrix} y_k & 0 & 0 & \cdots & 0 & -I_n & 0 \\ y_{k-1} & 0 & 0 & \cdots & -I_n & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ y_2 & 0 & -I_n & \cdots & 0 & 0 & 0 \\ y_1 & -I_n & 0 & \cdots & 0 & 0 & 0 \end{pmatrix}.$$

With this ω-structure we can rewrite (2) in the form:

$$\begin{cases} F(c(s)) & = 0 \\ \omega(c(s))c'(s) & = 0 \end{cases} \quad (4)$$

which we call a ω-*system* associated with equation (1).

The initial value problem for the differential system (4), is then naturally defined as:

$$\begin{cases} F(c(s)) & = 0 \\ \omega(c(s))c'(s) & = 0 \\ c(0) & = c_0 = (x_0, a_0, a_1, \ldots, a_k), \end{cases} \quad (5)$$

with $F(c_0) = 0$.

Differentiating the first equation in (5) with respect to s and defining

$$A(c(s)) = \begin{pmatrix} DF(c(s)) \\ \omega(c(s)) \end{pmatrix},$$

gives rise to the following initial value problem:

$$\begin{cases} A(c(s))c'(s) & = 0 \\ c(0) & = c_0 = (x_0, a_0, a_1, \ldots, a_k), \end{cases} \quad (6)$$

with $F(c_0) = 0$. We call (6) the *differential system* associated with equation (1).

Note that if $k = 0$, $A(c(s)) = DF(c(s))$. Also F being of class C^1 the two formulations above are equivalent.

Existence and uniqueness theorems

In this section we use the concepts of ω-structure and differential system introduced in the last section to prove several existence and uniqueness theorems.

Theorem 1. *If DF is Lipschitz in an open neighbourhood of c_0 and $A(c_0)$ is of maximum rank, then there is $r > 0$ such that the initial value problem (5) has a unique solution on $B = \{u; \| u - c_0 \| \leq r\}$.*

Remark: The solution is unique in the sense that its trace is unique.

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Proof.

Firstly we show that the equation (6) is equivalent to an initial value problem for an ordinary differential equation of the form :

$$\begin{cases} c'(s) & = \tau(A(c(s))) \\ c(0) & = c_0, \end{cases}$$

and secondly we show that the equation (6) is equivalent to equation (5).

As $A(c_0)$ has maximum rank, $\det(A(c_0)A^t(c_0)) \neq 0$. But DF is a continuous function in an open neighbourhood U of c_0, then $\det(A(u)A^t(u))$ is also continuous in U, hence there is an open set $V \subset U$ of c_0 such that $\det(A(u)A^t(u)) \neq 0$ ($A(u)$ has maximum rank) for all $u \in V$.

Let $r > 0$ be such that $B = \{u \in \mathbb{R}^{(k+1)n+1}; \| u - c_0 \| \leq r\} \subset V$.

As $A(u)$ has maximum rank in B there is an unique vector $\tau(A(u)) \in \mathbb{R}^{n+1}$ such that $A(u)\tau(A(u)) = 0$, $\| \tau(A(u)) \| = 1$ and

$$\det\begin{pmatrix} A(u) \\ \tau^t(A(u)) \end{pmatrix} > 0.$$

We shall show next that $\tau(A)$ is a locally Lipschitz function with respect to A, for all A with maximum rank.

Let

$$f(A, \tau) = \begin{pmatrix} A\tau \\ (\tau^t\tau - 1)/2 \end{pmatrix} \quad \text{and} \quad (A, \tau),$$

A maximum rank, be the solution of $f(A, \tau) = 0$. The implicit function theorem implies that τ can be written as a function of A, because

$$\det(f_\tau(A, \tau)) = \det\begin{pmatrix} A \\ \tau^t \end{pmatrix} \neq 0.$$

Furthermore $\begin{pmatrix} A \\ \tau^t \end{pmatrix}^{-1} = (A^+, \tau)$ where $A^+ = A^t(AA^t)^{-1}$ is the Moore-Penrose inverse of A. Also $A^+(A)$ is a continuous function of A.

Thus

$$\tau'(A) = -f_\tau^{-1}(A, \tau)f_A(A, \tau) =$$

$$= -(A^+, \tau(A)) \begin{pmatrix} \tau^t(A) & 0 & \cdots & 0 \\ 0 & \tau^t(A) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \tau^t(A) \\ 0 & 0 & \cdots & 0 \end{pmatrix}$$

is a continuous function of A.

It then follows that the initial value problem (6) is equivalent, in the set B, to the system

$$\begin{cases} c'(s) & = \tau(A(c(s))) \\ c(0) & = c_0. \end{cases} \quad (7)$$

Since $\tau'(A)$ is continuous, the set $\{A(v); v \in B\}$ is compact and $A(v)$ is Lipschitz in B, it follows that $\tau(A(v))$ is Lipschitz in B. Applying Picard theorem to equation (7) we conclude that it has a unique solution defined in B. Hence the equation (6) has also an unique solution in B, in sense that the trace is unique.

In order to show that the equation (5) has a unique solution in B, in sense that the trace is unique, one needs to observe that every solution of the equation (6) is also a solution of the equation (5) because $DF(c(s))c'(s) = 0$ implies that $F(c(s))$ is constant and as $F(c_0) = 0$ we have $F(c(s)) = 0$. ∎

Corollary 1. *If DF is Lipschitz in an open neighbourhood of $(x_0, a_0, a_1, \ldots, a_k)$ and $A(x_0, a_0, a_1, \ldots, a_k)$ has maximum rank, then there is $r > 0$ such that the initial value problem (3) has a unique general solution in $B = \{(X, Y_0, \ldots, Y_k); \| (Y, Y_0, \ldots, Y_k) - (x_0, a_0, \ldots, a_k) \| \leq r\}$.*

Singularities

Definition 5. *A point P_0 is a singularity of the implicit differential equation (1) if $F(P_0) = 0$ and $F_{Y^{(k)}}$ is singular at P_0 but not in any neighborhood of P_0.*

Proposition 1. *Let be given a general solution of equation (1) $c : I \to \mathbb{R}^{nk+1}$, $c(s) = (x(s), y_0(s), \ldots, y_k(s))$ with $c'(s_0) \neq 0$, DF Lipschitz in a neighborhood of $c(s_0)$:*

1) *If $x'(s_0) = 0$ then $y'_0(s_0) = 0, \ldots, y'_{k-1}(s_0) = 0$, $y'_k(s_0) \neq 0$ and $F_{y_k}(c(s_0))$ is singular.*

2) *If $A(c(s_0))$ is of maximal rank and $F_{y_k}(c(s_0))$ is singular then $x'(s_0) = 0$, $y'_0(s_0) = 0, \ldots, y'_{k-1}(s_0) = 0$, $y'_k(s_0) \neq 0$ and $F_{y_k}(c(s_0))$ has rank $n - 1$.*

Proof.

1) Suppose $x'(s_0) \neq 0$, and c a general solution of equation (1). By the equation (2) we have $y'_0(s_0) = 0, \ldots, y'_{k-1}(s_0) = 0$ but $y'_k(s_0) \neq 0$ since $c'(s_0) \neq 0$. Now

$$0 = F_x(c(s_0))x'(s_0) + F_{y_0}(c(s_0))y'_0(s_0) + \cdots$$
$$\cdots + F_{y_{k-1}}(c(s_0))y'_{k-1}(s_0) + F_{y_k}(c(s_0))y'_k(s_0).$$

Thus $F_{y_k}(c(s_0))y'_k(s_0) = 0$, and $F_{y_k}(c(s_0))$ is singular.

2) Let P and Q be non singular matrices such that

$$PF_{y_k}(c(s_0))Q = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}.$$

Let

$$\Lambda = \begin{pmatrix} P & & & \\ & Q^{-1} & & \\ & & \ddots & \\ & & & Q^{-1} \end{pmatrix}, \; \Gamma = \begin{pmatrix} I & & & \\ & Q & & \\ & & \ddots & \\ & & & Q \end{pmatrix}.$$

We have $\Lambda A(c(s))\Gamma\Gamma^{-1}c'(s) = 0$. Thus $B(c(s))d'(s) = 0$, where

$$B(c(s)) = \Lambda A(c(s))\Gamma =$$

$$= \begin{pmatrix} PF_x & PF_{y_0}Q & \cdots & PF_{y_{k-1}}Q & PF_{y_k}Q \\ Q^{-1}y_k & & & -I & \\ \vdots & & & & \\ Q^{-1}y_1 & -I & & & \end{pmatrix} =$$

$$= \begin{pmatrix} PF_x & PF_{y_0}Q & \cdots & PF_{y_{k-1}}Q & \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} \\ Q^{-1}y_k & & & -I & \\ \vdots & & & & \\ Q^{-1}y_1 & -I & & & \end{pmatrix}$$

and $d'(s) = \Gamma^{-1}c'(s)$.

Now for $s = s_0$ the rank of $B(c(s_0))$ is $(k+1)n$ because the rank of $A(c(s_0))$ is maximal. Thus $F_{y_k}(c(s_0))$ has rank $n-1$ and $x'(s_0) = 0, y'_0(s_0) = 0, \ldots, y'_{k-1}(s_0) = 0$. ∎

It follows from the last proposition that $x(s) = x(s_0) + x''(s_0)\frac{(s-s_0)^2}{2} + \cdots x^{(p)}(s_0)\frac{(s-s_0)^p}{p!} + O((s-s_0)^{p+1})$. If $x^{(i)}(s_0) = 0$, $i = 2, \ldots, p-1$ and $x^{(p)}(s_0) \neq 0$, then the $c(s)$ has a singularity of order p at s_0. If $p = 2$ then $c(s)$ has a simple fold as a singularity. By changing coordinates we can take $x(s) - x(s_0) = s^2$, thus in the $x, y_0, \ldots, y_{k-1}$ domain we have two solutions, one coming in and one going out of the point $(x(s_0), y_0(s_0), \ldots, y_{k-1}(s_0))$, which agrees with the result of Rabier (1989).

Implicit differential equations with $\text{rank}(\mathbf{F_{y_k}}) < \mathbf{n}$

If $F_{y_k}(c(s_0))$ is non singular then $A(c(s_0))$ has maximum rank, for

$$(c(s_0)) =$$

$$\begin{pmatrix} F_x(c(s_0)) & F_{y_0}(c(s_0)) & F_{y_1}(c(s_0)) & \cdots & F_{y_{k-1}}(c(s_0)) & F_{y_k}(c(s_0)) \\ y_k(s_0) & 0 & 0 & \cdots & -I & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ y_2(s_0) & 0 & -I & \cdots & 0 & 0 \\ y_1(s_0) & -I & 0 & \cdots & 0 & 0 \end{pmatrix}$$

Now, if $F_{y_k}(c(s_0))$ has rank $n-1$, $A(c(s_0))$ can still have maximum rank since the vector

$$\begin{pmatrix} F_x(c(s_0)) \\ y_k(s_0) \\ \vdots \\ y_1(s_0) \end{pmatrix}$$

can recover the rank of $A(c(s_0))$.

Proposition 2. *If the rank of $F_{y_k}(c_0)$ is less than or equal to $n-1$ in a neighborhood of c_0, then there are local changes of variables in the domain and in the range of F, where we can write (1) in the following form:*

$$\begin{cases} f(X, W(X), Z(X), \ldots, W^{(k-1)}(X), Z^{(k-1)}(X), W^{(k)}(X)) & = 0 \\ g(X, W(X), Z(X), \ldots, W^{(k-1)}(X), Z^{(k-1)}(X)) & = 0 \end{cases}$$
$$(8)$$

where $f : \Omega \to \mathbb{R}^m$, $g : \Omega \to \mathbb{R}^p$ are suficiently differentiable maps defined in the open connected set $\Omega \subset \mathbb{R}^{(k+1)m+kp+1}$ $(n = m + p)$, with $f_{W^{(k)}}$ non-singular.

Proof.

It has been indicated in Brenan, Campbell and Petzold (1989), but for the sake of competenness we repeat the proof here. Suppose that the rank of $F_{Y^{(k)}}$ is $m < n$. We can reorder both, equations and variables in (1), in such a way that

$$F_{Y^{(k)}} = \begin{pmatrix} f_{W^{(k)}} & f_{Z^{(k)}} \\ g_{W^{(k)}} & g_{Z^{(k)}} \end{pmatrix},$$

where $Y = (W, Z)$, $F = (f, g)$ and $f_{W^{(k)}}$ is non singular $m \times m$ matrix in a neighborhood of c_0.

By the implicit function theorem, we can solve $W^{(k)}$ with respect to $X, W, Z, \ldots, W^{(k-1)}, Z^{(k-1)}$ in the equation $f = 0$. By substituting $W^{(k)}$ in the equation $g = 0$, we have a relation between $W^{(k)}$ and $Z^{(k)}$. The main observation here is that $Z^{(k)}$ cannot be present in the equation $g = 0$ because if this is so the rank of $F_{Y^{(k)}}$ would be greater than m. By the same argument $Z^{(k)}$ cannot be present in the equation $f = 0$. Then we can rewrite equation (1) as in the statement of the proposition. ∎

For the equation (8), similar to previous definitions, we can define classical and general solutions.

Definition 6. *A map (W, Z) with $W : \mathscr{I} \to \mathbb{R}^m$, $Z : \mathscr{I} \to \mathbb{R}^p$ is said to be a classical solution of (8) if $W \in C^k$ and $Z \in C^{k-1}$ in $\mathscr{I} \subset \mathbb{R}$ and satisfies the equation (8).*

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Definition 7. *The image of a map $c : I \to \mathbb{R}^{(k+1)m+kp+1}$ is said to be a general solution of equation (8) if $c \in C^1$ in $I \subset \mathbb{R}$ and satisfies*

$$
\begin{cases}
f(c(s)) & = & 0 \\
g(c(s)) & = & 0 \\
w_1(s)x'(s) - w_0'(s) & = & 0 \\
z_1(s)x'(s) - z_0'(s) & = & 0 \\
\quad \vdots & & \\
w_{k-1}(s)x'(s) - w_{k-2}'(s) & = & 0 \\
z_{k-1}(s)x'(s) - z_{k-2}'(s) & = & 0 \\
w_k(s)x'(s) - w_{k-1}'(s) & = & 0
\end{cases}
$$

for all $s \in I$, where

$$c(s) = (x(s), w_0(s), z_0(s), \ldots, w_{k-1}(s), z_{k-1}(s), w_k(s)).$$

The ω-structure is now defined by the function $\omega : \Omega \to \mathbb{R}^N$ and $A : \Omega \to \mathbb{R}^M$, where $N = (km + (k-1)p)((k+1)m + kp + 1)$ and $M = ((k+1)m + kp)((k+1)m + kp + 1)$, be defined as

$\omega(x, w_0, z_0, \ldots, w_{k-1}, z_{k-1}, w_k) =$

$$
= \begin{pmatrix}
w_k & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -I_m & 0 & 0 \\
z_{k-1} & 0 & 0 & 0 & 0 & \cdots & 0 & -I_p & 0 & 0 & 0 \\
w_{k-1} & 0 & 0 & 0 & 0 & \cdots & -I_m & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & \vdots \\
z_2 & 0 & 0 & 0 & -I_p & \cdots & 0 & 0 & 0 & 0 & 0 \\
w_2 & 0 & 0 & -I_m & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
z_1 & 0 & -I_p & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
w_1 & -I_m & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
$$

and

$$
A(c(s)) = \begin{pmatrix} Df(c(s)) \\ Dg(c(s)) \\ \omega(c(s)) \end{pmatrix}.
$$

Then the following initial value problems

$$
\begin{cases}
f(X, W(X), Z(X), \ldots, W^{(k-1)}(X), Z^{(k-1)}(X), W^{(k)}(X)) & = 0 \\
g(X, W(X), Z(X), \ldots, W^{(k-1)}(X), Z^{(k-1)}(X)) & = 0 \\
W^{(i)}(x_0) = a_i, \ i = 0, 1, \ldots, k \\
Z^{(i)}(x_0) = b_i, \ i = 0, 1, \ldots, k-1,
\end{cases}
\tag{9}
$$

$$
\begin{cases}
f(c(s)) & = 0 \\
g(c(s)) & = 0 \\
\omega(c(s))c'(s) & = 0 \\
c(0) & = c_0 = (x_0, a_0, b_0, \ldots, a_{k-1}, b_{k-1}, a_k),
\end{cases}
\tag{10}
$$

and

$$
\begin{cases}
A(c(s))c'(s) & = 0 \\
c(0) & = c_0 = (x_0, a_0, b_0, \ldots, a_{k-1}, b_{k-1}, a_k),
\end{cases}
$$

with $f(c_0) = 0$ and $g(c_0) = 0$, are respectively equivalent to the equations (3), (5) and (6).

Lemma 2. *Consider a general solution of (8) given by $c : I \to \mathbb{R}^{(k+1)m+kp+1}$. If $x'(s) \neq 0$ in an interval $\mathscr{I} \subset I$, then $w_0(s) = W_0(x(s))$, $w_1(s) = \frac{d}{dx}W_0(x(s)), \ldots,$ $w_{k-1}(s) = \frac{d^{k-1}}{dx^{k-1}}W_0(x(s))$, $w_k(s) = \frac{d^k}{dx^k}W_0(x(s))$, $z_0(s) = Z_0(x(s)), z_1(s) = \frac{d}{dx}Z_0(x(s)), \ldots, z_{k-1}(s) = \frac{d^{k-1}}{dx^{k-1}}Z_0(x(s))$, in $\mathscr{I}$ and (W_0, Z_0) defined in $x(\mathscr{I})$ is a classical solution of the equation (8).*

Theorem 2. *If Df and Dg are Lipschitz in an open neighbourhood of c_0 and $A(c_0)$ has maximum rank, then there is $r > 0$ such that the initial value problem (10) has a unique solution in $B = \{v; \| v - c_0 \| \leq r\}$ (unique solution in the sense of unique trace).*

Corollary 2. *If Df and Dg are Lipschitz in an open neighbourhood of $(x_0, a_0, b_0, \ldots, a_{k-1}, b_{k-1}, a_k)$ and $A(x_0, a_0, b_0, \ldots, a_{k-1}, b_{k-1}, a_k)$ has maximum rank, then there is $r > 0$ such that the initial value problem (9) has a unique general solution in $B = \{(X, W_0, Z_0, \ldots, W_{k-1}, Z_{k-1}, W_k); \| (X, W_0, Z_0, \ldots, W_{k-1}, Z_{k-1}, W_k) - (x_0, a_0, b_0, \ldots, a_{k-1}, b_{k-1}, a_k) \| \leq r\}$.*

The proofs of Lemma 2, Theorem 2 and Corollary 2 follow those of Lemma 1, Theorem 1 and Corollary 1 closely and will thus be omitted.

Definition 8. *A point P_0 is a singularity of the implicit differential equation (8) if $f(P_0) = 0$, $g(P_0) = 0$ and $g_{z_{k-1}}$ is singular at P_0 but not in any neighborhood of P_0.*

Proposition 3. *Let be given a general solution of the equation (8) $c : I \to \mathbb{R}^{(k+1)m+kp+1}$, $c(s) = (x(s), w_0(s), z_0(s), \ldots, w_{k-1}(s), z_{k-1}(s), w_k(s))$ with $c'(s_0) \neq 0$, Df and Dg Lipcshitz in a neighborhood of $c(s_0)$:*

1) If $x'(s_0) = 0$ then $w_0'(s_0) = 0$, $z_0'(s_0) = 0$, $\ldots,$ $w_{k-1}'(s_0) = 0$, $z_{k-1}'(s_0) = 0$, $w_k'(s_0) \neq 0$ and $g_{z_{k-1}}(c(s_0))$ is singular.

2) If $A(c(s_0))$ is of maximal rank and $g_{z_{k-1}}(c(s_0))$ is singular then $x'(s_0) = 0$, $w_0'(s_0) = 0$, $z_0'(s_0) = 0$, $\ldots =$, $w_{k-1}'(s_0) = 0$, $z_{k-1}'(s_0) = 0$, $w_k'(s_0) \neq 0$ and $g_{z_{k-1}}(c(s_0))$ has rank $p - 1$.

Noting that if $\begin{pmatrix} A & B \\ C & 0 \end{pmatrix}$ is of maximal rank and B is nonsingular then C is of maximal rank, the proof of the proposition follows in a similar manner to the one given in Proposition 1.

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Examples

Example 1. *Let*

$$\begin{cases} X^2 + (Y(X))^2 & = 1 \\ Y(x_0) & = y_0 \end{cases}$$
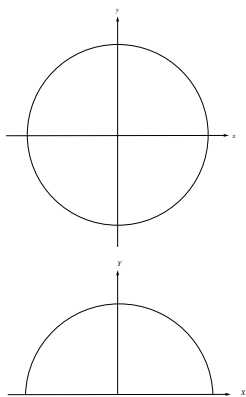
where $y_0 > 0$ and $x_0^2 + y_0^2 = 1$.

The classical solution of this equation is $Y(X) = (1-X^2)^{\frac{1}{2}}$ for $-1 < X < 1$ and $\{(-1,0),(1,0)\}$ is the set of singularities. The associated ω-system is

$$\begin{cases} y_0^2(s) + x^2(s) & = 1 \\ x(0) & = x_0 \\ y_0(0) & = y_0 \end{cases}$$

and the general solution is given by $c(s) = (cos(s + s_0), sin(s + s_0))$, $x_0 = cos(s_0)$ and $y_0 = sin(s_0)$, for $-\pi < s \le \pi$. Since $x'(-s_0) = x'(\pi - s_0) = 0$ and $c(0) = (x_0, y_0)$ we have that $c(s) = (X, Y(X))$ for $-s_0 < s < \pi - s_0$. See Figure 1.

Figure 1 – Example 1: General and classical solutions.

Example 2. *Let*

$$\begin{cases} (Y'(X))^2 & = Y(X) \\ Y(x_0) & = y_0 \\ Y'(x_0) & = z_0 \end{cases}$$

where $x_0 > 0$, $y_0 > 0$, $z_0 > 0$ and $z_0^2 = y_0$.

One of the classical solutions of this equation is $Y(X) = ((X - x_0)/2 + y_0^{1/2})^2$ for $X \in \mathbb{R}$ and the set of singularities is $\{(X,0) ; X \in \mathbb{R}\}$.
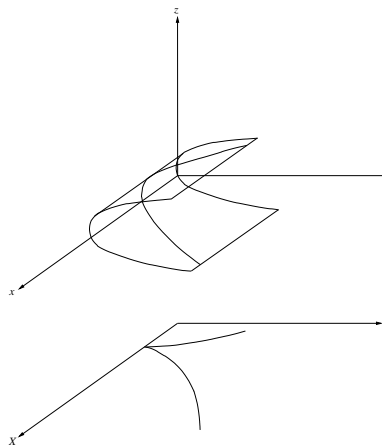
The associated ω-system is

$$\begin{cases} y_1^2(s) - y_0(s) & = 0 \\ y_1(s)x'(s) - y_0'(s) & = 0 \\ x(0) & = x_0 \\ y_0(0) & = y_0 \\ y_1(0) & = z_0 \end{cases}$$

and one of the the general solution is given by

$$c(s) = (s + x_0, (s/2 + y_0^{1/2})^2, s/2 + y_0^{1/2}),$$

for $s \in \mathbb{R}$. As $x'(s) = 1 \ne 0$ we have that $c(s) = (X, Y(X), Y'(X))$. See Figure 2.

Figure 2 – Example 2: General and classical solutions.

Note that the assumption of maximum rank imposed on $A(c_0)$ is essential as can be seen from this example.

In this example

$$A(c(s)) = \begin{pmatrix} 0 & -1 & 2y_1(s) \\ y_1(s) & -1 & 0 \end{pmatrix}$$

does not have maximum rank when $y_1(s) = 0$ and if $c_0 = (x_0, 0, 0)$ then example has many general solutions, two of then are given by $c(s) = (s + x_0, 0, 0)$ and $c(s) = (s + x_0, s^2/4, s/2)$.

Example 3. *Let*

$$\begin{cases} (Y'(X))^2 & = X \\ Y(x_0) & = y_0 \\ Y'(x_0) & = z_0 \end{cases}$$

where $x_0 > 0$, $y_0 > 0$, $z_0 > 0$ and $z_0^2 = x_0$.

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The classical solution of this equation is $Y(X) = y_0 + \frac{2}{3}(X^{3/2} - x_0^{3/2})$ for $X > 0$ and $\{(0,Y); \; Y \in \mathbb{R}\}$ is the set of singularities. The associated ω-system is

$$
\begin{cases}
y_1^2(s) - x(s) & = 0 \\
y_1(s)x'(s) - y_0'(s) & = 0 \\
x(0) & = x_0 \\
y_0(0) & = y_0 \\
y_1(0) & = z_0
\end{cases}
$$

and the general solution is given by $c(s) = ((s + x_0^{1/2})^2, y_0 + \frac{2}{3}((s + x_0^{1/2})^3 - x_0^{3/2}), s + x_0^{1/2})$ for $s \in \mathbb{R}$. Again as $x'(-x_0^{1/2}) = 0$ and $c(0) = (x_0, y_0, z_0)$ we have that $c(s) = (X, Y(X), Y'(X))$ for $s > -x_0^{1/2}$. See Figure 3.

Figure 3 – Example 3: General and classical solutions.
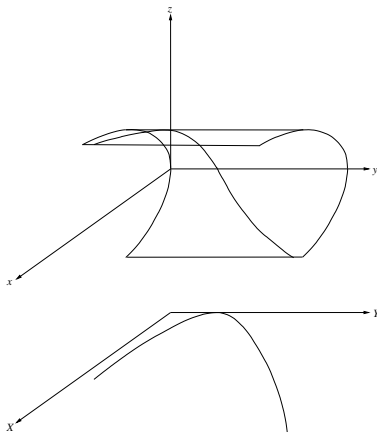
Source: The authors.

In the example above

$$
A(c(s)) = \begin{pmatrix} -1 & 0 & 2y_1(s) \\ y_1(s) & -1 & 0 \end{pmatrix}
$$

has maximum rank even in the case that $F_{y_1}(c(s)) = 2y_1(s) = 0$.

Numerical method

Numerical approaches for the solution of DAEs can be divided into roughly two classes: direct discretizations of the given system and methods which involve a reformulation combined with a discretization.

The desire for the most direct discretization possible arises because a redesign can be expensive and may require more user intervention. The reason for the popularity of reformulation approaches is that, as it turns out, direct discretizations are limited in their usefulness essentially to special DAE systems.

Many DAEs encountered in practical applications are index-1 or, if higher-index, can be expressed as a simple combination of Hessenberg systems. However, some worse-case difficulties may occur. The most robust direct applications of numerical ODE methods do not always work as one might hope, even for these restricted classes of problems.

Many codes emerged, mainly in the 90s, to solve initial value problems for DAEs (classic solutions). Among them we can mention the main codes:

- The code IDA is a part of the software package called SUNDIALS (SUite of Nonlinear and DIfferential/ALgebraic equation Solvers) which was developed by Serban, Hindmarsh and Cvodes (2005) at Lawrence Livermore National Laboratory, USA.

- The code RADAU5 by Hairer and Wannes (1996) is based on the 3-stage Radau collocation method.

- The code DASSL by Petzold (1982a) uses the BDF formulas to solve general index-1 DAEs, see Brenan, Campbell and Petzold (1996) for details.

- DAEPACK is a software library developed by Tolsma, Barton and Daepack (2000) and his group at MIT. DAEPACK is an acronym for Differential-Algebraic Equation Package.

- MEXX by Luvbich *et al*. (1992).

- LIMEX by Deuflhard, Hairer and Zugck (1987).

- GELDA and GENDA by Kunkel, Mehrmann and Weickert (1997) and Kunkel, Mehrmann and Seufer (2002), respectively.

Our focus is the description of an algorithm using continuation methods techniques combined with BDF methods to solve initial value problems (general solutions) for DAEs.

GSDAE is a code developed in C to obtain approximations of classic solutions (CSDAE routine) or general solutions (GSDAE routine) of DAE of any order (including order 0, which is a purely algebraic equation) in the form of implicit or in the semi-implicit form. The source code can be found at <https://github.com/antoniocastelofilho/GSDAE-CODE>.

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It uses the explicit Euler method defined as an initializer, since $c'(0)$ is not given as a condition initial, and the BDF method.

The strategies and methods used in the GSDAE are based on those of the DASSL (PETZOLD, 1982b) code for prediction, correction, and size control of step and order. Only when instability has detected the method and restarted using the linear multiple-step method again because close to a singularity, the explicit Euler method with step small provides a better approximation than the predictor polynomial.

The strategy of integration with the BDF method is that of fixed principal coefficients (BRENAN; CAMPBELL; PETZOLD, 1989; JACKSON; STAKS-DAVIS, 1980), which is an extension of the BDF method for variable steps. The idea of the strategy of fixed main coefficients and to apply the BDF method with step constant in the polynomial that interpolates the solution in the last k steps $(k = 1, \ldots, 5)$.

Below we describe the main strategies of the GSDAE.

We will solve for the general solution of the equation (5) by solving numerically the initial value problem is given in (7).

Let the equation

$$\sum_{i=0}^{r} \alpha_i c_{n-i} - h\beta_i \tau(A(c_{n-i})) = 0. \quad (11)$$

to evaluate τ we consider the QR-decomposition $A^t = Q \begin{pmatrix} R \\ 0^t \end{pmatrix}$. It gives $\tau(A) = \pm z$, where z is the last column of the matrix Q, since $\| z \| = 1$,

$$Az = (R^t \ 0) Q^t z = (R^t \ 0) \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} = 0 \text{ and } det \begin{pmatrix} A \\ z^t \end{pmatrix} =$$

$det(A^t \ z) = detQ \, detR$.

The computational cost of this decomposition is approximately $\frac{2}{3}(n(k+1))^3$, which can be lowered, by looking at the expression for ω, and writing

$$\begin{array}{rcccccc}
y_1(s)\tau_x - \tau_{y_0} & = & 0 & \Rightarrow & \tau_{y_0} & = & y_1(s)\tau_x \\
y_2(s)\tau_x - \tau_{y_1} & = & 0 & \Rightarrow & \tau_{y_1} & = & y_2(s)\tau_x \\
& & \vdots & & & & \\
& & \vdots & & & & \\
y_k(s)\tau_x - \tau_{y_{k-1}} & = & 0 & \Rightarrow & \tau_{y_{k-1}} & = & y_k(s)\tau_x \\
& & & & & & (12)
\end{array}$$

where $\tau = (\tau_x, \tau_{y_0}, \ldots, \tau_{y_k})$.

Substituting in $DF(c(s))\tau = 0$, we have

$$B(c(s))\psi = \begin{pmatrix} F_x + F_{y_0}y_1 + \cdots + F_{y_{k-1}}y_k & F_{y_k} \end{pmatrix} \begin{pmatrix} \tau_x \\ \tau_{y_k} \end{pmatrix} = 0.$$

Similarly we can obtain $\psi = \begin{pmatrix} \tau_x \\ \tau_{y_k} \end{pmatrix}$, using a QR-decomposition for B^t with an approximate computational cost $\frac{2}{3}n^3$. Thus, we can use the relations in the equation (12) to obtain τ.

This numerical scheme in the equation (11) can be used as a predictor/initializer method.

For the corrector step a BDF method can be used in equation (5):

$$\begin{cases} F(c_n) & = 0 \\ \omega(c_n)\dfrac{\rho c_n}{h} & = 0 \end{cases} \quad (13)$$

where $\rho c_n = \sum_{i=0}^{r} \gamma_i c_{n-i}$, with $\gamma_0 = 1$. To obtain c_n, a Newton type method for indeterminate systems is used; for this the derivative of the equation (13) has to be obtained and it has to be of maximal rank.

A modified Newton method for the equation (13) is given by

$$c_n^{i+1} = c_n^i - DG^+(c_n^0)G(c_n^i),$$

where

$$G(c_n) = \begin{pmatrix} F(c_n) \\ \omega(c_n)\dfrac{\rho c_n}{h} \end{pmatrix}.$$

By writing $\rho c_n = c_n + C_n$, $c_n = (x_n, y_{0,n}, \ldots, y_{k,n})$ and $C_n = (C_{x_n}, C_{y_{0,n}}, \ldots, C_{y_{k,n}})$, $DG(c_n)$ is given by

$DG(c_n) =$

$$= \begin{pmatrix}
F_x & F_{y_0} & F_{y_1} & F_{y_2} & \cdots & F_{y_{k-1}} & F_{y_k} \\
y_{1,n} & -I & x_n + C_{x_n} & 0 & \cdots & 0 & 0 \\
y_{2,n} & 0 & -I & x_n + C_{x_n} & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\
y_{k-1,n} & 0 & 0 & 0 & \cdots & x_n + C_{x_n} & 0 \\
y_{k,n} & 0 & 0 & 0 & \cdots & -I & x_n + C_{x_n}
\end{pmatrix}.$$

We have $DG(c_n) = A(c_n) + E(c_n)$, where

$E(c_n) =$

$$= \begin{pmatrix}
0 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & 0 & x_n + C_{x_n} & 0 & \cdots & 0 & 0 \\
0 & 0 & 0 & x_n + C_{x_n} & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & x_n + C_{x_n} & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & x_n + C_{x_n}
\end{pmatrix}.$$

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Since $\rho x(s_n) = hx'(s_n) + O(h^{r+1})$ for $c_{n-i} = c(s_{n-i})$, $i = 0, 1, \ldots, r$, we have $\| E(c(s_n)) \| = O(h)$. If h is sufficiently small such that

$$\| A^+(c(s_n)) \| \| E(c(s_n)) \| < 1.$$

It follows that $DG(c(s_n))$ is of maximal rank, see Allgower and Georg (1990).

To compute $v = D^+ u$, we can take a QR-decomposition of D^t:

$$D^t = Q \begin{pmatrix} R \\ 0^t \end{pmatrix}.$$

Thus

$$D^+ = D^t (D^t D)^{-1} = Q \begin{pmatrix} R^{-t} \\ 0^t \end{pmatrix}.$$

It follows

$$v = Q \begin{pmatrix} w \\ 0 \end{pmatrix},$$

where $R^t w = u$.

The computational cost for the modified Newton is approximatelly $\frac{2}{3}(n(k+1))^3 + j(n(k+1))^2$, where j is the number of iterations.

The computational cost can be optimized looking again into the expression for ω, since $\omega(c_n)\frac{\rho c_n}{h} = 0$ is written as

$$y_{1,n}(x_n + C_{x_n}) - (y_{0,n} + C_{y_0,n}) = 0 \Rightarrow$$
$$\Rightarrow y_{0,n} = y_{1,n}(x_n + C_{x_n}) - C_{y_0,n}$$
$$y_{2,n}(x_n + C_{x_n}) - (y_{1,n} + C_{y_1,n}) = 0 \Rightarrow$$
$$\Rightarrow y_{1,n} = y_{2,n}(x_n + C_{x_n}) - C_{y_1,n}$$
$$\vdots$$
$$y_{k,n}(x_n + C_{x_n}) - (y_{k-1,n} + C_{y_{k-1},n}) = 0 \Rightarrow$$
$$\Rightarrow y_{k-1,n} = y_{k,n}(x_n + C_{x_n}) - C_{y_{k-1},n}$$

or

$$y_{i,n} = y_{k,n}(x_n + C_{x_n})^{k-i} - \sum_{j=0}^{k-1-i} C_{y_{i+j,n}}(x_n + C_{x_n})^j,$$
$$i = 0, 1, \ldots, k-1.$$

$$(14)$$

Thus, from the first equation in (13) we have

$$H(x_n, y_{k,n}) =$$
$$= F(x_n, y_{0,n}, \ldots, y_{k-1,n}, y_{k,n}) = F(x_n, y_{k,n}(x_n + C_{x_n})^k -$$
$$- \sum_{j=0}^{k-1} C_{y_{j,n}}(x_n + C_{x_n})^j, \ldots, y_{k,n}(x_n + C_{x_n})$$
$$- C_{y_{k-1,n}}, y_{k,n}) = 0.$$

To compute c_n we solve $H(x_n, y_{k,n}) = 0$, with a computational cost given approximately by $\frac{2}{3}n^3 + jn^2$, where j is the number of iterations in the modified Newton's method. From this we obtain c_n using the relations given in the equation (14).
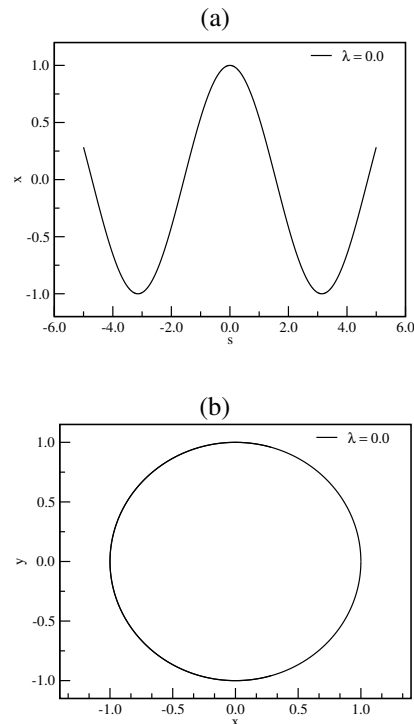
Results

Let a family of implicit differential equation

$$\begin{cases} \lambda Y'^2 + Y^2 + X^2 & = 1 \\ Y(x_0) & = y_0 \\ Y'(x_0) & = z_0. \end{cases}$$

This family for $\lambda = 0$ is a purely algebraic equation and for $\lambda \neq 0$, these DAE contain transverse singularities at $y' = 0$.

Case 1: Let $\lambda = 0.0$, $x_0 = 1.0$, $y_0 = 0.0$ e $z_0 = 0.0$. We have a purely algebraic equation. The GSDAE code is able to solve this type of equation. Results for the plans $s \times x$ and $x \times y$ are shown in the Figures 4(a) and(b) respectively.

**Figure 4 –** Case 1: (a) $s \times x$ plane, (b) $x \times y$ plane

(a)

(b)

Source: The authors.

Case 2: Let $\lambda = -1.0$, $x_0 = 1.0$, $y_0 = 0.0$ and $z_0 = 0.0$. The results for the plans $s \times x$, $x \times y$, $x \times y'$ and $y \times y'$, are shown in Figure 5 items (a)-(d) respectively. Item (b) shows the point where a transversal singularity occurs (red circle).

Case 3: Let $\lambda = 1.0$, $x_0 = 1.0$, $y_0 = 0.0$ and $z_0 = 0.0$ be. The results of this simulation are shown in items (a)-(d) of Figure 6 for the same planes as in Case 2. Note that transversal singularities are highlighted in item (b) (red circles).

Figure 5 – Case 2: (a) displays the plan $s \times x$; (b) shows the $x \times y$ plan, in (c) we have the $x \times y'$ plan and in (d) the $y \times y'$ plan.
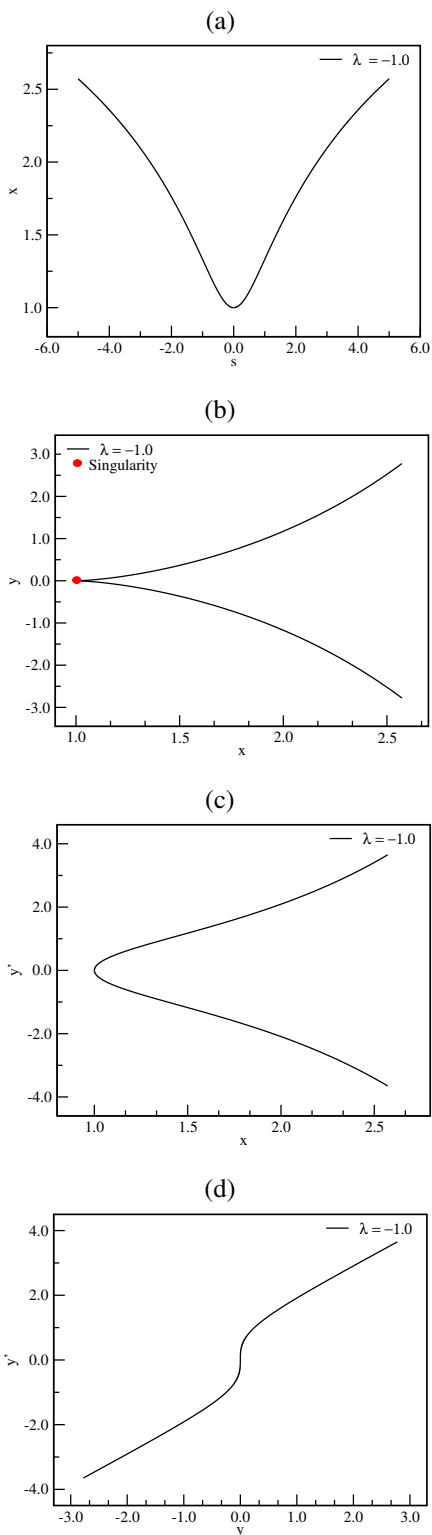
Figure 6 – Case 3: (a) displays the plan $s \times x$ and in (b) we have the plan $x \times y$ and in the item (c) we have the plans $x \times y$. In (d) we have, the plan $y \times y'$.

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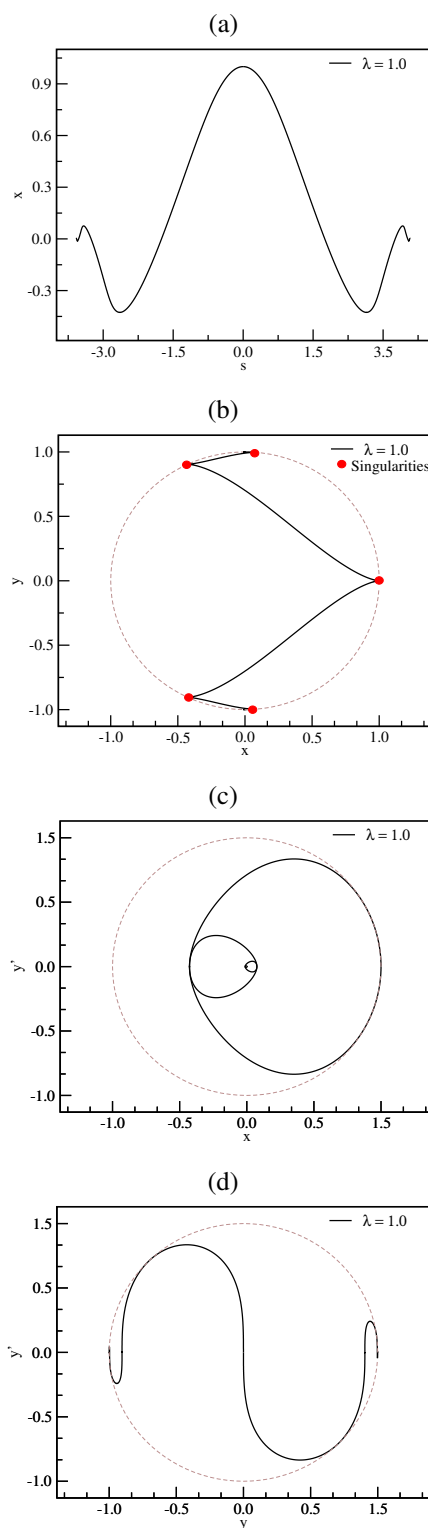
Case 4: Let $\lambda = 1.0$, $x_0 = 0.0$, $y_0 = 0.0$ and $z_0 = -1.0$. The plans $s \times x$, $x \times y$, $y \times y'$ and $x \times y'$ are shown in items (a)-(d) in Figure 7. Details with the singularities are shown in the item (b) (red circles). In the Figure 8 is show the magnification region of singularities to the plane $x \times y'$.

Figure 7 – Case 4: Figures $(a) - (d)$ show the plans $s \times x$, $x \times y$, $y \times y'$ and $x \times y'$, respectively.

(a)

(b)

(c)

(d)
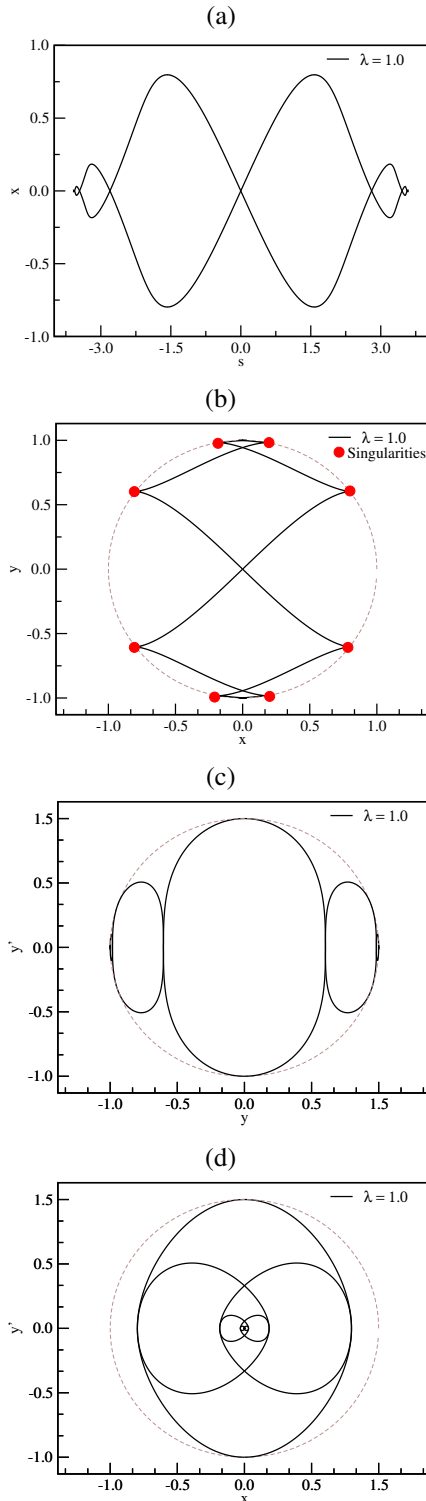
Figure 8 – Case 4: Zooming the plane $x \times y'$ around the non-transverse singularity.
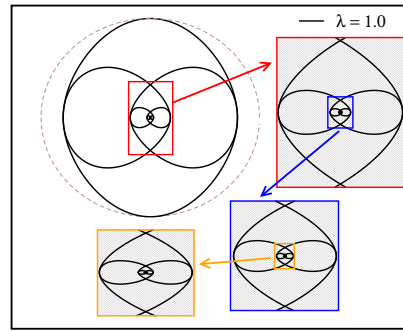
Conclusion

This work presents the solution of implicit differential equations with singularities. After presenting the basic concepts, we define the main theorems and show their proof. Some examples of classical differential equations with singularities were presented. In the section on implementation, we present the GSDAE code developed in C language that obtains approximations of the solutions for both classical and general solutions. Also, in the implementation section, we provide the link with the code and a manual for using the program, containing examples of its use. Finally, the results section shows four cases and their respective solutions for a family of implicit differential equations.

We believe that this work contributes to implicit differential equations and numerical methods; since the code provided is simple to use but very useful to solve differential-algebraic equations.

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