DIFFERENTIAL ALGEBRAIC EQUATIONS OF FILIPPOV TYPE

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Abstract: We will study discontinuous dynamical systems of Filippov-type. Mathematically, Filippov-type systems are defined as a set of first-order differential equations with discontinuous right-hand side. These systems arise in various applications, e.g. in control theory (so called relay feedback systems), in chemical engineering (an ideal gas–liquid system), or in biology (predator-prey models). We will show the way how to extend these models by a set of algebraic equations and then study the resulting system of differential-algebraic equations. All MATLAB simulations are performed in modified version of the program developed by Petri T. Piiroinen and Yuri A. Kuznetsov published in ACM Trans. Math. Software, 2008.

Keywords: Filippov systems, differential algebraic equations (DAEs), Filippov systems with DAEs, soft drink process

MSC: 34C60, 37N30, 65P30

1. Introduction

There are a variety of engineering problems involving dynamical systems. In recent years, the need to describe systems with a discontinuity in the state variables has emerged. The theory of the non-smooth systems has been introduced and thoroughly studied in [9]. From recent years, let us mention the book [5].

In addition to dynamical systems described by ordinary differential equations there are also models that require the use of differential equations along with algebraic ones. These are so-called differential algebraic equations (DAEs).

From the dynamical point of view, the essential differences between differential-algebraic equations (DAEs) and explicit ordinary differential equations (ODEs) arise in so-called singular problems, which lead to new dynamic phenomena such as those displayed at impasse points or singularity-induced bifurcations.

The origins of DAEs theory can be traced back to the work of K. Weierstrass and L. Kronecker on parameterized families of bilinear forms [20, 14]. In terms of

matrices, pencils were applied to the analysis of linear systems of ordinary differential equations with a possibly singular leading coefficient matrix by F. R. Gantmacher [10, 11]. Another milestone is the work of P. Dirac on generalized Hamiltonian systems [6, 7, 8]. The key ideas supporting what nowadays is known as the differentiation index of a semi-explicit DAEs can be found in these references. The work of Dirac was mainly motivated by applications in mechanics. A large amount of research on differential-algebraic equations has also been motivated by applications in circuit theory. The differential-algebraic form of circuit equations is naturally due to the combination of differential equations coming from reactive elements with algebraic (non-differential) relations modeling Kirchhoff laws and device characteristics.

To "measure" how difficult is to solve a DAEs system, the concept of indices has been introduced. There are different indices (Kronecker index, strangeness index, differentiation index, perturbation index, etc.), and the choice of the index depends on the DAEs and on the application, for which it is used (see [13, 19]).

If the model with DAEs features a discontinuity, then we have to modify the non-smooth dynamical systems theory to include DAEs. We will extend the theory of the non-smooth systems, namely the theory of Filippov systems, to the systems with DAEs. Finally, we will apply this theory to some application from chemical engineering.

2. Filippov systems

Let φ be a continuous and differentiable scalar function, $\varphi : \mathcal{D} \subseteq \mathbb{R}^n \to \mathbb{R}$, $n \geq 2$. The function φ divides the region $\mathcal{D}$ into three parts:

$$S_1 = \{\mathbf{x} \in \mathcal{D} \subseteq \mathbb{R}^n : \varphi(\mathbf{x}) > 0\},$$

$$S_2 = \{\mathbf{x} \in \mathcal{D} \subseteq \mathbb{R}^n : \varphi(\mathbf{x}) < 0\},$$

$$\Sigma = \{\mathbf{x} \in \mathcal{D} \subseteq \mathbb{R}^n : \varphi(\mathbf{x}) = 0\}.$$

Let us assume that the function φ has a non-vanishing gradient $\nabla \varphi$ on the boundary Σ. We define the Filippov system $\mathcal{F}$ on $\mathcal{D} = S_1 \cup S_2 \cup \Sigma$ as

$$\mathcal{F} : \dot{x} = \begin{cases} \mathbf{f}^{(1)}(\mathbf{x}) \,, & \mathbf{x} \in S_1 \,, \\ \mathbf{f}^{(0)}(\mathbf{x}) \,, & \mathbf{x} \in \Sigma \,, \\ \mathbf{f}^{(2)}(\mathbf{x}) \,, & \mathbf{x} \in S_2 \,, \end{cases} \tag{1}$$

where $\mathbf{x}(t) \in \mathbb{R}^n$, $\mathbf{f}^{(i)} : \mathbb{R}^n \to \mathbb{R}^n$, $i = 0, 1, 2$, are sufficiently smooth functions in all arguments, and $t \in \mathbb{R}$. We suppose that the state space $\mathcal{D} = S_1 \cup S_2 \cup \Sigma$, $\mathcal{D} \subset \mathbb{R}^n$, the vector fields $\mathbf{f}^{(1)}$ on S_1 and $\mathbf{f}^{(2)}$ on S_2 are given.

We have to define the vector field $\mathbf{f}^{(0)}$ that determines the behavior of the system (1) on the boundary Σ. There are several possible scenarios that occur if the trajectory with an initial condition $\mathbf{x}_0 \notin \Sigma$ reaches the boundary Σ. Let for example $\mathbf{x}_0 \in S_1$. The trajectory can cross the boundary from S_1 to S_2, turn back to S_1,

or it can even slide along the boundary Σ. The direction in which the trajectory continues after a contact with Σ is affected by both vector fields $\mathbf{f}^{(1)}$ and $\mathbf{f}^{(2)}$.

Let us define a scalar function $\sigma(\mathbf{x})$, $\mathbf{x} \in \Sigma$, as the product of dot products in $\mathbb{R}^n$

$$\sigma(\mathbf{x}) = \langle \nabla\varphi(\mathbf{x}), \mathbf{f}^{(1)}(\mathbf{x}) \rangle \cdot \langle \nabla\varphi(\mathbf{x}), \mathbf{f}^{(2)}(\mathbf{x}) \rangle. \tag{2}$$

The sign of the function $\sigma(\mathbf{x})$ determines the behavior of the trajectory after a contact with the boundary Σ. Let us use this sign as a criterion for the identification of two types of sets on the boundary Σ, a crossing set Σ_c and a sliding set Σ_s,

$$\Sigma_c \subseteq \Sigma = \{\mathbf{x} \in \Sigma : \sigma(\mathbf{x}) > 0\},$$

$$\Sigma_s \subseteq \Sigma = \{\mathbf{x} \in \Sigma : \sigma(\mathbf{x}) \leq 0\}.$$
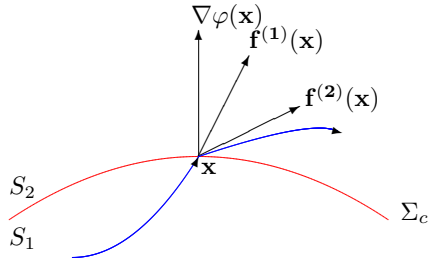
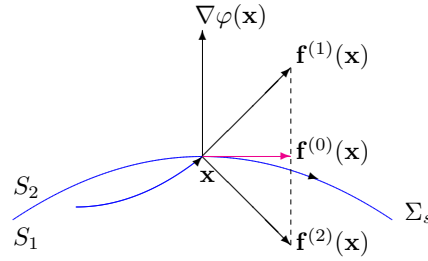The vector field $f^{(0)}$ on the boundary Σ is defined as follows:
• on Σ_c,

$$\mathbf{f}^{(0)} = \frac{1}{2}\left(\mathbf{f}^{(1)} + \mathbf{f}^{(2)}\right), \tag{3}$$

• on Σ_s, the vector field $f^{(0)}$ is defined as a convex combination

$$\mathbf{f}^{(0)} = (1-\lambda)\,\mathbf{f}^{(1)} + \lambda\,\mathbf{f}^{(2)}, \quad \lambda = \frac{\langle \nabla\varphi, \mathbf{f}^{(1)} \rangle}{\langle \nabla\varphi, \mathbf{f}^{(1)} - \mathbf{f}^{(2)} \rangle}, \quad 0 \leq \lambda \leq 1. \tag{4}$$

$$\Sigma_c = \{\mathbf{x} \in \Sigma : \sigma(\mathbf{x}) > 0\} \qquad \Sigma_s = \{\mathbf{x} \in \Sigma : \sigma(\mathbf{x}) \leq 0\}$$

Let us note that Σ_c contains those points $\mathbf{x} \in \Sigma$ in which both vectors $\mathbf{f}^{(1)}(\mathbf{x})$ and $\mathbf{f}^{(2)}(\mathbf{x})$ head to the same region. The set $\Sigma_s = \{\mathbf{x} \in \Sigma : \sigma(\mathbf{x}) \leq 0\}$ contains those points $\mathbf{x} \in \Sigma$ in which all other cases of configuration occur.

The equation (4) is called the Filippov convex combination. Let us note that it is not the only possibility how to define the vector field on the boundary Σ. Another possibility is for example to apply the so-called Utkin's equivalent control method, see e.g. [5].

Remark 2.1 Formula (4) follows from the fact that the trajectory slides along the sliding set, i.e., the vector field $\mathbf{f}^{(0)}(\mathbf{x})$ must be tangent to Σ_s,

$$\langle \nabla\varphi(\mathbf{x}), \mathbf{f}^{(0)}(\mathbf{x}) \rangle = 0, \quad \forall \mathbf{x} \in \Sigma_s. \tag{5}$$

On the sliding boundary Σ_s special points, so called sliding points, can be detected. Let us classify some of them.

- Singular sliding point is a point $\mathbf{x} \in \Sigma_s$ such that

$$\langle \nabla\varphi(\mathbf{x}), \mathbf{f}^{(1)}(\mathbf{x}) \rangle = 0 \quad \text{and also} \quad \langle \nabla\varphi(\mathbf{x}), \mathbf{f}^{(2)}(\mathbf{x}) \rangle = 0 \,.$$

  At these points, both vectors $\mathbf{f}^{(1)}(\mathbf{x})$ and $\mathbf{f}^{(2)}(\mathbf{x})$ are tangent to Σ_s.

- The point $\mathbf{x} \in \Sigma_s$ is a generic pseudo-equilibrium if

$$\mathbf{f}^{(0)}(\mathbf{x}) = \mathbf{0}, \quad \mathbf{f}^{(1)}(\mathbf{x}) \neq \mathbf{0}, \quad \mathbf{f}^{(2)}(\mathbf{x}) \neq \mathbf{0} \,.$$

  At these points, the vectors $\mathbf{f}^{(1)}(\mathbf{x})$ and $\mathbf{f}^{(2)}(\mathbf{x})$ are anti-collinear.

- In a boundary equilibrium $\mathbf{x} \in \Sigma_s$, one of the vectors $\mathbf{f}^{(i)}(\mathbf{x})$ vanishes,

$$\mathbf{f}^{(1)}(\mathbf{x}) = \mathbf{0} \quad \text{or} \quad \mathbf{f}^{(2)}(\mathbf{x}) = \mathbf{0} \,.$$

- The point $\mathbf{x} \in \Sigma_s$ is a tangent point if both $\mathbf{f}^{(1)}(\mathbf{x}) \neq \mathbf{0}$, $\mathbf{f}^{(2)}(\mathbf{x}) \neq \mathbf{0}$ and

$$\langle \nabla\varphi(\mathbf{x}), \ \mathbf{f}^{(1)}(\mathbf{x}) \rangle = 0 \quad \text{or} \quad \langle \nabla\varphi(\mathbf{x}), \ \mathbf{f}^{(2)}(\mathbf{x}) \rangle = 0 \,.$$

  In this case, both vectors $\mathbf{f}^{(1)}(\mathbf{x})$, $\mathbf{f}^{(2)}(\mathbf{x})$ are nonzero, but one of them is tangent to Σ. The tangent point terminates Σ_s in Σ, i.e., the sliding set Σ_s can be delimited solely by computing all tangent points.

3. Filippov systems with DAEs

Differential algebraic equations have become a widely accepted tool for the modeling and simulation of constrained dynamical systems in numerous applications, such as mechanical multibody systems, electrical circuit simulation, chemical engineering, control theory, fluid dynamics, and many other areas.

Let us have a general nonlinear system of differential-algebraic equations

$$\mathbf{F}(t, \mathbf{z}, \dot{\mathbf{z}}) = 0, \tag{6}$$

where $\mathbf{F} : I \times U \times V \to \mathbb{R}^n$, $t \in I$, $\mathbf{z}(t) \in U$, $\dot{\mathbf{z}}(t) \in V$, $\mathbf{z} : I \to \mathbb{R}^n$ is an unknown function, $\mathbf{z} \in \mathcal{C}^1(I, \mathbb{R}^n)$, $I \subseteq \mathbb{R}$ is a compact interval, $U, V \subseteq \mathbb{R}^n$ are open regions.

Let the equation (6) be equipped with the initial condition

$$\mathbf{z}(t_0) = \mathbf{z}_0, \ t_0 \in I, \ \mathbf{z}_0 \in \mathbb{R}^n. \tag{7}$$

Definition 3.1 Let the system of differential-algebraic equations (6), (7) be uniquely solvable. We define the so-called derivative array equations as

$$\mathbf{F}_\ell(t, \mathbf{z}, \dot{\mathbf{z}}, \ldots, \mathbf{z}^{(\ell+1)}) := \begin{bmatrix} \mathbf{F}(t, \mathbf{z}, \dot{\mathbf{z}}) \\ \frac{\mathrm{d}}{\mathrm{d}t} \mathbf{F}(t, \mathbf{z}, \dot{\mathbf{z}}) \\ \vdots \\ \frac{\mathrm{d}^\ell}{\mathrm{d}t^\ell} \mathbf{F}(t, \mathbf{z}, \dot{\mathbf{z}}) \end{bmatrix}, \tag{8}$$

where we can expand the term $\frac{\mathrm{d}}{\mathrm{d}t} \mathbf{F}(t, \mathbf{z}, \dot{\mathbf{z}})$ using the chain rule:

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathbf{F}(t, \mathbf{z}, \dot{\mathbf{z}}) = \mathbf{F}_t(t, \mathbf{z}, \dot{\mathbf{z}}) + \mathbf{F}_\mathbf{z}(t, \mathbf{z}, \dot{\mathbf{z}})\dot{\mathbf{z}} + \mathbf{F}_{\dot{\mathbf{z}}}(t, \mathbf{z}, \dot{\mathbf{z}})\ddot{\mathbf{z}}.$$

Other terms can be treated similarly.

In derivative array equations (8), let us formally replace $\dot{\mathbf{z}}(t)$ by $\mathbf{v}(t) \in \mathbb{R}^n$ and $(\ddot{\mathbf{z}}(t), \ldots, \mathbf{z}^{(\ell+1)}(t))$ by $\mathbf{w}(t) \in W$, $W \subseteq \mathbb{R}^{\ell n}$. In this setting, a given $(t, \mathbf{z})$ is said to be consistent if there exists a $(t, \mathbf{z}, \mathbf{v}, \mathbf{w}) \in I \times U \times V \times W$ for which $\mathbf{F}_\ell(t, \mathbf{z}, \mathbf{v}, \mathbf{w}) = 0$.

Definition 3.2 The smallest number $\nu \in \mathbb{N}_0$ for which $\mathbf{F}_\nu(t, \mathbf{z}, \mathbf{v}, \mathbf{w}) = 0$ holds for every consistent $(t, \mathbf{z})$, is called the differentiation index of (6).

The idea behind the differentiation index framework is, roughly speaking, to define the index of (6) as the number of differentiations needed to write $\dot{\mathbf{z}}$ in terms of $(t, \mathbf{z})$. Further details can be found in [13] or in [19].

In many technical applications a very common form of DAEs is the so called semi-explicit DAEs that provides a significant simplification of the fully nonlinear system. Therefore, in what follows we will explore this particular type of DAEs.

Let us consider DAEs (6). In $\mathbf{z}(t) = (\mathbf{x}(t), \mathbf{y}(t)) \in \mathbb{R}^{m+k}$ we distinguish two types of variables, in particular $\mathbf{x}(t) \in \mathbb{R}^m$ are called differential variables, and $\mathbf{y}(t) \in \mathbb{R}^k$, $k = n - m$, are called algebraic variables.

We rewrite (6) with the new variables $\mathbf{x}(t)$, $\mathbf{y}(t)$ as the semi-explicit DAEs:

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{y}), \tag{9}$$
$$\mathbf{0} = \mathbf{g}(\mathbf{x}, \mathbf{y}), \tag{10}$$

where $\mathbf{f} : U \times V \to \mathbb{R}^m$, $\mathbf{g} : U \times V \to \mathbb{R}^k$, $\mathbf{x} : I \to U$, $\mathbf{y} : I \to V$, $\mathbf{x} \in \mathcal{C}^1(I, \mathbb{R}^m)$ $I \subseteq \mathbb{R}$ is a compact interval, $U \subseteq \mathbb{R}^m$ and $V \subseteq \mathbb{R}^k$ are open regions, [18]

The proof of the following Theorem and more information can be found in e.g. [19, 13].

Theorem 3.1 Consider the semi-explicit differential algebraic equation (9)–(10). Then (9)–(10) has the differentiation index $\nu = 1$ if and only if the Jacobi matrix $\mathbf{g}_\mathbf{y}(\mathbf{x}, \mathbf{y})$ is regular for all consistent points $(\mathbf{x}, \mathbf{y}) \in U \times V$.

Remark 3.1 In (9),(10) the differential part of DAEs is denoted by $\mathbf{f}$, the algebraic part by $\mathbf{g}$.

Let us suppose that our system of DAEs (9),(10) has differentiation index $\nu = 1$. It implies that the Jacobi matrix $\mathbf{g_y}(\mathbf{x}, \mathbf{y})$ is regular for all consistent points $(\mathbf{x}, \mathbf{y}) \in U \times V$. Thus according to the Implicit Function Theorem, there exists a function $\mathbf{h} : \mathbb{R}^m \to \mathbb{R}^k$, such that $\mathbf{y} = \mathbf{h}(\mathbf{x})$, and

$$\mathbf{g}(\mathbf{x}, \mathbf{h}(\mathbf{x})) = \mathbf{0}, \quad \forall \mathbf{x} \in U \subseteq \mathbb{R}^m.$$

We substitute $\mathbf{y} = \mathbf{h}(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^m$, into (9) and obtain

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{h}(\mathbf{x})), \tag{11}$$

where $\mathbf{x} \in U \subseteq \mathbb{R}^m$.

The equation (11) is a system of ODEs on the $(n - k)$–dimensional manifold

$$\mathbb{M} = \{(\mathbf{x}, \mathbf{y}) \in \mathbb{R}^{m+k} : \mathbf{g}(\mathbf{x}, \mathbf{y}) = \mathbf{0}\}, \quad m + k = n. \tag{12}$$

Let again a continuous and differentiable scalar function $\varphi : \mathcal{D} \subseteq \mathbb{R}^{m+k} \to \mathbb{R}$ divide the region $\mathcal{D} \subseteq \mathbb{R}^{m+k}$ into three parts:

$$S_1 = \{(\mathbf{x}, \mathbf{y}) \in \mathcal{D} \subseteq \mathbb{R}^{m+k} : \varphi(\mathbf{x}, \mathbf{y}) > 0\},$$
$$S_2 = \{(\mathbf{x}, \mathbf{y}) \in \mathcal{D} \subseteq \mathbb{R}^{m+k} : \varphi(\mathbf{x}, \mathbf{y}) < 0\},$$
$$\Sigma = \{(\mathbf{x}, \mathbf{y}) \in \mathcal{D} \subseteq \mathbb{R}^{m+k} : \varphi(\mathbf{x}, \mathbf{y}) = 0\}.$$

We define a Filippov system $\mathcal{F}$ on $\mathcal{D} = S_1 \cup S_2 \cup \Sigma$ as

$$\mathcal{F} : \begin{bmatrix} \dot{\mathbf{x}} \\ \mathbf{0} \end{bmatrix} = \begin{cases} \mathbf{F}^{(1)}(\mathbf{x}, \mathbf{y}), & (\mathbf{x}, \mathbf{y}) \in S_1 \\ \mathbf{F}^{(0)}(\mathbf{x}, \mathbf{y}), & (\mathbf{x}, \mathbf{y}) \in \Sigma \\ \mathbf{F}^{(2)}(\mathbf{x}, \mathbf{y}), & (\mathbf{x}, \mathbf{y}) \in S_2 \end{cases} \quad \mathbf{F}^{(i)} = \begin{bmatrix} \mathbf{f}^{(i)} \\ \mathbf{g}^{(i)} \end{bmatrix}, \quad i = 0, 1, 2,$$

where $\mathbf{x}(t) \in \mathbb{R}^m$, $\mathbf{y}(t) \in \mathbb{R}^k$, $t \in \mathbb{R}$, $\mathbf{f}^{(i)} : \mathbb{R}^m \times \mathbb{R}^k \to \mathbb{R}^m$, $\mathbf{g}^{(i)} : \mathbb{R}^m \times \mathbb{R}^k \to \mathbb{R}^k$, $i = 0, 1, 2$, are sufficiently smooth functions in all arguments.

Similarly as in generic Filippov systems, we define the function

$$\sigma(\mathbf{x}, \mathbf{y}) = \langle \nabla\varphi(\mathbf{x}, \mathbf{y}), \mathbf{F}^{(1)}(\mathbf{x}, \mathbf{y}) \rangle \cdot \langle \nabla\varphi(\mathbf{x}, \mathbf{y}), \mathbf{F}^{(2)}(\mathbf{x}, \mathbf{y}) \rangle.$$

that divides the boundary Σ into a crossing set Σ_c and a sliding set Σ_s,

$$\Sigma_c \subseteq \Sigma = \{(\mathbf{x}, \mathbf{y}) \in \Sigma : \sigma(\mathbf{x}, \mathbf{y}) > 0\},$$

$$\Sigma_s \subseteq \Sigma = \{(\mathbf{x}, \mathbf{y}) \in \Sigma : \sigma(\mathbf{x}, \mathbf{y}) \leq 0\}.$$

On Σ_c, we set $\mathbf{F}^{(0)} = \dfrac{1}{2}\left(\mathbf{F}^{(1)} + \mathbf{F}^{(2)}\right)$, on Σ_s, we define the vector field $\mathbf{F}^{(0)}$ as a convex combination

$$\mathbf{F}^{(0)} = (1 - \lambda)\,\mathbf{F}^{(1)} + \lambda\,\mathbf{F}^{(2)}, \quad \lambda = \frac{\langle \nabla\varphi, \mathbf{F}^{(1)} \rangle}{\langle \nabla\varphi, \mathbf{F}^{(1)} - \mathbf{F}^{(2)} \rangle}, \quad 0 \le \lambda \le 1. \tag{13}$$

According to the convex combination (13), we can couple the differential parts of DAEs given by $\mathbf{f}^{(1)}$, $\mathbf{f}^{(2)}$, and separate them from the coupling of the algebraic parts given by $\mathbf{g}^{(1)}$, $\mathbf{g}^{(2)}$, i.e.,

$$\mathbf{f}^{(0)} = (1 - \lambda)\,\mathbf{f}^{(1)} + \lambda\,\mathbf{f}^{(2)}, \tag{14}$$

$$\mathbf{g}^{(0)} = (1 - \lambda)\,\mathbf{g}^{(1)} + \lambda\,\mathbf{g}^{(2)}. \tag{15}$$

The coupling of the differential equations of DAEs (14) is the same as in Section 2, but the coupling of the algebraic equations (15) is much more difficult. We don't a priori know which equations couple together, because here we don't have derivatives on the left side of the equations.

There are different ways to deal with this problem. Some authors prefer to pair only differential equations of DAEs and then add to them all algebraic equations.

We prefer to pair algebraic equations, too. This, however, requires more information about the system $\mathcal{F}$. Usually, we model some real applications and therefore each equation (differential or algebraic) has a physical meaning. In that case, we couple together the algebraic equations with the same physical meaning. Otherwise we could obtain unreasonable results. For more details and examples of coupling, see [13].

Let

$$\mathbb{M}_i = \{(\mathbf{x},\, \mathbf{y}) \in \mathbb{R}^{m+k} : \mathbf{g}^{(i)}(\mathbf{x},\, \mathbf{y}) = \mathbf{0}\}, \quad i = 1, 2, \tag{16}$$

be $(n-k)$-manifolds, where $n = m+k$. In Figure 1, the evolution of the trajectory on the manifolds $\mathbb{M}_1$ and $\mathbb{M}_2$ is shown. The trajectory starts with the initial condition $(\mathbf{x}(t_0),\, \mathbf{y}(t_0)) = (\mathbf{x}_0,\, \mathbf{y}_0) \in \mathbb{M}_1$ and crosses the boundary Σ to the manifold $\mathbb{M}_2$ at the crossing point $(\mathbf{x}(t_e),\, \mathbf{y}(t_e)) = (\mathbf{x}_e,\, \mathbf{y}_e)$. The subscript e denotes the so-called *event*, here the event is the contact of the trajectory with the boundary. In the following example, we illustrate the behavior of trajectories on manifolds $\mathbb{M}_1$ and $\mathbb{M}_2$.

Example 3.1 Let us have the Filippov system

$$\mathcal{F}: \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ 0 \end{bmatrix} = \begin{cases} \mathbf{F}^{(1)}(x_1,\, x_2,\, y)\,, & \varphi(x_1,\, x_2,\, y) < 0, \\[2mm] \mathbf{F}^{(2)}(x_1,\, x_2,\, y)\,, & \varphi(x_1,\, x_2,\, y) > 0, \end{cases} \tag{17}$$
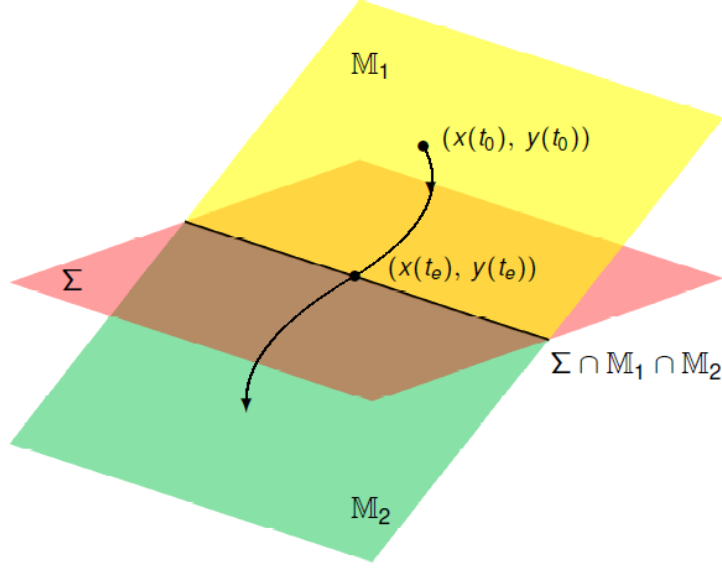
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Figure 1: Evolution of the trajectory on the manifolds $\mathbb{M}_1$ and $\mathbb{M}_2$.

where

$$\mathbf{F}_1(x_1,\, x_2,\, y) \;=\; \left.\begin{bmatrix} -x_1 & - & 3x_2 & + & y+15 \\ 3x_1 & - & x_2 & - & 2y \\ x_1 & & & - & y \end{bmatrix}\right\}\begin{array}{l}\mathbf{f}^{(1)} \\[6pt] \mathbf{g}^{(1)}\end{array}, \qquad (18)$$

$$\mathbf{F}_2(x_1,\, x_2,\, y) \;=\; \left.\begin{bmatrix} x_1 & + & 3x_2 & + & 2y-1 \\ 3x_1 & + & x_2 & - & 3y \\ x_1 & & & + & y \end{bmatrix}\right\}\begin{array}{l}\mathbf{f}^{(2)} \\[6pt] \mathbf{g}^{(2)}\end{array}, \qquad (19)$$

Let the function $\varphi : \mathbb{R}^{2+1} \to \mathbb{R}$ be defined as

$$\varphi(x_1,\, x_2,\, y) = x_1. \qquad (20)$$

Because $\nabla\varphi(x_1,\, x_2,\, y) = (1,\, 0,\, 0)$ and $x_1 = 0$ for $(x_1,\, x_2,\, y) \in \Sigma$, the scalar function $\sigma(x_1,\, x_2,\, y)$ has the form

$$\sigma(x_1,\, x_2,\, y) = (-3x_2 + y + 15)(3x_2 + 2y - 1).$$

The function σ divides the boundary Σ into two sets:

$$\Sigma_c \subseteq \Sigma = \{(x_1,\, x_2,\, y) \in \Sigma : \sigma(x_1,\, x_2,\, y) > 0\},$$

$$\Sigma_s \subseteq \Sigma = \{(x_1,\, x_2,\, y) \in \Sigma : \sigma(x_1,\, x_2,\, y) \leq 0\}.$$

On Σ_s, we set

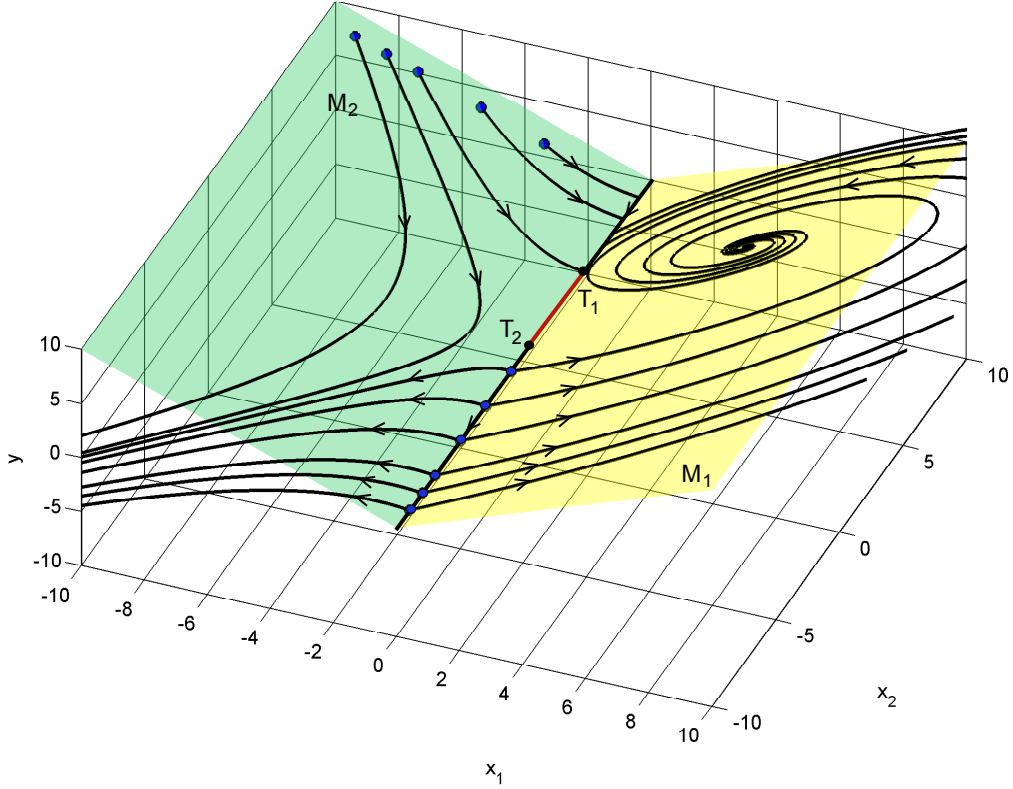$$\mathbf{F}^{(0)} = (1-\lambda)\,\mathbf{F}^{(1)} + \lambda\,\mathbf{F}^{(2)},$$

Figure 2: The phase portrait of the Filippov system in Example.

where

$$\lambda = \frac{-3x_2 + y + 15}{-6x_2 - y + 16}.$$

In Figure 2, the initial condition for each trajectory is depicted with the small blue circle. The yellow and green planes are the $(n - k)$–dimensional manifolds $\mathbb{M}_1$ and $\mathbb{M}_2$, $n = 3$, $k = 1$,

$$\mathbb{M}_1 = \{(x, y) \in \mathbb{R}^3 : y = x_1\}, \quad \mathbb{M}_2 = \{(x, y) \in \mathbb{R}^3 : y = -x_1\}. \tag{21}$$

The boundary Σ is depicted as the intersection of manifolds $\mathbb{M}_1$ and $\mathbb{M}_2$. On the boundary Σ, there are two tangent points T_1 and T_2 that delimit the set of sliding.

4. Soft drink process

The process of manufacturing soft-drink depicted in Figure 3 is based on the reaction between CO_2 and water:

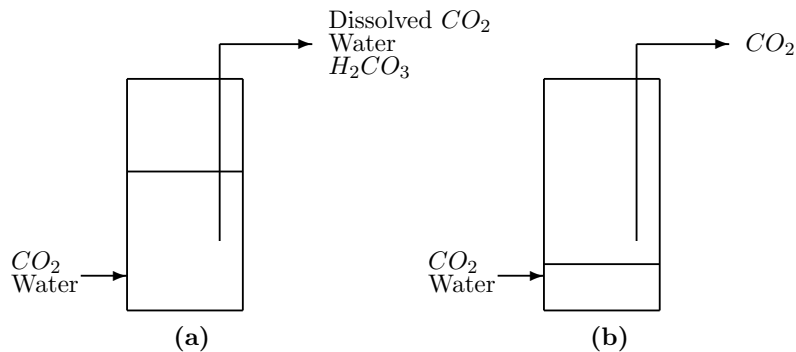$$CO_2 + H_2O \rightarrow H_2CO_3. \tag{22}$$

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Figure 3: The soft-drink process.

To simplify the model, we will suppose that

- The system contains only components CO_2, H_2O and H_2CO_3 (denoted by indices 1, 2 and 3, respectively).
- Intermediate ionisation reactions and dissociation of H_2CO_3 are ignored.
- In the liquid there are no gas bubbles.
- The valve dynamics is ignored.
- The flow rate through the valve is proportional to the difference of the tank pressure P and the outlet pressure P_{out}.
- The temperature T, the molar inflow rates F_1 and F_2, the outlet pressure, valve coefficients k_G and k_L and the valve opening X are all constant.

Let
$$M_1 = M_1(t), \qquad M_2 = M_2(t), \qquad M_3 = M_3(t),$$
be the total molar hold-ups of CO_2, H_2O and H_2CO_3, respectively. For a fixed t, let us define a scalar function $\varphi = \varphi(M_1, M_2, M_3)$,

$$\varphi(M_1, M_2, M_3) = \frac{M_2}{\rho_L} + \frac{M_3}{\rho_a} - V_d, \qquad (23)$$

where ρ_L, ρ_a are molar densities of water and acid, respectively. The volume of the whole tank is equal to V and the part of the volume that is below the opening of the dip tube is denoted as V_d, $0 < V_d < V$.

Similarly as in [4] and [2], in the tank two systems take place: the liquid model (the liquid leaves the tank) if $\varphi(M_1, M_2, M_3) > 0$ or the gas model (the gas leaves the tank) for $\varphi(M_1, M_2, M_3) < 0$. The acid phase consists of H_2CO_3, H_2O and dissolved CO_2 while the gas phase contains only CO_2. As a consequence, the liquid model is described by 3 ODEs and 6 algebraic equations, the gas model needs also 3 ODEs but only 4 algebraic equations. Let us give the list of these equations.

Differential equations:

Liquid model : $\varphi(M_1, M_2, M_3) > 0$ Gas model : $\varphi(M_1, M_2, M_3) < 0$

$$\frac{\mathrm{d}M_1}{\mathrm{d}t} = F_1 - L_1 - rV\,, \qquad\qquad \frac{\mathrm{d}M_1}{\mathrm{d}t} = F_1 - G - rV\,,$$

$$\frac{\mathrm{d}M_2}{\mathrm{d}t} = F_2 - L_2 - rV\,, \qquad\qquad \frac{\mathrm{d}M_2}{\mathrm{d}t} = F_2 - rV\,,$$

$$\frac{\mathrm{d}M_3}{\mathrm{d}t} = -L_3 + rV\,, \qquad\qquad \frac{\mathrm{d}M_3}{\mathrm{d}t} = rV\,,$$

The molar flow rates of the components through the valve are denoted L_1, L_2 and L_3 in the liquid model and G in the gas model. The rate r of the reaction (22) is given by

$$r = \kappa_c \frac{M_1 M_2}{V^2}, \qquad \text{where} \quad \kappa_c \quad \text{is the rate constant.} \qquad (24)$$

Algebraic equations:

Liquid model : $\varphi(M_1, M_2, M_3) > 0$ Gas model : $\varphi(M_1, M_2, M_3) < 0$

$$0 = M_1 - (M_\ell + M_g)\,, \qquad\qquad 0 = M_1 - (M_\ell + M_g)\,,$$

$$0 = P - \frac{\sigma M_\ell}{M_\ell + M_2 + M_3}\,, \qquad\qquad 0 = P - \frac{\sigma M_\ell}{M_\ell + M_2 + M_3}\,,$$

$$0 = V - \left(\frac{M_1 \mathrm{R} T}{P} + \frac{M_2}{\rho_L} + \frac{M_3}{\rho_a}\right)\,, \qquad 0 = V - \left(\frac{M_1 \mathrm{R} T}{P} + \frac{M_2}{\rho_L} + \frac{M_3}{\rho_a}\right)\,,$$

$$0 = \frac{M_2}{M_\ell + M_2 + M_3} - \frac{L_2}{L_1 + L_2 + L_3}\,, \qquad 0 = G - k_G X (P - P_{\text{out}})\,,$$

$$0 = \frac{M_3}{M_\ell + M_2 + M_3} - \frac{L_3}{L_1 + L_2 + L_3}\,,$$

$$0 = L_1 + L_2 + L_3 - k_L X (P - P_{\text{out}})\,,$$

P and T means pressure and temperature in the tank, the hold-ups of CO_2 in liquid and gas are denoted M_ℓ and M_g, the constant X is a valve opening, R is a gas constant and σ is Henry's constant for CO_2.

The straightforward computation shows that both the system of DAEs for the gas mode and the system of DAEs for the liquid model have differentiation index $\nu = 1$, [13].

Let us denote $\mathbf{x} = (x_1, x_2, x_3)$ the differential variables, $\mathbf{y} = (y_1, y_2, y_3, y_4, y_5, y_6)$ the algebraic ones.

For differential variables in both models we set

$$x_1 := M_1, \quad x_2 := M_2, \quad \text{and} \quad x_3 := M_3\,.$$

As the algebraic variables are concerned, we have to distinguish the models. In the gas model the algebraic variables are $\mathbf{y} = (y_1, y_4, y_5, y_6)$ and we substitute

$$y_1 := G, \quad y_4 := M_g, \quad y_5 := M_\ell, \quad \text{and} \quad y_6 := P\,.$$

In the liquid model $\mathbf{y} = (y_1, y_2, y_3, y_4, y_5, y_6)$, where we substitute

$$y_1 := L_1, \quad y_2 := L_2, \quad y_3 := L_3, \quad y_4 := M_g, \quad y_5 := M_\ell, \quad \text{and} \quad y_6 := P.$$

We extend the functions $\mathbf{f}^{(1)}$, $\mathbf{f}^{(2)}$, $\mathbf{g}^{(1)}$, $\mathbf{g}^{(2)}$ to all variables from liquid and gas model $(\mathbf{x}, \mathbf{y}) = (x_1, x_2, x_3, y_1, y_2, y_3, y_4, y_5, y_6)$. Then we can define the Filippov system $\mathcal{F}$

$$\mathcal{F}: \quad \begin{bmatrix} \dot{\mathbf{x}} \\ \mathbf{0} \end{bmatrix} = \begin{cases} \mathbf{F}^{(1)}(\mathbf{x}, \mathbf{y}), & (\mathbf{x}, \mathbf{y}) \in S_1, \\ \mathbf{F}^{(0)}(\mathbf{x}, \mathbf{y}), & (\mathbf{x}, \mathbf{y}) \in \Sigma, \\ \mathbf{F}^{(2)}(\mathbf{x}, \mathbf{y}), & (\mathbf{x}, \mathbf{y}) \in S_2 \end{cases} \qquad \mathbf{F}^{(i)} = \begin{bmatrix} \mathbf{f}^{(i)} \\ \mathbf{g}^{(i)} \end{bmatrix}, \quad i = 0, 1, 2, \quad (25)$$

where we set $\mathbf{x} = (x_1, x_2, x_3)$ and $\mathbf{y} = (y_1, y_2, y_3, y_4, y_5, y_6)$, and

$$\mathbf{f}^{(1)}(\mathbf{x}, \mathbf{y}) = \begin{bmatrix} F_1 - G - \kappa_c \dfrac{M_1 M_2}{V} \\[2ex] F_2 - \kappa_c \dfrac{M_1 M_2}{V} \\[2ex] \kappa_c \dfrac{M_1 M_2}{V} \end{bmatrix}, \quad \mathbf{f}^{(2)}(\mathbf{x}, \mathbf{y}) = \begin{bmatrix} F_1 - L_1 - \kappa_c \dfrac{M_1 M_2}{V} \\[2ex] F_2 - L_2 - \kappa_c \dfrac{M_1 M_2}{V} \\[2ex] -L_3 + \kappa_c \dfrac{M_1 M_2}{V} \end{bmatrix}. \quad (26)$$

$$\mathbf{g}^{(1)}(x, y) = \begin{bmatrix} y_1 - k_G X (y_6 - P_{\text{out}}) \\[2ex] x_1 - (y_5 + y_4) \\[2ex] y_6 - \dfrac{\sigma y_5}{y_5 + x_2 + x_3} \\[2ex] V - \left(\dfrac{x_1 RT}{y_6} + \dfrac{x_2}{\rho_L} + \dfrac{x_3}{\rho_a} \right) \end{bmatrix}, \quad (27)$$

$$\mathbf{g}^{(2)}(x, y) = \begin{bmatrix} \dfrac{x_2}{y_5 + x_2 + x_3} - \dfrac{y_2}{y_1 + y_2 + y_3} \\[2ex] \dfrac{x_3}{y_5 + x_2 + x_3} - \dfrac{y_3}{y_1 + y_2 + y_3} \\[2ex] y_1 + y_2 + y_3 - k_L X (y_6 - P_{\text{out}}) \\[2ex] x_1 - (y_5 + y_4) \\[2ex] y_6 - \dfrac{\sigma y_5}{y_5 + x_2 + x_3} \\[2ex] V - \left(\dfrac{x_1 RT}{y_6} + \dfrac{x_2}{\rho_L} + \dfrac{x_3}{\rho_a} \right) \end{bmatrix}. \quad (28)$$

We apply the routine described in Section 3 to our system and obtain the convex combination of the differential part:

$$\dot{x}_1 = F_1 - y_1 - \kappa_c \frac{x_1 x_2}{V}, \tag{29}$$

$$\dot{x}_2 = -\lambda y_2 + F_2 - \kappa_c \frac{x_1 x_2}{V}, \tag{30}$$

$$\dot{x}_3 = -\lambda y_3 + \kappa_c \frac{x_1 x_2}{V}, \tag{31}$$

where

$$\lambda = \frac{F_2 \rho_a + \kappa_c \frac{x_1 x_2}{V^2}(\rho_L - \rho_a)}{y_2 \rho_a + y_3 \rho_L}. \tag{32}$$

The convex combination of the algebraic part is

$$0 = \frac{x_2}{y_5 + x_2 + x_3} - \frac{y_2}{y_1 + y_2 + y_3},$$

$$0 = \frac{x_3}{y_5 + x_2 + x_3} - \frac{y_3}{y_1 + y_2 + y_3},$$

$$0 = (1 - \lambda)(y_1 - k_G X (y_6 - P_{\text{out}})) + \lambda (y_1 + y_2 + y_3 - k_L X (y_6 - P_{\text{out}})),$$

$$0 = x_1 - (y_5 + y_4),$$

$$0 = y_6 - \frac{\sigma y_5}{y_5 + x_2 + x_3}$$

$$0 = V - \left(\frac{x_1 \mathrm{R} T}{y_6} + \frac{x_2}{\rho_L} + \frac{x_3}{\rho_a} \right)$$

Parameter	Value	Meaning
F_1 (mol/s)	0.5	molar inflow of CO_2
F_2 (mol/s)	7.5	molar inflow of water
ρ_L (mol/ℓ)	50	molar density of water
ρ_a (mol/ℓ)	16	molar density of acid
V (ℓ)	10	volume of the tank
V_d (ℓ)	2.25	volume below the outlet tube
$T(K)$	293	absolute temperature
P_{out} (atm)	1	pressures in the outlet
X	1.0	valve opening
k_L (mol/atm/s)	2.5	valve coef. for the liquid flow
k_G (mol/atm/s)	3.0	valve coef. for the gas flow
κ_c (ℓ/mol/s)	0.433/4000	rate constant
σ (atm)	1640	Henry's constant for CO_2
R (ℓ atm/mol/K)	0.0820574587	gas constant

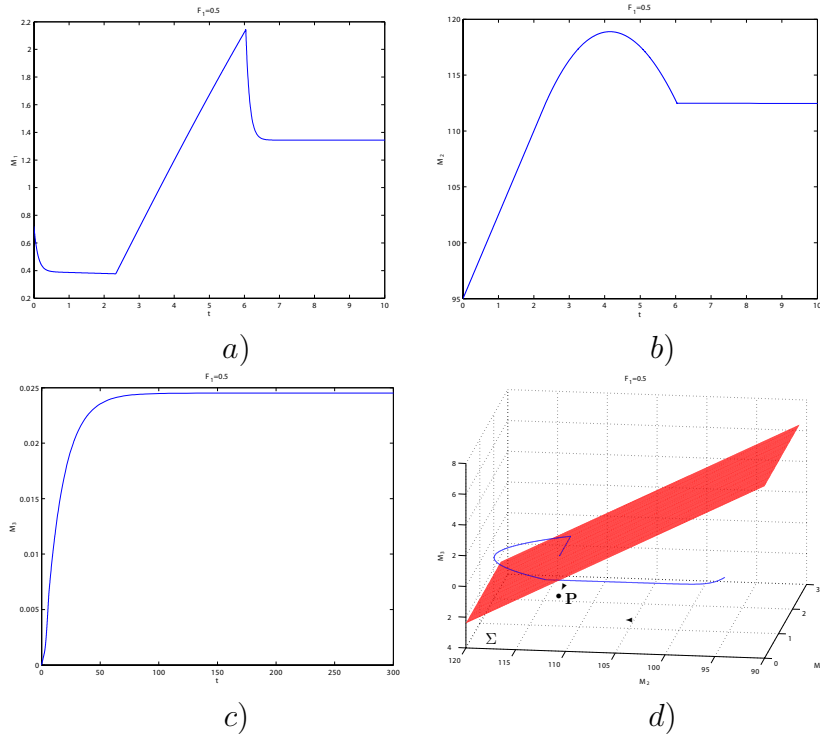Table 1: The parameters used for the simulation of the system.

Figure 4: Soft-drink process: a)–c) The integral curves of the state variables M_1, M_2 and M_3. d) The trajectory of the system (25) starting at the point $(0.72, 95, 0)$.

The behavior of the solution of the Filippov system (25) depends on thirteen parameters $F_1, F_2, \rho_L, \rho_a, V, V_d, T, P_{\text{out}}, X, k_L, k_G, \kappa_c, \sigma$, for a particular values used in simulations, see Table 1.

In Figure 4 a)–c), the integral curves of the state variables M_1, M_2 and M_3 are depicted. In Figure 4 d), the trajectory in coordinates (M_1, M_2, M_3) starting at the point $(0.72, 95, 0)$ is drown, and the boundary Σ (red plane) is shown. On the boundary Σ, the generic pseudo-equilibrium P was detected.

5. Conclusions

In the paper, we gave a brief overview of the theory of Filippov dynamical systems for ordinary differential equations. Many specific applications for example in chemical engineering are based on models of differential algebraic equations, i.e., the problem formulation contains both differential equations and algebraic equations. We show that also in this case the system can be seen as a dynamical system of Filippov type.

As a practical example, a model of the gas-liquid system with a reaction is pre-

sented. This system can't be formulated as a Filippov system with ODEs only. An extension of the Filippov systems theory is necessary. By using a modified Filippov convex method, the integral curves of both differential and algebraic variables can be obtained.

Let us remark that the study of the gas-liquid system is just the first step towards modeling of the real HDPE (High Density Polyethylene) reactor.

In the future, we intend to perform additional studies of Filippov systems with DAEs. Till now, there are assumptions that are too restrictive. Deeper understanding of the behavior of non-smooth dynamical systems defined by DAEs is required.

In simplified model, the generic pseudo-equilibrium P on the boundary Σ acted as an attractor for the whole state space, see [2, 3]. We want to find out whether this also applies in a more general model.

All MATLAB simulations were performed in a modified version of the program developed by Petri T. Piiroinen and Yuri A. Kuznetsov [17].

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