Positively invariant manifolds: concept and applications

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Abstract. In many applications of the system order reduction models, including those focused on spray ignition and combustion processes, it is assumed that all functions in corresponding differential equations are Lipschitzian. This assumption has not been checked in most cases and the cases when these functions were non-Lipschitzian have sometimes been overlooked. This allows us to question the results of application of the conventional theory of integral manifolds to some such systems. The aim of this paper is to demonstrate that even in the case of singular perturbed systems with non-Lipschitzian nonlinearities the order reduction can be performed, using a new concept of positively invariant manifolds. This is illustrated by several examples including the problem of heating, evaporation, ignition and combustion of Diesel fuel sprays.

1. Introduction

The modelling of many processes, including spray ignition and combustion processes in various engineering applications, has been based on the application of Computational Fluid Dynamics (CFD) codes [1, 2], although the limitations of this approach have been widely discussed in the literature [3]. An alternative approach to modelling these processes has been based on asymptotic methods for their analysis [4], applicable in the case when differences in the rates of change of variables are large. These methods can effectively complement the conventional approach to the problem, based on CFD modelling, by highlighting the physical background of individual processes [4]. One of these methods has been based on the theory of integral manifolds for singularly perturbed systems [5, 6, 7, 8], focused on the analysis of the following autonomous system:

\[ \dot{x} = f(x, y, \varepsilon), \quad \varepsilon \dot{y} = g(x, y, \varepsilon) \]  \hspace{1cm} (1)

where \(0 < \varepsilon \ll 1\), \(x \in \mathbb{R}^m\), \(y \in \mathbb{R}^n\), in \(\mathbb{R}^{m+n} = \mathbb{R}^m \times \mathbb{R}^n\). A surface \(y = \mathcal{R}(x, \varepsilon)\) is called a slow invariant manifold of System (1) if any trajectory \(x = x(t, \varepsilon)\), \(y = y(t, \varepsilon)\) of System (1) that has at least one common point \(x = x_0\), \(y = y_0\) with the surface \(y = \mathcal{R}(x, \varepsilon)\), i.e. \(y_0 = \mathcal{R}(x_0, \varepsilon)\), lies entirely on this surface, i.e. \(y(t, \varepsilon) = \mathcal{R}(x(t, \varepsilon), \varepsilon)\). In order to find this manifold, the functions \(f(x, y, \varepsilon)\) and \(g(x, y, \varepsilon)\) must be smooth and therefore satisfy the Lipschitzian condition:

\[ \|g(x_1, y_1) - g(x_2, y_2)\| \leq \mathcal{L} \|x_1 - x_2\| + \|y_1 - y_2\|, \]  \hspace{1cm} (2)
where \((x_1, y_1), (x_2, y_2)\) are arbitrary points in the domain and \(L > 0\).

In numerous papers, including [9, 4], the results of application of this theory to modelling of spray ignition and combustion processes are described. The analyses of spray ignition and combustion processes in these papers are based on the Arrhenius chemical model and these processes are indistinguishable from the point of view of modelling. The authors of [10] drew attention to the fact that in the model described in [4], Condition (2) is not satisfied which cast doubt on the validity of the results presented in [4]. In [10] an alternative approach to the analysis of the problem described in [4], using the new concept of positively invariant manifolds and the Tikhonov theorem, has been adopted (also see [3]).

Similarly to [10], our analysis will focus on the investigation of positively invariant manifolds for non-Lipschitzian systems, describing the processes of spray ignition and combustion. In contrast to [10] we will focus not on the model described in [4], but on a more advanced model, taking into account the volumetric absorption of the thermal radiation in droplets, developed in [11]. The positively invariant manifolds and Lyapunov functions will be used. Some preliminary results of our analysis were reported in [12].

2. Preliminary examples
To clarify the difficulties emerging during the analysis of differential systems with non-Lipschitzian nonlinearities and the differences between smooth and non-smooth functions we consider several simple examples.

Recall that function \(f(y)\) satisfies the Lipschitzian condition if for some positive \(L\) Inequality (2) is satisfied for all \((x_1, y_1)\) and \((x_2, y_2)\) from the interval under consideration. In this section the analysis will be focused on one-dimensional functions.

Example 1 (Smooth case). A solution to the initial value problem

\[
\frac{dy}{dx} = -y^2, \quad y(0) = 1
\]

can be presented as

\[
y(x) = \frac{1}{1 + x},
\]

where \(y(x) \to 0\) as \(x \to \infty\). It is necessary to use an infinite time interval to obtain this result. The plot of \(y(x)\) predicted by (3) is shown in Figure 1.

![Figure 1. The graph of \(y(x)\) predicted by (3) (smooth case).](image-url)
Example 2 *(Non-Lipschitzian case).* A solution to the initial value problem

\[ \frac{dy}{dx} = -\frac{1}{2}y, \quad y(0) = 1 \]

can be presented as

\[ y(x) = (1 - x/2)^2. \tag{4} \]

This solution is valid at the finite interval \([0, 2]\). This solution is smooth at \(x = 2\) but function \(F(y) = \frac{1}{2}y\) does not satisfy the Lipschitzian condition at any neighbourhood of \(y = 0\) as its derivative is infinitely large at \(y = 0\). The plot of \(y(x)\) predicted by (4) is shown in Figure 2. Equations leading to non-Lipschitzian solutions are referred to as equations with non-Lipschitzian non-linearities.

![Figure 2](image-url)

**Figure 2.** The graph of \(y(x)\) predicted by (4) (non-Lipschitzian case).

Example 3 *(Discontinuous case).* A solution to the initial value problem

\[ \frac{dy}{dx} = -\text{sgn}(y), \quad y(0) = 1 \]

can be presented as

\[ y(x) = (1 - x). \tag{5} \]

This solution is valid at the finite interval \([0, 1]\). It is not smooth at \(x = 1\). The plot of \(y(x)\) predicted by (5) is shown in Figure 3.

These examples show that, in a certain sense, differential equations with non-Lipschitzian non-linearities occupy an intermediate position between equations with smooth and discontinuous non-linearities (i.e. equations with solutions leading to smooth and discontinuous functions).

3. Finite time processes

The physical processes characterised by a finite period of existence are well known (e.g. droplet evaporation time). These processes are commonly described by non-smooth ODEs. In what follows this is illustrated by considering the scalar ODE:

\[ \frac{dy}{dt} = f(y), \quad f(0) = 0, \quad y(0) = y_0 > 0. \]
The integration of this equation, assuming that \( y(T) = 0 \), where \( T \) is the finite time, gives
\[
\int_{y_0}^{0} \frac{dy}{f(y)} = T.
\]
Assuming that \( f(y) = -y^\alpha \) one can see that the integral in the left hand side of this equation
\[
\int_{y_0}^{0} \frac{dy}{f(y)} = \frac{y_0^{1-\alpha}}{1-\alpha}
\]
converges if and only if \( \alpha < 1 \). Thus for a finite \( T \), function \( f(y) = -y^\alpha \) does not satisfy the Lipschitzian condition.

This conclusion can be generalised for
\[
f(y) = -y^\alpha (\varphi + f_1(y)),
\] where \( 0 < \varphi < \infty, |f_1(y)| \leq \mu < \varphi \). This is inferred from the fact that \( \varphi - \mu \leq \varphi + f_1(y) \leq \varphi + \mu \) and, therefore, \( T_- < T < T_+ \) where
\[
T = \int_{y_0}^{0} \frac{dy}{f(y)}, \quad y(T) = 0,
\]
and
\[
T_+ = \int_{y_0}^{0} \frac{dy}{-y^\alpha (\varphi - \mu)} = \frac{y_0^{1-\alpha}}{(1-\alpha)(\varphi - \mu)}, \quad T_- = \int_{y_0}^{0} \frac{dy}{-y^\alpha (\varphi + \mu)} = \frac{y_0^{1-\alpha}}{(1-\alpha)(\varphi + \mu)}.
\]

**Example 4** Let us consider the system
\[
dx/dt = 1, \quad dy/dt = -y^{1/2}; \quad x(0) = x_0, \quad y(0) = y_0
\] (7)
for which the trajectory \( y = 0 \) plays the role of a positively invariant manifold, i.e. the trajectory for any solution of (7) with \( y_0 = 0 \) lies on this manifold for all \( t > 0 \). The trajectory of any solution of (7) with \( y_0 > 0 \),
\[
y = \left(y_0^{1/2} + (x_0/2) - (x/2)\right)^2,
\]
reaches this manifold at \( x = 2y_0^{1/2} + x_0 \) and then stays on it at longer \( t \). Thus, \( y = 0 \) is positively invariant but it is not actually invariant since trajectories can leave this manifold when \( t \) decreases. An infinite number of trajectories with \( y_0 > 0 \) can pass through any point on \( y = 0 \).
4. Positively invariant manifolds
The concept of positively invariant manifolds will now be illustrated based on the following system:

\[ \begin{align*}
\dot{x} &= f(x, y), \\
\dot{y} &= \psi(y)g(x, y),
\end{align*} \tag{8, 9} \]

where \( x \) is a vector and \( y \) is a scalar. Scalar function \( \psi(y) \) is assumed to be non-Lipschitzian. We assume that \( 0 < \varphi_1 \leq g(x, y) \leq \varphi_2 \) for sufficiently small non-negative values of \( y \). \( f(x, y) \), and \( g(x, y) \) are continuous functions. The analysis will focus on \( \psi = -y^\alpha \) \((0 < \alpha < 1)\).

As the right hand side of (9) is zero at \( y = 0 \), any trajectory, described by (8)-(9), starting at \((x_0, 0)\) on the surface \( y = 0 \) lies on this surface for all \( t \geq 0 \). This surface is not invariant since not all trajectories of System (8)-(9) which have at least one point in common with this surface lie entirely on it; trajectories can leave this surface when \( t \) decreases. This surface, however, is positively invariant since any solution to System (8)-(9) starting at \((x_0, y_0)\) with sufficiently small positive \( y_0 \) reaches this surface during a finite time interval. Moreover, this surface is attractive. This can be proven, using the approach suggested in [13], by considering the Lyapunov function \( V(y) = y^2/2 \) with the derivative \( \dot{V}(y) = -y^{1+\alpha}g(x, y). \) \( \dot{V}(y) < 0 \) for \( y > 0 \) for all values of \( x \) under consideration. This implies the asymptotic stability of \( y = 0 \) with respect to \( y \) \((y \to 0 \text{ as } t \text{ increases})\).

The same analysis is applicable to the case when \( \psi = (\bar{y} - y)^\alpha \), where \( \bar{y} \) is a positive constant.

**Example 5** Consider now the initial-value problem

\[ \begin{align*}
\dot{y} &= (1 - y)^{1/2}(2 - y)^{1/2},
\end{align*} \tag{10} \]

with \( y(0) = y_0 \), the solution of which can be written in the form

\[ t = \log \frac{2y - 3 + 2\sqrt{(1 - y)(2 - y)}}{2y_0 - 3 + 2\sqrt{(1 - y_0)(2 - y_0)}}. \tag{11} \]

Equation (10) has two equilibria \( y = 1 \) and \( y = 2 \). The right hand side of (10), however, has physical meaning only for \( y < 1 \). Hence, the solution \( y(t) \) with \( y_0 < 1 \) attains the steady state \( y = 1 \) during the finite time

\[ t_1 = \log \frac{1}{3 - 2y_0 - 2\sqrt{(1 - y_0)(2 - y_0)}}, \]

which can be found from (11). For example, for \( y_0 = 0.5 \) this expression gives us

\[ t_1 = \log \frac{1}{2 - \sqrt{3}}. \]

A similar situation exists for the system of equations describing spray ignition and combustion which are discussed later.

**Example 6** Let us now consider the equation:

\[ \dot{y} = C_1(\bar{y} - y)^a(\bar{y} - y)^b \exp \left( \frac{y}{1 + \beta y}\right), \quad y(0) = y_0, \tag{12} \]

with the constants \( C_1 > 0, \; 0 < a < 1, \; 0 < b < 1, \; 0 < \bar{y} < \bar{y}. \) This can be considered as a generalisation of Example 5. Recall that the right hand side of Equation (12) has a physical meaning only for \( y < \bar{y} \). As in the case of the previous example, solution \( y(t) \) with \( y_0 < \bar{y} \) attains the steady state \( y = \bar{y} \) during a finite time, as shown in Figure 4.
5. Spray ignition and combustion model

Making some natural assumptions, spray heating, evaporation, ignition and combustion processes can be described by the following equations with dimensionless variables and parameters [11]:

\[
\frac{d\theta_g}{d\tau} = \frac{1}{\gamma} \left( P_1(\theta_g, \eta, \xi) - P_2(\theta_g, \theta_d, \frac{q}{3}) \right),
\]

\[
\frac{d\eta}{d\tau} = \frac{1}{\nu_f} \left[ -P_1(\theta_g, \eta, \xi) + \frac{\psi}{\nu_f} P_{23}(\theta_g, \theta_d, \frac{q}{3})(1 - \zeta(\theta_d)) \right],
\]

\[
\frac{d\xi}{dt} = -\frac{1}{\nu_{ox}} P_1(\theta_g, \eta, \xi),
\]

\[
\frac{d\theta_d}{d\tau} = \frac{\varepsilon_2}{\varepsilon_4q} P_{23}(\theta_g, \theta_d, \frac{q}{3})\zeta(\theta_d),
\]

\[
\frac{dq}{d\tau} = -\varepsilon_2 P_{23}(\theta_g, \theta_d, \frac{q}{3})(1 - \zeta(\theta_d)).
\]

where

\[
P_1(\theta_g, \eta, \xi) = \eta^a \xi^b \exp \left( \frac{\theta_g}{1 + \beta \theta_g} \right), \quad P_2(\theta_g, \theta_d, r) = \varepsilon_2 r \sqrt{\frac{T_{d0}(1 + \beta \theta_g)}{T_{g0}}} (\theta_g - \theta_d),
\]

\[
P_3(r) = \frac{\varepsilon_1 \varepsilon_3}{4\beta^{2+\beta}} (1 + \beta \theta_{gext})^4, \quad P_{23}(\theta_g, \theta_d, r) = P_2(\theta_g, \theta_d, r) + P_3(r),
\]

\[
\theta_{gext} = \frac{1}{\beta} \frac{T_{ext} - T_{d0}}{T_{d0}}, \quad \xi(\theta_d) = \frac{T_b - T_{d0}(1 + \beta \theta_d)}{T_b - T_{d0}},
\]

with the initial conditions:

\[
\theta_g(0) = \theta_{g0} \neq 0, \quad \theta_d(0) = \theta_{d0} = 0, \quad r(0) = r_0 = 1, \quad \eta(0) = \eta_0, \quad \xi(0) = \xi_0 = 1.
\]

Here \(\theta_g, \eta, \xi, \theta_d\) and \(r\) are dimensionless gas temperature, fuel concentration, oxidiser concentration, droplet temperature and droplet radius, respectively; \(q = r^3\).
5.1. Reduction of the model
In our previous paper [10], a system of equations similar to the one presented above was considered. The main difference between the physical models considered in [10] and described by System (13)-(17) is that the latter system takes into account the volumetric absorption of thermal radiation in droplets. The analysis of [10] was based on the assumption that the droplet radius is the fastest variable in the model, and on the Tikhonov theorem. The present analysis is based on the concept of positively invariant manifolds and the analysis of the Lyapunov functions.

We can prove that System (13)–(17) has the positively invariant manifold \( q \equiv 0 \). This proof is based on the observation that this system can be represented as (8), where \( q \) plays the role of \( y \) and the vector with coordinates \( \theta_g, \eta, \xi \) and \( \theta_d \) plays the role of vector \( x \). The right hand side of (17) can be presented as \(-q^{1/3}g(x, q)\) with
\[
g(x, q) = \varepsilon_2 \left( \varepsilon_1 \frac{T_{\theta b}(1 + \beta \theta_g)}{T_{0\theta}} (\theta_g - \theta_d) + \frac{\varepsilon_1 \varepsilon_3}{4\beta} q^{(1+\beta)/4} (1 + \beta \theta_g^{ext})^4 \right) (1 - \zeta(\theta_d)).
\]
The attractivity of this manifold follows from the analysis of Lyapunov function \( V(q) = q^2/2 \) with derivative \( \dot{V}(q) = -q^{2/3}P_{23}(\theta_g, \theta_d, q^{1/3})(1 - \zeta(\theta_d)). \) \( \dot{V}(q) < 0 \) for all \( \theta_g, \theta_d \) under consideration. This implies the asymptotic stability of \( q = 0 \) with respect to \( q \) (\( q \to 0 \) as \( t \to +\infty \)).

The partial integral of System (13)–(17) is \( q = (e^{\theta_d(\zeta(\theta_d))^{\beta_{db}}})^{\varepsilon_4} \) (see [11]). Note that \( \zeta(\theta_d) \to 0 \) as \( q \to 0 \), i.e. the droplet surface temperature approaches the boiling temperature \( (\theta_d \to \theta_{db}) \) when \( q \to 0 \). Having substituted \( q = 0 \) and \( \theta_d = \theta_{db} \) into (13)–(17), the latter can be rewritten as:
\[
\begin{align*}
\frac{d\theta_g}{d\tau} &= \frac{1}{\gamma} P_1(\theta_g, \eta, \xi), \\
\frac{d\eta}{d\tau} &= -\frac{1}{\nu_f} P_1(\theta_g, \eta, \xi), \\
\frac{d\xi}{dt} &= -\frac{1}{\nu_{ox}} P_1(\theta_g, \eta, \xi).
\end{align*}
\]
Two integrals
\[
\gamma \theta_g + \nu_f \eta = \gamma \theta_{g0} + \nu_f \eta_0
\]
and
\[
\gamma \theta_g + \nu_{ox} \xi = \gamma \theta_{g0} + \nu_{ox}
\]
of (18)–(20) make it possible to eliminate equations for \( \eta \) and \( \xi \) from the following analysis. The final equation for \( \theta_g \) can be presented as:
\[
\frac{d\theta_g}{d\tau} = \frac{1}{\gamma} P_1 \left( \theta_g, \eta_0 - \frac{\gamma}{\nu_f} (\theta_g - \theta_{g0}), 1 - \frac{\gamma}{\nu_{ox}} (\theta_g - \theta_{g0}) \right).
\]
To summarise our analysis, we have shown that application of the concept of positively invariant manifold \( q = 0 \) for (13)–(17) allows one to perform the order reduction of the original non-Lipschitzian system (13)–(17) and to obtain scalar Equation (23) for \( \theta_g \).

6. Conclusions
A concept of positively invariant manifolds for systems with non-Lipschitzian nonlinearities has been introduced and illustrated with several examples. The dynamics of thermal explosion in a fuel droplet/hot air mixture are investigated using this approach. Effects of radiative heating of droplets, semi-transparency of droplets and a limited amount of oxidiser are taken into account. The system of ODEs for gas/droplet temperatures, fuel vapour and oxygen concentrations, and droplet radii are reduced to a single ODE for gas temperature.
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