Parametric Qualitative Analysis of Ordinary Differential Equations: Computer Algebra Methods for Excluding Oscillations (Extended Abstract)

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Abstract. Investigating oscillations for parametric ordinary differential equations (ODEs) has many applications in science and engineering but is a very hard problem.
We review some recently developed criteria which give *sufficient conditions* to exclude oscillations by reducing them to problems on semi-algebraic sets—for polynomial vector fields. We will give some examples and we will discuss possible future work in the form of problems to be solved. Some of these problems might be rather immediate to be solved, some others might pose major challenges.

1 Introduction

Investigating oscillations for parametric ordinary differential equations (ODEs) has many applications in science and engineering but is a very hard problem. Already for two dimensional polynomial systems this question is related to Hilbert's 16th problem, which is still unsolved [1].

Using the theory of Hopf-bifurcations some non-numeric algorithmic methods have been recently developed to determine ranges of parameters for which some small stable limit cycle will occur in the system [2–8]. These algorithms give exact conditions for the existence of fixed points undergoing a Poincaré-Andronov-Hopf bifurcation that give birth to a small stable limit cycle under some general conditions which can be made algorithmic, too. If these conditions are not satisfied, one can be sure that there are no such fixed points, but unfortunately one cannot conclude that there are no limit cycles—which could arise by other means. Nevertheless, it is tempting to conjecture even in these cases that there are no oscillations, as has been done e.g. in [5, 6].

However, the ultimate goal of finding *exact algorithmic conditions* for the existence of oscillations, i. e. for determining for which parameter values there are non-constant limit cycles for a given system of parametric ordinary differential equations is a major challenge, so that considerable work has been spent—and will be also be invested in the future—for investigating sub-problems.

In this paper we deal with computer algebra methods for some of these sub-problems. Our techniques will be along the line of work reducing problems on the qualitative analysis of ordinary differential equations to semi-algebraic problems. This possibility might seem to be surprising on first sight, as even the description of flows induced by the simplest linear ordinary differential equations involves exponential functions. However, a significant part of the study of the qualitative behavior of differential equations can be done in the realm of algebraic or semi-algebraic sets: Starting from the rather trivial observation that for polynomial vector fields the study of the equilibria of the vector field is purely algebraic, also questions of the stability of the equilibria can in general be reduced to decidable questions on semi-algebraic sets (for polynomial vector fields) via the well known Routh-Hurwitz criterion [9]). Also the parametric question (for a parameterized polynomial vector field) whether fixed points undergo a *Hopf bifurcation* is not only known to be decidable but also lies within the realm of semi-algebraic sets [8, 10, 3].

We review some recently developed criteria which give sufficient conditions to exclude oscillations by reducing them to problems on semi-algebraic sets—for polynomial vector fields. We will give some examples and we will discuss possible future work in the form of problems to be solved. Some of these problems might be rather immediate to be solved, some others might pose major challenges.

2 Preliminaries

2.1 The Bendixson-Dulac criterion for 2-dimensional vector fields

Consider an autonomous planar vector field

$$\frac{dx}{dt} = F(x, y), \qquad \frac{dy}{dt} = G(x, y), \qquad (x, y) \in \mathbb{R}^2.$$

Bendixson in 1901 [11] was the first to give a criterion yielding sufficient conditions for excluding oscillations. For a modern proof we refer to [12, Theorem 1.8.2].

Theorem 1 (Bendixson's criterion). *If* $\operatorname{div}(F, G) = \frac{\partial(F)}{\partial x} + \frac{\partial(G)}{\partial y}$ *is not identically zero and does not change sign on a simply connected region* $D \subseteq \mathbb{R}^2$*, then* (F, G) *has no closed orbits lying entirely in* D.

Dulac in 1937 [13] was able to generalize the result of Bendixson as follows:

Theorem 2 (Dulac's criterion). *Let* $B(x, y)$ *be a scalar continuously differentiable function defined on a simply connected region* $D \subset \mathbb{R}^2$ *with no holes in it. If* $\frac{\partial(BF)}{\partial x} + \frac{\partial(BG)}{\partial y}$ *is not identically zero and does not change sign in* D*, then there are no periodic orbits lying entirely in* D.

Dulac's criterion is a generalization of Bendixson's criterion, which corresponds to $B(x, y) = 1$.

2.2 Quantifier elimination and positive quantifier elimination over the ordered field of the reals

In order to summarize the basic idea of real quantifier elimination, we introduce first-order logic on top of polynomial equations and inequalities.

We consider multivariate polynomials $f(u, x)$ with rational coefficients, where $u = (u_1 \dots, u_m)$ and $x = (x_1, \dots, x_n)$. We call u *parameters* and we call x *variables*. Equations will be expressions of the form $f = 0$, inequalities are of the form $f \leq 0$, $f < 0$, $f \geq 0$, $f > 0$, or $f \neq 0$. Equations and inequalities are called *atomic formulae*. *Quantifier-free formulae* are Boolean combinations of atomic formulae by the logical operators "$\wedge$," "$\vee$," and "$\neg$." *Existential formulae* are of the form $\exists x_1 \dots \exists x_n \psi(u, x)$, where ψ is a quantifier-free formula. Similarly, *universal formulae* are of the form $\forall x_1 \dots \forall x_n \psi(u, x)$. A general (prenex) *first-order formula* has several alternating blocks of existential and universal quantifiers in front of a quantifier-free formula.

The real *quantifier elimination problem* can be phrased as follows: Given a formula φ, find a quantifier-free formula φ' such that both φ and φ' are equivalent in the domain of the real numbers. A procedure computing such a φ' from φ is called a real *quantifier elimination procedure*.

Although real quantifier elimination is known to be a computationally hard problem [14, 15], there has been considerable and quite successful research on efficient implementations during the past decades, which has resulted in three major systems:

1. The commercial computer algebra system Mathematica includes an efficient implementation of CAD-based real quantifier elimination by Strzebonski [16, 17], the development of which started around 2000.
2. QEPCAD B [18], which implements partial cylindrical algebraic decomposition (CAD). The development of QEPCAD B started with the early work of Collins and his collaborators on CAD around 1973 and continues until today. QEPCAD B is supplemented by another software called SLFQ for simplifying quantifier-free formulas using CAD. Both QEPCAD B and SLFQ are freely available.[4]
3. REDLOG[5] [19, 20], which had been originally driven by the efficient implementation of quantifier elimination based on virtual substitution methods [14, 21, 22]. Meanwhile REDLOG includes also CAD and Hermitian quantifier elimination [23–25] for the reals as well as quantifier elimination for various other domains [26] including the integers [27, 28]. The development of REDLOG has been started in 1992 by one of the authors (T. Sturm) of this paper and continues until today. REDLOG is included in the computer algebra system REDUCE, which is open source.[6]

[4] http://www.usna.edu/Users/cs/qepcad/B/QEPCAD.html
[5] http://www.redlog.eu/
[6] http://reduce-algebra.sourceforge.net/

Besides regular quantifier elimination methods for the reals, REDLOG includes several variants of quantifier elimination. This includes in particular *extended quantifier elimination* [29], which yields in addition sample solutions for existential quantifiers, and *positive quantifier elimination* [4, 2], which includes powerful simplification techniques based on the knowledge that all considered variables are restricted to positive values.

As in many applications the region of interest is the positive cone of the state variables, and also the parameters of interest are known to be positive, the positive quantifier elimination is of special importance and will be used for many of the examples given below.

3 Some Algorithmic Global Criteria for Excluding Oscillations

The algorithmic criteria discussed in the following can be seen as generalizations of the Bendixson-Dulac criterion for 2-dimensional vector fields to arbitrary dimensions.

3.1 Muldowney's Criteria

The following theorem was proved by Muldowney [30, Theorem 4.1]: Suppose that one of the inequalities

$$\mu\left(\frac{\partial f^{[2]}}{\partial x}\right) < 0, \qquad \mu\left(-\frac{\partial f^{[2]}}{\partial x}\right) < 0 \tag{1}$$

holds for all $x \in \mathbb{R}^n$. Then the autonomous system with vector field $f : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ has no nonconstant periodic solutions. Here μ is some Lozinskiĭ norm and $f^{[2]}$ is one of the "compound matrices" of the Jacobian of the vector field f defined in [30]. As as also shown in [30] the criterion given in [30, Theorem 4.1] also holds when $x \in C$, where $C \subseteq \mathbb{R}^n$ is open and convex.

Remark. When $n = 2, \partial f^{[2]}/\partial x = \mathrm{Trace}\, \partial f/\partial x = \mathrm{div} f$, so that [30, Theorem 4.1] gives the results of Bendixson, i.e. the criterion of Muldowney can be seen as a generalization of the criterion of Bendixson from the planar case to arbitrary dimensions.

According to [30, (2.2)], any of the following expressions may be used as $\mu\left(\partial f^{[2]}/\partial x\right)$ in [30, Theorem 4.1].

$$\max\left\{ \frac{\partial f_r}{\partial x_r} + \frac{\partial f_s}{\partial x_s} + \sum_{q \neq r,s} \left|\frac{\partial f_q}{\partial x_r}\right| + \left|\frac{\partial f_q}{\partial x_s}\right| \,:\, r, s = 1, \ldots, n,\, r \neq s \right\}, \tag{2}$$

$$\max\left\{ \frac{\partial f_r}{\partial x_r} + \frac{\partial f_s}{\partial x_s} + \sum_{q \neq r,s} \left|\frac{\partial f_r}{\partial x_q}\right| + \left|\frac{\partial f_s}{\partial x_q}\right| \,:\, r, s = 1, \ldots, n,\, r \neq s \right\}. \tag{3}$$

Thus for a formula γ over the reals defining an open convex subset C of $\mathbb{R}^n$ and an autonomous polynomial vector field $f : \mathbb{R}^n \to \mathbb{R}^n$ the following first-order formula over the real closed field defines a sufficient condition such that the vector field defined by f has no non-constant periodic solution on C:

$$\begin{aligned}
\varphi \equiv\ & \forall x_1 \forall x_2 \cdots \forall x_n \Bigg(\gamma \Longrightarrow \\
& \max\left\{ \frac{\partial f_r}{\partial x_r} + \frac{\partial f_s}{\partial x_s} + \sum_{q \neq r,s} \left| \frac{\partial f_q}{\partial x_r} \right| + \left| \frac{\partial f_q}{\partial x_s} \right| \ : \ r, s = 1, \ldots, n,\ r \neq s \right\} < 0 \Bigg) \\
& \vee\ \forall x_1 \forall x_2 \cdots \forall x_n \Bigg(\gamma \Longrightarrow \\
& \max\left\{ -\frac{\partial f_r}{\partial x_r} - \frac{\partial f_s}{\partial x_s} + \sum_{q \neq r,s} \left| \frac{\partial f_q}{\partial x_r} \right| + \left| \frac{\partial f_q}{\partial x_s} \right| \ : \ r, s = 1, \ldots, n,\ r \neq s \right\} < 0 \Bigg) \\
& \vee\ \forall x_1 \forall x_2 \cdots \forall x_n \Bigg(\gamma \Longrightarrow \\
& \max\left\{ \frac{\partial f_r}{\partial x_r} + \frac{\partial f_s}{\partial x_s} + \sum_{q \neq r,s} \left| \frac{\partial f_r}{\partial x_q} \right| + \left| \frac{\partial f_s}{\partial x_q} \right| \ : \ r, s = 1, \ldots, n,\ r \neq s \right\} < 0 \Bigg) \\
& \vee\ \forall x_1 \forall x_2 \cdots \forall x_n \Bigg(\gamma \Longrightarrow \\
& \max\left\{ -\frac{\partial f_r}{\partial x_r} - \frac{\partial f_s}{\partial x_s} + \sum_{q \neq r,s} \left| \frac{\partial f_r}{\partial x_q} \right| + \left| \frac{\partial f_s}{\partial x_q} \right| \ : \ r, s = 1, \ldots, n,\ r \neq s \right\} < 0 \Bigg).
\end{aligned} \tag{4}$$

The maximum and absolute value functions are included in the language of ordered rings as it is commonly used for real quantifier elimination. They are, however, definable.

In [31] the problem of efficient automatic resolution of maxima and absolute values is addressed and computation examples are given.

3.2 An Algorithmic Global Criterion Excluding Oscillations Based on Algebraic First-Integrals

Computing algebraic first-integrals Another algorithmic method to parametrically investigate the absence of oscillations relies on the possibility to compute algebraic first integrals of polynomial vector fields. Those do not necessarily exist, but if there exists such first integrals up to a certain degree these can be computed by the following method described in the book by Goriely [32].

Consider an n-dimensional polynomial vector field $\mathbf{G}$ of degree d. In general, this vector field may depend on a certain number of parameters, say $(\nu_1, \ldots, \nu_p)$. The problem consists of finding the values of $(\nu_1, \ldots, \nu_p)$ such that the vector field admits a time-independent polynomial first integral of a given degree $\mathbf{D}$.

1. Start with $\mathbf{D} = 1$.

2. Consider the most general form of a polynomial first integral of degree $\mathbf{D}$

$$\mathbf{I}(\mathbf{x}) = \sum_{i,|i|=1}^{|i|=D} c_i \mathbf{x}^i. \tag{5}$$

3. Compute the time derivative of $\mathbf{I}(\mathbf{x})$.

$$\delta_{\mathbf{G}} \mathbf{I} = \sum_{i,|i|=0}^{|i|=D+d-1} \mathbf{Q}_i \mathbf{x}^i. \tag{6}$$

4. Since we are looking for $\mathbf{I}$ such that $\delta_{\mathbf{G}} \mathbf{I} = 0$, we have $\mathbf{Q}_i = 0$. This system of equations is a linear system for the coefficients c_i of dimension at most $\begin{pmatrix} n+d+D-1 \\ n \end{pmatrix}$. So, if there exist values of the parameter $(\nu_1, \ldots, \nu_p)$ and a set of constants c_i that are not all zero, such that $\mathbf{Q}_i = 0$ for all i, then $\mathbf{I}(\mathbf{x})$ is a first integral. Otherwise increase $\mathbf{D}$ by 1 and return to Step 2.

Notice that the linear system of equations constructed above are under determined in general, so that several different first integrals might arise when solving these systems.

A generalization of the Bendixson-Dulac criterion involving first-integrals For our algorithmic criteria we use the following generalization of the Bendixson-Dulac criterion for 2d-vector-fields to arbitrary dimensions proved by Tóth [33, Theorem 3.1]:

Theorem 3. *Let $M \in \{2, 3, 4, \ldots\}$ and let $T \subset \mathbb{R} \times \mathbb{R}^{M-1}$ be a domain such that for all $\bar{x} \in \mathbb{R}$ the set*

$$\Im(\bar{x}) := \{y \in \mathbb{R}^{M-1} \mid (\bar{x}, y) \in T\}$$

is convex. *Let $J : T \longrightarrow \mathbb{R}^M$ be continuous and suppose that there exists a sufficiently smooth function $P = (P_1, , ..., P_{M-1}) : T \longrightarrow \mathbb{R}^{M-1}$ such that its coordinate functions are (global) first integrals of the equation*

$$\dot{x} = J \circ x, \tag{7}$$

and let us suppose that for all $\bar{x} \in \mathbb{R}$ and $y^1, ..., y^{M-1} \in \Im(\bar{x})$

$$\begin{vmatrix} \partial_2 P_1(\bar{x}, y^1) \\ \vdots \\ \partial_2 P_{M-1}(\bar{x}, y^{M-1}) \end{vmatrix} \neq 0 \tag{8}$$

Then the differential equation (7) has no periodic solution.

If the convex set $\Im(\bar{x})$ is semi-algebraic and one can compute sufficiently many algebraic first-integrals then Theorem 3 yields a quantifier elimination problems over the ordered field of the reals.

4 Computation Examples

We have extended the Maple library QEHOPFLIB[7] implementing the methods in [8] by the following algorithmic methods:

1. Algorithms to produce from a system of ordinary differential equations essentially a formula corresponding to $\varphi_{\text{Muldowney}}$ as described by Equation (4). The formula can be generated for arbitrary vector fields, its symbolic analysis by quantifier elimination over the reals is only possible for systems of differential equations with a vector field described by parameterized multivariate rational functions.
2. Algorithms trying to compute algebraic first integrals up to a degree bound and to produce from a system of ordinary differential equations essentially a formula corresponding to the universally quantified condition in Theorem 3. Let us call this formula φ_{Toth}. The formula can be generated only for vector fields of dimension n which have at least $n-1$ algebraic first integrals up to the used degree bound d. Notice that the vector field can be described by parameterized multivariate rational functions.

In the examples discussed below we use the positive cone of the real n-space as convex subset, or the entire real n-space.

Actually, we produce the logical negation $\neg\varphi$ of φ rather than φ itself (for $\varphi_{\text{Muldowney}}$ as well as for φ_{Toth}), since the implementation of positive quantifier elimination in the current stable branch of REDLOG is restricted to existential formulas. It is, however, not hard to see that applying positive quantifier elimination to $\neg\varphi$ yielding, say, ψ and then positively simplifying $\neg\psi$, which involves re-adding the positivity conditions on all variables, yields exactly the desired result of applying to φ quantifier elimination subject to positivity assumptions on all variables. We are usually going to refer to this final result as φ'.

4.1 A non-parametric example

As a first simple example we take the following simple reaction that was already studied in [33]:

Simple reaction system: It is the induced kinetic differential equation (cf. [34]) of the reaction

$$3\,\mathrm{OH} \xrightarrow{1} \mathrm{H_2O} + \mathrm{HO_2}, \qquad \mathrm{H_2O} + \mathrm{HO_2} \xrightarrow{1} 3\,\mathrm{OH} \tag{9}$$

i.e.

$$\dot{x} = -3x^3 + 3yz, \qquad \dot{y} = x^3 - yz, \qquad \dot{z} = x^3 - yz \tag{10}$$

where the concentrations of the components are denoted by x, y and z with $x := [\mathrm{OH}], y := [\mathrm{H_2O}], z := [\mathrm{HO_2}]$.

This model does not seem to have oscillatory behavior. Although it does not depend on parameters the question of a *proof* that there are no oscillations

[7] http://cg.cs.uni-bonn.de/project-pages/symbolicanalysis/

for any values of the concentrations of the reactants, i.e. the state variables, is already beyond the scope of pure numerical computations.

Using the undetermined coefficients method one find two first-integrals of degree one algorithmically. The generated first-order formula φ_{Toth} describing the negation of the criterion of Tóth can be reduced by REDLOG to *false* within some milliseconds on a current standard PC. Thus this example can be solved fully algorithmically by the method computing first integrals.

Using the criterion of Muldowney [30, Theorem 4.1] (for the L^1 norm and L^∞ norm) one can also come up easily with a first order-formula (describing the negation of the Muldowney criterion for excluding oscillations). This formula $\varphi_{\mathrm{Muldowney}}$ can be reduced by REDLOG to *true* within a few milliseconds, which unfortunately is the non-conclusive answer: one cannot prove the absence of oscillations in this way—a result not contradicting the result stated above, as the Muldowney criterion is a sufficient but not a necessary condition for the absence of oscillations.

4.2 Parametric examples

The question whether there are oscillations or not is a parametric question in general. As the generated formula φ' can be parametric and the result of the quantifier elimination procedure will be a condition on the parameters in general—i.e. a first-order formula involving the parameters only.

Models of Genetic Circuits For the family of examples arising out of a simple quasi-steady state approximation of a model of genetic circuits investigated in [5] the Muldowney criteria in its realization of the framework of [31] can proof the absence of oscillations for several relevant values of parameters. We refer to [5, 31] for an exposition of the models and to [31] for the results.

Using the first-integral based method described in this paper we could not come up with any conclusive result for any of the examples from [5].

A model of viral dynamics The following example is also discussed in more depth in [31]. It consists of a simple mathematical model for the populations dynamics of the human immunodefficiency type 1 virus (HIV-1) investigated in [35]. There a three-component model is described involving uninfected CD4 + T-cells, infected such cells and free virus, whose densities at time t are denoted by $x(t), y(t), v(t)$.

In [35] a simplified two-component model employed by Bonhoeffer et al. [36] is investigated analytically.

For the two-component model the equilibria are computed analytically for biologically relevant non-negative parameter values and their local stability properties are parametrically investigated in [35]. Moreover, using the general Bendixson-Dulac criteria for 2D-vector fields with an ad hoc Dulac function $B(x, y) = 1/y$ it is shown that there are no periodic solutions for the system

```
eq1 := diff(x(t),t) = s - mu*x(t) - beta*x(t)*v(t);
eq2 := diff(y(t),t) = beta*x(t)*v(t) - alpha*y(t);
eq3 := diff(v(t),t) = c*y(t)-gamma1*v(t);
fcns:={x(t),y(t),v(t)};
params:={s,mu,beta,alpha,c,gamma1};
paramcondlist:={s>0,mu>0,beta>0,alpha>0,c>0,gamma1>0};
DELimitCycleMuldowney({eq1,eq2,eq3},
      fcns,params,{},paramcondlist);
od;
```

Fig. 1. A Maple script for generating the first-order formulas $\neg\varphi$ for the three-component model of viral dynamics from [35].

for positive parameter values and positive values of the state variables, i.e. the biologically relevant ones.

Using our algorithms, we can easily construct the formula for the Muldowney criteria even for the three-component model, cf. Figure 1—but we could not compute first-integrals for this system. Using REDLOG quantifier elimination and formula simplification of the obtained first-order formula can be performed within some milliseconds. Unfortunately, the obtained result for the negated Muldowney criteria is a non-parametric *true*, i. e. the non-conclusive answer, as they give sufficient conditions for excluding oscillations, but no indication about a necessary condition.

Also when applying our framework to the two-component model, we obtain the non-conclusive *true* within some milliseconds of computation time.

In our framework we can easily use Dulac functions for 2D-cases, too. When using the Dulac function $B(x, y) = 1/y$ for the two-component model, we obtain the conclusive *false* as an answer, i.e. we can prove that there are no oscillations for the two-component model (for any values of the parameters).

So the hand computations using Dulac functions can be widely simplified by our framework—however,one has to specify the Dulac function in addition to the vector field.

5 Some Possible Future Directions

In the examples given above sometimes one of the given criteria was successful, sometimes the other one, and very often none of them. So a first problem is the following.

Problem 1. What is the relative strength of the Muldowney criteria for different norms? What are their combined strengths compared to the criteria involving first integrals?

In one of our computation examples (cf. Sect. 4.2) it was necessary to use an appropriate Dulac function in order to come up with a criterion proving the absence of oscillations.

An inspection of the proof of [30, Theorem 4.1] seems to indicate that the answer to the following problem is “yes”.

Problem 2. Are there generalizations of the criterion of Muldowney involving Dulac functions?

In the positive case one might ask how to find appropriate Dulac functions. For polynomial functions (or rational functions) one could use the approach to specify those with undetermined coefficients up to a certain degree—and then use these in the quantifier-elimination step. However, in its naive realization the computational complexity does not only seem to be prohibitive under worst case considerations, but also for most but the most trivial cases. So the following problem occurs:

Problem 3. Are there constructive and efficient ways for generating appropriate Dulac functions for the criterion of Muldowney?

The Bendixson-Dulac criteria are not only generalizable using first-integrals as has been done in [33] or also e.g. in [37], but also to systems with invariant hypersurfaces.

Problem 4. Specify algorithmic methods for excluding oscillations using algebraic invariant hypersurfaces.

A standard technique for excluding oscillations in hand computations is to find Lyapunov functions, which also prohibit the existence of oscillations. As the existence of Lyapunov functions of certain form can also be proven by quantifier elimination techniques [38] the following problem shall be formulated:

Problem 5. Are there constructive and efficient ways for generating appropriate Lyapunov functions? Can these be defined semi-algebraically for polynomial vector fields?

Finally the following problems, which are presumably much more challenging, shall be posed:

Problem 6. For autonomous polynomial vector fields are there algorithmic criteria that are *sufficient and necessary* for excluding oscillations?

All of the questions also generalize to differential algebraic equations [39, 40]. Although having an additional “algebraic part” seems to be compatible with the semi-algebraic context, which the qualitative investigations of the ODEs have been reduced to, many new definitional and theoretical problems arise. Of particular interest is here the possibility of various forms of singularities [41] leading for example to singularity induced bifurcations.

Problem 7. Generalize the problems to differential algebraic equations (possibly with singularities).

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