Solving Parametric Polynomial Systems by RealComprehensiveTriangularize

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Abstract. In the authors' previous work, the concept of comprehensive triangular decomposition of parametric semi-algebraic systems (RCTD for short) was introduced. For a given parametric semi-algebraic system, say S, an RCTD partitions the parametric space into disjoint semi-algebraic sets, above each of which the real solutions of S are described by a finite family of triangular systems. Such a decomposition permits to easily count the number of distinct real solutions depending on different parameter values as well as to conveniently describe the real solutions as continuous functions of the parameters. In this paper, we present the implementation of RCTD in the RegularChains library, namely the Re-alComprehensiveTriangularize command. The use of RCTD is illustrated by the stability analysis of several biological systems.

Keywords: Parametric polynomial system, real comprehensive triangular decomposition, RegularChains

1 Introduction

Parametric polynomial systems arise naturally in many applications. For this reason, the computer algebra community has contributed many techniques to deal with such systems, by means of various tools such as cylindrical algebraic decomposition [9], quantifier elimination [2, 1], comprehensive Gröbner bases [14], discriminant varieties [11] or border polynomials [15], as well as comprehensive triangular decomposition (CTD).

The concept of comprehensive triangular decomposition was introduced in [5] in order to study the specialization properties of regular chains. As a byproduct, one can determine for which parameter values, a parametric polynomial system has complex solutions, or, in general, compute the projection of a constructible set, or do quantifier elimination over an algebraically closed field. In [3], different variants of CTDs were proposed, including disjoint squarefree CTD and real

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CTD (RCTD). The former is used to count and describe distinct complex solutions depending on parameters, whereas the latter is used to count and describe distinct real solutions depending on parameters.

Informally speaking, an RCTD of a parametric semi-algebraic system S is a partition of the parametric space into disjoint semi-algebraic sets together with a family of triangular systems, such that above each cell in the partition, the real solutions of S are disjoint (if finitely many) and are described by a sub-family of the triangular systems. RCTD is implemented as RealComprehensiveTriangularize in the RegularChains library.

In Section 2, we illustrate the functionality of RCTD through the analysis of the stability of a simple dynamical system. In Section 3, we present some more advanced applications of RCTD. In Sections 4 and 5, we briefly explain the theory behind RCTD and list the related RegularChains commands.

2 Functionality

In the field of biology, a very important problem is to study the stability of the equilibria (or steady states) of a biological system. For a biological system, say BS, modeled by a system of autonomous differential equations, say

$$DS: \frac{d\mathbf{x}(t)}{dt} = F(\mathbf{u}, \mathbf{x}),$$

the equilibria of BS (or DS) are defined as the real zeros of $F(\mathbf{u}, \mathbf{x})$. Here **u** denotes parameters.

Assuming that F is a vector of rational functions in $\mathbb{Q}[\mathbf{u}, \mathbf{x}]$, the study of the equilibria of BS can often be reduced to solving a parametric semi-algebraic system. Taking also into consideration the fact that certain degenerated behaviors have no practical interest, in [6,3], the authors introduced the concept of *real comprehensive triangular decomposition* (RCTD). Broadly speaking, for a parametric semi-algebraic system S, a RCTD is given by

- (a) a partition of the whole parameter space such that above each cell
 - (i) either the corresponding constructible system induced by S has infinitely many complex solutions,
 - (ii) or S has no real solutions,
 - (iii) or S has finitely many real solutions which are continuous functions of the parameters and with disjoint graphs.
- (b) in Case (iii), a description of the solutions of S as functions of the parameters by means of triangular systems.

RealComprehensiveTriangularize is the RegularChains command computing RCTDs. We apply it to the stability analysis of the dynamical system below, an instance of the *multiple switch model* proposed in [8] by Cinquin and Demongeot:

$$\begin{aligned} \frac{dx}{dt} &= -x + \frac{s}{1+y^2} \\ \frac{dy}{dt} &= -y + \frac{s}{1+x^2}, \end{aligned}$$

where x, y denote concentrations of two proteins and s denotes the strength of unprocessed protein expression. One wishes to determine the values of the parameter s for which this system is bistable, that is, those parameter values for which the system has two asymptotically stable equilibria. Figure 1 shows how to set up the problem while Figure 2 illustrates the stability analysis conducted through RCTD computation. On this latter, one can see that the biological system is bistable if and only if s > 2 holds. Moreover, in this case, the concentrations x and y are expressed as functions of s. The following plots illustrate the bi-stability.



Let us explain now the usage of RealComprehensiveTriangularize as shown in Figure 2. The function takes three arguments: (1) a semi-algebraic system, (2) the number of its parameters and (3) a polynomial ring for which the list of its variables are sorted in descending order. For this example, the second argument "1" means that the last variable, that is s, is the only parameter. The output consists of (i) two squarefree semi-algebraic systems in a triangular shape and, (ii) three semi-algebraic sets forming the partition of the parameter space. In this output, the list of indices following a semi-algebraic set C specifies the triangular systems describing the solutions above C. If this list of indices is empty, then the input parametric system has no real solutions above C.

After an RCTD is computed, the different numbers of real solutions (depending on the parameter values) are stored in a data-structure. To know the parameter values corresponding to a particular number of real solutions, one can call RealComprehensiveTriangularize with the computed RCTD as input, as well as the polynomial ring and the prescribed number of real solutions.

The real solutions are encoded by squarefree semi-algebraic systems. As we can see on Figure 2, such system consists of a set of equations in a triangular shape and a set of positive inequalities. Moreover, the (real) zero set of any squarefree semi-algebraic system is non-empty and, its dimension is the same as the number of parameters.

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The biological system is described by the following system of differential equations. Its right hand side encodes the equilibria: $\begin{bmatrix} > \text{ ode } := \{\text{diff}(x(t),t) = -x(t)+s/(1+y(t)^2), \text{ diff}(y(t),t)=-y(t)+s/(1+x(t)^2)\}:\\ F := [-x+s/(1+y^2), -y+s/(1+x^2)]: \end{bmatrix}$ The following two Hurwitz determinants determine the stability of the hyperbolic equilibria: $\begin{bmatrix} > \text{ D1 } := -(\text{diff}(F[1], x)+\text{diff}(F[2], y)): \#\text{D1 is 2}\\ D2 := \text{ diff}(F[1], x)+\text{diff}(F[2], y)-\text{diff}(F[1], y)+\text{diff}(F[2], x): \end{bmatrix}$ The semi-algebraic system below encodes the asymtotically stable hyperbolic equilibria: $\begin{bmatrix} > P := [numer(normal(F[1]))=0, numer(normal(F[2]))=0, x>0, y>0, s>0, numer(D2)>0];\\ P:= [-y^2 x - x + s = 0, -y x^2 - y + s = 0, 0 < x, 0 < y, 0 < s, 0 < 1 + 2 x^2 + x^4 + 2 y^2 + 4 y^2 x^2 + 2 y^2 x^4 + y^4 + 2 y^4 x^2 + y^4 x^4 - 4 y x s^2] \end{bmatrix}$

Fig. 1. Study of the stability of equilibria of a biological system: problem set-up.

3 Application

In this section, we show how RealComprehensiveTriangularize is used to analyze the stability of a real life biological system from [13], which was also solved by other parametric solving tools in [12].

The system models the antagonistic interactions between cyclin-dependent kinases and the anaphase promoting complex. It is described by the following dynamical system.

$$\frac{kx}{dt} = k_1 - (k'_2 + k''_2 y)x$$

$$\frac{ky}{dt} = \frac{(k'_3 + k'_3 A)(1-y)}{J_3 + 1 - y} - \frac{k_4 mxy}{J_4 + y}$$

where x and y denotes the concentrations of cyclin B/Cdk dimers and active Cdh1/APC complexes, $k_1, k'_2, k''_2, k''_3, k''_3, k_4$ are rate constants, J_3, J_4 are Michaelis constants, and m is a real parameter representing cell "mass". Figure 3 shows how to compute conditions on m such that the system is bistable by RealComprehensiveTriangularize. The whole computational process is similar to that of Section 2. Isolating the real roots of the univariate polynomial in the output, we obtain three real roots: 0.1097139798, 0.5273193027, 1.132028425. So the system is bistable if and only if 0.1097139798 < m < 0.5273193027 or m > 1.132028425.

4 Related notions and commands

The notion of a regular chain, introduced independently in [10] and [16], is closely related to that of a triangular decomposition of a polynomial system. Broadly speaking, a triangular decomposition³ of a polynomial system S is a set of simpler (in a precise sense) polynomial systems S_1, \ldots, S_e such that

$$p \text{ is a solution of } S \Leftrightarrow \exists i : p \text{ is a solution of } S_i.$$
 (1)

 3 http://en.wikipedia.org/wiki/Triangular_decomposition

Compute a real comprhensive triangular decomposition of P w.r.t. the parameter s: $\begin{bmatrix} R := PolynomialRing([y, x, s]): ctd := RealComprehensiveTriangularize(P, 1, R); ctd := [[[1, squarefree_semi_algebraic_system]], [[semi_algebraic_set, []]], [semi_algebraic_set, [2]]] \\ Derive the values of s such that P has 2 positive real solutions, that is the biological system is bistable:$ $<math display="block">\begin{bmatrix} > ctd2 := RealComprehensiveTriangularize(ctd, R, 2);Display(ctd2[2][1][1],R); Display(ctd2[1][1] [2],R); ctd2 := [[[1, squarefree_semi_algebraic_system]], [[semi_algebraic_set, [1]]]] \\ [2 < s] \\ xy - 1 = 0 \\ x^2 - sx + 1 = 0 \\ y > 0 \\ x > 0 \\ 8xs^3 - 6xs^5 - 4s^2 + 5s^4 - s^6 + xs^7 > 0 \end{bmatrix}$



When the purpose is to describe all the solutions of S, whether their coordinates are real numbers or not, (in which case S is said to be *algebraic*) those simpler systems are required to be regular chains⁴. If the coefficients of S are real numbers and if only the real solutions are required (in which case S is said to be *semi-algebraic*), then those real solutions can be obtained by a triangular decomposition into so-called *regular semi-algebraic systems*, a notion introduced in [4]. In both cases, each of these simpler systems has a triangular shape and remarkable properties, which justifies the terminology. We refer to [7] for a formal presentation on the concepts of a regular chain and a triangular decomposition of a polynomial system

Consider a multivariate semi-algebraic system

$$f_1 = 0, \dots, f_m = 0, h_1 \neq 0, \dots, h_t \neq 0, p_1 > 0, \dots, p_s > 0, \tag{2}$$

with $f_1, \ldots, f_m, h_1, \ldots, h_t, p_1, \ldots, p_s \in \mathbb{Q}[u_1, \ldots, u_d, y_1, \ldots, y_\ell]$. where u_1, \ldots, u_d are regarded as parameters and y_1, \ldots, y_ℓ are regarded as unknowns. Various ways of solving System (2) are available and implemented in the RegularChains library.

One may want to express y_1, \ldots, y_ℓ as functions of u_1, \ldots, u_d . This is essentially done by the command RealComprehensiveTriangularize which was presented in the previous sections.

Alternatively, one may want to simply determine the (u_1, \ldots, u_d) -values for which there exists at least one (y_1, \ldots, y_ℓ) -value satisfying System (2). This

⁴ More generally, a triangular decomposition into regular chains of a polynomial system S with coefficients in an arbitrary field \mathbb{K} describes the solutions of S whose coordinates are in the algebraic closure of \mathbb{K} .

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 $\begin{bmatrix} > F := [k1-(k21+k22*y)*x, (k31+k32*A)*(1-y)/(J3+1-y)-k4*m*x*y/(J4+y)]: \\ F := normal(subs({k1=1/25, k21=1/25, k22=1, k31=1, k32=10, k4=35, J3=1/25, J4=1/25, A=0}, F)); \\ F := \left[\frac{1}{25} - xy - \frac{1}{25}x, -\frac{25(875 xy^2 m - 910 xy m - 25y^2 + 24y + 1)}{(25y - 26)(25y + 1)}\right] \\ > D1 := humer(normal(-(diff(F[1],x)+diff(F[2],y))): D2 := numer(normal(diff(F[1],x)*diff(F[2],y))-diff(F[1],y)*diff(F[2],x))): \\ D2 := numer(normal(diff(F[1],x)*diff(F[2],y)-diff(F[1],y)*diff(F[2],x))): \\ > P := [numer(F[1])=0, numer(F[2])=0, x>0, y>0, m>0, 25*y-26<>0, D1>0, D2>0]: \\ > R := PolynomialRing([x, y, m]): \\ ctd := RealComprehensiveTriangularize(P, 1, R, 2); \\ ctd := [[1, squarefree_semi_algebraic_system]], [[semi_algebraic_set, [1]]]] \\ > out := Info(ctd[2][1][1], R); \\ out := [And(RootOf(28983500 _Z^3 - 51273600 _Z^2 + 22577975 _Z - 1898208, index = real_1) \\ < m, m < RootOf(28983500 _Z^3 - 51273600 _Z^2 + 22577975 _Z - 1898208, index = real_2))], \\ [RootOf(28983500 _Z^3 - 51273600 _Z^2 + 22577975 _Z - 1898208, index = real_3) < m]] \\ \end{bmatrix}$

Fig. 3. Determine when a biological system is bistable.

question is often refered as *existential quantifier elimination* and can be answered by RealComprehensiveTriangularize as well. However, the commands QuantifierElimination and Projection are more specialized answers to this question. In some circumstances, they may run faster than RealComprehensive-Triangularize or provide more compact answers.

Of practical interest is a variant of the previous question, which is specified as follows. Given a non-negative integer range $[k_1, k_2]$, with $k_1 \leq k_2$, determine the (u_1, \ldots, u_d) -values for which there exist at least k_1 and at most k_2 (y_1, \ldots, y_ℓ) -values satisfying System (2). This question is often referred as *real root classification* [15] and can be answered by the RealRootClassification command of the RegularChains library.

Finally, we observe that, in practice, parametric semi-algebraic systems are often given by linear polynomials, that is, multivariate polynomials of total degree 1. For this case, the LinearSolve command of the RegularChains library implements a variant of the Fourier-Motzkin Algorithm.

5 Theoretical concepts underlying RCTDs

This section gathers the mathematical definitions and properties underlying the notion of RCTD. Recall that K is a field; we denote by **K** its algebraic closure. A (squarefree) regular chain T of K[**u**, **y**] specializes well at a point $u \in \mathbf{K}^d$ if T(u) is a (squarefree) regular chain of **K**[**y**] and $\operatorname{init}(T)(u) \neq 0$ holds, where $\operatorname{init}(T)$ denotes the product of the initials of T.

For instance, the regular chain $T = \begin{cases} (s+1)z \\ (x+1)y+s \\ x^2+x+s \end{cases}$ with s < x < y < z

does not specialize well at s = 0 or s = -1. Indeed, we have:

$$T(0) = \begin{cases} z \\ (x+1)y \\ (x+1)x \end{cases} \quad T(-1) = \begin{cases} 0 \\ (x+1)y-1 \\ x^2+x-1 \end{cases}$$

Definition 1 Let $F \subset \mathbb{K}[\mathbf{u}, \mathbf{y}]$. A CTD of the zero set V(F) of F is given by:

- a finite partition C of the parameter space into constructible sets,
- above each $C \in C$, there is a set of regular chains \mathcal{T}_C such that:
 - each regular chain $T \in \mathcal{T}_C$ specializes well at any $u \in C$ and
 - for any $u \in C$, we have $V(F(u)) = \bigcup_{T \in \mathcal{T}_C} W(T(u))$.

where W(T(u)) denotes the zeros of T(u) which do not cancel init(T)(u).

Example 1 A CTD of $F := \{x^2(1+y) - s, y^2(1+x) - s\}$ is as follows:

1. $s \neq 0 \longrightarrow \{T_1, T_2\}$ 2. $s = 0 \longrightarrow \{T_2, T_3\}$

where

$$T_1 = \begin{cases} x^2y + x^2 - s \\ x^3 + x^2 - s \end{cases} \quad T_2 = \begin{cases} (x+1)y + x \\ x^2 - sx - s \end{cases} \quad T_3 = \begin{cases} y+1 \\ x+1 \\ s \end{cases}$$

Definition 2 Let $F \subset \mathbb{K}[\mathbf{u}, \mathbf{y}]$. A DSCTD of V(F) is given by :

- a finite partition C of the parameter space,
- each cell $C \in C$ is associated with a set of squarefree regular chains \mathcal{T}_C such that:
 - each squarefree regular chain $T \in \mathcal{T}_C$ specializes well at any $u \in C$ and
 - for any $u \in C$, $V(F(u)) = \bigcup_{T \in \mathcal{T}_C} W(T(u))$, where \cup denotes disjoint union.

Example 2 A DSCTD of $F := \{x^2(1+y) - s, y^2(1+x) - s\}$ is as follows (where T_1, T_2, T_3 are as above):

 $\begin{array}{l} 1. \ s \neq 0, \ s \neq 4/27 \ and \ s \neq -4 \longrightarrow \{T_1, T_2\} \\ 2. \ s = -4 \longrightarrow \{T_1\} \\ 3. \ s = 0 \longrightarrow \{T_3, T_4\} \\ 4. \ s = 4/27 \longrightarrow \{T_2, T_5, T_6\} \\ T_4 = \begin{cases} y \\ x \\ s \end{cases} T_5 = \begin{cases} 3y - 1 \\ 3x - 1 \\ 27s - 4 \end{cases} T_6 = \begin{cases} 3y + 2 \\ 3x + 2 \\ 27s - 4 \end{cases}.$

We conclude by stating a sketch of the algorithm computing an RCTD. Let $S \subset \mathbb{Q}[\mathbf{u}][\mathbf{y}]$ be a parametric semi-algebraic system. For simplicity, we assume that S consists of equations only.

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- (1) Compute a DSCTD $(\mathcal{C}, (\mathcal{T}_C, C \in \mathcal{C}))$ of S.
- (2) Refine each constructible set cell $C \in C$ into connected semi-algebraic sets by cylindrical algebraic decomposition.
- (3) For each connected cell C above which S has finitely many complex solutions: compute the number of real solutions of $T \in \mathcal{T}_C$ at a sample point u of Cand remove those Ts which have no real solutions at u.

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References

- 1. S. Basu, R. Pollack, and M.-F. Roy. Algorithms in real algebraic geometry, volume 10 of Algorithms and Computations in Mathematics. Springer-Verlag, 2006.
- B. Caviness and J. Johnson, editors. Quantifier Elimination and Cylindical Algebraic Decomposition, Texts and Mongraphs in Symbolic Computation. Springer, 1998.
- 3. C. Chen. Solving Polynomial Systems via Triangular Decomposition. PhD thesis, University of Western Ontario, 2011.
- C. Chen, J. H. Davenport, J. May, M. Moreno Maza, B. Xia, and R. Xiao. Triangular decomposition of semi-algebraic systems. J. Symb. Comp, 49: 3-26, 2013.
- C. Chen, O. Golubitsky, F. Lemaire, M. Moreno Maza, and W. Pan. Comprehensive triangular decomposition. In *Proc. of CASC'07*, volume 4770 of *Lecture Notes in Computer Science*, pages 73–101. Springer Verlag, 2007.
- C. Chen and M. Moreno Maza. Semi-algebraic description of the equilibria of dynamical systems. In Proc. CASC' 2011, 2011.
- 7. C. Chen and M. Moreno Maza. Algorithms for computing triangular decomposition of polynomial systems. J. Symb. Comput. 47(6): 610-642, 2012.
- O. Cinquin and J. Demongeot. Positive and negative feedback: striking a balance between necessary antagonists, 2002.
- G. E. Collins. Quantifier elimination for real closed fields by cylindrical algebraic decomposition. Springer Lecture Notes in Computer Science, 33:515–532, 1975.
- M. Kalkbrener. Three contributions to elimination theory. PhD thesis, Johannes Kepler University, Linz, 1991.
- D. Lazard and F. Rouillier. Solving parametric polynomial systems. J. Symb. Comput., 42(6):636–667, 2007.
- W. Niu and D. M. Wang. Algebraic approaches to stability analysis of biological systems. *Mathematics in Computer Science*, 1:507–539, 2008.
- J. Tyson and B. Novak. Regulation of the eukaryotic cell cycle: Molecular antagonism, hysteresis, and irreversible transitions. *Journal of Theoretical Biology*, 210(2):249 – 263, 2001.
- 14. V. Weispfenning. Comprehensive Gröbner bases. J. Symb. Comp., 14:1–29, 1992.
- L. Yang, X. R. Hou, and B. Xia. A complete algorithm for automated discovering of a class of inequality-type theorems. *Science in China, Series* F, 44(6):33–49, 2001.
- L. Yang and J. Zhang. Searching dependency between algebraic equations: an algorithm applied to automated reasoning. Technical Report IC/89/263, International Atomic Energy Agency, Miramare, Trieste, Italy, 1991.