Advances in Applied Mathematics 71 (2015) 52–67

Contents lists available at ScienceDirect

Advances in Applied Mathematics

www.elsevier.com/locate/yaama

Detecting binomiality ☆

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ARTICLE INFO

Article history:
Received 23 March 2015
Received in revised form 27 August 2015
Accepted 28 August 2015
Available online 7 September 2015

MSC:
primary 13P15, 37N25
secondary 92C42, 13P25, 13P10

Keywords:
Polynomial systems in biology
Binomial ideal
Steady states
Chemical reaction networks

ABSTRACT

Binomial ideals are special polynomial ideals with many algorithmically and theoretically nice properties. We discuss the problem of deciding if a given polynomial ideal is binomial. While the methods are general, our main motivation and source of examples is the simplification of steady state equations of chemical reaction networks. For homogeneous ideals we give an efficient, Gröbner-free algorithm for binomiality detection, based on linear algebra only. On inhomogeneous input the algorithm can only give a sufficient condition for binomiality. As a remedy we construct a heuristic toolbox that can lead to simplifications even if the given ideal is not binomial.

1. Introduction

Non-linear algebra is a mainstay in modern applied mathematics and across the sciences. Very often non-linearity comes in the form of polynomial equations which are much more flexible than linear equations in modeling complex phenomena. The price to be paid is that their mathematical theory—commutative algebra and algebraic geometry—is

☆ The authors are supported by the research focus dynamical systems of the state Saxony-Anhalt.
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http://dx.doi.org/10.1016/j.aam.2015.08.004
0196-8858/

much more involved than linear algebra. Fortunately, polynomial systems in applications often have special structures. In this paper we focus on *sparsity*, that is, polynomials having few terms.

The sparsest polynomials are monomials. Systems of monomial equations are a big topic in algebraic combinatorics, but in the view of modeling they are not much help. Their solution sets are unions of coordinate hyperplanes. The next and more interesting class are *binomial systems* in which each polynomial is allowed to have two terms. Binomials are flexible enough to model many interesting phenomena, but sparse enough to allow a specialized theory [9]. The strongest classical results about binomial systems require one to seek solutions in algebraically closed field such as the complex numbers. However, for the objects in applications (think of concentrations or probabilities) this assumption is prohibitive. One often works with non-negative real numbers and this leads to the fields of real and semi-algebraic geometry. New theory in combinatorial commutative algebra shows that for binomial equations field assumptions can be skirted and that the dependence of binomial systems on their coefficients is quite weak [15]. For binomial equations one can hope for results that do not depend on the explicit values of the parameters and are thus robust in the presence of uncertainty.

The main theme of this paper is how to detect binomiality, that is, how to decide if a given polynomial system is equivalent to a binomial system. The common way to decide binomiality is to compute a Gröbner basis since an ideal can be generated by binomials if and only if any reduced Gröbner basis is binomial [9, Corollary 1.2]. For polynomial systems arising in applications, however, computing a reduced Gröbner basis is often too demanding: as parameter values are unknown, computations have to be performed over the field of rational functions in the parameters. Even though this is computationally feasible, it is time consuming and usually yields an output that is hard to digest for humans. This added complexity comes from the fact that Gröbner bases contain a lot more information than what may be needed for a specific task such as deciding binomiality of a polynomial system. Hence Gröbner-free methods are desirable.

Gröbner-free methods. Gröbner bases started as a generalization of Gauss elimination to polynomials. They have since come back to their roots in linear algebra by the advent of F4 and F5 type algorithms which try to arrange computations so that sparse linear algebra can exploited [7]. Our method draws on linear algebra in bases of monomials too, and is inspired by these developments in computer algebra.

Deciding if a set of polynomials can be brought into binomial form using linear algebra is the question whether the coefficient matrix has a *partitioning kernel basis* (Definition 2.1 and Proposition 2.5). Deciding this property requires only row reductions and hence is computationally cheap compared to Gröbner bases. It was shown in [19] that, if the coefficient matrix of a suitably extended polynomial system admits a partitioning kernel basis, then the polynomial system is generated by binomials. As a first insight we show that the converse of this need not hold (Example 2.8).