DETECTING BINOMIALITY

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Abstract. Detection of binomiality of polynomial systems is discussed. The focus is on linear-algebraic methods which are applicable to a class of large examples where Gröbner basis methods fail. The results are illustrated on steady state equations in chemical reaction network theory.

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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 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

Date: February 26, 2015.
2010 Mathematics Subject Classification. Primary: 13P15, 37N25; Secondary: 92C42, 13P25, 13P10.
Key words and phrases. polynomial systems in biology, binomial ideal, steady states, chemical reaction networks.

The authors are supported by the research focus dynamical systems of the state Saxony-Anhalt.
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 [14]. It can also be shown that the dependence of binomial systems on their coefficients is quite weak. 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. For example, if a polynomial system is equivalent to a binomial system, then its positive real part can be parameterized by monomials. Analysis of these toric steady states yields much more effective results than in the general situation [19].

The main theme of this paper is how to detect binomiality, that is, how to decide if a given polynomial system is equivalent to 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 be 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).

In general computer algebra profits from homogeneity. This is true for Gröbner bases where, for example, Hilbert function driven algorithms can be used to convert a basis for a cheap term-order into one for an expensive order. We also observe this phenomenon in our Gröbner-free approach: a satisfying answer to the binomial detection problem can be found if the given system of polynomials is homogeneous. In Section 3 we discuss this case which eventually leads to Algorithm 3.3.
In the inhomogeneous case things are more complicated. Gröbner basis computations can be reduced to the homogeneous case by an easy trick. Detection of binomiality can not (Example 4.1). We address this problem by collecting heuristic approaches that, in the best case, yield binomiality without Gröbner bases. Our approaches can also be used if the system is not entirely binomial, but has some binomials. In Example 4.4 we demonstrate this on a polynomial system from [3] which describes ERK signaling.

**Deciding multistationarity in systems biology.** While the method works for any polynomial system, our motivation comes from chemical reaction network theory where ordinary differential equations with polynomial right-hand sides are used to model dynamic processes in systems biology. The mathematics of these systems is extremely challenging, in particular since realistic models are huge and involve uncertain parameters. As a consequence of the latter, studying dynamical systems arising in biological applications often amounts to studying parameterized families of polynomial ODEs. The first order of business (and concern of a large part of the work in the area) is to determine steady states which are thus zero sets of families of parameterized polynomial equations. Moreover, the structure of the polynomial ODEs entails the existence of affine linear subspaces that are invariant for solutions. Hence questions concerning existence and uniqueness of steady states or existence of multiple steady states are equivalent to questions regarding the intersection of the zero set of a parameterized family of polynomials with a family of affine linear subspaces [3]. Even though this is difficult in general, a variety of results for precluding multiple steady states has appeared in recent years (see [12, 20] for methods employing the determinant of the Jacobian and [5, 2] for graph based methods). Similarly, a variety of results concerning the existence of multiple steady states have emerged (for example [6, 3]).

If a system is modeled by a polynomial system equivalent to a binomial one, then the problem is much more tractable. Specifically, the positive real part of its zero set can be parameterized by monomials. Whenever this is the case, multistationarity can be precluded by [17, Theorem 1.4] and established by [19, Theorem 5.5]. Both of these results require only the study of systems of linear inequalities. Since zero sets of general polynomial systems need not have parametrizations at all, we view the task of detecting binomiality as an important step in analyzing polynomials from systems biology.

**Notation.** In this paper we work with the polynomial ring $\mathbb{k}[x_1, \ldots, x_n]$ in $n$ variables. The coefficient field $\mathbb{k}$ is usually $\mathbb{R}$, or the field of real rational functions in a set of parameters. Our methods are agnostic towards the field. A system of polynomial equations $f_1 = f_2 = \cdots = f_s = 0$ in the variables $x_1, \ldots, x_n$ is encoded in the ideal $\langle f_1, \ldots, f_s \rangle \subset \mathbb{k}[x_1, \ldots, x_n]$. A binomial is a polynomial with at most two terms. In particular, a monomial is a binomial. It is important to distinguish between binomial ideals and binomial systems. A binomial system $f_1 = \cdots = f_s = 0$ is a polynomial system such that each $f_i$ is a binomial. In contrast, an ideal $\langle f_1, \ldots, f_s \rangle$ is a binomial ideal if there exist binomials that generate the same ideal. Thus general non-binomials
do not form a binomial system, even if they generate a binomial ideal. For the sake of brevity we will not give an introduction to commutative algebra here, but refer to standard text books like [4, 1]. The very modest amount of matroid theory necessary in Section 2 can be picked up from the first pages of [18].

Acknowledgment. We thank David Cox for discussions on the role of homogeneity in computer algebra. We are grateful to Alicia Dickenstein for pointing out a crucial error in an earlier version of this paper. TK is supported by CDS the Center for Dynamical Systems at Otto-von-Guericke University.

2. Gröbner-free criteria for binomiality

The most basic criterion to decide if an ideal is binomial is to compute a Gröbner basis. This works because the Buchberger algorithm is binomial-friendly: an S-pair of binomials is a binomial. Since the reduced Gröbner basis is unique and must be computable from the binomial generators, it consists of binomials if and only if the ideal is binomial. However, Gröbner bases can be very hard to compute, so other criteria using only linear algebra are also desirable. Linear algebra enters, when we write a polynomial system as $A\Psi(x)$, the product of a coefficient matrix $A$ with entries in $\mathbb{k}$, and a vector of monomials $\Psi(x)$. Clearly, if we use row operations on the matrix to bring it into a form where each row has at most two entries, then the ideal is generated by binomials and monomials. This criterion is too naive to detect all binomial ideals since it allows only $\mathbb{k}$-linear combinations of the given polynomials. We show here that, at least for homogeneous ideals, it can be extended to a characterization. Before we embark into the details, we formalize the condition on the matrix.

Definition 2.1. A matrix $A$ has a partitioning kernel basis if its kernel admits a basis of vectors with disjoint supports, that is if there exists a basis $b^{(1)}, \ldots, b^{(d)}$ of ker($A$) such that supp($b^{(i)}$) $\cap$ supp($b^{(j)}$) = $\emptyset$ for all $i \neq j$.

The following proposition allows one to check for a partitioning kernel basis with linear algebra. The underlying reason is the very restricted structure of the kernel, expressed best in matroid language.

Proposition 2.2. The following are equivalent for any matrix $A$.

1) $A$ has a partitioning kernel basis.
2) The matroid of $A$ is a direct sum of uniform matroids $U_{r-1,r}$ of corank one, and possibly several coloops $U_{1,1}$.
3) The reduced row-echelon form of $A$ has at most two entries in each row.

Proof. 1 $\Rightarrow$ 2: Let $c_1, \ldots, c_k$ be the partitioning kernel basis. This basis satisfies the circuit axioms. Indeed, non-containment and circuit elimination are satisfied trivially because there is no overlap between any two circuits. For any element $\tilde{c} \in \text{ker}(A)$, we have $\tilde{c} = \sum_i \lambda_i c_i$. By the partitioning kernel basis property supp($\tilde{c}$) = $\bigcup_i \{\text{supp}(c_i) :
\( \lambda_i \neq 0 \), so \( \tilde{c} \) either \( \tilde{c} \) is proportional to one of the \( c_i \), or its support contains the support of a circuit, so it cannot be a circuit. The columns of \( A \) which do not appear in any circuit are coloops and the remaining columns form a direct sum of \( k \) uniform matroids of corank one.

2 \( \Rightarrow \) 3: If the column matroid of \( A \) is direct sum of matroids, then the unique reduced row echelon form has block structure corresponding to the direct sum decomposition. Therefore it suffices to consider a single block which has one-dimensional kernel of full support (the coloops are \((1 \times 1)\)-identity blocks). Ignoring zero rows, the reduced row echelon form of such a matrix is \((I_{r-1}|c)\) where \( r-1 \) is the rank and \( c \in k^{r-1} \).

3 \( \Rightarrow \) 1: Coloops are columns that appear with coefficient zero in every element of the kernel. Thus we can assume that that there are none and each row of \( A \) has exactly two entries. Let \( c_r \) be a non-pivotal column with \( r-1 \) non-zero entries. Let \( c_1, \ldots, c_{r-1} \) be the corresponding pivotal columns. By construction, the block \((I_{r-1}|c_r)\) has only zeros above and below it, so its unique kernel vector is orthogonal to the kernel of the remaining columns. This procedure can be applied to any non-pivotal column.

\[ \square \]

**Remark 2.3.** Proposition 2.2 shows that the complexity of deciding if a matrix has a partitioning kernel basis is essentially the same as that of Gauss-Jordan elimination. One needs \( O(n^3) \) field operations where \( n \) is the larger of the dimensions of the matrix.

**Remark 2.4.** A direct sum of (arbitrary) uniform matroids is called a partition matroid.

We now translate Proposition 2.2 to polynomial systems.

**Proposition 2.5.** If \( A \) has a partitioning kernel basis, and \( \Psi(x) \) is any vector of monomials, then the ideal \( \langle A\Psi(x) \rangle \subset k[x_1, \ldots, x_n] \) is binomial. If \( A\Psi(x) \) is any system that can be transformed into a binomial system using only \( k \)-linear combinations, then \( A \) has a partitioning kernel basis.

**Proof.** Up to coloops the first part is [19, Theorem 3.3] and the coloops only give monomials. The second statement is clear since \( k \)-linear combinations of polynomials are row operations on the coefficient matrix and those do not change the kernel. \( \square \)

Our general strategy is to suitably extend a given system with redundant polynomials such that linear algebra also works for systems that are binomial, but where \( A\Psi(x) \) does not have a partitioning kernel basis. This happens in the following example.

**Example 2.6.** Let \( f_1 = x - y \), \( f_2 = z - w \), and \( f_3 = x(f_1 + f_2) = x^2 - xy + xz - xw \). Ordering the monomials \( \Psi = (x, y, z, w, x^2, xy, xz, xw) \), the system linearizes as

\[
\begin{pmatrix}
1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & -1 & 1 & -1 & 1 \\
\end{pmatrix}
\cdot
\Psi^T.
\]

The coefficient matrix does not have a partitioning kernel basis since \( f_3 \) is a linear combination of monomial multiples of the binomial generators, but not the generators themselves. Algorithm 3.3 takes this problem into account, working degree by
Theorem 2.7 ([19, Theorem 3.19]). Let \( f_1 = f_2 = \cdots = f_s = 0 \) be a polynomial system. If there exist monomials \( x^{\alpha_1}, \ldots, x^{\alpha_m} \) such that, for some \( i_1, \ldots, i_m \in [s] \), the system
\[
(2.1) \quad f_1 = f_2 = \cdots = f_s = x^{\alpha_1} f_{i_1} = \cdots = x^{\alpha_m} f_{i_m} = 0
\]
has a coefficient matrix with a partitioning kernel basis, then \( \langle f_1, \ldots, f_s \rangle \) is binomial.

Theorem 2.7 is true since the additional generators in (2.1) do not change the ideal that the system generates. This together with the explicit description of the binomial generators in the case of a partitioning kernel basis [19, Theorem 3.3] yields the result. If the condition in Theorem 2.7 was also necessary, then a test for binomiality could be build on trying to systematically identify the monomials \( x^\alpha \). However, the converse of Theorem 2.7 is not true.

Example 2.8. Let \( I = \langle f_1, f_2 \rangle \) be the homogeneous binomial ideal generated by the non-binomials \( f_1 = x - y + x^2 + y^2 + z^2 \), \( f_2 = x^2 + y^2 + z^2 \). For no choice of monomials \( x^{\alpha_1}, \ldots, x^{\alpha_1}, x^{\alpha_2}, \ldots, x^{\alpha_2} \) does the coefficient matrix of the system
\[
(2.2) \quad f_1 = x^{\alpha_1} f_1 = \cdots = x^{\alpha_2} f_1 = f_2 = x^{\alpha_2} f_2 = \cdots = x^{\alpha_2} f_2 = 0
\]
have a partitioning kernel basis.

For the proof Example 2.8 we first need the following curious little fact.

Lemma 2.9. The ideal \( I = \langle x^2 + y^2 + z^2 \rangle \subset k[x, y, z] \) does not contain a binomial.

Proof. Let \( \overline{k} \) be the algebraic closure of \( k \) and consider the extension \( \overline{T} \) of \( T \) to \( \overline{k}[x, y, z] \). Assume \( \overline{T} \) contains a binomial \( b = f(x^2 + y^2 + z^2) \), where \( f \in \overline{k}[x, y, z] \). Since \( b \) can be assumed monic, the part of this equation that lies in \( k[x, y, z] \) is not zero and yields a binomial in \( I \). Consequently, we can assume \( k = \overline{k} \). We can also assume that \( b \) is homogeneous and that it is not divisible by any variable. Indeed, if a variable divides \( b \), then it divides \( f \) and we find a lower degree binomial in \( I \). Since the symmetric group on the variables \( x, y, z \) leaves \( I \) invariant we can assume \( b = x^d - \lambda y^s z^{d-s} \) for some \( 0 \leq s < d \) and \( \lambda \in k \). Since \( k \) is algebraically closed, there is a solution \( \xi \) to the equation \( x^d = -1 \). The generator \( x^2 + y^2 + z^2 \) vanishes at \( (\xi, 1, 0) \) but \( b \) does not. This contradiction shows that \( I \) can not contain a binomial. \( \Box \)

Proof of Example 2.8. Let \( d \) be the highest degree among monomials in the system (2.2) and consider the restriction of all involved polynomials to degree \( d \). By the explicit form of \( f_1 \) and \( f_2 \) only monomial multiples of \( x^2 + y^2 + z^2 \) can contribute to the degree \( d \) part. If the coefficient matrix of the system (2.2) had a partitioning kernel basis, then by Proposition 2.2 row reductions on it would yield a binomial in degree \( d \) which is impossible by Lemma 2.9. \( \Box \)
Example 2.8 may seem contrived, but this kind of “trivial obfuscation” of binomials does happen in applications. Of course, for humans it is obvious that one should first isolate the linear binomial $x - y$ and then search for implied quadratic binomials which reduce the trinomial. Our next aim is Algorithm 3.3 which implements this idea, at least in the homogeneous case. The homogeneity assumption can not be skirted, unfortunately. It is true that an ideal is binomial if and only if its homogenization is binomial [9, Corollary 1.4], but the homogenization is not accessible without a Gröbner basis. It would be superb for our purposes if homogenizing the generators of a binomial ideal would yield a binomial ideal. Unfortunately this is not the case as Example 4.1 shows.

3. The homogeneous case

If a given ideal $I$ is homogeneous, the graded vector space structure of the quotient $\mathbb{k}[x_1, \ldots, x_n]/I$ allows one to check binomiality degree by degree. For this we need some basic facts about quotients modulo binomials (see [9, Section 1] for details). Any set of binomials $B$ in $\mathbb{k}[x_1, \ldots, x_n]$ induces an equivalence relation on the set of monomials in $\mathbb{k}[x_1, \ldots, x_n]$ under which $m_1 \sim m_2$ if and only if $m_1 - \lambda m_2 \in \langle B \rangle$ for some non-zero $\lambda \in \mathbb{k}$. As a $\mathbb{k}$-vector space the quotient ring $\mathbb{k}[x_1, \ldots, x_n]/\langle B \rangle$ is spanned by the equivalence classes of monomials and those are all linearly independent [9, Proposition 1.11]. If the binomials are homogeneous, then the situation is particularly nice. For example, the equivalence classes are finite and elements of the quotient have well-defined degrees. The notions of monomial, binomial, and polynomial are extended to the quotient ring. For example, a binomial is a polynomial that uses at most two equivalence classes of monomials. The unified mathematical framework to deal with quotients modulo binomials are are monoid algebras, but we refrain from introducing this notion here.

As a consequence of the discussion above a polynomial system $f_1 = \cdots = f_s = 0$ can be considered modulo binomials, and the coefficient matrix of the quotient system is well-defined. It arises from the coefficient matrix of the original system by summing columns for monomials in the same equivalence class.

Example 3.1. In $\mathbb{k}[x, y]$, let $f = x^3 + xy^2 + y^3$ and $b = x^2 - y^2$. In degree three, $b$ makes $x^3$ equivalent to $xy^2$ and $x^2y$ equivalent to $y^3$. The degree three part in the quotient $\mathbb{k}[x, y]/\langle b \rangle$ is two-dimensional with one basis vector per equivalence class. The trinomial $f$ maps to a binomial with coefficient matrix $[2, 1]$. This matrix arises from the matrix $[1, 1, 1]$ by summing the columns corresponding to $x^3$ and $xy^2$.

The reduction modulo lower degree binomials in Example 3.1 can be done in general.

Lemma 3.2. Let $f_1, \ldots, f_s \in \mathbb{k}[x_1, \ldots, x_n]$ be homogeneous polynomials of degree $d$, and $B \subset \mathbb{k}[x_1, \ldots, x_n]$ a set of homogeneous binomials of degree at most $d$. Then in the quotient ring $\mathbb{k}[x_1, \ldots, x_n]/\langle B \rangle$ the ideal $\langle f_1, \ldots, f_s \rangle/\langle B \rangle$ is binomial if and only if the coefficient matrix of the images of $f_1, \ldots, f_s$ in $\mathbb{k}[x_1, \ldots, x_n]/\langle B \rangle$ has a partitioning kernel basis.
Proof. By the graded version of Nakayama’s lemma [8, Exercise 4.6], a homogeneous ideal has a well-defined number of minimal generators in each degree. Since the $f_i$ generate a binomial ideal, there are degree $d$ binomials $b_1, \ldots, b_t$ that generate the same ideal. Since the images of the $f_i$ span the $k$-vector space of degree $d$ polynomials in $\langle f_1, \ldots, f_s \rangle / B$ as well as the $b_i$, the result follows from Proposition 2.5. \qed

Lemma 3.2 is the basis for the following binomial detection algorithm.

**Algorithm 3.3.**

**Input:** Homogeneous polynomials $f_1, \ldots, f_s \in k[x_1, \ldots, x_n]$.  
**Output:** Yes and a binomial generating set of $\langle f_1, \ldots, f_s \rangle$ if one exists, No otherwise.

1) Let  
   - $B := \emptyset$  
   - $R := k[x_1, \ldots, x_n]$.  

2) While $G$ is not empty,  
   a) Let $G_{\text{min}}$ be the set of elements of minimal degree in $G$.  
   b) Redefine $G := G \setminus G_{\text{min}}$.  
   c) Compute the reduced row echelon form of the coefficient matrix $A$ of $G_{\text{min}}$.  
   d) If $A$ does not have a partitioning kernel basis, output No and stop.  
   e) Find a set $B'$ of binomials that generate $\langle G_{\text{min}} \rangle$ and redefine $B := B \cup B'$.  
   f) Redefine $R := R / \langle B' \rangle$.  
   g) Redefine $G$ as its image in $R$.  

3) Output Yes and $B$.

**Proof of correctness and termination.** Termination is obvious. In fact, the maximum number of iterations in the while loop equals the number of different degrees among $g_1, \ldots, g_s$. Lemma 3.2 shows that the while loop either exhausts $G$ if $\langle g_1, \ldots, g_s \rangle$ is binomial, or stops when this is not the case. \qed

**Remark 3.4.** In the homogeneous case there is a natural choice of finite-dimensional vector spaces to work in: polynomials of a fixed degree. In each iteration of the while loop in Algorithm 3.3, the rows of $A$ span the vector space of polynomials of degree $d$ in the ideal (modulo the binomials in $\langle B \rangle$). In the general inhomogeneous situation extra work is needed to construct a suitable finite-dimensional vector space. In particular, one needs to select from the infinite list of binomials in the ideal not too many, but enough to reduce all given polynomials to binomials whenever this is possible. An interesting problem for the future is to adapt one of the selection strategies from the F4 algorithm for Gröbner bases [10] for this task.

**Remark 3.5.** Coefficient matrices of polynomial systems are typically very sparse. An efficient implementation of Algorithm 3.3 has to take this into account.

**Remark 3.6.** Algorithm 3.3 could also be written completely in the polynomial ring without any quotients. Then in each new degree, one would have to consider the coefficient matrix of $G_{\text{min}}$ together with all binomials of degree $d$ in the ideal $\langle B \rangle$. This
list grows very quickly and so does the list of monomials appearing in these binomials. Thus it is not only more elegant to work with the quotient, but also more efficient.

To implement Algorithm 3.3 completely without Gröbner bases some refinements are necessary. Simply using $R = \mathbb{k}[x_1, \ldots, x_n]/B$ in Macaulay2 will make it compute a Gröbner basis of $B$ to effectively work with the quotient. For our purposes, however, this is not necessary.

**Proposition 3.7.** Algorithm 3.3 can be implemented Gröbner-free.

**Proof.** The critical steps are 2.g, when the algorithm reduces $G$ modulo the binomials already found, and 2.c where elements of $G_{\text{min}}$ need to be written in terms of a basis of the finite-dimensional vector space $R_{\deg(G_{\text{min}})}$ of degree $\deg(G_{\text{min}})$ monomials modulo the binomials in $B$. Both of these computations can be carried out graph-theoretically. The equivalence relation introduced in the beginning of this section can also be thought of as a graph on monomials. Restricting to monomials of degree $\deg(G_{\text{min}})$, the connected components are a vector space basis of $R_{\deg(G_{\text{min}})}$ and can thus be used to gather coefficients in step 2.g. Consequently an element of $G_{\text{min}}$ is a binomial if its monomials come from at most two connected components. This test can either be used to replace step 2.c, or it can be used to find the coefficient matrix with respect to the basis of connected components. \qed

**Remark 3.8.** The feasibility of graph-theoretic computations in cases where Gröbner bases can not be computed has been demonstrated in [15]. Example 4.9 there contains a binomial ideal with unknown Gröbner basis whose non-radicality was proved using a graph-theoretic computation. This yielded a negative answer to the question of radicality of conditional independence ideals in algebraic statistics.

**Remark 3.9.** Using Gröbner bases one represents each connected component of the graph defined by $\langle B \rangle$ by its least monomial with respect to the term order. Our philosophy is that this is not necessary: one should work with the connected components per se. Why bother with picking and finding a specific representative in each component if any representative works. In an implementation one could choose a data structure that for each monomial stores an index of the connected component it belongs to.

**Remark 3.10.** It is trivial to generate classes of examples where Gröbner bases methods fail, but Algorithm 3.3 is quick. For example, take any set of binomials whose Gröbner basis cannot be computed and add any polynomial in the ideal. Algorithm 3.3 immediately goes to work on reducing the polynomial modulo the binomials, while any implementation of Gröbner bases embarks into its hopeless task.

**Remark 3.11.** Remark 3.10 highlights the Gröbner-free spirit of our method. The Gröbner basis of an ideal contains much more information than binomiality. One should avoid expensive computation to decide this simple question.
4. Heuristics for the inhomogeneous case

The ideals one encounters in chemical reaction network theory are often not homogeneous, so that the results from Section 3 do not apply. The first idea that one may have for the inhomogeneous case is to work with some (partial) homogenization. Gröbner bases are quite robust in relation to homogenization. For example, to compute a Gröbner basis of a non-homogeneous ideal it suffices to homogenize the generators, compute a Gröbner basis of this homogeneous ideal, and then dehomogenize. Although the intermediate homogeneous ideal is not equal to the homogenization of the original ideal, the dehomogenized Gröbner basis is a Gröbner basis of the dehomogenized ideal [1, Exercise 1.7.8].

Unfortunately the notion of binomiality does not lend itself to that kind of tricks. Geometrically, homogenizing (all polynomials in) an ideal yields the projective closure and dehomogenizing restricts to one affine piece. Homogenizing only the generators creates extra components at infinity and these components need not be binomial.

Example 4.1. The ideal \( \langle ab - x, ab - y, x + y + 1 \rangle \subset k[a, b, x, y] \) is binomial as it equals \( \langle 2y + 1, 2x + 1, 2ab + 1 \rangle \). Homogenizing the generators, however, yields the non-binomial ideal \( \langle ab - xz, ab - yz, x + y + z \rangle \).

We now present some alternatives that do not give complete answers but are quick to check. They can be applied before resorting to an expensive Gröbner basis computation.

The quickest (but least likely to be successful) approach is to try linear algebraic manipulations of the given polynomials. Equivalently one applies row operations to the coefficient matrix, for instance, computing the reduced row echelon form. If it has a partitioning kernel basis, then the ideal is binomial and all non-binomial generators are \( k \)-linear combinations of the binomials. While it may seem very much to ask for this, it does happen for the family of networks in [19, Section 4].

If just linear algebra is not successful, one can homogenize the generators and run Algorithm 3.3. If the result comes out binomial, then the original ideal was binomial by the following simple fact, proven for instance in [1, Corollary A.4.16].

Proposition 4.2. Let \( I \) be an ideal and \( I' \) the homogeneous ideal generated by the homogenizations of the generators of \( I \). Then \( I \) is generated by the dehomogenization of any generating set of \( I' \).

We now illustrate a phenomenon leading to failure of the above heuristics.
Example 4.3. Consider the network from [19, Example 3.15]. Its steady state ideal is binomial, but applying Algorithm 3.3 to a homogenization of the generators yields a non-binomial result. The steady states are positive real zeros of the following polynomials.

\[ f_1 = -k_{12}x_1 + k_{21}x_2 - k_{1112}x_1x_7 + (k_{1211} + k_{1213})x_9, \]
\[ f_2 = k_{12}x_1 - k_{21}x_2 - k_{23}x_2 + k_{32}x_3 + k_{67}x_6, \]
\[ f_3 = k_{23}x_2 - k_{34}x_3 - k_{34}x_3 - k_{89}x_3x_7 + k_{910}x_8 + k_{98}x_8, \]
\[ f_4 = k_{34}x_3 - k_{56}x_4x_5 + k_{65}x_6, \]
\[ f_5 = -k_{56}x_4x_5 + k_{65}x_6 + k_{910}x_8 + k_{1213}x_9, \]
\[ f_6 = k_{56}x_4x_5 - (k_{65} + k_{67})x_6, \]
\[ f_7 = k_{67}x_6 - k_{1112}x_1x_7 - k_{89}x_3x_7 + k_{98}x_8 + k_{1211}x_9, \]
\[ f_8 = k_{89}x_3x_7 - (k_{910} + k_{98})x_8, \]
\[ f_9 = k_{1112}x_1x_7 - (k_{1211} + k_{1213})x_9. \]

The binomials \( f_6, f_8, \) and \( f_9 \) can be used to express, respectively, \( x_6, x_8, \) and \( x_9 \) in the remaining polynomials.

\[ f_1' = -k_{12}x_1 + k_{21}x_2, \]
\[ f_2' = k_{12}x_1 - k_{21}x_2 - k_{23}x_2 + k_{32}x_3 + \frac{k_{56}k_{67}x_4x_5}{k_{65} + k_{67}}, \]
\[ f_3' = k_{23}x_2 - (k_{32} + k_{34})x_3, \]
\[ f_4' = k_{34}x_3 - \frac{k_{56}k_{67}x_4x_5}{k_{65} + k_{67}}, \]
\[ f_5' = \frac{k_{56}k_{67}x_4x_5}{k_{65} + k_{67}} + \frac{k_{1112}k_{1213}x_1x_7}{k_{1211} + k_{1213}} + \frac{k_{89}k_{910}x_3x_7}{k_{910} + k_{98}}, \]
\[ f_7' = \frac{k_{56}k_{67}x_4x_5}{k_{65} + k_{67}} - \frac{(k_{1112}k_{1213}(k_{910} + k_{98})x_1 + (k_{1211} + k_{1213})k_{89}k_{910}x_3)x_7}{(k_{1211} + k_{1213})(k_{910} + k_{98})}. \]

Using the linear relations \( f_1' \) and \( f_3' \) the remaining system is recognized to consist of only two independent binomials:

\[ f_2'' = -\frac{k_{23}k_{34}x_2}{k_{32} + k_{34}} + \frac{k_{56}k_{67}x_4x_5}{k_{65} + k_{67}}, \]
\[ f_4'' = \frac{k_{23}k_{34}x_2}{k_{32} + k_{34}} - \frac{k_{56}k_{67}x_4x_5}{k_{65} + k_{67}}, \]
\[ f_5'' = -\frac{k_{56}k_{67}x_4x_5}{k_{65} + k_{67}} + \left(\frac{k_{1112}k_{1213}k_{21}}{k_{12}(k_{1211} + k_{1213})} + \frac{k_{23}k_{89}k_{910}}{(k_{32} + k_{34})(k_{910} + k_{98})}\right)x_2x_7, \]
\[ f_7'' = \frac{k_{56}k_{67}x_4x_5}{k_{65} + k_{67}} + \left(-\frac{k_{1112}k_{1213}k_{21}}{k_{12}(k_{1211} + k_{1213})} - \frac{k_{23}k_{89}k_{910}}{(k_{32} + k_{34})(k_{910} + k_{98})}\right)x_2x_7. \]
This analysis shows that the steady state ideal under consideration equals the binomial ideal \( \langle f'_1, f'_2, f'_3, f'_5, f_6, f_8, f_9 \rangle \). The Gröbner basis computation in [19, Example 3.15] also yields the result, but it is arguably less instructive. Note also that naive homogenization does not yield binomiality. The element \( f_2 \) is linear. After homogenization, Algorithm 3.3 would pick only this element as \( G_{\min} \) and stop since it is not a binomial.

The effect in Example 4.3 motivates our final method: term replacements using known binomials. We expect this to be very useful in applications from system biology for the following reasons.

- It often happens that non-binomial generators are linear combinations of binomials, as in Example 4.3 where \( f_1 = f'_1 + f_9 \).
- Steady state ideals of networks with enzyme-substrate complexes always have some binomial generators. These complexes are produced by only one reaction and thus their rate of change is binomial.
- In MAPK networks one often finds binomials of the form \( k x_a x_b - k' x_c \).
- Frequently binomials in steady state ideals are linear. Equivalently some of the concentrations are equal up to a scaling (which may depend on kinetic parameters). This happens for all examples in [16].

We now illustrate term replacements in a larger example which comes from the network for ERK activation embedded in two negative feedback loops (see [3, Section 5]).

**Example 4.4.** Consider the following steady state ideal generated by 29 polynomials.

\[
\begin{align*}
    f_1 &= -k_1 x_1 x_2 + k_2 x_3 + k_6 x_6, \\
    f_2 &= -k_1 x_1 x_2 + k_2 x_3 + k_3 x_3, \\
    f_3 &= k_1 x_1 x_2 - k_2 x_3 - k_3 x_3, \\
    f_4 &= k_1 x_1 x_10 + k_1 x_10 + k_3 x_25 + k_2 x_27 + k_3 x_3 - k_3 x_18 x_4, \\
        &+ k_4 x_4 x_5 + k_5 x_6 - k_7 x_4 x_7 + k_9 x_8 + k_9 x_8 - k_10 x_4 x_9, \\
    f_5 &= k_1 x_{12} + k_1 x_{12} + k_1 x_{13} + k_1 x_{13} + k_3 x_{24} + k_3 x_{24} + k_3 x_{27} + k_3 x_{27} - k_3 x_{11} x_5 - k_3 x_{16} x_5, \\
        &+ k_4 x_{26} x_5 - k_4 x_{26} x_5 + k_5 x_6 + k_6 x_6 - k_6 x_5, \\
    f_6 &= k_4 x_5 + k_5 x_5 - k_5 x_6 - k_6 x_6, \\
    f_7 &= k_1 x_{13} + k_7 x_{14} x_7 + k_8 x_8, \\
    f_8 &= k_7 x_{14} x_7 - k_9 x_8 - k_9 x_8, \\
    f_9 &= k_1 x_{10} + k_1 x_{12} + k_1 x_{13} + k_3 x_8 - k_10 x_4 x_9, \\
        &- k_10 x_4 x_9 - k_10 x_4 x_9, \\
    f_{10} &= -k_1 x_{10} - k_1 x_{10} - k_1 x_{10} + k_1 x_{10} x_9, \\
    f_{11} &= k_1 x_{10} + k_1 x_{12} - k_1 x_{12} + k_1 x_{12} + k_1 x_{12} + k_2 x_{15} + k_2 x_{15} - k_2 x_{11} x_6, \\
        &+ k_3 x_{17} + k_3 x_{17} + k_1 x_{13} x_5, \\
    f_{12} &= -k_1 x_{12} - k_1 x_{12} + k_1 x_{11} x_5, \\
    f_{13} &= -k_1 x_{13} - k_1 x_{13} + k_1 x_{13} x_5, \\
    f_{14} &= -k_1 x_{11} x_3 + k_2 x_{15} + k_3 x_{21} + k_3 x_{24}, \\
        &- k_5 x_{19} - k_5 x_{19} x_4, \\
    f_{15} &= k_1 x_{11} x_5 - k_3 x_{15} - k_1 x_{15}, \\
    f_{16} &= k_1 x_{15} - k_2 x_{11} x_5 + k_3 x_{17} - k_3 x_{16} x_5 + k_3 x_20 + k_2 x_20 + k_2 x_21 + k_3 x_23 + k_3 x_24 + k_3 x_24 - k_3 x_4 x_5, \\
    f_{17} &= k_2 x_{11} x_16 - k_2 x_{17} - k_2 x_{17}, \\
    f_{18} &= k_2 x_{17} - k_2 x_{13} x_5 + k_3 x_{20} - k_4 x_{18} x_5 + k_3 x_{23} + k_3 x_{25} + k_3 x_{25}, \\
        &- k_4 x_{18} x_5 + k_4 x_{29} + k_4 x_{29} - k_3 x_{18} x_4, \\
    f_{19} &= -k_4 x_{19} - k_4 x_{19} + k_3 x_{19} x_{19} - k_3 x_{19} x_{19} + k_3 x_{20} + k_2 x_{20} + k_2 x_{21} + k_3 x_{21} + k_4 x_{19}, \\
    f_{20} &= k_2 x_{18} x_5 - k_2 x_{20} - k_2 x_{20}, \\
    f_{21} &= -k_2 x_{18} x_5 - k_2 x_{21} + k_3 x_{21}, \\
    f_{22} &= -k_3 x_{18} x_5 + k_3 x_{22} + k_3 x_{23}, \\
    f_{23} &= -k_3 x_{18} x_5 + k_3 x_{21} + k_3 x_{23}, \\
    f_{24} &= -k_3 x_{24} - k_3 x_{24} + k_3 x_{16} x_5, \\
    f_{25} &= -k_3 x_{25} - k_3 x_{25} + k_3 x_{18} x_4, \\
    f_{26} &= -k_3 x_{25} + k_4 x_{27} - k_4 x_{26} x_5, \\
    f_{27} &= -k_4 x_{27} - k_4 x_{27} + k_4 x_{26} x_5
\end{align*}
\]
After some obvious factorization, the following elements are binomials: \( f_2, f_6, f_8, f_{10}, f_{12}, f_{13}, f_{15}, f_{17}, f_{20}, f_{21}, f_{22}, f_{23}, f_{24}, f_{25}, f_{27}, f_{29} \). The system has seven conservation relations, which can be found by linear algebra. According to our strategy to use binomials to simplify the system, we eliminate, if possible, non-binomials using the conservation relations. This is not always possible, as some of the conservation relations stem from duplicate equations like \( f_2 = -f_3 \). We eliminate \( f_3, f_4, f_5, f_8, f_9, f_{18} \), and \( f_{19} \). The remaining non-binomial part consists of \( f_1, f_7, f_{11}, f_{14}, f_{16}, f_{26}, \) and \( f_{28} \). Dividing by reaction constants, each of the binomials is of the form \( x_i = K x_j x_l \). Using these in the non-binomials yields

\[
\begin{align*}
 f'_{1} &= -\frac{k_1 k_3 x_1 x_2}{k_2 + k_3} + \frac{k_4 k_6 x_4 x_5}{k_5 + k_6}, \\
f'_{11} &= -\frac{k_{13} k_{15} x_{11} x_{12}}{k_{14} + k_{15}} + \frac{k_{10} k_{12} x_4 x_9}{k_{11} + k_{12}}, \\
f'_{14} &= -\frac{k_{19} k_{21} x_{11} x_{14}}{k_{20} + k_{21}} + \frac{k_{28} k_{30} x_{16} x_{19}}{k_{29} + k_{30}} + \frac{k_{34} k_{36} x_{16} x_{5}}{k_{35} + k_{36}}, \\
f'_{16} &= \frac{k_{19} k_{21} x_{11} x_{14}}{k_{20} + k_{21}} - \frac{k_{22} k_{24} x_{11} x_{16}}{k_{23} + k_{24}} - \frac{k_{28} x_{16} x_{19}}{k_{29} + k_{30}} + \frac{k_{28} k_{29} x_{16} x_{19}}{k_{26} + k_{27}} \\
 &\quad + \frac{k_{31} k_{33} x_{18} x_{22}}{k_{32} + k_{33}} - \frac{k_{34} x_{16} x_{5}}{k_{35} + k_{36}}, \\
f'_{26} &= \frac{k_{37} k_{39} x_{18} x_{4}}{k_{38} + k_{39}} - \frac{k_{40} k_{42} x_{26} x_{5}}{k_{41} + k_{42}}, \\
f'_{28} &= k_{46} x_{19} - \frac{k_{43} k_{45} x_{18} x_{28}}{k_{44} + k_{45}}.
\end{align*}
\]

In particular, we find five new binomials \( f'_{1}, f'_{7}, f'_{11}, f'_{14}, \) and \( f'_{28} \). Adding \( f'_{14} \) to \( f'_{16} \) yields the trinomial

\[
\begin{align*}
f''_{16} &= -\frac{k_{22} k_{24} x_{11} x_{16}}{k_{23} + k_{24}} + \frac{k_{25} k_{27} x_{18} x_{19}}{k_{26} + k_{27}} + \frac{k_{31} k_{33} x_{18} x_{22}}{k_{32} + k_{33}}.
\end{align*}
\]

Consequently, the original system is equivalent to a system consisting of 27 binomials and two trinomials of a relatively simple shape. For comparison we computed the Gröbner basis in in Macaulay2 with rational functions in the reaction rates as coefficients. Although the computation finished in just 18 minutes, the result is practically unusable. The Gröbner basis consists of 169 elements each of it with huge rational functions as coefficients. The structure that we observed above is completely lost.

The lesson learned from Example 4.4 is that term replacements using binomials are useful in solving a polynomial system, even if the end result is not binomial. Especially in the non-homogeneous case where the notion of minimal generators is absent, computations with the Binomials package [13] in Macaulay2[11] can probably only assist, but not automatically do useful reductions.
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