Experiments on the Conradi-Kahle Algorithm for Detecting Binomiality for Biological Models

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1 Introduction

Given a polynomial ideal, we consider the problem of existence of a basis for the ideal consisting of polynomials with at most two monomials. Binomial ideals offer clear computational advantages over arbitrary ideals. They appear in various applications. Binomial ideals have been extensively studied in the literature [6,10,11]. It has been shown that Gröbner bases [3] can be used to test binomiality (see e.g., [6]). Millán, et al. in [14] present a sufficient condition for binomiality of the steady state ideal. Conradi and Kahle [5] proved that this condition is necessary for homogeneous ideals and proposed an algorithm, which was implemented in Macaulay2 [9].

2 Remarks on the Complexity of Conradi-Kahle Algorithm

- **Steps** (3) **and** (4)**.** can be ignored in terms of complexity, as they are at most linear.
- **Step** (5)**.** Let t denote the number of distinct monomials in $F_{\min}$ and $m := \max(s, t)$. Computing the reduced row echelon form of A can be done in at most m^ω steps, where ω is the constant in the complexity of matrix multiplication.
- **Step** (6)**.** needs at most st operations which is less or equal than m^ω, so we ignore this term.
- **Step** (9)**.** requires at most t operations, where t is as in Step (5). This can be ignored as it is strictly less than the number of operations in Step (5).
- **Step** (10)**.** can be bounded by tm, which itself can be bounded by m^ω, hence ignored.
- **Step** (11)**.** can be obviously ignored.
- **Step** (12)**.** The number of operations for computing this quotient can be bounded by the the number of operations for computing a Gröbner basis for $\langle B \rangle$. This is because having computed a Gröbner basis for $\langle B \rangle$, one can obtain a basis for the quotient ring.

Algorithm 1 (Conradi and Kahle, 2015)

Input: Homogeneous polynomials $f_1, \ldots, f_s \in \mathbb{K}[x_1, \ldots, x_n]$, where $\mathbb{K}$ is a field.
Output: *Yes* if the ideal $\langle f_1, \ldots, f_s \rangle$ is binomial. *No* otherwise.

1: Let $B := \emptyset, R := \mathbb{K}[x_1, \ldots, x_n]$ and $F := \{f_1, \ldots, f_s\}$.
2: **while** $F \neq \emptyset$ **do**
3: Let $F_{\min}$ be the set of elements of minimal degree in F.
4: $F := F \setminus F_{\min}$.
5: Compute the reduced row echelon form A of the coefficient matrix of $F_{\min}$.
6: **if** A has a row with three or more non-zero entries **then**
7: **return** *No* and stop
8: **end if**
9: Let M be the vector of monomials in $F_{\min}$.
10: Let B' be the set of entries of AM.
11: $B := B \cup B'$.
12: $R := \mathbb{K}[x_1, \ldots, x_n]/\langle B \rangle$.
13: Redefine F as the image of F in R.
14: **end while**
15: **return** *Yes*.

– **Step** (13)**.** is equivalent to reducing F modulo $\langle B \rangle$, which can be done via reducing F modulo a Gröbner basis of $\langle B \rangle$.

In conclusion, major part of the operations in the algorithm are done in steps (12) and (13). Following Mayr and Meyer's work on the complexity of computing Gröbner bases [13], computations in steps 12 and 13 of the algorithm can be EXP-SPACE. Equivalently, this can be done by means of Gaussian elimination on the corresponding Macaulay matrix of B in step 12 or $B \cup F$ in step 13, respectively. Conradi and Kahle observe through experiments that these steps can be performed via graph enumeration algorithms like breadth first search, which makes it more efficient than Gröbner bases in practice [5]. In our implementation we have not used such graph enumeration algorithms.

3 Macaulay2 and Maple experiments

We consider 20 biomodels from the BioModels repository [4,7] and ODEbase [12]. We use Algorithm 1 to test binomiality of these biomodels. We emphasise that in our computations we do not assign values to the parameters $k_1, \ldots, k_r$ and we work in $\mathbb{Q}(k_1, \ldots, k_r)[x_1, \ldots, x_n]$. All of the polynomials considered are of degree 2. We have implemented Algorithm 1 in Maple [8] and also use a slight variant of the implementation of the algorithm in the Macaulay2 package Binomials [9,10]. We also test binomiality via computing a Gröbner basis of the ideal. Our computations are done on a 3.5 GHz Intel Core i7 with 16 GB RAM. In our computations we used Macaulay2 1.12 and Maple 2019.1.

Table 1 shows the results of our computations. The columns C-K (M2) and C-K (Maple) show the CPU timings in seconds of executing Algorithm 1 in

Biomodel	#var,#par	C-K(M2)	C-K(Maple)	Bin(C-K)	GB(M2)	GB(Maple)	Bin(GB)
2	13, 37	0.1	1	–	–	–	–
9	26, 39	0.04	0.2	Yes	0.5	0.001	Yes
28	16, 31	0.04	0.1	–	–	–	–
30	18, 36	0.5	0.2	–	–	–	–
46	16, 22	0.02	0.2	–	100	80	No
85	17, 42	0.04	0.6	–	–	–	–
86	17, 56	0.08	6	–	–	–	–
102	13, 42	0.04	0.2	–	–	–	–
103	17, 50	0.1	0.9	–	–	–	–
108	9, 19	0.01	0.03	–	–	–	–
152	64, 7	0.3	400	–	–	–	–
153	75, 7	0.4	500	–	–	–	–
187	11, 17	0.02	0.07	–	0.06	0.1	No
200	22, 54	0.05	1	–	–	–	–
205	194, 351	0.6	50	–	–	–	–
243	23, 19	0.04	0.3	–	0.01	0.05	No
262	11, 28	0.05	0.02	Yes	0.01	0.02	Yes
264	14, 31	0.7	0.03	Yes	2	0.04	Yes
315	20, 52	0.02	0.2	–	–	–	–
335	34, 54	0.04	0.8	–	30	90	No

Table 1. CPU times (in seconds) for Algorithm 1 and Gröbner bases.

Macaulay2 and Maple, respectively. In the column Bin (C-K), *Yes* means that the algorithm successfully determined that the ideal is binomial, while – means that the algorithm cannot determine whether the ideal is binomial or not. The columns GB (M2) and GB (Maple) are the timings of Gröbner bases computations of the input polynomials in Macaulay2 and Maple, respectively. In the Bin (GB) column – means that the Gröbner basis computation did not finish after 600 seconds. *Yes* in the latter column means that the Gröbner basis computation finished and shows that the ideal is binomial, while *No* shows that the Gröbner basis computation finished but it detected that the ideal is not binomial.

None of the ideals in the biomodels that we have studied are homogeneous. Therefore, in order to use Algorithm 1 we need to homogenise the ideals. Consequently, if the algorithm applied to our homogenised systems returns *No*, we are not able to say whether the ideal is binomial or not (see [5, Section 4]), therefore, we show this case by – in the table. As one can see from the column Bin (C-K), the Conradi-Kahle Algorithm is able to test binomiality only for Biomodels 9, 262 and 264. However, Gröbner bases are able to test binomiality for every given ideal. One can see from the table that whenever Gröbner bases computations give a Yes answer to the binomiality question, then the Conradi-Kahle Algorithm can detect this as well. In the Yes cases, the timings for both methods in both Macaulay2 and Maple are very close.

Algorithm 1 returns the output within at most a few seconds, however, most of the Gröbner bases computations did not finish in 600 seconds. The advan-

tage of testing binomiality using Gröbner bases computations can be seen in Biomodels 46, 187, 243 and 335, where Gröbner bases computations–although slower–show that the ideal is not binomial, but the Conradi-Kahle Algorithm cannot detect this in spite of its fast execution. With a few exceptions, we do not observe significant difference between Macaulay2 and Maple computations, neither for the Conradi-Kahle Algorithm nor for the Gröbner bases computations.

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