Speeding up Cylindrical Algebraic Decomposition by Gröbner Bases

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Abstract. Gröbner Bases [Buc70] and Cylindrical Algebraic Decomposition [Col75,CMMXY09] are generally thought of as two, rather different, methods of looking at systems of equations and, in the case of Cylindrical Algebraic Decomposition, inequalities. However, even for a mixed system of equalities and inequalities, it is possible to apply Gröbner bases to the (conjoined) equalities before invoking CAD. We see that this is, quite often but not always, a beneficial preconditioning of the CAD problem.

It is also possible to precondition the (conjoined) inequalities with respect to the equalities, and this can also be useful in many cases.

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1 Introduction

Solving systems of equations, or equations and inequations (\neq) /inequalities (>,<) is an old subject. Deciding the truth of, or more generally eliminating quantifiers from, quantified Boolean combinations of such statements, is more recent [Tar51]. We can distinguish many families of methods, even if we restrict attention to the real numbers, or possibly the complex numbers.

$$\{\mathbf{x}: p_1(\mathbf{x}) = 0 \land p_2(\mathbf{x}) = 0 \land \dots \land p_l(\mathbf{x}) = 0\}. \tag{1}$$

We have concentrated on purely lexicographical orders, since these seem to be the most useful to us.

 $=_{\Delta}$ The method of triangular decomposition via regular chains [ALMM99,MM05]. Here the output is a set of regular chains of polynomials

$$\{(p_{1,1}, p_{1,2}, \ldots), (p_{2,1}, p_{2,2}, \ldots), \ldots\},$$
 (2)

and the solution is the union of the set of regular zeros of these regular chains:

$$\left\{ \mathbf{x} : p_{1,1}(\mathbf{x}) = p_{1,2}(\mathbf{x}) = \dots = 0 \land \left(\prod_{i} \operatorname{init}(p_{1,i}) \right) (\mathbf{x}) \neq 0 \right\} \cup \dots . \quad (3)$$

 $<_{\text{Col}}$ The method of Cylindrical (semi-)Algebraic Decomposition for real closed fields, computed via repeated projection to \mathbf{R}^1 and repeated lifting [Col75, and many improvements].

=_{Col} The previous case restricted to equality.

 $<_{\Delta \mathbf{R}}$ The method of Cylindrical (semi-)Algebraic Decomposition for real closed fields via triangular decomposition [CMMXY09].

 $\neq_{\Delta \mathbf{C}}$ The method of Cylindrical Decomposition over the complexes via triangular decomposition, which was introduced in [CMMXY09] as a stepping-stone to the previous method, but which probably has independent interest.

△CH Quantifier Elimination by partial (i.e. taking account of the Boolean structure and quantifier structure) Cylindrical Algebraic Decomposition [CH91].

Others such as Weispfenning's Virtual Term Substitution [Bro05, is a readable introduction], or Tarski's original method [Tar51].

Conversely instead of asking for solutions \mathbf{x} to $\exists \mathbf{x} f_1(\mathbf{x}) \geq 0 \wedge \cdots$, we may use a Positivstellensatz to show that no such \mathbf{x} exist, as in [PQR09]. We do not discuss this direction further here.

It should be noted that both $<_{\text{Col}}$ and $<_{\Delta\mathbf{R}}/\neq_{\Delta\mathbf{C}}$ (but not $\not\supseteq_{\text{CH}}$) have the draw-back that the Cylindrical Algebraic Decomposition produces decompositions for, not only the question posed, e.g. $\forall y \exists z p(x,y,z) = 0 \land q(x,y,z) = 0 \land r(x,y,z) > 0$, but also all other questions involving the same polynomials, provided the quantifiers are over variables in the same order, e.g. $\exists y \forall z p(x,y,z) < 0 \lor (q(x,y,z) > 0 \land r(x,y,z) = 0)$.

This paper asks the question: "can these methods usefully be combined?" The combinations we are thinking about are those of conjunction: Can the fact that B is in the context of $a_1 = 0 \land \cdots \land a_k = 0 \land B$ be used to simplify B? In particular, we look at the use of Gröbner base methods to simplify the equalities in the conjunction and to simplify the inequalities in the light of the equalities.

Technical Note: all computations ($=_G$, $<_{\Delta \mathbf{R}}$ and $\neq_{\Delta \mathbf{C}}$) were performed in Maple 16 β on a 3.1GHz Intel processor, except for the $<_{\mathrm{Col}}$, $=_{\mathrm{Col}}$ and $\not\equiv_{\mathrm{CH}}$ ones, which were performed on a 2.83GHz Intel processor with QEPCAD B version 1.65 [Bro03]. Times for a hybrid calculation, e.g. $=_G/<_{\mathrm{Col}}$, are either quoted as the total time or a decomposition a+b=c where a is the time (in milliseconds) for $=_G$, b for $<_{\mathrm{Col}}$, and c is the sum. We have run QEPCAD in three modes:

1. on the problem as given in [BH91], implementing \mathbb{A}_{CH} ;

- 2. as above but with the full-cad option to ignore the Boolean structure of the expression;
- 3. with no quantifiers stated, and the full-cad option, implementing < Col.

2 Examples in this paper

2.1 [BH91]

This paper has a variety of examples for $\not\supseteq_{\mathrm{CH}}$, all of a form to which $=_G$ is applicable.

2.2 [CMMXY09]

This paper has a variety of examples for $<_{\Delta \mathbf{R}}$. We chose some of those to which $=_G$ is applicable.

2.3 Two Spheres and A Cylinder

Let the following be spheres in \mathbb{R}^3 :

$$S_1: \qquad (x-1)^2 + y^2 + z^2 - 3;$$

$$S_2: \qquad (x+1)^2 + y^2 + z^2 - 3;$$

$$S_3: \qquad (x-1)^2 + \left(y - \frac{1}{2}\right)^2 + z^2 - 3;$$

$$S_4: \qquad (x+1)^2 + \left(y + \frac{2}{3}\right)^2 + \left(z + \frac{3}{4}\right)^2 - 3.$$

Denote the infinite cylinder centred on the z-axis with radius 1 by C, so that the equation defining the cylinder is:

$$C: \quad x^2 + y^2 - 1.$$

Now we investigate intersecting pairs of spheres (roughly increasing in CAD 'difficulty') under conditions based on the cylinder. We assume the spheres' equation will always be required to equal 0 but make no assumptions on the condition on the cylinder. That is, we wish to solve the problem:

$$S_i = 0 \land S_{i+1} = 0 \land C * 0 \qquad * \in \{=, \neq, <, >, \leq, \geq\}, i = 1, 2, 3.$$
 (4)

We use the underlying variable ordering (z, y, x).

² This is the QEPCAD notation, meaning that we will project from (z,y,x)-space to (z,y)-space to (z)-space. We therefore end up with polynomials in z alone, so this is equivalent to a purely lexicographical Gröbner base with $z \prec y \prec x$, i.e. plex([z,y,x]) in Maple: $=_{GC}$ is used to indicate Gröbner bases with this (compatible) ordering. The CAD package in Maple [CMMXY09] requires PolynomialRing([x,y,z]) to achieve the same effect as QEPCAD's (z,y,x). $=_{GR}$ denotes the reverse plex order.

3 Prior Art

Needless to say, we are not the first to have had this idea.

3.1 Buchberger-Hong

[BH91] considers the case of $=_G$ ([BGK85] re-implemented in C) applied to $<_{\text{Col}}$ (an early version of [CH91] re-implemented in C), i.e., rather than computing a CAD for the zeros of a system of equations E (i.e. $e_1 = 0 \land e_2 = 0 \land \cdots$) and inequalities F, compute it for G, a (purely lexicographical) Gröbner base for E, and F. They generally found a very substantial speed-up in the total computation time, e.g. "Solotareff A"³

$$\exists x \exists y \ 3x^2 - 2x - a = x^3 - x^2 - ax - 2b + a - 2 =$$
 (5)

$$3y^2 - 2y - a = y^3 - y^2 - ay - 2b + a - 2 = 0$$
 (6)

$$4a \in [1,7] \land 4b \in [-3,3] \land x \in [-1,0] \land y \in [0,1] \tag{7}$$

(with the variable ordering (b, a, x, y)) took them 11500 ms for $\not\supseteq_{\mathrm{CH}}$, but 717 for $=_G$, and 117 for $\not\supseteq_{\mathrm{CH}}$ applied to the result, a total of 834 ms, or a 13-fold speed-up. "Solotareff B" is the same problem but with (a, b, x, y) as the variable ordering, and here the $\not\supseteq_{\mathrm{CH}}$ time was again greatly reduced, but the $=_G$ time was excessive. Of course, there have been substantial improvements in the implementation of all these algorithms since [BH91] was published, and Table 2 shows that the $=_G$ time is now less than 1/3 of the $\not\supseteq_{\mathrm{CH}}$ time. We choose rather to focus on the number of cells generated, which is closely connected to the $=_{\mathrm{Col}}$ time, and also affects the time taken to make use of the output. The cell counts are shown in Table 1.

Table 1. Cell counts for Solotareff

| | Ord | ering A | Orde | ring B |
|---------------|---|---------------|-------------|-----------------------|
| | <col :<="" th=""/> <th>$=_G/<_{Col}$</th> <th>$<_{Col} =$</th> <th>$_G/<_{\mathrm{Col}}$</th> | $=_G/<_{Col}$ | $<_{Col} =$ | $_G/<_{\mathrm{Col}}$ |
| (5–7) Partial | 153 | 63 | 375 | 41 |
| Full | 349 | 625 | 1063 | 237 |
| (5–6) Partial | 29 | 15 | 97 | 17 |
| Full | 29 | 33 | 97 | 17 |

More reruns of [BH91] are given in Table 2. We see that, with today's technology, the conclusion of [BH91], viz. that $=_G$ generally improves $\not\supseteq_{CH}$ for the class of problems to which it is applicable, is still generally valid, but the details differ: notably the Gröbner base time is generally insignificant today.

³ There are various problems labelled "Solotareff": for a description of this class see [Wil12] and the links therein.

Table 2. [BH91] with today's technology

| | ∄c | Н | $=_G$ | /∄сн | | ∄ _{CH} /f | ull-cad | $=_G/\mathbb{A}_{\mathrm{CH}}$ | $_{ m I}/{ m full}$ | -cad |
|-----|-------|------------------|------------|--------------|------------------|--------------------|------------------|--------------------------------|---------------------|------------------|
| | Time | \mathbf{Cells} | Tim | \mathbf{e} | \mathbf{Cells} | Time | \mathbf{Cells} | \mathbf{Tim} | e | \mathbf{Cells} |
| IΑ | 190 | 503 | 22+72= | 94 | 23 | 188 | 503 | 22 + 73 = | 95 | 51 |
| ΙВ | 199 | 369 | 21 + 74 = | 95 | 17 | 191 | 369 | 21 + 75 = | 96 | 33 |
| RA | 85 | 1 | 24 + 73 = | 97 | 1 | 86 | 1 | 24 + 71 = | 95 | 1 |
| RB | 129 | 1 | 24 + 72 = | 96 | 1 | 125 | 1 | 24 + 72 = | 96 | 1 |
| E A | 297 | 621 | 25 + 134 = | 159 | 621 | 576 | 11139 | 25 + 394 = | 419 | 11139 |
| ΕВ | Error | ? | 50+?= | Error | ? | Error | ? | 50+?= | Error | ? |
| S A | 89 | 153 | 22 + 72 = | 94 | 63 | 199 | 349 | 22+185= | 207 | 625 |
| SB | 113 | 375 | 23 + 75 = | 98 | 41 | 228 | 1063 | 23+180= | 203 | 237 |
| C A | 133 | 19 | 42 + ? = | Error | ? | 235 | 19 | 42 + ? = | Error | ? |
| СВ | Error | ? | 132 + ? = | Error | ? | Error | ? | 132 + ? = | Error | ? |

Table 3. [BH91] Examples for full CADs

| | = | Col | $=_{G}$ | $/=_{\text{Col}}$ | | <_\D | R | $=_G/<$ | $\Delta \mathbf{R}$ |
|---------|-------|------------------|-------------|-------------------|------------------|---------|------------------|---------|---------------------|
| | Time | \mathbf{Cells} | Time | 9 | \mathbf{Cells} | Time | \mathbf{Cells} | Time | \mathbf{Cells} |
| IΑ | 236 | 3723 | 22+77= | 99 | 273 | 29426 | 3763 | 2470 | 273 |
| ΙВ | 212 | 3001 | 21 + 76 = | 97 | 189 | 36262 | 2795 | 1482 | 189 |
| RA | 150 | 2101 | 24 + 86 = | 110 | 105 | 17355 | 1267 | 570 | 165 |
| RB | 21091 | 7119 | 24 + 80 = | 104 | 141 | 356670 | 7119 | 470 | 141 |
| E A* | 7390 | 114541 | 25 + 3189 = | 3214 | 53559 | 262623 | 28557 | 62496 | 14439 |
| E B* | Error | ? | 50+?= | Error | ? | > 1000s | ? | > 1000s | ? |
| $S A^*$ | 115 | 1751 | 22+82= | 104 | 297 | 16014 | 1751 | 2025 | 297 |
| $S B^*$ | 253 | 6091 | 23+82= | 105 | 243 | 43439 | 6091 | 1647 | 243 |
| C A* | 820 | 8387 | 42+?= | Error | ? | 216028 | 7895 | > 1000s | ? |
| C B* | Error | ? | 132 + ? = | Error | ? | > 1000s | ? | > 1000s | ? |

 $[\]ast$ indicates that the linear inequalities have been omitted in this version.

There is one point which is not explicit in [BH91]. As the computation of Gröbner bases in one variable is just equivalent to Euclid's algorithm, i.e. Gaussian elimination in Sylvester's matrix, Gröbner base computations which are not genuinely multi-variate do not affect the set of resultants etc. generated in $<_{\text{Col}}$, and hence are of limited use in the projection phase. They might still reduce the work done in the lifting phase, of course.

Table 3 re-runs the examples of [BH91], but asking for complete cylindrical algebraic decompositions, and hence we can compare $<_{\text{Col}}$ with $<_{\Delta\mathbf{R}}$ legitimately. Given that the algorithms are fundamentally different, the similarities in cell counts are striking. The differences in cell counts (where present) reflect differences in the cylindrical algebraic decompositions for the same input problem.

3.2 Phisanbut

Phisanbut [Phi11], considering branch cuts in the complex plane, observed that $g=0 \land f>0$ could be reduced to $g=0 \land \operatorname{prem}(f,g)>0$ under suitable conditions, where prem denotes the pseudo-remainder operation. More precisely, if f and g are regarded as polynomials in the main variable x, of degrees d and e respectively, then $\operatorname{prem}(f,g)=\operatorname{rem}(e^{d-e+1}f,g)$, where e is the leading coefficients of e. When e0 and e0, or when e0, where e1 is even, $\operatorname{prem}(f,g)$ 1 has the same sign as e1. Unfortunately e2 might have variable sign, and e4 and e6 and e7 is e8 in e9, where e9 and e9 are e9 are e9, where e9 is e9, where e9 is e9, where e9 is the smallest integer such that the division is exact, and by analogy we have sprecond(e9, e9 are e9. Note that sprecond(e9, e9 are precond(e9, e9 or a strict divisor of it, i.e. sprecond is never worse. She generally, but not always, saw [Phi11, Tables 8.13, 8.14] a significant decrease in the number of cells, and the time taken to compute sprecond was minimal.

4 Further developments

4.1 = $_G$ with $<_{\Delta R}$

It would seem natural to apply $=_G$ to $<_{\Delta \mathbf{R}}$, as [BH91] did to $\not\equiv_{\mathrm{CH}}$. The results are in Table 3, and show a speed-up in all instances except the Collision problems. We also note the substantial speed advantage enjoyed by $<_{\mathrm{Col}}$, and this is a subject for further study.

$4.2 =_G \text{ with } \neq_{\Delta C}$

We can also $\min =_G \text{ with } \neq_{\Delta \mathbf{C}}$, and these results are shown in Table 4, which also compares $\neq_{\Delta \mathbf{C}}$ with $<_{\Delta \mathbf{R}}$. $<_{\Delta \mathbf{R}}$ involves doing $\neq_{\Delta \mathbf{C}}$ first, and then running the MakeSemiAlgebraic algorithm from [CMMXY09]. For these examples, the MakeSemiAlgebraic step is the most expensive initially, but often not after we apply $=_G$.

4.3 =_G with inequalities in $<_{\Delta R}$

Having reduced the equalities to a Gröbner base G, it is now possible to reduce the inequalities by G, since adding/subtracting a multiple of an element of G is adding/subtracting 0. We can reduce with respect to the main variable, denoted $=_G/\to_x^G$, with respect to secondary variables, denoted $=_G/\to_y^G$, or with respect to all variables (Maple's NormalForm), denoted $=_G/\to_y^G$. If we compare tables 6 and 7 we see that the number of cells produced is the same across the two methods.

Table 4. Timings for [BH91] Examples: $<_{\Delta \mathbf{R}}/\neq_{\Delta \mathbf{C}}$

| | $\neq_{\Delta \mathbf{C}}$ | | | , . | $=_G/<_{\Delta \mathbf{R}}$ | |
|----------------|----------------------------|---------|-------|---------|-----------------------------|-------|
| | Time | Time | Ratio | Time | Time | Ratio |
| Intersection A | 5691 | 29426 | 4.17 | 1168 | 2470 | 1.11 |
| Intersection B | 5584 | 36262 | 5.49 | 886 | 1482 | 0.67 |
| Random A | 4614 | 17355 | 2.76 | 310 | 570 | 0.84 |
| Random B | 67343 | 356670 | 4.30 | 318 | 470 | 0.48 |
| Ellipse A* | 85425 | 262623 | 2.07 | 27916 | 62496 | 1.24 |
| Ellipse B* | 441245 | > 1000s | - | > 1000s | > 1000s | - |
| Solotareff A* | 6666 | 16014 | 1.40 | 1760 | 2025 | 0.15 |
| Solotareff B* | 9536 | 43439 | 3.56 | 1404 | 1647 | 0.17 |
| Collision A* | 41085 | 216028 | 4.26 | > 1000s | > 1000s | _ |
| Collision B* | > 1000s | > 1000s | - | > 1000s | > 1000s | - |

[&]quot;Ratio" = $(<_{\Delta \mathbf{R}} - \neq_{\Delta \mathbf{C}})/\neq_{\Delta \mathbf{C}}$, i.e. the relative cost of MakeSemiAlgebraic.

Table 5. Examples from [CMMXY09]

| | <_\D | R | $=_G/<$ | $\Delta \mathbf{R}$ | | Ra | tio |
|----------|------------|-------|-----------------|---------------------|------|--------|------------------|
| | Time Cells | | \mathbf{Time} | ${f Time}$ | | | \mathbf{Cells} |
| | | | 20 + 245 = | | | | 18.14 |
| Cyclic-4 | > 1000s | ? | 64 + 5813 = | 5877 | 621 | ? | ? |
| 2 | 2249 | 895 | 22 + 1845 = | 1867 | 579 | 1.20 | 1.55 |
| 4 | 3225 | 421 | 24 + 19738 = | 19762 | 1481 | 0.16 | 0.28 |
| 6 | 363 | 41 | 20 + 918 = | 938 | 89 | 0.39 | 0.46 |
| 7 | 3667 | 895 | 26 + 6537 = | 6563 | 1211 | 0.56 | 0.74 |
| 8 | 3216 | 365 | 21 + 174 = | 195 | 51 | 16.49 | 7.16 |
| 13 | 14342 | 4949 | 18 + 220 = | 238 | 81 | 60.26 | 61.10 |
| 14 | 334860 | 27551 | 21 + 971 = | 992 | 423 | 337.56 | 65.13 |

Table 6. Spheres and Cylinders: $<_{\Delta R}$

| | $<_{\Delta {f R}}$ | | $=_G/$ | $<_{\Delta {f R}}$ | $=_G/\rightarrow_3$ | $_{y}^{G}/<_{\Delta \mathbf{R}}$ | $=_G/\rightarrow_x^G$ | $G/<_{\Delta {f R}}$ | $=_G/\overset{*}{\rightarrow}^0$ | $^{G}/<_{\Delta {f R}}$ |
|---------------|--------------------|------------------|-----------------|--------------------|---------------------|----------------------------------|-----------------------|----------------------|----------------------------------|-------------------------|
| | Time | \mathbf{Cells} | \mathbf{Time} | \mathbf{Cells} | Time | \mathbf{Cells} | \mathbf{Time} | \mathbf{Cells} | \mathbf{Time} | \mathbf{Cells} |
| S_1, S_2, C | | | | | | 91 | 528 | 183 | 298 | 99 |
| S_2, S_3, C | | | | | | 627 | 2149 | 517 | 506 | 213 |
| S_3, S_4, C | 247458 | 11957 | 8164 | 1359 | 9177 | 1123 | 5476 | 881 | 590 | 213 |

Table 7. Spheres and Cylinders: $<_{Col}$

| | < _{Col} | $=_G/<_{\text{Co}}$ | $=_G/\overset{*}{\to}^G/<_{\text{Col}}$ | | |
|---------------|------------------|---------------------|---|-----------------|-------|
| | Time Cells | Time | Cells | \mathbf{Time} | Cells |
| S_1, S_2, C | 30 1073 | 23 + 8 = 31 | 267 | 24 + 4 = 28 | 99 |
| S_2, S_3, C | 763 12097 | 27 + 36 = 63 | 1299 | 28 + 13 = 41 | 213 |
| S_3, S_4, C | 1760 11957 | 28 + 37 = 65 | 1359 | 29 + 14 = 43 | 213 |

5 Choice of Method

Suppose we are given a problem, which we may formulate as

quantified variables
$$e_1 = 0 \land \dots \land e_k = 0 \land B(f_1, \dots, f_l),$$
 (8)

where B is a Boolean combination of conditions $= 0, \neq 0, < 0$ etc. on some polynomials f_j , then we may be able, by applying Gröbner techniques to the e_j , producing $e_j^{(i)}$, and then reducing the f_j , to produce various alternative formulations

quantified variables
$$e_1^{(i)} = 0 \wedge \dots \wedge e_{k(i)}^{(i)} = 0 \wedge B(f_1^{(i)}, \dots, f_l^{(i)}),$$
 (8⁽ⁱ⁾)

and each of these may have several variable orderings compatible with the constraints implied by the quantification (if any). Which should we choose? Of course, in the presence of arbitrary parallelism, we can start them all, and accept the first to finish, but we may wish to be less extravagant.

In the contexts of $\not\supseteq_{\text{CH}}$ (strictly speaking, the REDLOG implementation), and where the only choice was in the variable order, this question was considered by [DSS04]. Retrospectively, there are two measures for the difficulty of a CAD computation: the time taken and the number of cells produced. For a given $\not\supseteq_{\text{CH}}$ problem, they observed that two are usually correlated for different formulations, and we observe the same here for $<_{\Delta \mathbf{R}}$ — see our tables. However, we would like a measure that could be calculated in advance, rather than retrospectively.

The processes of [Col75,CH91] starts with a set A_n of polynomials in n (ordered) variables x_1, \ldots, x_n , and

- 1. repeatedly project A_i into A_{i-1} in one fewer variable, until A_1 has only one variable.
- * (denote the set $\{A_n, \ldots, A_1\}$ by $A(x_1, \ldots, x_n)$)
- 2. isolate the roots of these polynomials to get a decomposition of \mathbb{R}^1 ,
- 3. repeatedly lift the decomposition until we get a (partial for [CH91]) cylindrical algebraic decomposition of \mathbb{R}^n .

The third step is, both theoretically and practically, by far the most expensive. Hence the question arises: what can we measure at the end of step 1, i.e. depending on A only, which is well-correlated with the final cost? Three things come to mind.

$$\begin{array}{l} \operatorname{card}(A(x_1,\ldots,x_n)) &= \sum_{i=1}^n |A_i|. \\ \operatorname{td}(A(x_1,\ldots,x_n)) &= \sum_{i=1}^n \sum_{p_{i,j} \in A_i} \operatorname{td}(p_{i,j}) \text{ where td denotes total degree.} \\ \operatorname{sotd}(A(x_1,\ldots,x_n)) &= \sum_{i=1}^n \sum_{p_{i,j} \in A_i} \sum_{\text{monomials } m \text{ of } p_{i,j}} \operatorname{td}(m). \end{array}$$

[DSS04] discard td, observing that td and sotd are highly correlated and sotd "has the advantage of favouring sparse polynomials". They then observe that $sotd(A(x_1,...,x_n))$ is significantly more correlated with the retrospective measures for any given problem than card. This gives a first algorithm for deciding how to project: for all admissible (i.e. compatible with the quantifier structure, if

any) permutations π of (x_1, \ldots, x_n) , compute $A(x_{\pi(1)}, \ldots, x_{\pi(n)})$, and choose the one with the least sotd value. The drawback of this is that it requires potentially (n-1)n! projection operations. They show that (at least on their examples) this always produces a good projection order, and frequently the optimal.

| | | $<_{\Delta {f R}}$ | $=_G/<$ | $\leq_{\Delta \mathbf{R}}$ | $=_G/\overset{*}{\to}^G/<_{\Delta\mathbf{R}}$ | | |
|---------------|---|--------------------|---------|----------------------------|---|------------------|--|
| | | Time Cells | Time | \mathbf{Cells} | Time | \mathbf{Cells} | |
| S_1, S_2, C | С | 8654 1073 | 905 | 267 | 270 | 99 | |
|] | R | | 902 | 267 | 453 | 183 | |
| S_2, S_3, C | С | 189202 12097 | 5911 | 1299 | 499 | 213 | |
|] | R | | 18941 | 2639 | 5307 | 859 | |
| S_3, S_4, C | С | 248340 11957 | 8159 | 1359 | 580 | 213 | |
| | R | | 160171 | 9091 | 196714 | 11203 | |

Table 8. Spheres and Cylinders: $<_{\Delta \mathbf{R}}$ — choice of orderings

They therefore propose a greedy algorithm, where for all permissible choices of the first variable to be projected, we compute $sotd(A_{n-1})$, and choose the variable which gives the least value. Having fixed this as the first variable to project, for all permissible choices of the second variable to be projected, we compute $sotd(A_{n-2})$, and choose the variable which gives the least value, and so on. Hence, assuming all projection orders are possible, the **number** of projections done is $n + (n-1) + \cdots = O(n^2)$ rather than n!. It is currently an open question whether the **cost** of projections behaves similarly.

We proposed taking this idea still further, and suggested that, for several different formulations A_n, B_n, \ldots of a problem, we should compute $sotd(A_n)$, $sotd(B_n), \ldots$ and take the formulation that yields the lowest sotd. We observed, however, that neither td nor sotd are good predictors in Table 11, despite seeming useful in Table 10.

6 The metric TNoI

When we apply Gröbner techniques to a set of equations (either by calculating a basis or a normal form) we are, in some sense, trying to simplify the set of equations. In a zero-dimensional ideal, as shown in the Gianni-Kalkbrener Theorem [Gia89,Kal89], a purely lexicographic Gröbner basis has a very distinct, triangular structure.

With this in mind we thought it may be of some use to consider the number of variables present in a certain problem and so defined the following quantity, TNoI, which stand for "Total Number of Indeterminates":

$$TNoI(F) = \sum_{f \in F} NoI(f), \tag{9}$$

where NoI(f) is the number of indeterminates present in a polynomial f.

Table 9. [BH91]: effect of orderings $=_{GC}$ versus $=_{GR}$

| | | <_\D | R | $=_G/<$ | $\Delta \mathbf{R}$ |
|----------------|--------------|---------|------------------|---------|---------------------|
| | | Time | \mathbf{Cells} | Time | \mathbf{Cells} |
| Intersection A | \mathbf{C} | 29426 | 3763 | 2470 | 273 |
| | R | | | > 1000s | ? |
| Intersection B | С | 36262 | 2795 | 1482 | 189 |
| | R | | | > 1000s | ? |
| Random A | С | 17355 | 1219 | 570 | 165 |
| | R | | | > 1000s | ? |
| Random B | С | 356670 | 7119 | 470 | 141 |
| | R | | | > 1000s | ? |
| Ellipse A* | С | 262623 | 28557 | 62496 | 14439 |
| | R | | | 271726 | 29939 |
| Ellipse B* | С | > 1000s | ? | > 1000s | ? |
| | R | | | > 1000s | ? |
| Solotareff A* | С | 16014 | 1751 | 2025 | |
| | R | | | > 1000s | ? |
| Solotareff B* | С | 43439 | 6091 | 1647 | - |
| | R | | | > 1000s | ? |
| Collision A* | С | 216028 | 7895 | > 1000s | ? |
| | R | | | > 1000s | ? |
| Collision B* | С | > 1000s | ? | > 1000s | ? |
| | R | | | > 1000s | ? |

We note that $=_{GR}$ is definitely worse than $=_{GC}$.

Table 10. Spheres and Cylinders: $<_{\Delta \mathbf{R}}$ —degrees

| | $<_{\Delta {f R}}$ | | | | | | | | $=_G/$ | | |
|---------------|--------------------|--------|------------------|---------|------|------------------|---------|-----------------|------------------|--|--|
| | degrees | Time | \mathbf{Cells} | degrees | Time | \mathbf{Cells} | degrees | \mathbf{Time} | \mathbf{Cells} | | |
| S_1, S_2, C | | | | | | | | | | | |
| S_2, S_3, C | | | | | | | | | | | |
| S_3, S_4, C | 6 / 21 | 248340 | 11957 | 5 / 15 | 8159 | 1359 | 5 / 15 | 580 | 213 | | |

'degrees' is $td(A_n)/sotd(A_n)$.

Table 11. [BH91]: degrees

| | | $<_{\Delta {f R}}$ | | = | $G/<_{\Delta \mathbf{R}}$ | |
|----------------|---------|--------------------|------------------|----------|---------------------------|------------------|
| | degrees | \mathbf{Time} | \mathbf{Cells} | degrees | \mathbf{Time} | \mathbf{Cells} |
| Intersection A | 6 / 14 | 29426 | 3763 | 17 / 50 | 2470 | 273 |
| Intersection B | 6 / 14 | 36262 | 2795 | 15 / 41 | 1482 | 189 |
| Random A | 9 / 16 | 17355 | 1219 | 19 / 68 | 570 | 165 |
| Random B | 9 / 16 | 356670 | 7119 | 19 / 73 | 470 | 141 |
| Ellipse A* | 6 / 24 | 262623 | 28557 | 6 / 26 | 62496 | 14439 |
| Ellipse B* | 6 / 24 | > 1000s | ? | 25 / 253 | >1000s | ? |
| Solotareff A* | 10 / 25 | 16014 | 1751 | 10 / 28 | 2025 | 297 |
| Solotareff B* | 10 / 25 | 43439 | 6091 | 21 / 69 | 1647 | 243 |
| Collision A* | 6 / 23 | 216028 | 7895 | 27 / 251 | >1000s | ? |
| Collision B* | 6 / 23 | > 1000s | ? | 36 / 875 | >1000s | ? |

6.1 TNoI data

The results of calculating such a quantity are given in Table 8, Table 9 and Table 10, showing a promising correlation to whether our preconditioning (with compatible ordering) is beneficial or not. In particular we note the following points:

- In every example where preconditioning reduces TNoI (15 cases) there is a significant reduction in timing (a decrease factor ranging from 4.20 to 757.26) and number of cells produced (a decrease factor ranging from 1.98 to 65.13).
- When preconditioning increases TNoI (7 cases) then generally there is an increase in time (an increase factor ranging from 1.79 to 6.13) and the number of cells created (an increase factor ranging from 1.35 to 3.52) or the problem remains infeasible. There is one 'false positive' result ([CMMXY09, Example 2]) where there is an increase in TNoI but a slight improvement in the time (a decrease factor of 1.20) and cells produced (a decrease factor of 1.55).
- TNoI alone does not measure the abstract difficulty of the calculations: Intersection A has a higher TNoI than Ellipse A yet the latter takes 25 times longer and produces over 50 times as many cells. We have only shown how to use it to compare variants of the same problem.

As mentioned above, calculating TNoI alone is not of a huge use, and even considering the difference or ratio does little to predict the degree of improvement to expect. However, if we take the logarithm of the ratio (equivalently the difference of the logarithms) of TNoI and compare to the time or number of cells we get some interesting results.

Plotting these quantities against each other certainly suggested there was a positive correlation. Recall that the sample correlation coefficient is defined as

$$r_{X,Y} = \frac{\sum_{i=1}^{n} (X_i - \overline{X})(Y_i - \overline{Y})}{\sqrt{\sum_{i=1}^{n} (X_i - \overline{X})^2} \sqrt{\sum_{i=1}^{n} (Y_i - \overline{Y})^2}}$$
(10)

and is a number between -1 and 1 that indicates how correlated data is. A sample coefficient of 1 indicates perfect positive correlation and a coefficient of -1 indicates perfect negative correlation. Although we are only working with a small bank of data (22 examples) and partially incomplete data (timings of > 1000s were replaced by 10000 seconds and unknown cell numbers were replaced by 100000 to allow for coefficient calculation) there were still promising results.

Let S be the polynomial input, \mathcal{D}_S its corresponding CAD, t_S the time taken to calculate \mathcal{D}_S and c_S the number of cells in \mathcal{D}_S . Let G be the Gröbner basis calculated with respect to the compatible ordering and define \mathcal{D}_G , t_G and c_G in a similar fashion. With the data set we obtained the sample correlation coefficients were as follows:

- comparing $\log(\mathtt{TNoI}(S)) - \log(\mathtt{TNoI}(G))$ with $\log(t_S) - \log(t_G)$ gives a sample coefficient r = 0.821 which indicates strong correlation (for our limited sample set).

- comparing $\log(\mathtt{TNoI}(S)) - \log(\mathtt{TNoI}(G))$ with $\log(c_S) - \log(c_G)$ gives a sample coefficient r = 0.829 which again indicate a strong correlation (for our limited sample set).

Of course correlation does not imply causation, especially with a relatively small data set, so let us look more deeply at what TNoI is measuring.

Table 12. TNoI for Spheres

| ĺ | | $<_{\Delta \mathbf{R}}$ $=_G/<_{\Delta \mathbf{R}}$ | | | | R | $=_G$ | $/\overset{*}{\rightarrow}^{G}/$ < | $<_{\Delta {f R}}$ | |
|---|---------------|---|--------|------------------|------|-----------------|------------------|------------------------------------|--------------------|------------------|
| | | TNoI | Time | \mathbf{Cells} | TNoI | \mathbf{Time} | \mathbf{Cells} | TNoI | \mathbf{Time} | \mathbf{Cells} |
| Ī | S_1, S_2, C | | 8654 | 1073 | 5 | 905 | 267 | 4 | 270 | 99 |
| | S_2, S_3, C | 8 | 189202 | 12097 | 6 | 5911 | 1299 | 6 | 499 | 213 |
| | S_3, S_4, C | 8 | 248340 | 11957 | 7 | 8159 | 1359 | 7 | 580 | 213 |

Table 13. TNoI for [BH91]

| | | $<_{\Delta {f R}}$ | | $=_G/<_{\Delta \mathbf{R}}$ | | |
|----------------|------|--------------------|-------|-----------------------------|--------------|-------|
| | TNoI | \mathbf{Time} | Cells | TNoI | Time | Cells |
| Intersection A | 8 | 29426 | 3763 | 7 | 2470 | 273 |
| Intersection B | 8 | 36262 | 2795 | 7 | 1482 | 189 |
| Random A | 9 | 17355 | 1219 | 5 | 570 | 165 |
| Random B | 9 | 356670 | 7119 | 5 | 471 | 141 |
| Ellipse A* | 7 | 262623 | 28557 | 6 | 62496 | 14439 |
| Ellipse B* | 7 | > 1000s | ? | 21 > | $\sim 1000s$ | ? |
| Solotareff A* | 9 | 16014 | 1751 | 8 | 2025 | 297 |
| Solotareff B* | 9 | 43439 | 6091 | 7 | 1647 | 243 |
| Collision A* | 7 | 216028 | 7895 | 18 > | $\sim 1000s$ | ? |
| Collision B* | 7 | > 1000s | ? | 22 > | $\sim 1000s$ | ? |

6.2 What is TNoI measuring?

Consider what causes TNoI to decrease. Let S be a set of polynomials in variables x_1, \ldots, x_n ordered $x_1 < x_2 < \cdots < x_n$. The following are three possible reasons for a decrease in TNoI:

- 1. The number of polynomials in a specific set of variables, $\{x_{i_1}, \ldots, x_{i_l}\}$, is decreased. If x_k is the most important variable then reducing the number of these polynomials will simplify the decomposition in the (x_1, \ldots, x_k) -plane. This will simplify the overall CAD, reducing the number of cells produced and hence the time taken to calculate the decomposition.
- 2. At least one variable is eliminated from a polynomial. If the variable x_k is eliminated from a polynomial p then the decomposition based around p

Table 14. TNoI for [CMMXY09]

| | $<_{\Delta {f R}}$ | | | $=_G/<_{\Delta \mathbf{R}}$ | | | |
|----------|--------------------|-----------------|-------|-----------------------------|--------------------|-------|--|
| | TNoI | \mathbf{Time} | Cells | TNoI | \mathbf{Time} | Cells | |
| Cyclic-3 | 9 | 3136 | 381 | 6 | 20 + 245 = 265 | 21 | |
| Cyclic-4 | 16 | > 1000s | ? | 6 | 64 + 5813 = 5877 | 621 | |
| 2 | 7 | 2249 | 895 | 14 | 22 + 1845 = 1867 | 579 | |
| 4 | 6 | 3225 | 421 | 11 | 24 + 19738 = 19762 | 1481 | |
| 6 | 4 | 363 | 41 | 5 | 20 + 918 = 938 | 89 | |
| 7 | 8 | 3667 | 895 | 22 | 26 + 6537 = 6563 | 1211 | |
| 8 | 6 | 3216 | 365 | 5 | 21 + 174 = 195 | 51 | |
| 13 | 9 | 14342 | 4949 | 4 | 18 + 220 = 238 | 81 | |
| 14 | 11 | 334860 | 27551 | 9 | 21 + 971 = 992 | 423 | |

will be greatly simplified. This will again simplify the overall CAD, reducing the number of cells produced and hence the time taken to calculate the decomposition.

3. A polynomial in a large number of variables, say k, is replaced by j polynomials each with n_i variables such that $\sum n_i < k$. Intuitively this would increase the number of discriminants and resultants calculated, be it in the projection phase of $<_{\text{Col}}$ or in $\neq_{\Delta \mathbf{C}}$, but the results appear in lower levels of the projection tree, and this effect is more potent than the apparent increase in the number of discriminants and resultants. We have yet to build a good model of this, though.

Obviously, in general, a combination of these factors will be the reason for the decrease in TNoI. Also, there may be opposing increases in TNoI, which presumably explains why the 'false positive' of [CMMXY09, Example 2] shows an increase in TNoI but an improvement in the CAD efficiency.

7 Conclusions

- For both $<_{\text{Col}}$ and $<_{\Delta \mathbf{R}}$ and $\neq_{\Delta \mathbf{C}}$, pre-conditioning the equations (where applicable) by means of a Gröbner calculation is often well worth doing.
- Gröbner reduction of inequalities with respect to equalities has never, in our examples, made things worse.
- A priori, it can be quite difficult to see which combinations of Gröbner base and Gröbner reduction will be best, but the Gröbner side is generally cheap⁴.
- We therefore have multiple equivalent formulations of a given problem. We have investigated the metrics of [DSS04], but have concluded that, at the level of choice of formulation, TNoI is a better predictor. It does not help for predicting the best ordering of variables, for which [DSS04] or the Brown heuristic [Bro04] are appropriate. Phisanbut [Phi11, Chapter 8] found the Brown heuristic sufficiently good, and simpler to compute.

⁴ This is a significant change from [BH91], who had examples where the Gröbner calculations was much more expensive than the Cylindrical Algebraic Decomposition.

- In Section 3.2 we saw how $g = 0 \land f > 0$ could be reduced to $g = 0 \land$ sprecond(f,g) > 0. In principle, given $s_1 = 0 \land \cdots \land s_k = 0 \land f > 0$, after computing a Gröbner base G for the s_i , we could attempt a more general reduction of f by G. Pure NormalForm reduction has proved useful (Tables 6, 7), but we do not have enough good examples to measure the utility of a more general pseudoremainder-like reduction.

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