Varieties of Doubly-Exponential behaviour in Quantifier Elimination and Cylindrical Algebraic Decomposition

#### James Davenport<sup>1</sup> Job at https: //www.bath.ac.uk/jobs/Vacancy.aspx?ref=CC9078

University of Bath

February 2022

<sup>1</sup>Partially Supported by EPSRC Grant EP/T015713/1

James DavenportJob at https://www.bath.ac.uk/jobs/Vacanc 1/32

- Introduction
- Oubly Exponential?
- 8 Resultant-based projection
- Ochordality
- **6** Equational Constraints
- **o** Virtual Term Substitution
- Omprehensive Gröbner Bases
- 8 Regular Chains
- Summary

## Notation

- *d* The maximum degree (in each variable separately) of the input polynomials.
- / The maximum bit-length of the integer coefficients
- *m* The number of (distinct) polynomials.
- *n* The number of variables.
- *a* The number of alternations of quantifiers.  $a \le n 1$ .
- *q* The number of equational constraints.
- This is the standard theory setting. Real problems tend to involve rational functions, and rational, or even algebraic, numbers.
- (M, D) At most M sets, each of combined degree  $\leq D$  [McC84].

## Doubly Exponential?

The complexity of QE (and hence CAD) is doubly exponential in n, more precisely  $d^{2^{e_d}}m^{2^{e_m}}$  where  $e_d$  and  $e_m$  depend non-trivially on n (or on a).

[Col75] 
$$e_m \le n + O(1); e_d \le \log_2 3n + O(1).$$

- [McC84] Both bounded by n + O(1), conditional on no (awkward) nullification.
  - [Laz94] (justified by [MPP19]) n + O(1) unconditionally.
  - [DH88] both  $e_d$  and  $e_m$  were at least n/5 + O(1), with a being  $\Theta(n)$ (in fact 2n/5 + O(1))
  - [BD07] (again with a being  $\Theta(n)$ , this time 2n/3 + O(1)) that  $e_m$  was at least n/3 + O(1), even if d = 1.
  - [BD07]  $e_m$  was at least n/3 + O(1), even if d = 1 (again with a being  $\Theta(n)$ , this time 2n/3 + O(1)).

Numerous heuristics [HEW<sup>+</sup>19, e.g.], generally based on degrees of polynomials, for choosing order of elimination etc..

Instead of considering degrees of the polynomials in F, consider the graph  $\mathcal{G}(F)$  on  $\{x_1, \ldots, x_n\}$  with an edge betwen  $(x_i, x_j)$  iff there is a polynomial in F containing both  $x_i$  and  $x_j$ . Connectedness?

- Gröbner If  $\mathcal{G}(F)$  is not connected, the problems are independent, and [Buc79, Criterion 1] will treat them as such.
  - CAD Essentially independent, but this is hard to describe: we have "the outer product" of the two (or more) CADs. We definitely need to project one component at a time.

- A graph  $\mathcal{G}$  is *chordal* if every every > 3-cycle has a chord.
- Equivalently, every induced cycle has length 3. Every graph  $\mathcal{G}$  has a chordal completion  $\overline{\mathcal{G}}$ .
- Minimum chordal completion is NP-complete [Yan81], but that doesn't really worry me.
- If this is the complete graph, then graph theory doesn't seem to help us: the exciting case is when  $\overline{\mathcal{G}}$  is smaller.
- An ordering  $\succ$  on the vertices  $x_1, \ldots, x_n$  is a *perfect elimination* ordering if  $\forall i \ x_i$  and its neighbours  $x_j : x_j \prec x_i$  form a clique. This, and chordality, can be found efficiently [RTL76].

Non-trivial chordality has been exploited.

Regular Chains [Che20] shows how it can be exploited efficiently.

- Gröbner Bases [CP16] consider "chordal elimination". The challenge here is that an S-polynomial can introduce new edges in  $\mathcal{G}$ .
  - CAD [LXZZ21] consider chordality here, ordering x<sub>i</sub> in a perfect elimination ordering.
  - Here  $e_d$  (and I think  $e_m$ ) becomes the "tree depth"  $\leq n$ , assuming that these paths are compatible with any quantifier structure.

What we currently lack is any view of how common in practice these non-trivial chordal structures are.

## Equational Constraints and $e_m$

Any CAD algorithm based on iterated resultants is bound to have  $e_m = n + O(1)$  in the worst case, because this is how the number of polynomials grows as we take iterated resultants and discriminants: from m to  $\frac{m(m+1)}{2}$  as we eliminate one variable. Starting with [McC99], we explore how, in constructing a CAD to do QE for  $f(\mathbf{x}) = 0 \land \Phi(g_i(\mathbf{x}))$ , i.e. a CAD of  $f(\mathbf{x}) = 0$  rather than the whole of  $\mathbb{R}^n$ , it may not be necessary to consider  $\operatorname{res}_x(g_i, g_j)$ , but merely the  $\operatorname{res}_x(f, g_i)$ . Geometrically, we do not care how  $g_i$  and  $g_j$  interact off the variety, and algebraically we have rules for commuting resultants/discriminants.

If applicable (these ideas were developed for the McCallum projection, i.e. no nullification, and adapting to Lazard is challenging [Nai21]), these reduce  $e_m$  from n + O(1) to n - q + O(1).

There's a snag if  $res(f_i, f_j)$  (the derived equational constraint in fewer variables) has non-trivial content, which corresponds to  $\vee$  — back to QE?

Any CAD algorithm based on iterated resultants is bound to have  $e_d = n + O(1)$  in the worst case, because this is how resultant degrees grow.

If f, g, h have degree d, then  $\operatorname{res}_x(f, g)$  has degree  $2d^2$  and  $P_z := \operatorname{res}_y(\operatorname{res}_x(f, g), \operatorname{res}_x(f, h))$  has degree  $8d^4$ . This despite the fact that Bézout says there are  $O(d^3)$  common zeroes. P(z) has as roots, not just the z-coordinates of common zeros  $\{z : \exists y \exists x f(x, y, z) = g(x, y, z) = h(x, y, z)\}$ , but also  $\{z : \exists y (\exists x_1 f(x_1, y, z) = g(x_1, y, z) \land \exists x_2 f(x_2, y, z) = h(x_2, y, z))\}$  — spurious zeroes.

[BM09] show that there is a suitable multivariate resultant which has the "right" degree.

We have seen that equational constraints can reduce  $e_m$ . But they can also reduce  $e_d$  as well.

[ED16, DE16, EBD20] consider the use of either multivariate resultants [BM09] or Gröbner bases, and show that, under generic assumptions, this will also reduce  $e_d$  to n - q + o(1). We need the "generic assumptions", as there are issues when the resultants (or Gröbner basis elements) are not primitive [DE16]. Nevertheless, all these techniques bring substantial improvements in practice.

# VTS=Virtual Term Substitution, [Wei88] for linear

Here  $\cdots Q_n y_n \Phi(y_1, \dots, y_n)$  in which  $y_n$  occurs linearly can be replaced by  $\cdots \hat{\Phi}(y_1, \dots, y_{n-1})$ . This was extended in [Wei94, Wei97] to the quadratic case and beyond, with details of the cubic case being in [Koš16]. An extension to unbounded degree is given in [LPJ14].

A crude description would be "substituting in the critical values and their neighbours", but the details are more subtle, hence Weispfenning's concept of *virtual* term substitution.

In particular, if  $y_n$  occurs quadratically, with corresponding critical values  $y_n = \frac{1}{2a} \left( -b \pm \sqrt{b^2 - 4ac} \right)$ , there might be 0, 1 or 2 critical values, and we also need to worry about the case a = 0: hence VTS has substitutions with guards, and the result of eliminating an  $\exists$  quantifier, and hence a block of  $\exists$ , is a disjunction, often large. However, VTS treats  $\forall$  as  $\neg_1 \exists \neg_2$ , so  $\neg_2$  turns the disjunction into a conjunction, processing the  $\exists$  builds a further disjunction on top of this, which  $\neg_1$  turns back into a conjunction. Each could have exponential blowup, so  $a \geq 2^{2^a}$  behaviour for  $e_m$ .

James DavenportJob at https://www.bath.ac.uk/jobs/Vacanc 11/32

# CGB=Comprehensive Gröbner Bases (I) [Wei98, FIS15]

The key idea is this. We consider an "innermost block" in this form:

$$\exists \overline{x} \left( \begin{array}{c} f_1(\overline{y},\overline{x}) = 0 \land \cdots f_r(\overline{y},\overline{x}) = 0 \land \\ p_1(\overline{y},\overline{x}) > 0 \land \cdots p_s(\overline{y},\overline{x}) > 0 \land \\ q_1(\overline{y},\overline{x}) \neq 0 \land \cdots q_t(\overline{y},\overline{x}) \neq 0 \end{array} \right)$$

where  $\overline{y}$  represents the remaining variables, and  $f_i, p_j, q_k \in \mathbb{Q}[\overline{y}, \overline{x}] \setminus \mathbb{Q}[\overline{y}]$ . We introduce new variables  $\overline{z}$  and  $\overline{w}$ , with  $\overline{z}, \overline{w} \succ \overline{x}$ , and consider the polynomials

$$\{f_1, \ldots, f_r, \underbrace{z_1^2 p_1 - 1, \ldots, z_s^2 p_s - 1}_{\text{forcing positive}}, \underbrace{w_1 q_1 - 1, \ldots, w_t q_t - 1}_{\text{forcing nonzero}}\}.$$

Let  $\mathcal{G} = (S_i, G_i)$  be a Comprehensive Gröbner System (with parameters  $\overline{y}$ ) for this so that  $\overline{y}$  space is partitioned by the  $S_i$ . We claim each  $G_i$  will be  $\{f'_1, \ldots, f'_{r'}, u_1 z_1^2 - p'_1, \ldots, u_s z_s^2 - p'_s, v_1 w_1 - q'_1, \ldots, v_t w_t - q'_t\}$ . Our answer will be  $\bigvee_i \Psi_i(S_i, G_i)$ : next two slides explain  $\Psi_i$ . If  $G_i = (1)$  then we return false. Otherwise recall  $G_i = \{f'_1, \dots, f'_{r'}, u_1 z_1^2 - p'_1, \dots, u_s z_s^2 - p'_s, v_1 w_1 - q'_1, \dots, v_t w_t - q'_t\}.$ Let  $I = \langle f'_1, \dots, f'_{r'} \rangle$ ,

$$\chi(x) = \prod_{(e_1,\ldots,e_s)\in\{0,1\}^s} \chi'_{(p'_1/u_1)^{e_1},\cdots,(p'_s/u_s)^{e_s}}(x) = x^{2^sd} + \sum_{0}^{2^sd-1} a_i x^i.$$

The answer is  $\Psi_i := \mathcal{F}(S_i) \wedge I_{2^s d}(a_i)$ .

JHD: at least that's my reconstruction. I can't see where the  $w_i$  (the  $\neq 0$ ) terms come in. Also, the subscript of  $\chi_{...}^{I}$ , the characteristic polynomial of  $M_{...}^{I}$ , is not a polynomial.

# $\exists \phi: G_i > 0$ -dimensional ( $\overline{z}, \overline{w}$ irrelevant for dimension)

 $\overline{u} :=$ maximal independent variables ( $\overline{x}, G_i, \succ$ ). (B) If  $\overline{u} = \overline{x}$  return SYNRAC( $\mathcal{F}(S) \land \exists \overline{x} \phi$ ) [Wei98]  $\overline{x}' := \overline{x} \setminus \overline{u}; \ \phi_1 := \operatorname{Free}(\phi, \overline{x}'); \ \phi_2 := \operatorname{NonFree}(\phi, \overline{x}');$  $\varphi := \phi_1 \land \mathsf{Recurse}(S_i, \exists \overline{x}' \phi_2) \qquad (1)(\mathsf{A})$ JHD: I think this means  $\varphi$  now only contains  $\overline{u}$ -variables Let  $\varphi_1 \vee \cdots \vee \varphi_l$  be a disjunctive normal form of  $\varphi$ . (C) for 1 < i < l do  $\varphi_i^{(1)} := \operatorname{Free}(\varphi, \overline{u}); \ \varphi_i^{(2)} := \operatorname{NonFree}(\varphi_i, \overline{u});$  $\psi_i := \varphi_i^{(1)} \land \mathsf{Recurse}(\underline{S}_i, \exists \overline{u} \phi_i^{(2)}) \tag{2}(E)$ Return  $\Psi := \mathcal{F}(S_i) \land (\psi_1 \lor \cdots \lor \psi_l)$ JHD: "Recurse" goes right back to the MainQE, note that call (1) has pushed the  $\overline{u}$ -variables into being parameters (I think) (D). But somehow  $S_i$  gets lost in these recursions: I hope I've added it in the right place. Their Theorem 16 states that this does terminate — far from obvious (F).

# CGB=Comprehensive Gröbner Bases (IV) [Wei98, FIS15]

- Recursing with S is, I think, my interpolation to make sense of the recursions we'll see later. S initially is ℝ<sup>#ȳ</sup>.
- There's a lot of freedom here: ML?
- Onte that our main recursion is on φ in conjunctive normmal form (CNF), whereas here we convert to disjunctive normal form (DNF) and implicitly back at the end of the block. Since CNF↔DNF naïvely is exponential, this would provide an exponential blowup at each ∃/∀ boundary, similar to [DH88].
- Therefore this recursion is on strictly fewer variables, since dim > 0.
- But the two previous notes are probably key.

I know no results on the complexity of Comprehensive Gröbner Bases.

Since we are doing Gröbner Bases, we might *hope for* singly exponential behaviour at each block, and hence  $e_d = O(a)$  rather than O(n), but worst-case Gröbner bases can be doubly exponential [MR13]. *If* we get O(a) behaviour, though, this does not depend on having a lot of equational constraints. We are doing CNF/DNF conversions at each quantifier alternation, as with VTS, so this could be expected to give us  $e_m = O(a)$ rather than O(n). Regular Chains/Triangular Decompositions are an alternative to Gröbner bases, and write the solution as a union of triangular sets. Very little is known about the complexity of Triangular Decompositions. I *believe* that the upper bounds for Gröbner bases [Dub90, etc.] still apply, but I haven't seen a formal proof. In the presence of equational constraints [BCD<sup>+</sup>14], we should get the same improvement as Gröbner bases deliver. There is probably a relationship between the different triangular sets in a Triangular Decomposition and the sets  $S_i$  in a Comprehensive Gröbner Basis, but again I don't know what this is.

# Black-swans [AL17]

"Average-case complexity without the black swans": i.e. without an exponentially-rare family that is worse than exponentially bad.

#### Definition

For  $k \in \mathbf{N}$  let  $(M_k, \mu_k)$  be a probability space and let  $T_k : M_k \to \mathbb{R}$ be a  $\mu_k$ -measurable function. We say that the family  $\{T_k\}$  has a weak expectation of O(f(k)) if there exists a family of sets of exceptional inputs,  $E_k \subseteq M_k$ , such that  $\mu_k(E_k) = e^{-\Omega(k)}$  and the conditional expectation  $E[T_k(x)|x \notin E_k]$  is bounded by O(f(k)).

- Condition numbers inversely proportional to a distance to a homogeneous algebraic set of ill-posed inputs;
- Renegar's condition number for conic optimization;
- The running time of power iteration for computing a leading eigenvector of a Hermitian matrix.
- ? Any such result in our area?

Idea  $e_m$  $e_d$ Collins n + O(1) $(\log_2 3)n + O(1)$ McCallum (but nullification) n + O(1)n + O(1)Lazard [MPP19] n + O(1)n + O(1)(?) n - q + O(1)Equational Constraints (?) n - q + O(1)Virtual Term Substitution (?) O(a)challenges Comprehensive Gröbner Bases (??) O(a) (??) O(a)-n+O(1)Regular Chains (??) n - q + O(1) (??) n - q + O(1)But Virtual Term Substitution (where applicable), Comprehensive Gröbner Bases and Regular Chains all seem to be very fast in practice.

## Conclusions/Questions

- We need to understand the complexity of Virtual Term Substitution.
- What about unbounded degree: [LPJ14]? It is restricted to univariates — is this inherent?
- We need to understand the complexity of Comprehensive Gröbner Bases.
- We need to understand the complexity of Regular Chains.
- We need to understand the inter-relationships between these methods.
- Are there any "weak average case complexity" results? The examples of [BD07, DH88] seem very special.

D. Amelunxen and M. Lotz. Average-case complexity without the black swans. J. Complexity, 41:82–101, 2017.

 R.J. Bradford, C. Chen, J.H. Davenport, M. England, M. Moreno Maza, and D.J. Wilson. Truth Table Invariant Cylindrical Algebraic Decomposition by Regular Chains.

In Proceedings CASC 2014, pages 44-58, 2014.

 C.W. Brown and J.H. Davenport. The Complexity of Quantifier Elimination and Cylindrical Algebraic Decomposition. In C.W. Brown, editor, *Proceedings ISSAC 2007*, pages 54–60, 2007.

# **Bibliography II**

#### L. Busé and B. Mourrain.

Explicit factors of some iterated resultants and discriminants. *Math. Comp.*, 78:345–386, 2009.

## B. Buchberger.

A Criterion for Detecting Unnecessary Reductions in the Construction of Groebner Bases.

In Proceedings EUROSAM 79, pages 3-21, 1979.



#### Changbo Chen.

Chordality Preserving Incremental Triangular Decomposition and Its Implementation.

In A.M. Bigatti, J. Carette, J.H. Davenport, M. Joswig, and T. de Wolff, editors, *Mathematical Software — ICMS 2020*, volume 12097 of *Springer Lecture Notes in Computer Science*, pages 27–38. Springer, 2020.

# **Bibliography III**

URL: https://www.researchgate.net/publication/ 342758264\_Chordality\_Preserving\_Incremental\_ Triangular\_Decomposition\_and\_Its\_Implementation, doi:10.1007/978-3-030-52200-1\_3.

C. Chen and M. Moreno Maza. Cylindrical Algebraic Decomposition in the RegularChains Library.

In *Proceedings Mathematical Software — ICMS 2014*, pages 425–433, 2014.

- C. Chen and M. Moreno Maza.

Quantifier Elimination by Cylindrical Algebraic Decomposition Based on Regular Chains.

In K. Nabeshima, editor, *Proceedings ISSAC 2014*, pages 91–98, 2014.

# Bibliography IV

G.E. Collins.

Quantifier Elimination for Real Closed Fields by Cylindrical Algebraic Decomposition.

In Proceedings 2nd. GI Conference Automata Theory & Formal Languages, pages 134–183, 1975.

D. Cifuentes and P. Parrilo.

Exploiting chordal structure in polynomial ideals: A Grobner bases approach.

SIAM Journal on Discrete Mathematics, 30:1534–1570, 2016.

- J.H. Davenport and M. England.
   Need Polynomial Systems be Doubly-exponential?
   In Proceedings ICMS 2016, pages 157–164, 2016.
- J.H. Davenport and J. Heintz. Real Quantifier Elimination is Doubly Exponential. J. Symbolic Comp., 5:29–35, 1988.

#### T.W. Dubé.

The structure of polynomial ideals and Gröbner Bases. *SIAM J. Comp.*, 19:750–753, 1990.

M. England, R.J. Bradford, and J.H. Davenport. Cylindrical Algebraic Decomposition with Equational Constraints.

In J.H. Davenport, M. England, A. Griggio, T. Sturm, and C. Tinelli, editors, *Symbolic Computation and Satisfiability Checking: special issue of Journal of Symbolic Computation*, volume 100, pages 38–71. 2020.

# **Bibliography VI**

#### 

#### M. England and J.H. Davenport.

The Complexity of Cylindrical Algebraic Decomposition with Respect to Polynomial Degree.

In V.P. Gerdt, W. Koepf, W.M. Seiler, and E.V. Vorozhtsov, editors, *Proceedings CASC 2016*, Springer Lecture Notes in Computer Science 9890, pages 172–192. Springer, 2016. URL: http://arxiv.org/abs/1605.02494, doi:10.1007/978-3-319-45641-6\_12.

 R. Fukasaku, H. Iwane, and Y. Sato.
 Real Quantifier Elimination by Computation of Comprehensive Gröbner Systems.
 In D. Robertz, editor, *Proceedings ISSAC 2015*, pages 173–180, 2015.

# **Bibliography VII**

Z. Huang, M. England, D. Wilson, J.H. Davenport, and L.C. Paulson.

Using Machine Learning to Improve Cylindrical Algebraic Decomposition.

Mathematics in Computer Science, 11:461-488, 2019.

M. Košta.

New concepts for real quantifier elimination by virtual substitution.

PhD thesis, Universität des Saarlandes, 2016.

## D. Lazard.

An Improved Projection Operator for Cylindrical Algebraic Decomposition.

In C.L. Bajaj, editor, *Proceedings Algebraic Geometry and its Applications: Collections of Papers from Shreeram*  *S. Abhyankar's 60th Birthday Conference*, pages 467–476, 1994.

K. Liiva, G.O. Passmore, and P.B. Jackson.

A note on real quantifier elimination by virtual term substitution of unbounded degree.

https:

//homepages.inf.ed.ac.uk/pbj/papers/pas14.pdf,
2014.

 H. Li, B. Xia, H. Zhang, and T. Zheng.
 Choosing the Variable Ordering for Cylindrical Algebraic Decomposition via Exploiting Chordal Structure.
 ISSAC '21: Proceedings of the 2021 International Symposium on Symbolic and Algebraic Computation, pages 281–288, 2021.

## S. McCallum.

An Improved Projection Operation for Cylindrical Algebraic Decomposition.

PhD thesis, University of Wisconsin-Madison Computer Science, 1984.

S. McCallum.

On Projection in CAD-Based Quantifier Elimination with Equational Constraints.

In S. Dooley, editor, *Proceedings ISSAC '99*, pages 145–149, 1999.

S. McCallum, A. Parusiński, and L. Paunescu.
 Validity proof of Lazard's method for CAD construction.
 J. Symbolic Comp., 92:52–69, 2019.

#### E.W. Mayr and S. Ritscher.

Dimension-dependent bounds for Gröbner bases of polynomial ideals.

J. Symbolic Comp., 49:78–94, 2013.

### A.S. Nair.

Curtains in Cylindrical Algebraic Decomposition. PhD thesis, University of Bath, 2021. URL: https: //researchportal.bath.ac.uk/en/studentTheses/ curtains-in-cylindrical-algebraic-decomposition.



Donald J Rose, R Endre Tarjan, and George S Lueker. Algorithmic aspects of vertex elimination on graphs. SIAM Journal on computing, 5(2):266–283, 1976.

# Bibliography XI

#### V. Weispfenning. The Complexity of Linear Problems in Fields. *J. Symbolic Comp.*, 5:3–27, 1988.

## V. Weispfenning.

Quantifier elimination for real algebra — the cubic case. In *Proceedings ISSAC 1994*, pages 258–263, 1994.

## V. Weispfenning.

Quantifier elimination for real algebra — the quadratic case and beyond.

AAECC, 8:85-101, 1997.

## V. Weispfenning.

A New Approach to Quantifier Elimination for Real Algebra. Quantifier Elimination and Cylindrical Algebraic Decomposition, pages 376–392, 1998.



Mihalis Yannakakis. Computing the minimum fill-in is NP-complete. SIAM Journal on Algebraic Discrete Methods, 2(1):77–79, 1981.