

# Real Quantifier Elimination Technology and Optimisations via Machine Learning

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Computational Algebraic Geometry Research Network

**University of Warwick**

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# Outline

- 1 The Real QE Problem
  - Quantifier Elimination
  - Real QE via CAD
  - Alternatives to Traditional CAD
- 2 Optimising CAD via Machine Learning
  - ML for Computer Algebra
  - ML for CAD Variable Ordering
  - Beyond Efficiency Gains
- 3 Applications (time permitting)
  - Biology
  - Economics

# Overview

(Slide 1/48)

**Summary:** the talk will describe the Real Quantifier Elimination Problem and the Cylindrical Algebraic Decomposition method to tackle it. We will introduce what these things are, how machine learning may be used to optimise them, and how explainable AI may be used to gain ideas to improve software without embedding machine learning models.

**Key message:** potential for fruitful interplay between computational mathematics and machine learning.

**Joint work with:** Rashid Barket, James Bridge, James Davenport, Tereso del Río, Forian Florescu, Zongyang Huang, Laurence Paulson, and Lynn Pickering.

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# Real QE

(Slide 2/48)

## Real Quantifier Elimination (Real QE)

**Given:** A quantified formulae (in prenex normal form) whose atoms are (integral) polynomial constraints;

**Produce:** a quantifier free formula logically equivalent over  $\mathbb{R}$ .

Fully quantified examples:

In:  $\exists x, x^2 + 3x + 1 > 0$

Out: True e.g. when  $x = 0$

In:  $\forall x, x^2 + 3x + 1 > 0$

Out: False e.g. when  $x = -1$

In:  $\forall x, x^2 + 1 > 0$

Out: True

Partially quantified example:

In:  $\forall x, x^2 + bx + 1 > 0$

Out: ???

The answer depends on the unquantified variable,  $b$ .

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## Partially quantified Tarski formulae example

(Slide 3/48)

Consider  $\forall x, x^2 + bx + 1 > 0$ .

When  $b = 0$  and  $b = 3$ :

$\forall x, x^2 + 1 > 0$  is True,

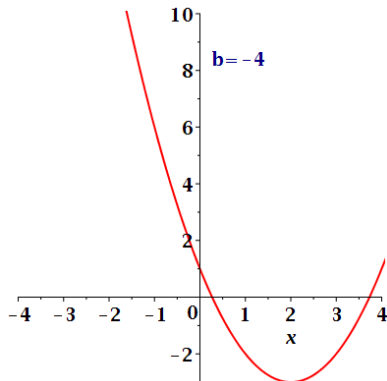
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So in general the answer  
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Input:  $\forall x, x^2 + bx + 1 > 0$

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The technology we look at  
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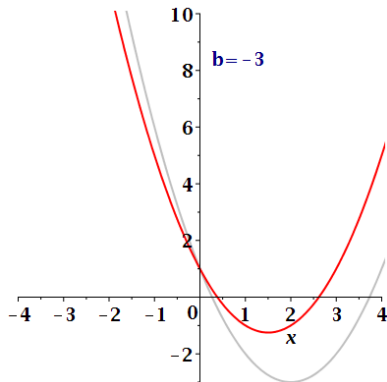
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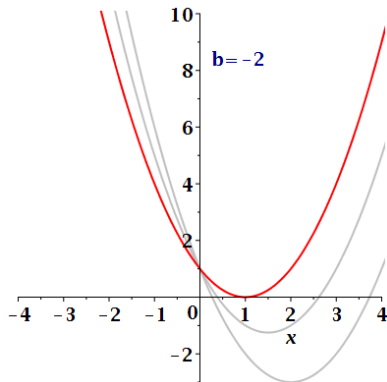
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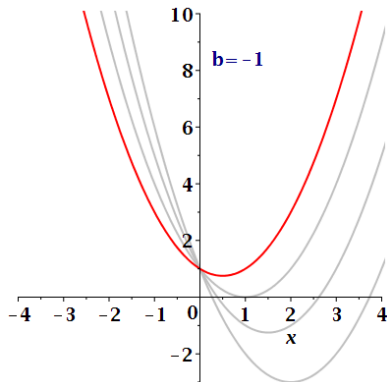
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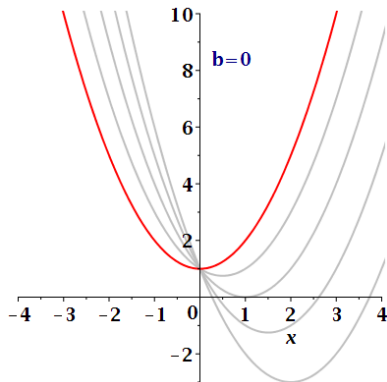
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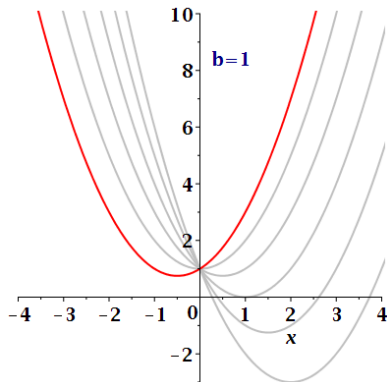
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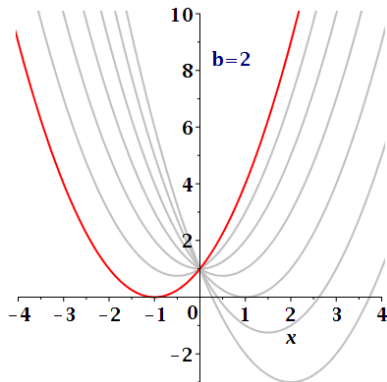
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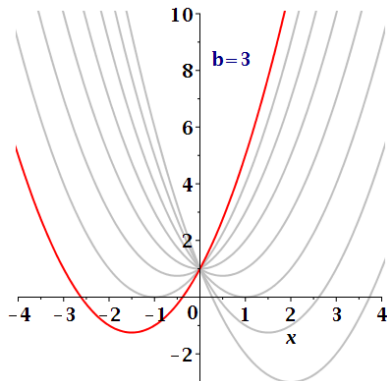
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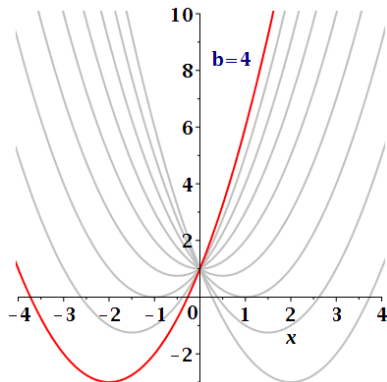
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## Numeric vs. Symbolic solution?

(Slide 4/48)

The solution in the previous slide was essentially numeric: try what happens for many different values and interpolate a solution.

The alternative is to use **Symbolic Computation**: algorithms and data-structures for manipulating exact mathematical expressions and objects. Traditionally implemented in *Computer Algebra Systems* (e.g. Macaulay2, Maple, Mathematica, Sage).

Advantages of Symbolic Computation:

- Can solve numerically ill-conditioned problems.
- Provide guarantees for safety critical systems.
- Provide fundamental insight into the system.

Disadvantage of Symbolic Computation: much more expensive!

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# Cylindrical Algebraic Decomposition

(Slide 5/48)

A **Cylindrical Algebraic Decomposition (CAD)** is:

- a **decomposition** of  $\mathbb{R}^n$  into a set of cells  $C_i$  (i.e.  $\bigcup_i C_i = \mathbb{R}^n$  and  $C_i \cap C_j = \emptyset$  if  $i \neq j$ ) such that:
- cells are **semi-algebraic** meaning they may be described by a finite sequence of polynomial constraints;
- cells are **cylindrical** meaning the projection of any two onto a lower coordinate space *in the variable ordering* are identical or disjoint (i.e. the cells in  $\mathbb{R}^m$  stack up in cylinders over cells from CAD in  $\mathbb{R}^{m-1}$ ).



G.E. Collins.

*Quantifier elimination for real closed fields by cylindrical algebraic decomposition.*

In Proc. 2nd GI Conf. Automata Theory and Formal Languages, pp. 134–183. Springer-Verlag, 1975.

# CAD Invariance Property

(Slide 6/48)

CAD may also refer to an algorithm that produces the CAD object.

The traditional CAD algorithm introduced by Collins in the 1970s takes a set of input polynomials and produces a CAD such that each polynomial has constant sign in each cell: this additional property is called **sign-invariance**.

Such a CAD allows us to uncover properties of polynomials over infinite space by examining finite set of sample points.

Most applications (e.g. QE) actually provide as input a **logical formulae built from polynomial constraints** and require as output a **truth-invariant CAD**: one such that each formula has **constant truth value** in each cell.

Such a CAD allows us to find solution sets from the descriptions of true cells: semi-algebraic; easy to visualise and check membership.

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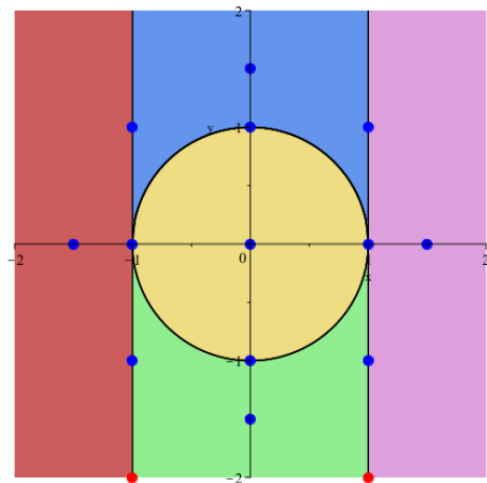
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## Example: Circle – visualisation

(Slide 7/48)

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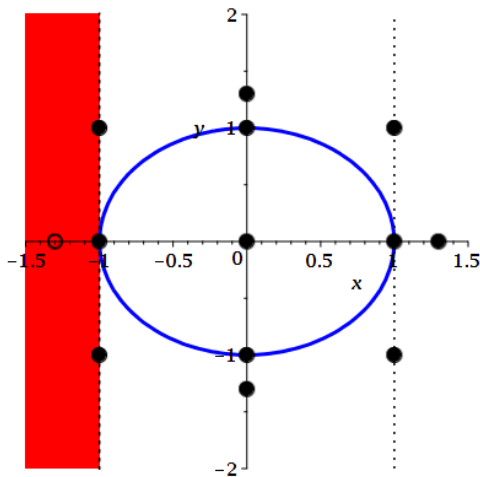
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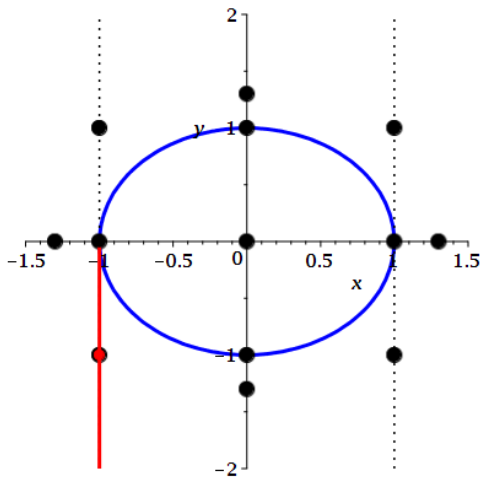
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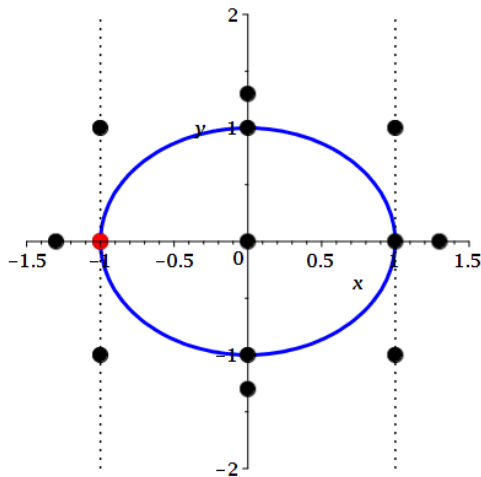




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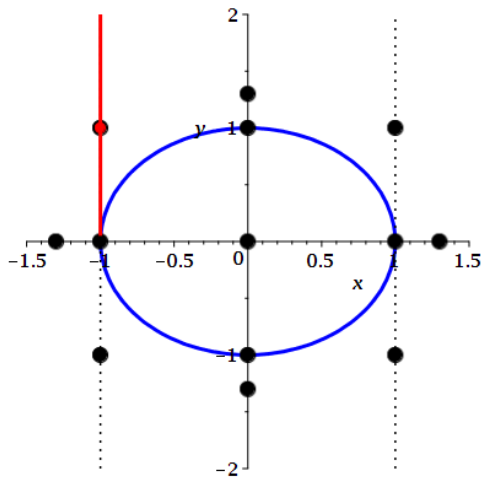
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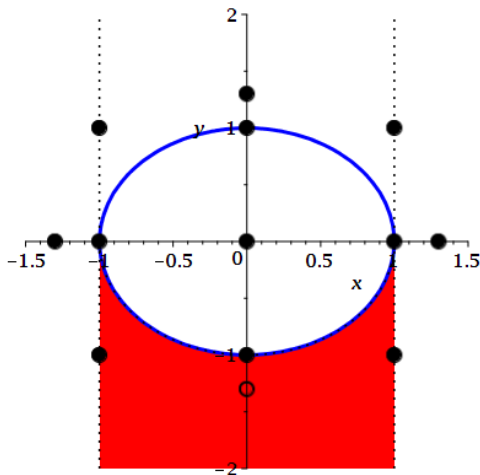
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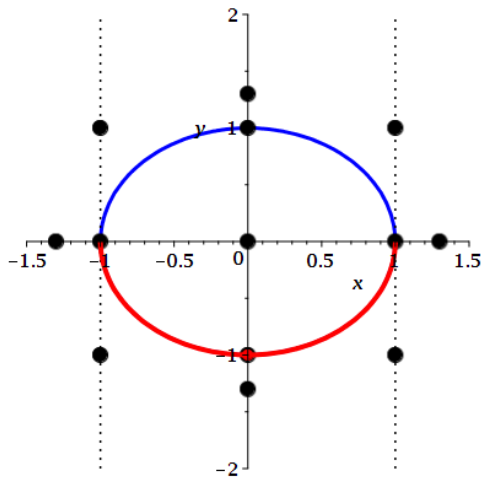
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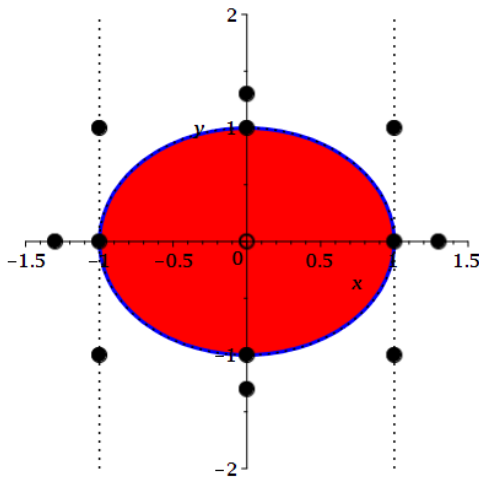
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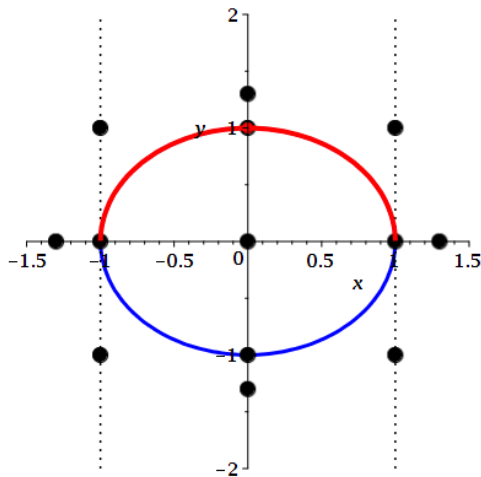
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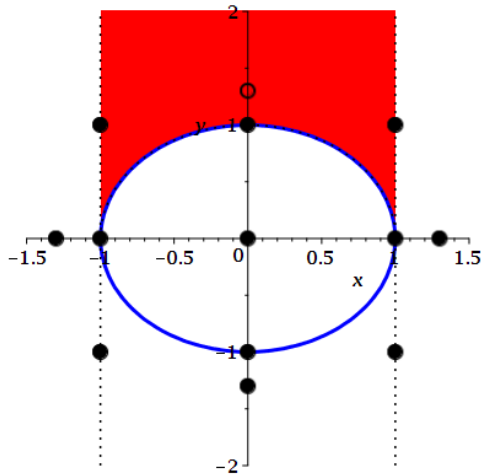
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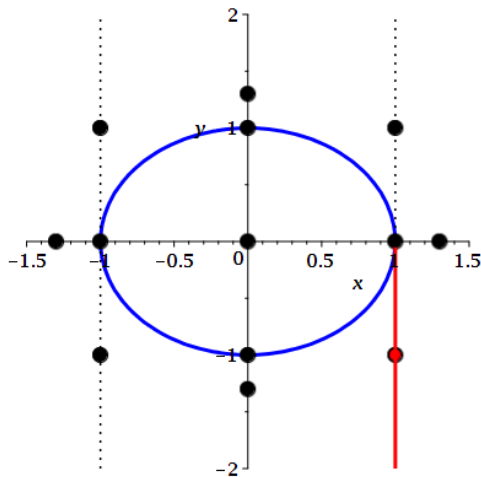
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- Cell 10:  $x = 1, y < 0$
- Cell 11:  $x = 1, y = 0$
- Cell 12:  $x = 1, y > 0$
- Cell 13:  $x > 1, y$  free



# Example: Circle – visualisation

(Slide 7/48)

- Cell 1:  $x < -1, y$  free
- Cell 2:  $x = -1, y < 0$
- Cell 3:  $x = -1, y = 0$
- Cell 4:  $x = -1, y > 0$
- Cell 5:  $-1 < x < 1,$   
 $y^2 + x^2 - 1 > 0, y < 0$
- Cell 6:  $-1 < x < 1,$   
 $y^2 + x^2 - 1 = 0, y < 0$
- Cell 7:  $-1 < x < 1,$   
 $y^2 + x^2 - 1 < 0$
- Cell 8:  $-1 < x < 1,$   
 $y^2 + x^2 - 1 = 0, y > 0$
- Cell 9:  $-1 < x < 1,$   
 $y^2 + x^2 - 1 > 0, y > 0$
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- Cell 13:  $x > 1, y$  free

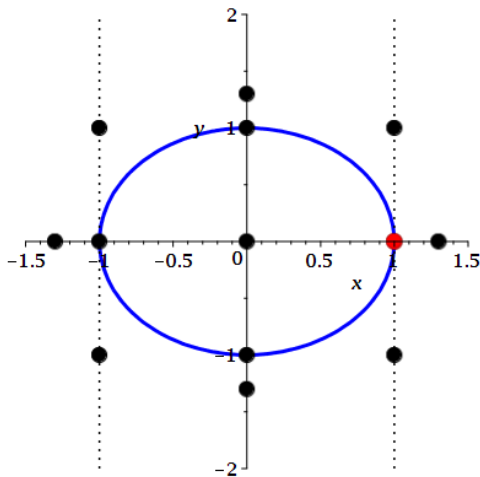




## Example: Circle – visualisation

(Slide 7/48)

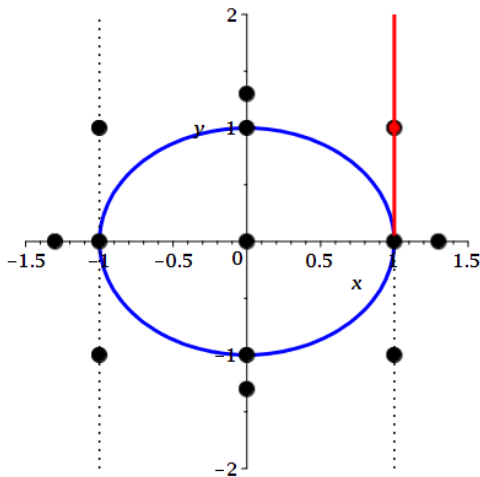
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(Slide 7/48)

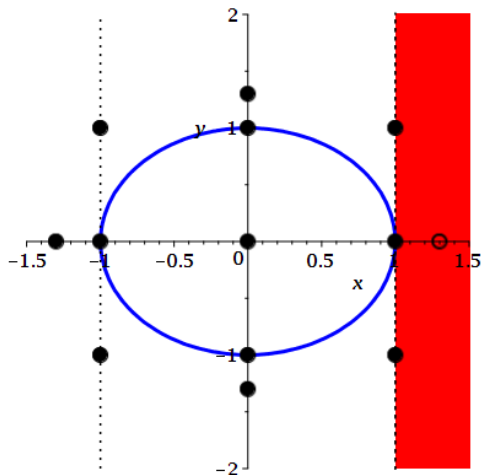
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## Example: Circle – visualisation

(Slide 7/48)

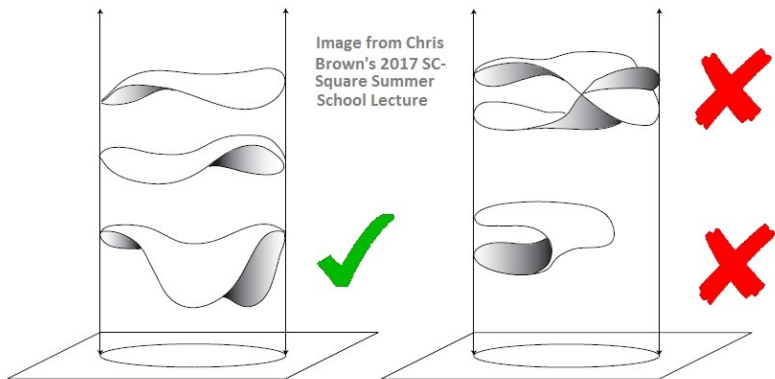
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- Cell 13:  $x > 1, y$  free



## How to build a CAD?

(Slide 8/48)

The usual approach is to calculate projection polynomials whose roots indicate changes in the behaviour of the input set; decompose with respect to these and then lift back working at a sample point. Sound if the projection provides **delineability**.

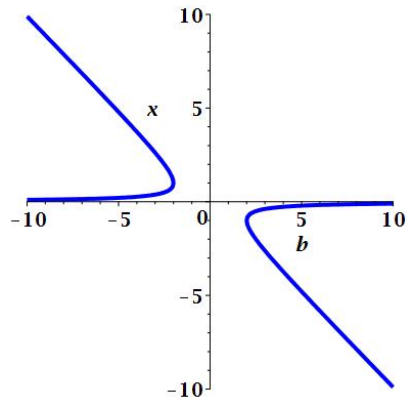


# QE via CAD Example

(Slide 9/48)

How to determine with CAD?

$$\exists x, x^2 + bx + 1 \leq 0$$



## QE via CAD Example

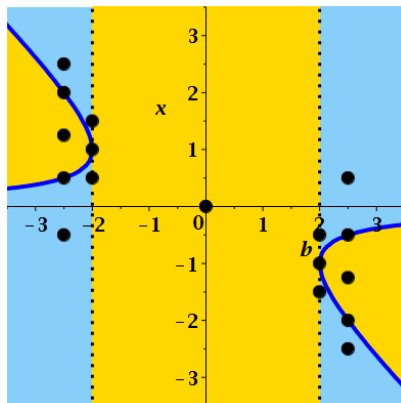
(Slide 9/48)

How to determine with CAD?

$$\exists x, x^2 + bx + 1 \leq 0$$

To solve we:

Build a sign-invariant CAD for  
 $f = x^2 + bx + 1$ .



## QE via CAD Example

(Slide 9/48)

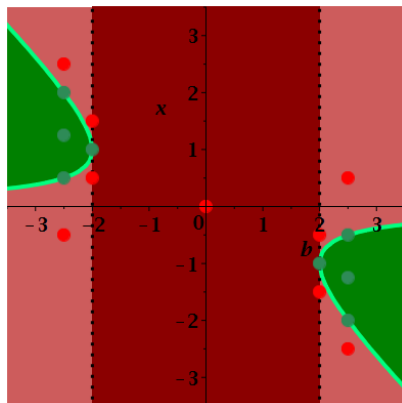
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To solve we:

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Tag each cell true or false  
according to  $f \leq 0$ .



# QE via CAD Example

(Slide 9/48)

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$$\exists x, x^2 + bx + 1 \leq 0$$

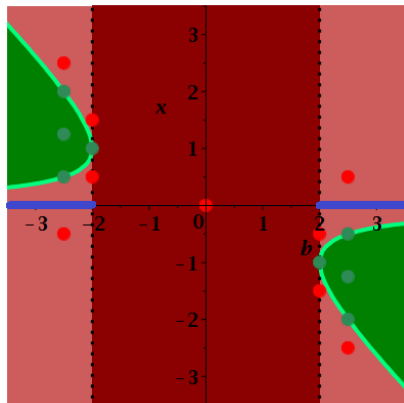
To solve we:

Build a sign-invariant CAD for  
 $f = x^2 + bx + 1$ .

Tag each cell true or false  
 according to  $f \leq 0$ .

Take disjunction of projections of  
 true cells:

$$b < -2 \vee b = -2 \\ \vee b = 2 \vee b > 2$$





## QE via CAD Example

(Slide 9/48)

How to determine with CAD?

$$\exists x, x^2 + bx + 1 \leq 0$$

To solve we:

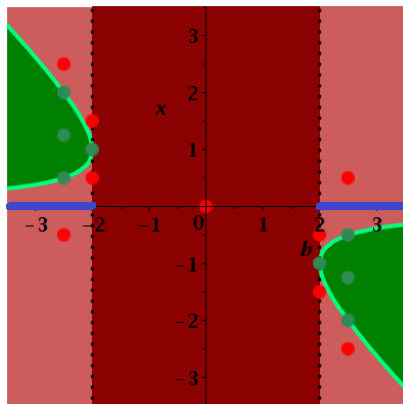
Build a sign-invariant CAD for  
 $f = x^2 + bx + 1$ .

Tag each cell true or false  
according to  $f \leq 0$ .

Take disjunction of projections of  
true cells:

$\implies$

$$b \leq -2 \vee b \geq 2$$



## QE via CAD in General

(Slide 10/48)

In general we can perform Real QE on a decomposition as follows.

- Eliminate existential quantifiers by projecting the true cells, as in the previous example.
- Eliminate universal quantifiers by using the relation

$$\forall x P(x) = \neg \exists x \neg P(x)$$

and then proceeding with existential QE.

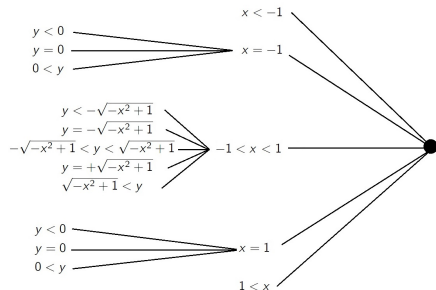
Recall our original example was  $\forall x, x^2 + bx + 1 > 0$ . The above leads us to study  $\exists x, x^2 + bx + 1 \leq 0$  which from the previous slide we know has solution  $b \leq -2 \vee b \geq +2$ . The solution to our universally quantified problem is then the negation of this:  $-2 < b \wedge b < +2$  (as we found numerically earlier).

# Cylindricity Property

(Slide 11/48)

Decompositions allow us to understand infinite space with a finite number of samples and (semi-) algebraic cells allows us to construct solution formulae easily. But why cylindricity?

The Real QE solution process requires us to project cells (and combine those projections) and to calculate the complement of cells: both of these things are trivial for cells arranged cylindrically.



Cylindricity means we can think of CAD as a tree branching by variable.

## Warning: CAD Complexity

(Slide 12/48)

By the end of projection you have doubly exponentially many polynomials of doubly exponential degree (in the number of projections, i.e. variables). Hence also the number of real roots, cells and time to compute them grows doubly exponentially!



C. Brown and J.H. Davenport.

*The complexity of quantifier elimination and cylindrical algebraic decomposition.*

In Proc. ISSAC '07, pages 54–60. ACM, 2007.

Thus in practice applications are only realistic for 4 variables, unless specific optimisations are utilised:

$$2^{2^3} = 256 \quad 2^{2^4} = 65,536 \quad 2^{2^5} = 4,294,967,296$$

# The Doubly Exponential Wall

(Slide 13/48)

## Images by Tereso del Rio



Exponential Growth



Doubly Exponential Growth

# Real QE Applications

(Slide 14/48)

QE can solve problems throughout engineering & science. E.g.

- derivation of optimal numerical schemes.
- artificial intelligence to pass university entrance exam.
- automated theorem proving.
- automated loop parallelisation.
- structural design (minimising the weight of trusses).
- $\vdots$

There is no lack of potential applications: the problem is scaling up in the face of high complexity!

## QE Applications References



M. Erascu and H. Hong.

Real quantifier elimination for the synthesis of optimal numerical algorithms  
(Case study: Square root computation).

*Journal of Symbolic Computation*, 75:110–126, 2016.



N.H. Arai, T. Matsuzaki, H. Iwane, and H. Anai.

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In Proc. ISSAC '14, pages 1–8. ACM, 2014.



L.C. Paulson.

Metitarski: Past and future.

In Proc ITP '12, pages 1–10. Springer, 2012.



A. Grosslinger, M. Griebel, and C. Lengauer.

Quantifier elimination in automatic loop parallelization.

*Journal of Symbolic Computation*, 41(11):1206–1221, 2006.



A.E. Charalampakis and I. Chatzigiannelis.

Analytical solutions for the minimum weight design of trusses by cylindrical  
algebraic decomposition.

*Archive of Applied Mechanics*, 88(1):39–49, 2018.

## QE via CAD Implementations

(Slide 15/48)

Both of the big proprietary Computer Algebra Systems have QE implementations: MATHEMATICA (the `Resolve` command) and MAPLE (`RegularChains:-SemiAlgebraicSetTools; QuantifierElimination:-CylindricalAlgebraicDecompose; and RootFinding:-Parametric:-CellDecomposition`).

The specialist computer algebra system QEPCAD-B is dedicated to QE via CAD and is available for free. It can be used via an intelligent interface TARSKI, is available as a sub-package of SAGE, and can now even run in your browser!



Z. Kovács, C.W. Brown, T. Recio, and R. Vajda

*A web version of Tarski, a system for computing with Tarski formulas and semialgebraic sets.*

In Proc. SYNASC 2022, pages 59–62, IEEE, 2022.

<https://doi.org/10.1109/SYNASC57785.2022.00019>



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## Alternatives to CAD for QE

(Slide 16/48)

There exists algorithms to achieve Real QE other than via CAD:

- Virtual Term Substitution: more efficient but degree limitations. Implementations in MATHEMATICA and REDLOG.
- QE via Comprehensive Gröbner Bases: more efficient, especially if there are many equations. Implementation in SYNRRAC package for MAPLE.
- Family of algorithms for Real QE with complexity doubly exponential in the number of quantifier eliminations. No implementations and analysis suggests that the crossover point where the asymptomatic growth becomes relevant is too far away for practical use at the moment.
- Variety of specialist Real QE algorithms for input of certain shape.

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## Alternatives to CAD for QE References



T. Sturm.

*Thirty years of virtual substitution: Foundations, techniques, applications.*  
In Proc. ISSAC 2018, pages 11–16, ACM, 2018.



R. Fukasaku, H. Iwane, and Y. Sato.

Real quantifier elimination by computation of comprehensive Gröbner systems.  
In Proc. ISSAC '15, pages 173–180. ACM, 2015.



J. Renegar.

Recent progress on the complexity of the decision problem for the reals.  
In B.F. Caviness and J.R. Johnson, editors, *Quantifier Elimination and Cylindrical Algebraic Decomposition*, pages 220–241. Springer-Verlag, 1998.



H.P. Le and M. Safey El Din.

Faster one block quantifier elimination for regular polynomial systems of equations.  
In Proc. ISSAC '21, pages 265–272. ACM, 2021.

# Alternatives to Traditional CAD Computation I (Slide 17/48)

There are now various alternative computational schemes for CAD:

- 1 **CAD adapted for SMT:** CAD as a theory solver in the CDCL(T) paradigm for problems where all variables are existentially quantified.

The logic space is searched efficiently via a SAT-solver with CAD used to analyse whether subsets of constraints can be satisfied together.

Open source implementations exist in the SMT-solvers, SMT-RAT, YICES2, Z3 and CVC5.



G. Kremer and E. Ábrahám.

*Fully incremental cylindrical algebraic decomposition.*

J. of Symbolic Computation, 100, pages 11–37. Elsevier, 2020.

<https://doi.org/10.1016/j.jsc.2019.07.018>

## Alternatives to Traditional CAD Computation II (Slide 18/48)

- 2 **CAD theory redesigned for SMT:** the theorems that underpin CAD reused to validate search-based algorithms that generalise bad guesses to CAD-cells.



D. Jovanovic and L. de Moura

*Solving Non-linear Arithmetic*

Proc. IJCAR 2012, LNCS 7364, pp. 339–354.

[https://doi.org/10.1007/978-3-642-31365-3\\_27](https://doi.org/10.1007/978-3-642-31365-3_27)



E. Ábrahám, J.H. Davenport, M. England and G. Kremer.

*Deciding the consistency of non-linear real arithmetic constraints with a conflict driven search using cylindrical algebraic coverings.*

JLAMP 119, pages 2352–2208. Elsevier, 2021.

<https://doi.org/10.1016/j.jlamp.2020.100633>

## Alternatives to Traditional CAD Computation III (Slide 19/48)

- 3 **SMT inspired CAD algorithms for QE:** Generalisations of the new SMT-based algorithms to tackle the full Real QE problem.



C. W. Brown

*Open Non-uniform Cylindrical Algebraic Decompositions*

Proc. ISSAC 2015, pp. 85–92. ACM, 2015

<https://doi.org/10.1145/2755996.2756654>



G. Kremer and J. Nalbach.

*Cylindrical Algebraic Coverings for Quantifiers.*

Proc. SC<sup>2</sup> 2022, CEUR-WS 3458, pp. 1–9, 2023.

<https://ceur-ws.org/Vol-3458>

# Alternatives to Traditional CAD Computation IV (Slide 20/48)

- ④ **CAD via Regular Chains:** First performs a decomposition in  $\mathbb{C}^n$  using regular chains (triangular sets) theory and then refines this to a decomposition of  $\mathbb{R}^n$ .



C. Chen and M. Moreno Maza and B. Xia and L. Yang.

*Computing cylindrical algebraic decomposition via triangular decomposition.*

Proc. ISSAC 2009, pp. 95–102. ACM, 2009.

<https://doi.org/10.1145/1576702.1576718>



# Alternatives to Traditional CAD Computation V (Slide 21/48)

- 5 **Geometric CAD:** A new view of CAD proposed made using Geometric Fiber Classification that suggests a computation scheme using Gröbner Bases in place of iterated resultants.



Rizeng Chen.

*Geometric Fiber Classification of Morphisms and a Geometric Approach to Cylindrical Algebraic Decomposition.*

Preprint, arXiv:2311.10515 (Dec 2023).

<https://doi.org/10.48550/arXiv.2311.10515>

# Optimising CAD

(Slide 22/48)

All of the alternative CAD computation schemes above still have doubly exponential complexity in the worst case.

They also all have a sensitivity to the variable ordering which:

- Determines the meaning of cylindricity in the definition;
- Determines the order of operations in the algorithm.

It is well observed that this choice can dramatically effect the efficiency or even tractability of CAD, but there does not exist any theoretical method to make the choice – it is commonly decided by heuristics. This is one key area in which a CAD implementation may be optimised.

We will consider whether this can be achieved via machine learning.

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# Machine Learning Mathematics

(Slide 23/48)

**Machine Learning** (ML) uses statistics upon data to learn how to perform tasks that have not been explicitly programmed. ML technology is behind recent Artificial Intelligence (AI) applications. It is increasingly used in industry and academia.

**(Q) How can ML assist mathematicians?**

There have been a variety of papers suggesting that ML can guide pure mathematicians to potential conjectures.



Davies, Alex and Veličković, Petar and Buesing, Lars and Blackwell, Sam and Zheng, Daniel and Tomašev, Nenad and Tanburn, Richard and Battaglia, Peter and Blundell, Charles and Juhász, András and Lackenby, Marc and Williamson, Geordie and Hassabis, Demis and Kohli, Pushmeet  
*Advancing mathematics by guiding human intuition with AI.*

Nature, 600, pp. 70—74.

<https://doi.org/10.1038/s41586-021-04086-x>

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# Machine Learning Matrix Multiplication

(Slide 24/48)

Reinforcement learning found an improvement on Strassen's algorithm to multiply matrices:



A. Fawzi and M. Balog and A. Huang and T. Hubert and B. Romera-Paredes and M. Barekatin and A. Novikov and F.J.R. Ruiz and J. Schrittwieser and G. Swirszcz and D. Silver and D. Hassabis and P. Kohli.

*Discovering faster matrix multiplication algorithms with reinforcement learning.*

Nature, 610, pp. 47—53, 2022.

<https://doi.org/10.1038/s41586-022-05172-4>

That solution seeded a new random walk based algorithm which found an even better one!



Manuel Kauers and Jakob Moosbauer.

*Flip Graphs for Matrix Multiplication.*

Proc. ISSAC 2023, pp. 381 — 388. ACM, 2023.

<https://doi.org/10.1145/3597066.3597120>





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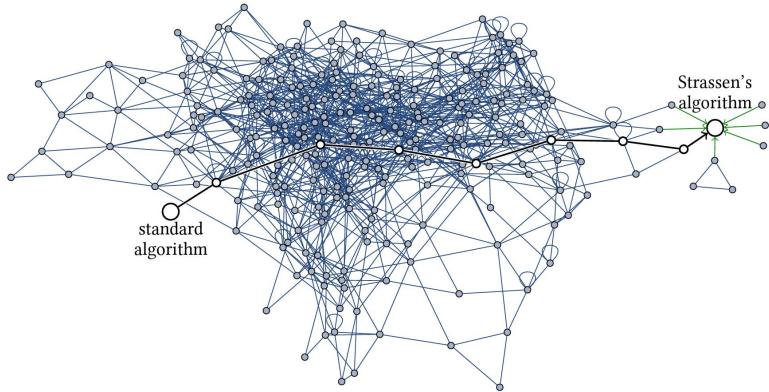


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Proc. ISSAC 2023, pp. 381 — 388. ACM, 2023.

<https://doi.org/10.1145/3597066.3597120>



# Machine Learning to make Algorithms

(Slide 25/48)



Romera-Paredes, B. and Barekatin, M. and Novikov, A. and Balog, M. and Kumar, M.P. and Dupont, E. and Ruiz, F.J.R. and Ellenberg, J.S. and Wang, P. and Fawzi, O. and Kohli, P. and Fawzi, A.

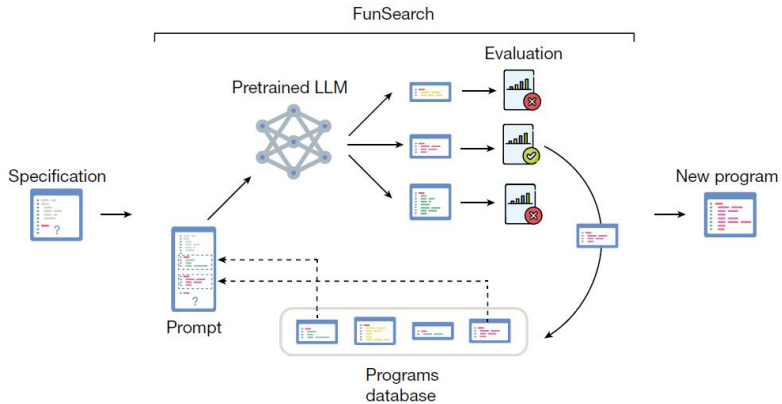
*Mathematical discoveries from program search with large language models.*

Nature, 625, pp. 468—475, 2023.

<https://doi.org/10.1038/s41586-023-06924-6>

Starts with a database of heuristic methods for the problems and evolves them by feeding two at a time as a prompt to an LLM (Codey) which is asked to merge them; with the outputs evaluated for fitness and the best added into the database.

Does not train the LLM themselves! The LLM is simply the merger tool. They produce programs that describe how to solve a problem, rather than the problem solution itself.



# Symbolic Computation vs Machine Learning

(Slide 26/48)

(Q) So can ML replace symbolic computation?

There is a growing body of research on the use of ML in place of expensive symbolic computation. E.g. for integration and the solution of differential equations.



G. Lample and D. Charton

*Deep Learning for Symbolic Mathematics.*

Proc. ICLR 2020.

<https://doi.org/10.48550/arXiv.1912.01412>

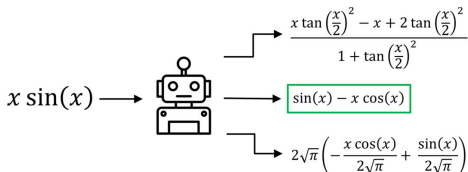
These tasks are well-suited because it is cheap to symbolically check the correctness of the answer! However, this is not the case for most symbolic computation.

# ML for Symbolic Algorithm Selection

(Slide 27/48)

The types of integrals dealt with in that paper were very simple. The integrator in a Computer Algebra System like Maple can integrate far more general functions but does so using a wide variety of different algorithms.

(Q) How to select the right algorithm to use for an input?



Coventry University PhD student Rashid Barket is sponsored by Maplesoft to build an ML-based algorithm selector.

## Symbolic Computation WITH Machine Learning (Slide 28/48)

ML can only offer probabilistic guidance, but symbolic computation prizes exact results. 99% accuracy is great for image recognition but would not be acceptable for a mathematical proof.

However, ML can be applied to symbolic computation and still ensure exact results; by having it select or otherwise guide existing algorithms rather than replace them entirely.

Symbolic Computation algorithms often come with choices that need to be made, which do not effect the mathematical correctness of the final result, but which do effect the resources required to find that result (and often how the result is presented).

Such choices are often either left to the user, hard coded by the developer, or made based on a simple heuristic. ML may be able to offer a superior choice.

# This is INTERESTING Machine Learning

(Slide 29/48)

**Summary:** ML should be of interest to those developing mathematical algorithms.

**But also,** ML researchers should also be interested in this application. It is a particularly challenging (interesting) domain:

- No a priori limit on the input space.
- Supervised learning hard: because labelling dataset needs lots of expensive symbolic computation.
- Unsupervised learning is hard: because it is unclear if a particular outcome is good or bad without seeing the rest.
- What constitutes a meaningful and representative data set?
- Insufficient quantities of real world data for deep learning.
- How to perform data augmentation / synthetic data generation to allow for generalisability on problems of interest?



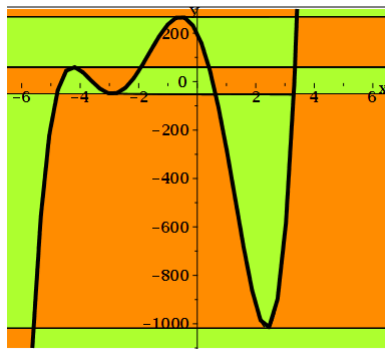
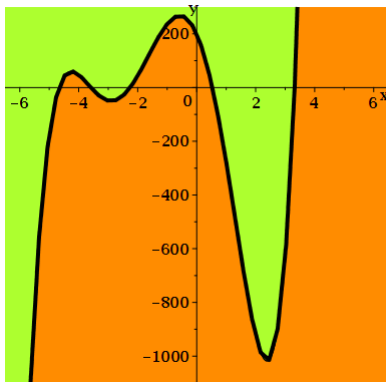
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  - Economics

# Variable Ordering for CAD

(Slide 30/48)

CAD requires a variable ordering: there can be multiple valid orderings which lead to an acceptable decomposition, but some lead to smaller decompositions via less computation.



# CAD Variable Ordering Choice

(Slide 31/48)

Depending on our application we may have a free or constrained choice in variable ordering. When using CAD for QE we must project variables in the order of quantification, but we are free to change order within quantifier blocks (and with the free variables).

The variable ordering has been long known to effect the number of cells produced in a CAD or even the tractability of a problem.

There are various *human-designed heuristics* to make the choice:

- Simple heuristics which use only simple measures of polynomials (degrees, sparsity etc.)
- Expensive heuristics which use more involved algebraic computations.

# Simple human-designed heuristics

(Slide 32/48)

**Brown's Heuristic:** chooses variable based on overall degree; breaking ties with total degree of the terms with that variable; breaking ties with number of terms the variable is in.



C. Brown

*Companion to the Tutorial: Cylindrical Algebraic Decomposition, presented at ISSAC 2004.*

[www.usna.edu/Users/cs/wcbrown/research/ISSAC04/handout.pdf](http://www.usna.edu/Users/cs/wcbrown/research/ISSAC04/handout.pdf)

**gmods:** chooses variable based on the sum of its degree in each polynomial.



T. del Río and M. England

*New Heuristic to Choose a Cylindrical Algebraic Decomposition Variable Ordering Motivated by Complexity Analysis*

Proc. CASC 2022, LNCS 13366, pp. 300—317. Springer, 2022.

[https://doi.org/10.1007/978-3-031-14788-3\\_17](https://doi.org/10.1007/978-3-031-14788-3_17)

## First use of ML for CAD variable ordering choice (Slide 33/48)

First attempt used a support vector machine classifier to choose which of the three variable ordering heuristics we had implemented in our CAD code to follow for a given problem instance: no one heuristic dominated the others; ML choice did better than any one.



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

*Applying machine learning to the problem of choosing a heuristic to select the variable ordering for cylindrical algebraic decomposition.*

Intelligent Computer Mathematics (LNCS 8543), pp. 92-107. Springer Berlin Heidelberg, 2014.

[http://dx.doi.org/10.1007/978-3-319-08434-3\\_8](http://dx.doi.org/10.1007/978-3-319-08434-3_8)

The first use of Machine Learning to optimise computer algebra.

# EPSRC ML4QE Project

(Slide 34/48)

Experiments with ML methodology to choose the ordering directly.  
In particular:

- Classifier model choice.
- New feature extraction methods to represent polynomials to Machine Learning models: brute force combinations of simple statistics followed by selection
- Tailored hyper-parameter selection to runtime rather than classification accuracy.



D. Florescu and M. England.

*A Machine Learning Based Software Pipeline to Pick the Variable Ordering for Algorithms with Polynomial Inputs.*

Mathematical Software (LNCS 12097), pp. 302–311. Springer International Publishing, 2020.

[https://doi.org/10.1007/978-3-030-52200-1\\_30](https://doi.org/10.1007/978-3-030-52200-1_30)

## Dataset Considerations

(Slide 35/48)

The above work used the QF\_NRA SMT-LIB benchmarks: a collection of satisfiability problems whose atoms are non-linear polynomial constraints over the reals.

Chosen as the largest (only substantial) existing set of benchmarks for CAD. Problems are meaningful: come from “*industry*” (theorem provers MetiTarski and Keymaera), biology, economics, dynamic geometry proofs, etc. **However:**

- Dataset is highly imbalanced with respect to CAD variable ordering. Risk of over-fitting given no reason to expect imbalance in general data.
- Data is highly dominated by one source of problems.
- Dataset contains many problems that are very similar (e.g. differ by a constant). Thus a risk of data leakage between testing and training.

# Dataset Lessons

(Slide 36/48)

- 1 Use variable permutations on problem instances to:
  - Balance dataset (random permutation on each instance).
  - Augment dataset (from each problem instance create a set of instances from all possible permutations).
- 2 Merge problem instances who have the same CAD tree structure in each variable ordering.

We find the loss of “accuracy” from (1a) is offset from (1b); while (2) allows for similar learning from a dataset a fraction of the size.



Tereso del Río and M. England.

*Data Augmentation for Mathematical Objects.*

Proc. SC<sup>2</sup> 2023, CEUR-WS 3455, pp. 29—38, 2023.

<https://ceur-ws.org/Vol-3455/>



# From Classification to Regression

(Slide 37/48)

Prior work framed this as ML *Classification* (choose from discrete set of variable orderings). May be reframed as ML *Regression* predict the time taken with a particular ordering: multiple predictions then compared to choose the final ordering. Why?

- A model trained with regression has access to more information: not just which ordering did best but also which came second, which third etc.
- However, regression is a more difficult task (but we only need to be good enough at it to make a ranking).

So we hypothesised that regression would outperform classification.



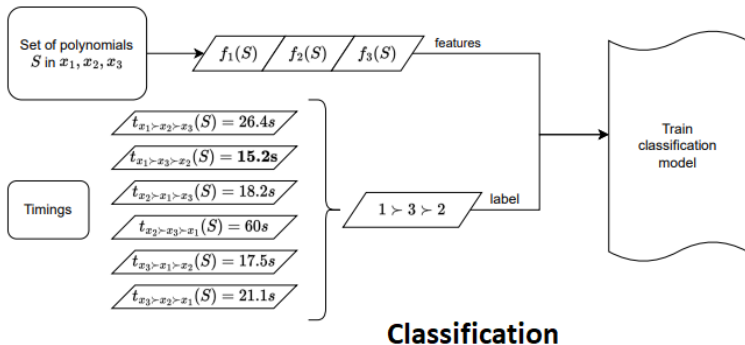
T. del Río and M. England.

*Lessons on Datasets and Paradigms in Machine Learning for Symbolic Computation: A Case Study on CAD..*

Submitted, 2024. <https://doi.org/10.48550/arXiv.2401.13343>

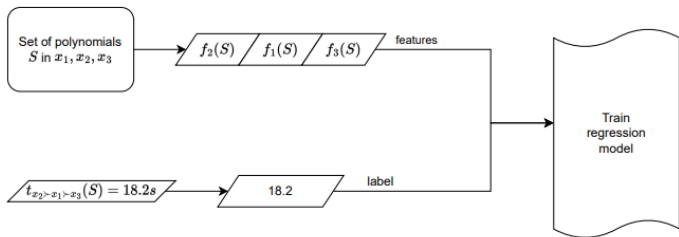
# Classification vs Regression Flowcharts

(Slide 38/48)



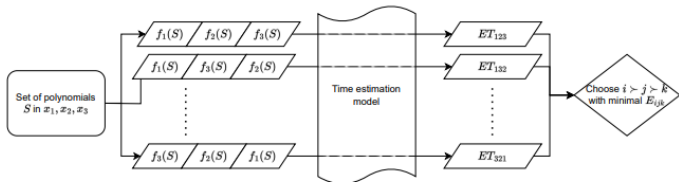
# Classification vs. Regression Flowcharts

(Slide 38/48)



**Regression Training**  
**Regression Testing**

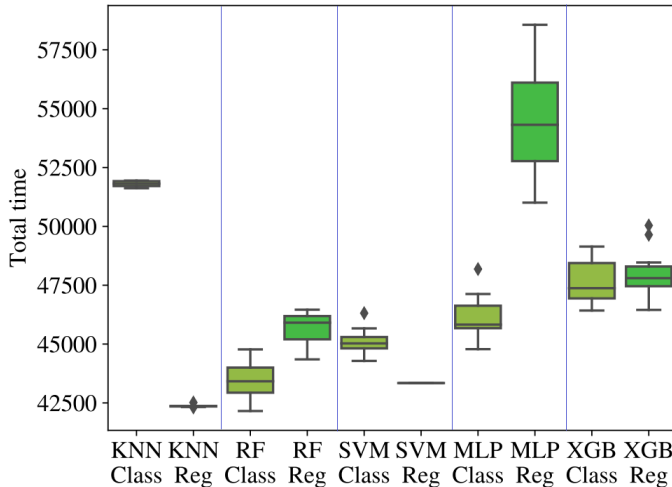
x6



# Classification vs. Regression Results

(Slide 39/48)

Regression not universally beneficial, but new state-of-the-art ML.



## Remaining Challenges

(Slide 40/48)

None of the above used Deep Learning. The dataset size, even after augmentation, did not really support this.

Key remaining challenges:

- 1 How to create synthetic data sufficient for training deep learning but representative of the problems to be solved in reality?
- 2 Better representations of the mathematics to the ML models than feature extraction. E.g. Graph Neural Networks.

Some progress on similar challenges in the context of symbolic integration algorithm selection.

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# Inspiration

(Slide 41/48)



D. Peifer, M. Stillman, and D. Halpern-Leistner.

*Learning selection strategies in Buchberger's algorithm,*

In: *Proc. ICML 2020*, pages 7575-7585, PMLR, 2020.

Applied reinforcement learning to choose the order in which to process S-pairs in Buchberger's algorithm for a Gröbner Basis.

Human analysis of their model revealed a simple, "*human level*" strategy that explained most of the choices. Simple, but very different the human-designed heuristics.

Suggests that ML can reveal new mathematical truths about the algorithm, and direct future non-ML algorithm development.

How to automate such analysis?

# Explainable AI (XAI)

(Slide 42/48)

The field of **Explainable AI (XAI)** covers ML techniques whose decisions can be explained to a human expert. XAI is increasingly important: both as an error check on the ML process; and to build trust in new AI technologies.

- **Ante-hoc explainable models** are transparent by design in their decisions, e.g. linear regression and support vector machines which fit a line to maximise an objective.
- **Post-hoc explainability** is where an ML model is trained as normal, and then a secondary analysis provides an interpretation.



# Post-hoc XAI for CAD Variable Ordering

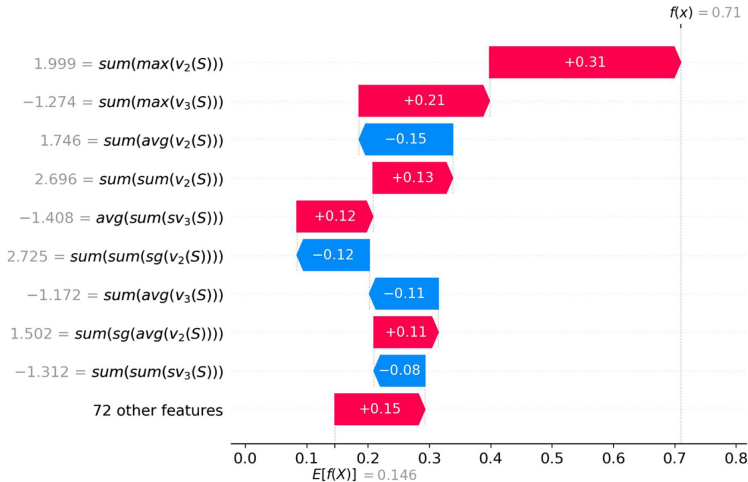
(Slide 43/48)



L. Pickering, T. Del Rio Almajano, M. England and K. Cohen.  
*Explainable AI Insights for Symbolic Computation: A case study on selecting the variable ordering for cylindrical algebraic decomposition.*  
*Journal of Symbolic Computation*, **123**, Article Number 102276, 2024.

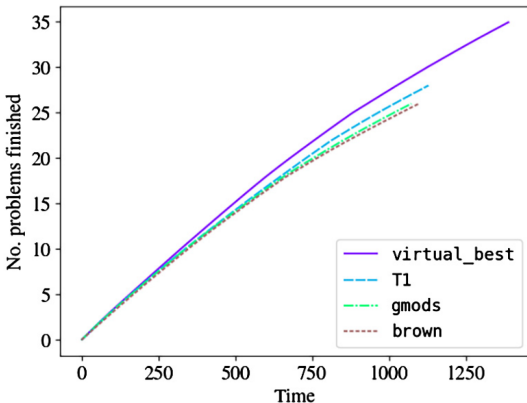
We applied the SHAP XAI tool to analyse the features used by ML classifiers to choose the CAD variable ordering. Some features identified as impactful had been known before; others were new.

# Example SHAP Waterfall Plot



## Designing a heuristics from SHAP output

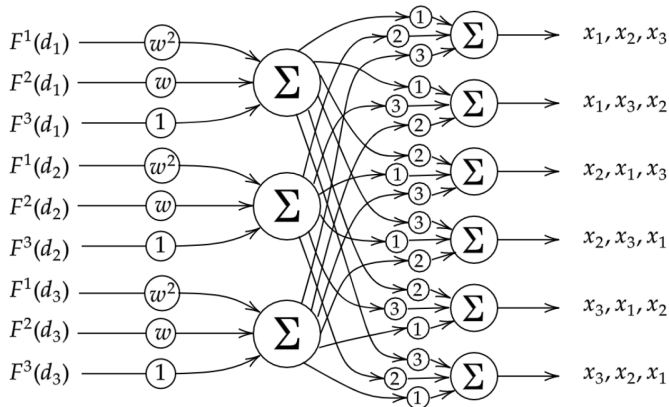
We aggregated across the dataset; had models vote on features to create overall feature ranking; took the top 6 voted features and studied ordered triples of them (similar to Brown's heuristic).



# Ante-hoc XAI for CAD Variable Ordering

(Slide 46/48)

Started by formulating Brown's heuristic as a neural network:



Where  $w$  is chosen so that  $F^i(d_v) < 2 - 1$  for all features and variables.

## Searching the space of similar networks

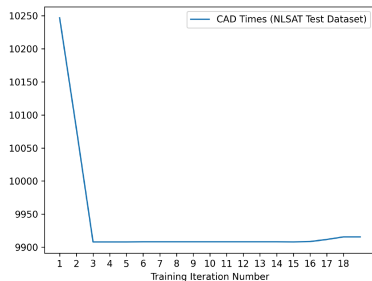
(Slide 47/48)

Starting from the Brown NN we optimise by ML training to:

- use different features  $F^i$  (i.e. different feature triples);
- use different weights (more complicated combinations of the same three pieces of information).

What results is a heuristic informed by a ML process but no more complicated than the human designed one.

This one is ongoing work with Dorian Florescu (not yet published).



## Summary of the Two XAI Experiments

(Slide 48/48)

Both experiments took a *human-designed* heuristic as a starting point and then used ML processes to produce another heuristic.

The latter is not human-designed but is *human-level*:

- can be expressed in natural language in a similar amount of text as a heuristic designed by a human;
- can be implemented without any ML architecture.

Potentially these could be new methodologies for heuristic design.

# Thanks for Listening



## Contact Details

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`https://matthewengland.coventry.domains/`

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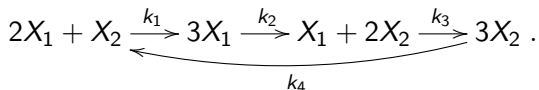
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## Chemical Reaction Networks

(Slide 50/48)

A **Chemical Reaction Network** (CRN) models the behaviour of a chemical system. Toy Example:



From this we define a dynamical system:

$$\begin{cases} \dot{x}_1 = (3 - 2)k_1x_1x_1x_2 - 2k_2x_1^3 - k_3x_1x_2^2 + 2k_4x_2^3, \\ \dot{x}_2 = -k_1x_1^2x_2 + 2k_2x_1^3 + k_3x_1x_2^2 - 2k_4x_2^3. \end{cases}$$

Steady states when all the derivatives are zero:

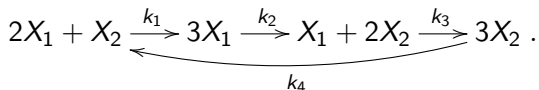
$$\begin{cases} k_1x_1^2x_2 - 2k_2x_1^3 - k_3x_1x_2^2 + 2k_4x_2^3 = 0, \\ x_1 + x_2 - k_5 = 0. \end{cases}$$

Parametric real semi-algebraic geometry problem.

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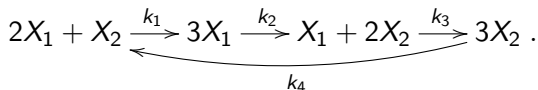
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Parametric real semi-algebraic geometry problem.

# Multistationarity

(Slide 51/48)

A CRN exhibits **multistationarity** if there exists a choice of parameter values for which the system has more than one (positive real) solution.

Why care about multistationarity?

- Used for switch behaviour.
- Instrumental to cellular memory and cell differentiation during development.
- Used by micro organisms in survival strategies.
- Used in decision making processes in the cell division cycle.

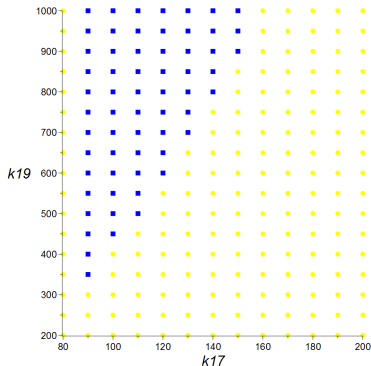
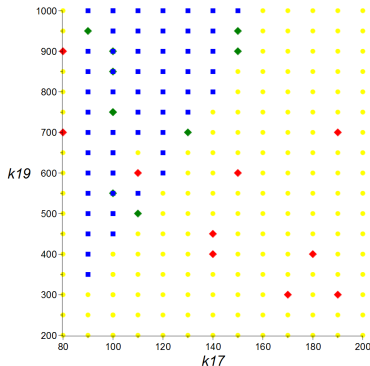
There are a variety of efficient methods for answering the Boolean question as to whether or not a system can exhibit multistationarity. Less studied is the question of determining the actual parameter values where multistationarity occurs.

# Numeric Methods for Multistationarity 1

(Slide 52/48)

Numeric sampling of the parameter space is used. However:

- Incorrect results can be obtained at ill-conditioned points.
- No guarantee all areas of interest will be sampled.



## Numeric Methods for Multistationarity 2

(Slide 53/48)

Numeric sampling of the parameter space is used. However:

- Incorrect results can be obtained at ill-conditioned points.
- No guarantee all areas of interest will be sampled.

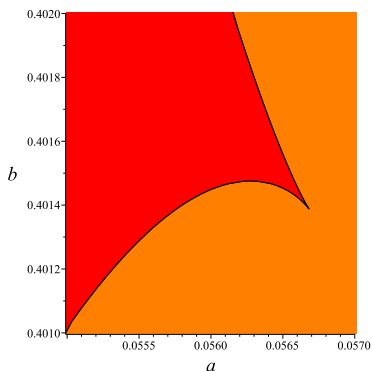
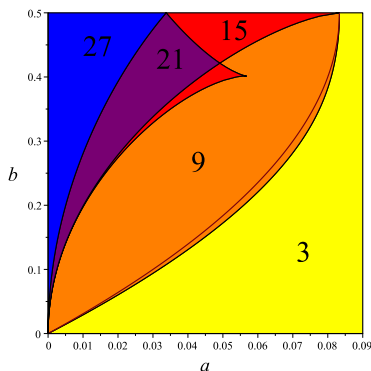


Image courtesy of AmirHosein SadeghiManesh.

## Biology Example References



R. Bradford, J.H. Davenport, M. England, H. Errami, V. Gerdt, D. Grigoriev, C. Hoyt, M. Košta, O. Radulescu, T. Sturm, and A. Weber.

Identifying the parametric occurrence of multiple steady states for some biological networks.

*Journal of Symbolic Computation*, 98:84–119, 2020.



D. Lazard and F. Rouillier.

Solving parametric polynomial systems.

*Journal of Symbolic Computation*, 42(6):636–667, 2007.



G. Röst and A. Sadeghimanesh.

Exotic bifurcations in three connected populations with Allee effects.

*International Journal of Bifurcation and Chaos*, 31(13):2150202, 2021.



A. Sadeghimanesh and M. England.

*Polynomial Superlevel Set Representation of the Multistationarity Region of Chemical Reaction Networks.*

BMC Bioinformatics, 23 Article number 391, 26 pages, 2022.



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# Framework for Reasoning in Economics

(Slide 54/48)

Determine whether, with variables  $\Lambda = (v_1, \dots, v_n)$ , the hypotheses  $H(\Lambda)$  follow from the assumptions  $A(\Lambda)$ . I.e. answer

$$\forall \Lambda. A(\Lambda) \Rightarrow H(\Lambda)?$$

Logically the answer must be True or False. But economists are interested also in the following:

- Are the assumptions themselves contradictory?
- If False, can additional assumptions be made to give True?
- If True, can any assumptions be removed?

Such questions can be answered by Real QE in many cases.

# TheoryGuru Framework

(Slide 55/48)

THEORYGURU package for MATHEMATICA led by Casey Milligan (Chicago). For a proposed economics theorem, we check both:

- the existence of an example  
 $\exists \Lambda, A \wedge H,$
- and the existence of a counterexample  
 $\exists \Lambda, A \wedge \neg H.$

Then categorize the proposed theorem as:

	$\neg \exists \Lambda, A \wedge \neg H$	$\exists \Lambda, A \wedge \neg H$
$\exists \Lambda, A \wedge H$	True	Mixed
$\neg \exists \Lambda, A \wedge H$	Contradictory Assumptions	False

An economist can explore: e.g. strengthen assumptions of Mixed result, or weaken assumptions of True result.

## Example #0013 Context

(Slide 56/48)

**Context:** Disagreement between Mulligan and Krugman on causes of recession. In particular, latter asserted that whenever taxes on labour supply are primarily responsible for a recession then wages increase. Benchmark Example #0013 considers this claim.

Two scenarios to track: what actually happens (*act*) when taxes ( $t$ ) and demand forces ( $a$ ) together create a recession, and what would have happened (*hyp*) if taxes on labour supply had been the only factor affecting the market.



The labour demand and supply functions  $D(w, a)$  and  $S(w, t)$  meet at the labour market equilibrium to supply quantity of labour  $q$ .

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## Example #0013 Logic

(Slide 57/48)

$$\begin{aligned}
 A &\equiv \frac{\partial D(w, a)}{\partial w} < 0 \wedge \frac{\partial S(w, t)}{\partial w} > 0 \\
 &\wedge \frac{\partial D(w, a)}{\partial a} = 1 \wedge \frac{\partial S(w, t)}{\partial t} = 1 \\
 &\wedge \frac{d}{dact} (D(w, a) = q = S(w, t)) \\
 &\wedge \frac{d}{dhyp} (D(w, a) = q = S(w, t)) \\
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 &\wedge \frac{dq}{dhyp} < \frac{1}{2} \frac{dq}{dact} < 0 \\
 H &\equiv \frac{dw}{dact} > 0.
 \end{aligned}$$

### Assumptions:

- Usual slope restrictions.
- Standard normalizations.
- Scenarios both move labour market equilibrium over course of recession.
- Scenarios have the same tax change but only the *act* scenario has a demand shift.
- Majority of the reduction in labour was due to supply.

Hypothesis: wages are higher at the end of the recession.

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- Scenarios both move labour market equilibrium over course of recession.
- **Scenarios have the same tax change but only the *act* scenario has a demand shift.**
- Majority of the reduction in labour was due to supply.

Hypothesis: wages are higher at the end of the recession.

## Example #0013 Logic

(Slide 57/48)

$$\begin{aligned}
 A &\equiv \frac{\partial D(w, a)}{\partial w} < 0 \wedge \frac{\partial S(w, t)}{\partial w} > 0 \\
 &\wedge \frac{\partial D(w, a)}{\partial a} = 1 \wedge \frac{\partial S(w, t)}{\partial t} = 1 \\
 &\wedge \frac{d}{dact} (D(w, a) = q = S(w, t)) \\
 &\wedge \frac{d}{dhyp} (D(w, a) = q = S(w, t)) \\
 &\wedge \frac{dt}{dact} = \frac{dt}{dhyp} \wedge \frac{da}{dhyp} = 0 \\
 &\wedge \frac{dq}{dhyp} < \frac{1}{2} \frac{dq}{dact} < 0 \\
 H &\equiv \frac{dw}{dact} > 0.
 \end{aligned}$$

### Assumptions:

- Usual slope restrictions.
- Standard normalizations.
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- Usual slope restrictions.
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Hypothesis: **wages are higher at the end of the recession.**

## Example #0013 Result

(Slide 58/48)

We may view this as a Tarski formula in 12 variables,

$$\Lambda = \left\{ \begin{array}{l} \frac{da}{dact}, \frac{da}{dhyp}, \frac{dt}{dact}, \frac{dt}{dhyp}, \\ \frac{dq}{dact}, \frac{dq}{dhyp}, \frac{dw}{dact}, \frac{dw}{dhyp}, \\ \frac{\partial D(w, a)}{\partial a}, \frac{\partial S(w, t)}{\partial t}, \frac{\partial D(w, a)}{\partial w}, \frac{\partial S(w, t)}{\partial w} \end{array} \right\},$$

Each is representing a partial derivative describing the supply and demand function or a total derivative indicating a change over time within a scenario.

Evaluating the two existential problems shows that both examples and counterexamples exist: the theorem is not universally true.

## Example #0013 Exploration

(Slide 59/48)

If we leave  $\frac{\partial D(w,a)}{\partial w}$  and  $\frac{\partial S(w,t)}{\partial w}$  as free variables then QE recovers a disjunction of three quantifier-free formulae. Two of them contradict the assumptions, but the third, below, could be added to  $A$  to guarantee the truth of  $H$ .

$$\frac{\partial S(w,t)}{\partial w} \geq -\frac{\partial D(w,a)}{\partial w} > 0.$$

The added assumption states that labour supply is at least as sensitive to wages as labour demand.

**The algebra and logical reasoning above is not political!** Any politics comes with whether the assumptions hold. We cannot remove the politics, but at least gain clarity over which arguments are political and which not.

## Economics Example References



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# Thanks for Listening



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