Graph structure in polynomial systems: chordal networks

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Based on joint work
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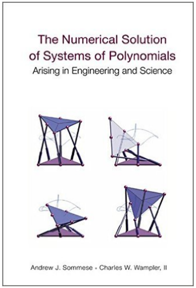
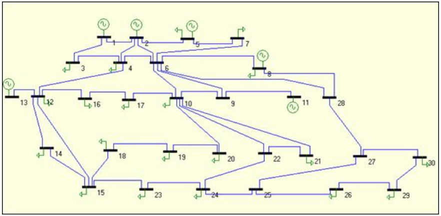
Background: structured polynomial systems

Many application domains require the solution of large-scale systems of polynomial equations.

Among others: robotics, power systems, chemical engineering, cryptography, etc.





$$S + E \underset{k_{-1}}{\overset{k_{+1}}{\rightleftharpoons}} ES \underset{k_{-2}}{\overset{k_{+2}}{\rightleftharpoons}} P + E$$

$$\frac{d[S]}{dt} = -k_1[E][S] + k_{-1}[ES]$$

$$\frac{d[E]}{dt} = -k_1[E][S] + (k_{-1} + k_2)[ES] - k_{-2}[E][P]$$

$$\frac{d[ES]}{dt} = k_1[E][S] - (k_{-1} + k_2)[ES] + k_{-2}[E][P]$$

$$\frac{d[P]}{dt} = k_2[ES] - k_{-2}[E][P]$$

Polynomial systems and graphs

A polynomial system defined by m equations in n variables:

$$f_i(x_0, \ldots, x_{n-1}) = 0, \qquad i = 1, \ldots, m$$

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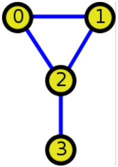
Example:

$$I = \langle x_0^2 x_1 x_2 + 2x_1 + 1, \quad x_1^2 + x_2, \quad x_1 + x_2, \quad x_2 x_3 \rangle$$



Questions

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- Can the graph structure help *solve* this system?
- For instance, to optimize, or to compute Groebner bases?
- Or, perhaps we can do something *better*?
- Preserve graph (sparsity) structure?
- Complexity aspects?

(Hyper)Graphical modelling

Pervasive idea in many areas, in particular: numerical linear algebra, graphical models, constraint satisfaction, database theory, . . .

Key notions: chordality and treewidth.

Many names: Arnborg, Beeri/Fagin/Maier/Yannakakis, Blair/Peyton, Bodlaender, Courcelle, Dechter, Freuder, Lauritzen/Spiegelhalter, Pearl, Robertson/Seymour, . . .

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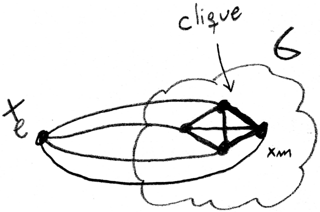
Reasonably well-known in discrete (0/1) optimization, what happens in the continuous side?
(e.g., Waki et al., Lasserre, Bienstock, Vandenberghe, Lavaei, etc)

Chordality

Let G be a graph with vertices $x_0, \ldots, x_{n-1}$.
A vertex ordering

$$x_0 > x_1 > \cdots > x_{n-1}$$

is a perfect elimination ordering if for all ℓ, the set



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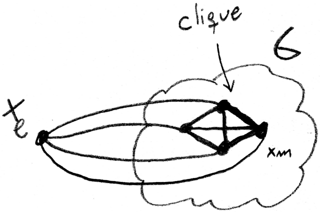

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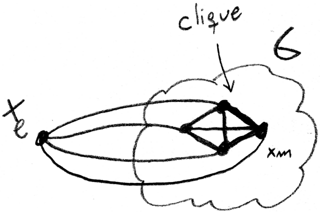

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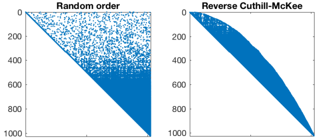
(Equivalently, in numerical linear algebra: Cholesky factorization has no “fill-in”)



Chordality, treewidth, and a meta-theorem

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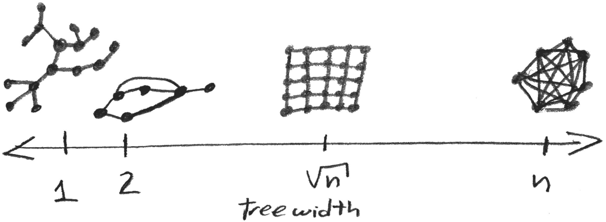

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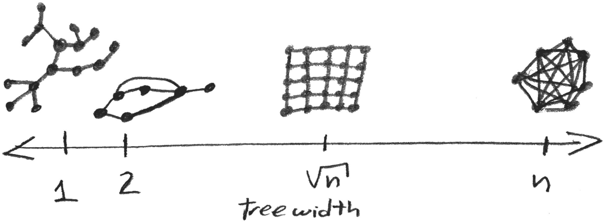

Meta-theorem:
NP-complete problems are "easy" on graphs of small treewidth.

(Simple) example: stable set on trees

Given a graph, a *stable* (or *independent*) set is a subset of vertices, such that no two are pairwise neighbors.

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Fix a root, and solve this recursion starting from the leaves:

$$S(i) = \max\Big(\sum_{j \in \text{children}(i)} S(j), \quad 1 + \sum_{j \in \text{grandchildren}(i)} S(j) \Big),$$

$$S(\text{leaf}) = 1,$$

where $S(i)$ represents the size of the largest independent set of the corresponding subtree.

Bad news? (I)

Recall the *subset sum* problem, with data $A = \{a_1, \dots, a_n\} \subset \mathbb{Z}$.
Is there a subset of A that adds up to 0?

Letting s_i be the partial sums, we can write a polynomial system:

$$\begin{aligned} 0 &= s_0 \\ 0 &= (s_i - s_{i-1})(s_i - s_{i-1} - a_i) \\ 0 &= s_n \end{aligned}$$

The graph associated with these equations is a path (treewidth=1)

But, subset sum is NP-complete... :(

Bad news? (II)

For *linear* equations, “good” elimination preserves graph structure (perfect!)

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For polynomials, however, Groebner bases can destroy chordality.

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Q: Are there alternative descriptions that "play nicely" with graphical structure?

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Key: "nice" graphical structure allows DP to work *in principle*. But, we also need to control the *complexity* of the objects DP is propagating. Without this, we're doomed!

[Ubiquitous theme: "complicated" value functions in optimal control, "message complexity" in statistical inference, . . .]

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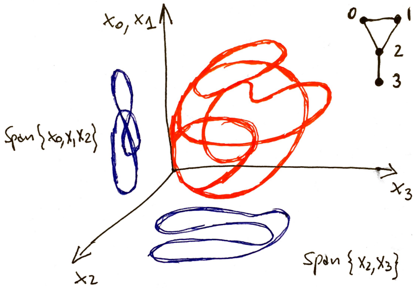
Consider the full solution set (an algebraic variety).

Require the projections onto the subspaces spanned by the maximal cliques to have bounded degree.



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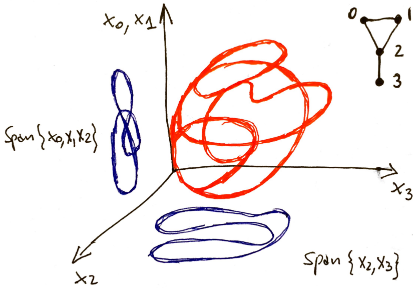


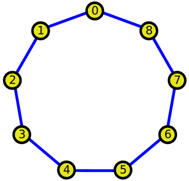
- For discrete domains (e.g., 0/1 problems), always satisfied.
- Holds in other cases, e.g., low-rank matrices (determinantal varieties).

Two approaches

- Chordal elimination and Groebner bases (arXiv:1411:1745)
  - New *chordal elimination* algorithm, to exploit graphical structure
  - Conditions under which chordal elimination succeeds
  - For a certain class, complexity is *linear* in number of variables! (exponential in treewidth)
  - Implementation and experimental results
- *Chordal networks* (arXiv:1604.02618)
  - New representation/decomposition for polynomial systems
  - Efficient algorithms to compute them. Can use them for root counting, dimension, radical ideal membership, etc.
  - Links to BDDs (binary decision diagrams) and extensions

Example 1: Coloring a cycle

Let $C_n = (V, E)$ be the cycle graph and consider the ideal I given by the equations



$$x_i^3 - 1 = 0, \qquad i \in V$$
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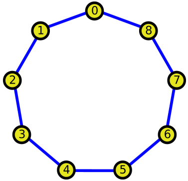

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\end{aligned}
$$

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However, a Gröbner basis is not so simple: one of its 13 elements is

$$
\begin{gathered}
x_0x_2x_4x_6 + x_0x_2x_4x_7 + x_0x_2x_4x_8 + x_0x_2x_5x_6 + x_0x_2x_5x_7 + x_0x_2x_5x_8 + x_0x_2x_6x_8 + x_0x_2x_7x_8 + x_0x_2x_8^2 + x_0x_3x_4x_6 + x_0x_3x_4x_7 \\
+x_0x_3x_4x_8 + x_0x_3x_5x_6 + x_0x_3x_5x_7 + x_0x_3x_5x_8 + x_0x_3x_6x_8 + x_0x_3x_7x_8 + x_0x_3x_8^2 + x_0x_4x_6x_8 + x_0x_4x_7x_8 + x_0x_4x_8^2 + x_0x_5x_6x_8 \\
+x_0x_5x_7x_8 + x_0x_5x_8^2 + x_0x_6x_8^2 + x_0x_7x_8^2 + x_0 + x_1x_2x_4x_6 + x_1x_2x_4x_7 + x_1x_2x_4x_8 + x_1x_2x_5x_6 + x_1x_2x_5x_7 + x_1x_2x_5x_8 \\
+x_1x_2x_6x_8 + x_1x_2x_7x_8 + x_1x_2x_8^2 + x_1x_3x_4x_6 + x_1x_3x_4x_7 + x_1x_3x_4x_8 + x_1x_3x_5x_6 + x_1x_3x_5x_7 + x_1x_3x_5x^8 + x_1x_3x_6x_8 + x_1x_3x_7x_8 \\
+x_1x_3x_8^2 + x_1x_4x_6x_8 + x_1x_4x_7x_8 + x_1x_4x_8^2 + x_1x_5x_6x_8 + x_1x_5x_7x_8 + x_1x_5x_8^2 + x_1x_6x_8^2 + x_1x_7x_8^2 + x_1 + x_2x_4x_6x_8 + x_2x_4x_7x_8 \\
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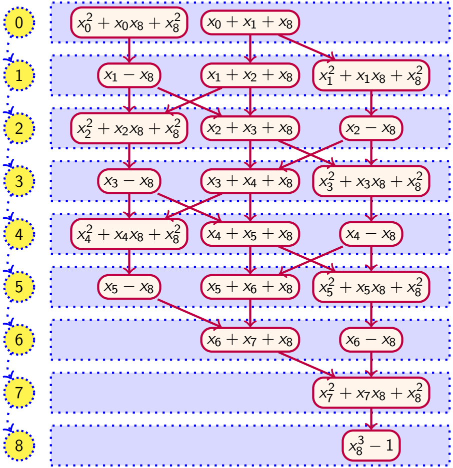
\end{gathered}
$$

Example 1: Coloring a cycle

There is a nicer representation, that respects its graphical structure.
The solution set can be *decomposed* into *triangular* sets:

$$\mathcal{V}(I) = \bigcup_{T} \mathcal{V}(T)$$

where the union is over all *maximal directed paths* in the figure.
The number of triangular sets is 21, which is the 8-th Fibonacci number.



Chordal networks

A new representation of structured polynomial systems!

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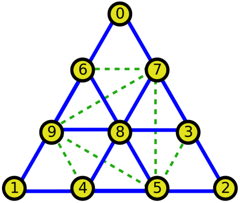
  - Remarkably, many polynomial systems admit "small" chordal networks, even though the number of components may be exponentially large.
- What are they good for?
  - Can be effectively used to solve feasibility, counting, dimension, elimination, radical membership, ...
  - Linear time algorithms (exponential in treewidth)
  - Implementation and experimental results.

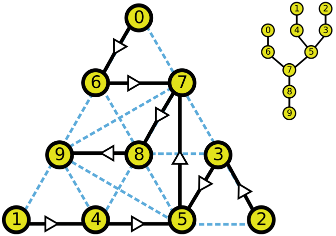
Elimination tree of a chordal graph

The elimination tree of a graph G is the following *directed spanning tree*:

For each ℓ there is an arc from x_ℓ towards the largest x_p that is adjacent to x_ℓ and $p > \ell$.

Note that the elimination tree is rooted at x_{n-1}.





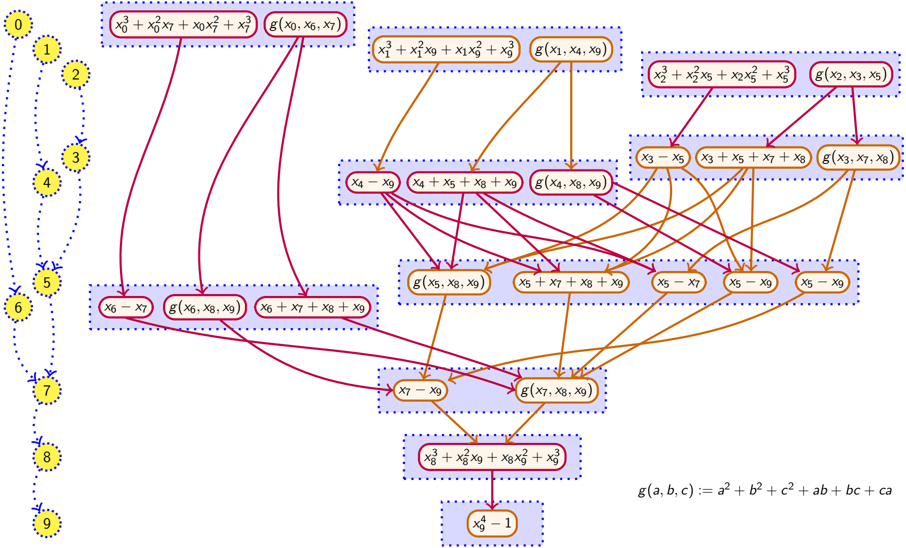
Chordal networks (definition)

A G-chordal network is a directed graph $\mathcal{N}$, whose nodes are polynomial sets in $\mathbb{K}[X]$, such that:

- Graded: Each node F is given a $\text{rank}(F) \in \{0, \ldots, n-1\}$, s.t. $F \subset \mathbb{K}[X_{\text{rank}(F)}]$.
- Tree-like: For any arc (F_ℓ, F_p) we have that x_p is the parent of x_ℓ in the elimination tree of G, where $\ell = \text{rank}(F_\ell), p = \text{rank}(F_p)$.

A chordal network is triangular if each node consists of a single polynomial f, and either $f = 0$ or its largest variable is $x_{\text{rank}(f)}$.

Chordal networks (Example)

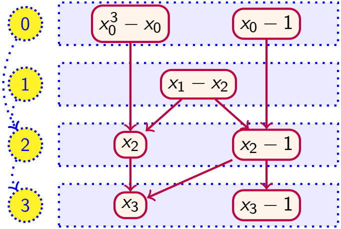


$$g(a, b, c) := a^2 + b^2 + c^2 + ab + bc + ca$$

Computing chordal networks (Example)

$$I = \langle x_2 - x_3, x_1 - x_2, x_1^2 - x_1, x_0x_2 - x_2, x_0^3 - x_0 \rangle$$

The output of the algorithm will be



This represents the decomposition of I into the triangular sets

$$(x_3, x_2, x_1 - x_2, x_0^3 - x_0),$$
$$(x_3, x_2 - 1, x_1 - x_2, x_0 - 1),$$
$$(x_3 - 1, x_2 - 1, x_1 - x_2, x_0 - 1).$$

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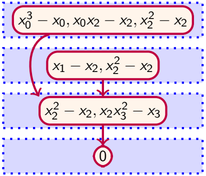

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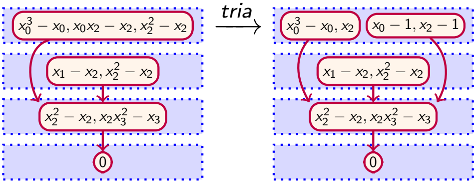

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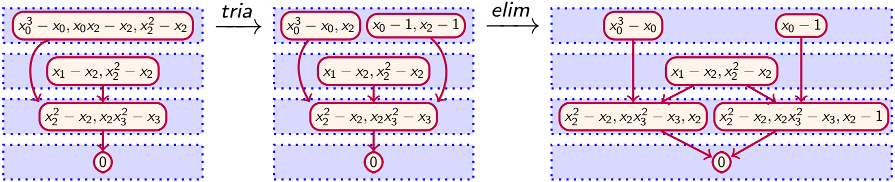

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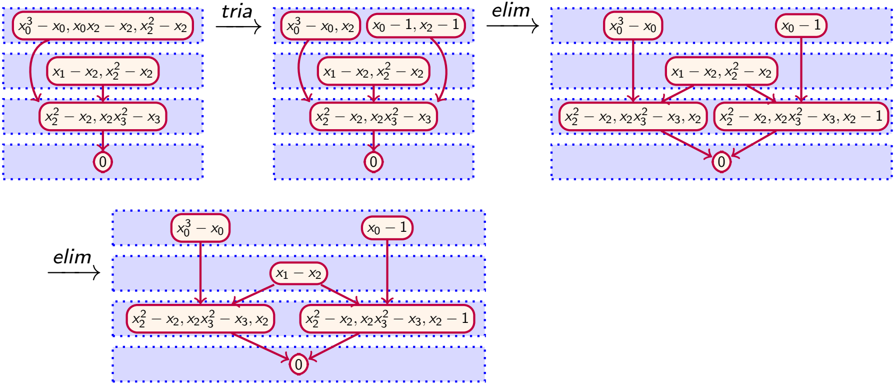

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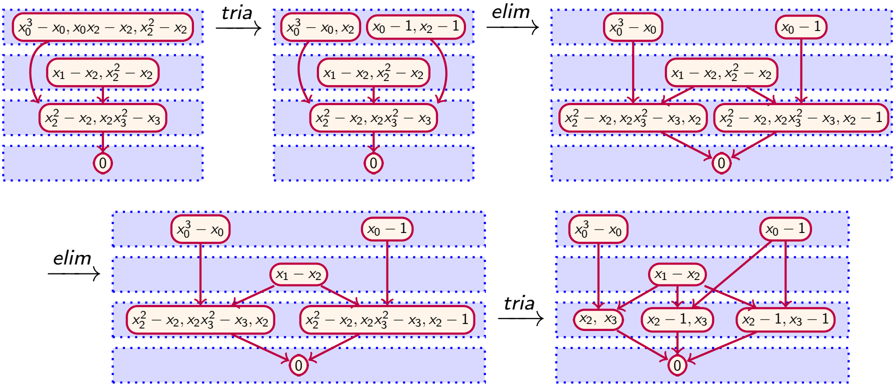
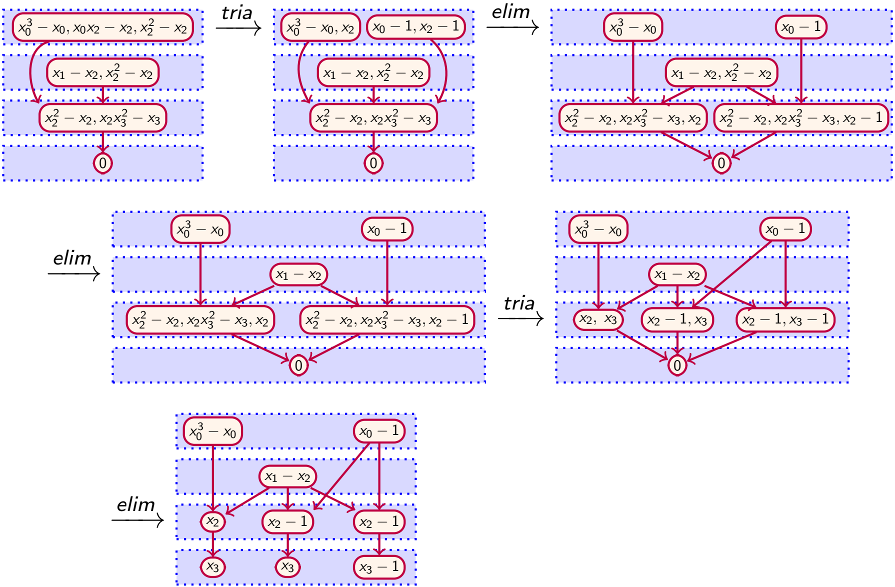


Computing chordal networks (Example)



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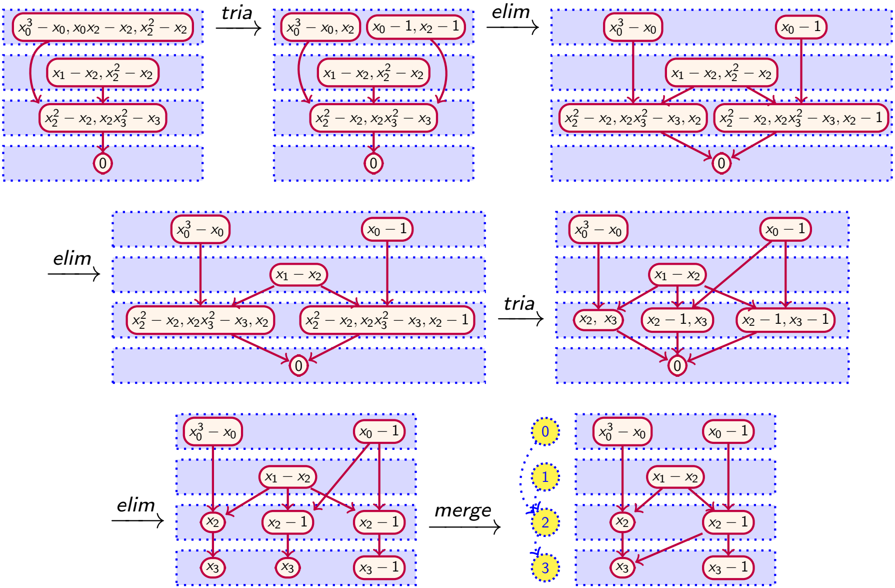


Chordal networks in computational algebra

Given a triangular chordal network $\mathcal{N}$ of a polynomial system, the following problems can be solved in linear time:

- Compute the cardinality of $\mathcal{V}(I)$.
- Compute the dimension of $\mathcal{V}(I)$
- Describe the top dimensional component of $\mathcal{V}(I)$.

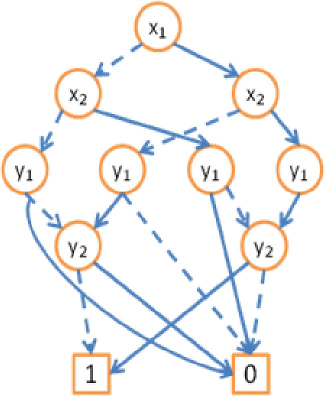
We also developed efficient algorithms to

- Solve the radical ideal membership problem ($h \in \sqrt{I}$?)
- Compute the equidimensional components of the variety.

Links to BDDs

Very interesting connections with *binary decision diagrams* (BDDs).

- A clever representation of Boolean functions/sets, usually much more compact than naive alternatives
- Enabler of very significant practical advances in (discrete) formal verification and model checking
- "One of the only really fundamental data structures that came out in the last twenty-five years" (D. Knuth)



For the special case of *monomial ideals*, chordal networks are equivalent to (reduced, ordered) BDDs. But in general, more powerful!

Implementation and examples

Implemented in Sage, using Singular and PolyBoRi (for $\mathbb{F}_2$).
Upcoming package for Macaulay2.

- Graph colorings (counting q-colorings)
- Cryptography ("baby" AES, Cid *et al.*)
- Sensor Network localization
- Discretization of polynomial equations
- Reachability in vector addition systems
- Algebraic statistics

Example: Vector addition systems

Given a set of vectors $\mathcal{B} \subset \mathbb{Z}^n$, construct a graph with vertex set $\mathbb{N}^n$ in which $u, v \in \mathbb{N}^n$ are adjacent if $u - v \in \pm\mathcal{B}$.

Ex: Determine whether $f_n \in I_n$, where

$$f_n := x_0 x_1^2 x_2^3 \cdots x_{n-1}^n - x_0^n x_1^{n-1} \cdots x_{n-1},$$
$$I_n := \{x_i x_{i+3} - x_{i+1} x_{i+2} : 0 \leq i < n\},$$

and where the indices are taken modulo n.

We compare our radical membership test with Singular (Gröbner bases) and Epsilon (triangular decompositions).

n	5	10	15	20	25	30	35	40	45	50	55
ChordalNet	0.7	3.0	8.5	14.3	21.8	29.8	37.7	48.2	62.3	70.6	84.8
Singular	0.0	0.0	0.2	17.9	1036.2	-	-	-	-	-	-
Epsilon	0.1	0.2	0.4	2.0	54.4	160.1	5141.9	17510.1	-	-	-

Summary

- (Hyper)graphical structure *may* simplify optimization/solving
- Under assumptions (treewidth + algebraic structure), tractable!
- New data structures: chordal networks
- Yields practical, competitive, implementable algorithms
- Ongoing and future work: other polynomial solving approaches (e.g., homotopies, full numerical algebraic geometry...)

Summary

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If you want to know more:

- D. Cifuentes, P.A. Parrilo, Exploiting chordal structure in polynomial ideals: a Groebner basis approach. *SIAM J. of Discrete Mathematics*, 30(3), 1534–1570, 2016. `arXiv:1411.1745`.
- D. Cifuentes, P.A. Parrilo, An efficient tree decomposition method for permanents and mixed discriminants, *Linear Algebra and Appl.*, 493:45–81, 2016. `arXiv:1507.03046`.
- D. Cifuentes, P.A. Parrilo, Chordal networks of polynomial ideals. *SIAM Journal on Applied Algebra and Geometry*, 1(1), 73–110, 2017. `arXiv:1604.02618`.

Thanks for your attention!