Graph structure in polynomial systems

Pablo A. Parrilo

Laboratory for Information and Decision Systems
Electrical Engineering and Computer Science
Massachusetts Institute of Technology

Based on joint work
with Diego Cifuentes (MIT)

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

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

A polynomial system defined by $m$ equations in $n$ variables:

$$f_i(x_0, \ldots, x_{n-1}) = 0, \quad i = 1, \ldots, m$$
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Construct a graph \( G \) (“primal graph”) with \( n \) nodes:

- Nodes are variables \( \{x_0, \ldots, x_{n-1}\} \).
- For each equation, add a clique connecting the variables appearing in that equation.
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Example:

\[
I = \langle x_0^2x_1x_2 + 2x_1 + 1, \; x_1^2 + x_2, \; x_1 + x_2, \; x_2x_3 \rangle
\]
“Abstracted” the polynomial system to a (hyper)graph.

Questions

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?
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- 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

$$X_l := \{x_l\} \cup \{x_m : x_m \text{ is adjacent to } x_l, \ x_l > x_m\}$$

is such that the restriction $G|_{X_l}$ is a clique.
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(Equivalently, in numerical linear algebra: Cholesky factorization has no “fill-in”)

Cifuentes, Parrilo (MIT)
Chordality, treewidth, and a meta-theorem

A chordal completion of $G$ is a chordal graph with the same vertex set as $G$, and which contains all edges of $G$. 

The treewidth of a graph is the clique number (minus one) of its smallest chordal completion. Informally, treewidth quantitatively measures how “tree-like” a graph is.

Meta-theorem: NP-complete problems are “easy” on graphs of small treewidth.
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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 the recursion below starting from the leaves:

\[
S(i) = \max \left( \sum_{j \in \text{children}(i)} S(j), \quad 1 + \sum_{j \in \text{grandchildren}(i)} S(j) \right),
\]

\[
S(\text{leaf}) = 1,
\]

where \( S(i) \) represents the size of the largest independent set of the corresponding subtree.
Recall the *partition* problem, with data \( A = \{a_1, \ldots, a_n\} \subset \mathbb{Z}_+ \).
Can we split \( A \) in two subsets with equal sum?

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

\[
\begin{align*}
0 &= s_0 \\
0 &= (s_i - s_{i-1} + a_i)(s_i - s_{i-1} - a_i) \\
0 &= s_n
\end{align*}
\]

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

\[ S_0 \longrightarrow S_1 \longrightarrow S_2 \longrightarrow \cdots \longrightarrow S_n \]

But, partition is NP-complete… :(
Bad news? (I)

Recall the *partition* problem, with data $A = \{a_1, \ldots, a_n\} \subset \mathbb{Z}_+$. Can we split $A$ in two subsets with equal sum?

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$$
\begin{array}{c}
\circ S_0 \quad S_1 \quad S_2 \quad \cdots \quad S_n \\
\end{array}
$$

But, partition is NP-complete... :(  

(DGTA: equivalent to 1-dim realizability of cycle... [Saxe79])
Bad news? (II)

For \textit{linear} equations, “good” elimination preserves graph structure (perfect!)

For polynomials, however, Groebner bases can destroy chordality.

Ex: Consider \( I = \langle x_0 x_2 - 1, x_1 x_2 - 1 \rangle \), whose associated graph is the path \( x_0 \rightarrow x_2 \rightarrow x_1 \).

Every Groebner basis must contain the polynomial \( x_0 - x_1 \), breaking the sparsity structure.

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

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**Q:** Are there *alternative descriptions* that “play nicely” with graphical structure?
How to resolve this (apparent) contradiction?

“Trees are good”  \iff  “Trees can be NP-hard”
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Underlying hero/culprit: dynamic programming (DP), and more refined cousins (nonserial DP, belief propagation, etc).
How to resolve this (apparent) contradiction?

“Trees are good” ⇔ “Trees can be NP-hard”

Underlying hero/culprit: dynamic programming (DP), and more refined cousins (nonserial DP, belief propagation, etc).

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, …]
How to get around this?

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In the algebraic setting, a natural condition: degree of *projections onto clique subspaces*.

Consider the full solution set (an algebraic variety).

 Require the *projections* onto the subspaces spanned by the *maximal cliques* to have bounded degree.
How to get around this?

Need to impose conditions on the geometry!

In the algebraic setting, a natural condition:
degree of projections onto clique subspaces.

Consider the full solution set
(an algebraic variety).

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

- 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
Chordal elimination (sketch)

Given equations, construct graph $G$, a chordal completion, and a perfect elimination ordering.

Will produce a decreasing sequence of ideals $I = I_0 \supseteq I_1 \supseteq \cdots \supseteq I_{n-1}$.

Given current ideal $I_l$, split the generators

$$I_l = \underbrace{J_l}_{\in \mathbb{K}[X_l]} + K_{l+1}^{\notin \mathbb{K}[X_l]}$$

and eliminate variable $x_l$

$$I_{l+1} = \text{elim}_{l+1}(J_l) + K_{l+1}$$

“Ideally” (!), $I_l$ should be the $l$-th elimination ideal $\text{elim}_l(I)$...

By chordality, graph structure is always preserved!

Also, all elimination operations are performed on “small” rings!
Example: chordal elimination

\[ I = \langle x_0^4 - 1, x_0^2 + x_2, x_1^2 + x_2, x_2^2 + x_3 \rangle \]

Zero-dimensional system, 8 solutions.

Elimination order: \((x_0, x_1, x_2, x_3)\)

\[
\begin{align*}
&\begin{array}{l}
x_0^4 - 1 \\
x_0^2 + x_2
\end{array} \\
&\begin{array}{l}
x_1^2 + x_2 \\
x_2^2 + x_3
\end{array}
\end{align*}
\]

Solving backwards (e.g.): \(x_3 = -1 \rightarrow x_2 = 1 \rightarrow x_1 = i \rightarrow x_0 = i\).
But, naive chordal elimination may fail!

\[ I = \langle x_0x_2 + 1, \ x_1^2 + x_2, \ x_1 + x_2, \ x_2x_3 \rangle \]

Groebner basis:

\[ \{ x_0 - 1, \ x_1 - 1, \ x_2 + 1, \ x_3 \} \]

Elimination:

\[
\begin{align*}
& x_0x_2 + 1 \\
& x_1^2 + x_2 \\
& x_1 + x_2 \\
& x_2x_3 \\
& x_2^2 + x_2 \\
& x_2 + x_3 \\
& 0
\end{align*}
\]

We got \( I_3 = \langle 0 \rangle \), but really \( \text{elim}_3(I) = \langle x_3 \rangle \).
When does chordal elimination succeed?

We need conditions for this to work, i.e., for $V(I) = V(\text{elim}_I(I))$.

**Thm 1:** Let $I$ be an ideal and assume that for each $l$ such that $X_l$ is a maximal clique of $G$, the ideal $J_l \subseteq K[X_l]$ is zero dimensional. Then, chordal elimination succeeds.

In particular, finite fields $\mathbb{F}_q$, and 0/1 problems.
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**Def:** A polynomial $f$ is *simplicial* if for each variable $x_l$, the monomial $m_l$ of largest degree in $x_l$ is unique and has the form $m_l = x^{d_l}$.

**Thm 2:** Let $I = \langle f_1, \ldots, f_s \rangle$ be an ideal such that for each $1 \leq i \leq s$, $f_i$ is generic simplicial. Then, chordal elimination succeeds.
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We need conditions for this to work, i.e., for $\mathbf{V}(I_l) = \mathbf{V}(\text{elim}_I(l))$.

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[Intuition: interaction of (iterated) “closure/extension thm” + chordality]
[Intuition: variety has “small” coordinate projections, can compute those, and glue them]
Example 1: Coloring a cycle

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

\[
x_i^3 - 1 = 0, \quad i \in V \\
x_i^2 + x_ix_j + x_j^2 = 0, \quad ij \in E
\]

These equations encode the proper 3-colorings of the graph. Note that coloring the cycle graph is very easy!
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However, a Gröbner basis is not so simple: one of its 13 elements is

\[
\begin{align*}
&x_0 x_2 x_4 x_6 + x_0 x_2 x_4 x_7 + x_0 x_2 x_4 x_8 + x_0 x_2 x_5 x_6 + x_0 x_2 x_5 x_7 + x_0 x_2 x_5 x_8 + x_0 x_2 x_6 x_8 + x_0 x_2 x_7 x_8 + x_0 x_2 x_8^2 + x_0 x_3 x_4 x_6 + x_0 x_3 x_4 x_7 \\
&+ x_0 x_3 x_4 x_8 + x_0 x_3 x_5 x_6 + x_0 x_3 x_5 x_7 + x_0 x_3 x_5 x_8 + x_0 x_3 x_7 x_8 + x_0 x_3 x_8^2 + x_0 x_4 x_6 x_8 + x_0 x_4 x_7 x_8 + x_0 x_4 x_8^2 + x_0 x_5 x_6 x_8 \\
&+ x_0 x_5 x_7 x_8 + x_0 x_5 x_8^2 + x_0 x_6 x_8^2 + x_0 x_7 x_8^2 + x_0 + x_1 x_2 x_4 x_6 + x_1 x_2 x_4 x_7 + x_1 x_2 x_4 x_8 + x_1 x_2 x_5 x_6 + x_1 x_2 x_5 x_7 + x_1 x_2 x_5 x_8 \\
&+ x_1 x_2 x_6 x_8 + x_1 x_2 x_7 x_8 + x_1 x_2 x_8^2 + x_1 x_3 x_4 x_6 + x_1 x_3 x_4 x_7 + x_1 x_3 x_4 x_8 + x_1 x_3 x_5 x_6 + x_1 x_3 x_5 x_7 + x_1 x_3 x_5 x_8 + x_1 x_3 x_6 x_8 + x_1 x_3 x_7 x_8 \\
&+ x_1 x_3 x_8^2 + x_1 x_4 x_6 x_8 + x_1 x_4 x_7 x_8 + x_1 x_4 x_8^2 + x_1 x_5 x_6 x_8 + x_1 x_5 x_7 x_8 + x_1 x_5 x_8^2 + x_1 x_6 x_8^2 + x_1 x_7 x_8^2 + x_0 + x_1 x_2 x_4 x_8 + x_2 x_4 x_7 x_8 \\
&+ x_2 x_4 x_8^2 + x_2 x_5 x_6 x_8 + x_2 x_5 x_7 x_8 + x_2 x_5 x_8^2 + x_2 x_6 x_8^2 + x_2 x_7 x_8^2 + x_2 + x_3 x_4 x_6 x_8 + x_3 x_4 x_7 x_8 + x_3 x_4 x_8^2 + x_3 x_5 x_6 x_8 + x_3 x_5 x_7 x_8 \\
&+ x_3 x_5 x_8^2 + x_3 x_6 x_8^2 + x_3 x_7 x_8^2 + x_3 + x_4 x_6 x_8^2 + x_4 x_7 x_8^2 + x_4 + x_5 x_6 x_8^2 + x_5 x_7 x_8^2 + x_5 + x_6 + x_7 + x_8
\end{align*}
\]
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!

- What do they look like?
  - “Enlarged” elimination tree, with polynomial sets as nodes.
  - Efficient encoding of components in paths/subtrees.

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.

Cifuentes, Parrilo (MIT)
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- How can you compute them?
  - A nice algorithm to compute chordal networks.
  - Remarkably, many polynomial systems admit “small” chordal networks, even though the number of components may be exponentially large.

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  - Linear time algorithms (exponential in treewidth)
  - Implementation and experimental results.
The elimination tree of a graph $G$ is the following directed spanning tree:

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

Note that the elimination tree is rooted at $x_{n-1}$.
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 rank($F$) $\in \{0, \ldots, n-1\}$, s.t. $F \subset \mathbb{K}[X_{\text{rank}(F)}]$.  

- **Tree-like**: For any arc $(F_\ell, F_p)$, $x_p$ is the parent of $x_\ell$ 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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\[ x_0^3 - x_0, x_0x_2 - x_2, x_2^2 - x_2 \]
\[ x_1 - x_2, x_2^2 - x_2 \]
\[ x_2^2 - x_2, x_2x_3^2 - x_3 \]

0
Computing chordal networks (Example)

\[ x_0^3 - x_0, x_0 x_2 - x_2, x_2^2 - x_2, x_1 - x_2, x_2^2 - x_2, x_2^2 - x_2 x_3^2 - x_3 \]

\[ 0 \]

\[ x_0^3 - x_0, x_2 \]

\[ x_0 - 1, x_2 - 1 \]

\[ x_1 - x_2, x_2^2 - x_2 \]

\[ x_2^2 - x_2, x_2 x_3^2 - x_3 \]

\[ 0 \]
Computing chordal networks (Example)

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\[ x_1 - x_2, x^2_2 - x_2 \]
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\[ \xrightarrow{\text{tria}} \]

\[ x^3_0 - x_0, x_2 \]
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\[ x^2_2 - x_2, x_2x^2_3 - x_3 \]
\[ 0 \]

\[ \xrightarrow{\text{elim}} \]

\[ x^3_0 - x_0 \]
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&0
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\[\text{tria}\]

\[
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&x_0^3 - x_0, x_2 \\
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&x_1 - x_2, x_2^2 - x_2 \\
&x_2 - x_2, x_2x_3^2 - x_3
\end{align*}
\]

\[\text{elim}\]

\[
\begin{align*}
&x_0^3 - x_0 \\
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\end{align*}
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\[\text{elim}\]

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\end{align*}
\]
Computing chordal networks (Example)

\[
\begin{align*}
&x_0^3 - x_0, x_0x_2 - x_2, x_2^2 - x_2 \\
&x_1 - x_2, x_2^2 - x_2 \\
&x_2 - x_2, x_2x_3^2 - x_3 \\
&0
\end{align*}
\]

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\begin{align*}
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&0
\end{align*}
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Computing chordal networks (Example)

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\begin{align*}
x_0^3 - x_0, x_0x_2 - x_2, x_2^2 - x_2 \\
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x_2^2 - x_2, x_2x_3^2 - x_3 \\
0
\end{align*}
\]

\[
\begin{align*}
x_0^3 - x_0, x_0 \xrightarrow{\text{tria}} x_0 - 1, x_2 - 1 \\
x_1 - x_2, x_2^2 - x_2 \\
x_2^2 - x_2, x_2x_3^2 - x_3 \\
0
\end{align*}
\]

\[
\begin{align*}
x_0^3 - x_0, x_0 \xrightarrow{\text{elim}} x_0 - 1 \\
x_1 - x_2, x_2^2 - x_2 \\
x_2^2 - x_2, x_2x_3^2 - x_3, x_2 - 1 \\
0
\end{align*}
\]

\[
\begin{align*}
x_0^3 - x_0 \xrightarrow{\text{tria}} x_0 - 1 \\
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x_2^2 - x_2, x_2x_3^2 - x_3, x_2 - 1 \\
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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.
Radical ideal membership (Sketch)

\[ h(x) = \left\{ \begin{array}{ll}
0 & \text{if } x_9 = 0 \\
\frac{1}{2} h^a_6 & \text{if } x_7 - x_9 \\
\frac{1}{2} h^b_6 & \text{if } x_7 + x_8 + x_9 \\
\frac{1}{2} h^b_7 & \text{if } x_8^2 + x_8 x_9 + x_9^2 \\
\frac{1}{2} h^a_7 & \text{if } x_8^3 + x_8^2 x_9 + x_8 x_9^2 + x_9^3 \\
1 & \text{if } x_9^4 - 1 
\end{array} \right. \]
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!
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).

<table>
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<th>10</th>
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</tr>
</tbody>
</table>
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...)

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If you want to know more:


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Thanks for your attention!
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