Graph structure in polynomial systems: chordal networks

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Based on joint work with Diego Cifuentes (MIT)

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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.
Polynomial systems and graphs

A polynomial system defined by \( m \) equations in \( n \) variables:

\[
f_i(x_0, \ldots, x_{n-1}) = 0, \quad i = 1, \ldots, m
\]
A polynomial system defined by $m$ equations in $n$ variables:

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

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:

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

$$X_\ell := \{x_\ell\} \cup \{x_m : x_m \text{ is adjacent to } x_\ell, \ x_\ell > x_m\}$$

is such that the restriction $G|_{X_\ell}$ is a clique.
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A graph is chordal if it has a perfect elimination ordering.

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

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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 $G$. 

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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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.

**STABLE SET problem:** Compute a stable set of maximum cardinality.
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For general graphs, **NP-complete**.
On trees, **linear-time** solvable!

\[ S(i) = \max \left( \sum_{j \in \text{children}(i)} S(j), 1 + \sum_{j \in \text{grandchildren}(i)} S(j) \right), \]
\[ S(\text{leaf}) = 1, \]
where \( S(i) \) represents the size of the largest independent set of the corresponding subtree.
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Fix a root, and solve this recursion starting from the leaves:

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\]

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

where \( S(i) \) represents the size of the largest independent set of the corresponding subtree.
Recall the *subset sum* problem, with data $A = \{a_1, \ldots, a_n\} \subset \mathbb{Z}$. Is there a subset of $A$ that adds up to 0?

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

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

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

$$
\begin{array}{cccccccc}
S_0 & \rightarrow & S_1 & \rightarrow & S_2 & \rightarrow & \cdots & \rightarrow & S_n \\
\end{array}
$$

But, subset sum is NP-complete... :(
Bad news? (II)

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

For polynomials, however, Groebner bases can destroy chordality. Ex: Consider $I = \langle x_0x_2 - 1, x_1x_2 - 1 \rangle$, 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”

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!


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[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.

- 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

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

These equations encode the proper 3-colorings of the graph. Note that coloring the cycle graph is very easy!
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These equations encode the proper 3-colorings of the graph. Note that coloring the cycle graph is very easy!

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

\[
x_0x_2x_4x_6 + x_0x_2x_4x_8 + x_0x_2x_5x_6 + x_0x_2x_5x_7 + x_0x_2x_5x_8 + x_0x_2x_6x_8 + x_0x_2x_7x_8 + x_0x_2x_8^2 + x_0x_3x_4x_6 + x_0x_3x_4x_7 + x_0x_3x_5x_6 + x_0x_3x_5x_7 + x_0x_3x_5x_8 + x_0x_3x_6x_8 + x_0x_3x_7x_8 + x_0x_4x_6x_8 + x_0x_4x_7x_8 + x_0x_4x_8^2 + x_0x_5x_6x_8 + x_0x_5x_7x_8 + x_0x_6x_8^2 + x_0x_7x_8^2 + x_0 + x_1x_2x_4x_6 + x_1x_2x_4x_7 + x_1x_2x_4x_8 + x_1x_2x_5x_6 + x_1x_2x_5x_7 + x_1x_2x_5x_8 + x_1x_2x_6x_8 + x_1x_2x_7x_8 + x_1x_3x_4x_6 + x_1x_3x_4x_8 + x_1x_3x_5x_6 + x_1x_3x_5x_7 + x_1x_3x_5x_8 + x_1x_3x_6x_8 + x_1x_3x_7x_8 + x_1x_3x_8^2 + x_1x_4x_6x_8 + x_1x_4x_7x_8 + x_1x_4x_8^2 + x_1x_5x_6x_8 + x_1x_5x_7x_8 + x_1x_5x_8^2 + x_1x_6x_8^2 + x_1x_7x_8^2 + x_1 + x_2x_4x_6x_8 + x_2x_4x_7x_8 + x_2x_4x_8^2 + x_2x_5x_6x_8 + x_2x_5x_7x_8 + x_2x_5x_8^2 + x_2x_6x_8^2 + x_2x_7x_8^2 + x_2 + x_3x_4x_6x_8 + x_3x_4x_7x_8 + x_3x_4x_8^2 + x_3x_5x_6x_8 + x_3x_5x_7x_8 + x_3x_5x_8^2 + x_3x_6x_8^2 + x_3x_7x_8^2 + x_3 + x_4x_6x_8^2 + x_4x_7x_8^2 + x_4 + x_5x_6x_8^2 + x_5x_7x_8^2 + x_5 + x_6 + x_7 + x_8
\]
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.

Linear time algorithms (exponential in treewidth)

Implementation and experimental results.

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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.

What are they good for?
- Can be effectively used to solve feasibility, counting, dimension, elimination, radical membership, . . .
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- What are they good for?
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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 $x_{n-1}$.
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 rank(\( F \)) \( \in \{ 0, \ldots, n - 1 \} \), s.t. 
  \[ F \subset \mathbb{K}[X_{\text{rank}(F)}]. \]

- **Tree-like**: For any arc \( (F_\ell, F_p) \) we have that \( x_p \) 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)

\[ I = \langle x_2 - x_3, x_1 - x_2, x_1^2 - x_1, x_0 x_2 - x_2, x_0^3 - x_0 \rangle \]

The output of the algorithm will be

This represents the decomposition of \( I \) into the triangular sets

\[ (x_3, x_2, x_1 - x_2, x_0^3 - x_0), \]
\[ (x_3, x_2 - 1, x_1 - x_2, x_0 - 1), \]
\[ (x_3 - 1, x_2 - 1, x_1 - x_2, x_0 - 1). \]
Computing chordal networks (Example)

\[ x_3^3 - x_0, x_0 x_2 - x_2, x_2^2 - x_2 \]
\[ x_1 - x_2, x_2^2 - x_2 \]
\[ x_2^2 - x_2, x_2 x_3^2 - x_3 \]
\[ 0 \]
Computing chordal networks (Example)

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

\[
\begin{align*}
    x_0^3 - x_0, x_2 \\
    x_1 - x_2, x_2^2 - x_2 \\
    x_2^2 - x_2, x_2x_3^2 - x_3 \\
    0
\end{align*}
\]
Computing chordal networks (Example)

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

\[ x_0^3 - x_0, x_0 x_2 - x_2, x_0 - 1, x_2 - 1, x_1 - x_2, x_2^2 - x_2, x_2^2 - x_2, x_2 x_3^2 - x_3 \]

\[ x_0^3 - x_0, x_0 x_2 - x_2, x_2^2 - x_2, x_2^2 - x_2, x_2 - x_2, x_2 x_3^2 - x_3, x_2 - 1 \]
Computing chordal networks (Example)

\[
\begin{align*}
\text{tria} & : x_0^3 - x_0, x_0 x_2 - x_2, x_2^2 - x_2 \\
& \quad \rightarrow x_1 - x_2, x_2^2 - x_2 \\
& \quad \rightarrow x_2 - x_2, x_2 x_3^2 - x_3 \\
& \quad \quad \quad 0
\end{align*}
\]

\[
\begin{align*}
\text{elim} & : x_0^3 - x_0, x_0 - 1, x_2 - 1 \\
& \quad \rightarrow x_1 - x_2, x_2^2 - x_2 \\
& \quad \rightarrow x_2 - x_2, x_2 x_3^2 - x_3, x_2 \\
& \quad \quad \quad 0
\end{align*}
\]

\[
\begin{align*}
\text{elim} & : x_0^3 - x_0, x_0 - 1 \\
& \quad \rightarrow x_1 - x_2 \\
& \quad \rightarrow x_2 - x_2, x_2 x_3^2 - x_3, x_2 \\
& \quad \quad \quad 0
\end{align*}
\]
Computing chordal networks (Example)

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

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

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

\[ 0 \]

\[ x_0^3 - x_0, x_0 - 1, x_2 - 1 \]

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

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

\[ x_2^2 - x_2, x_2 x_3^2 - x_3, x_2 - 1 \]

\[ 0 \]

\[ x_0^3 - x_0 \]

\[ x_0 - 1 \]

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

\[ x_2^2 - x_2, x_2 x_3^2 - x_3, x_2 - 1 \]

\[ 0 \]
Computing chordal networks (Example)

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

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

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

\[ 0 \]

\[ \text{tria} \rightarrow \]

\[ x_0^3 - x_0, x_0 - 1, x_2 - 1 \]

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

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

\[ x_2^2 - x_2, x_2 x_3^2 - x_3, x_2 - 1 \]

\[ 0 \]

\[ \text{elim} \rightarrow \]

\[ x_0^3 - x_0 \]

\[ x_0 - 1 \]

\[ x_1 - x_2 \]

\[ x_2^2 - x_2, x_2 x_3^2 - x_3, x_2 - 1 \]

\[ 0 \]

\[ \text{tria} \rightarrow \]

\[ x_0^3 - x_0 \]

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\[ x_2 - 1, x_3 \]

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\[ 0 \]
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\[
x_0^3 - x_0, x_0x_2 - x_2, x_2^2 - x_2, \\
x_1 - x_2, x_2^2 - x_2, \\
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\]

\[
x_0^3 - x_0, x_0 - 1, x_2 - 1, \\
x_1 - x_2, x_2^2 - x_2, \\
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x_0^3 - x_0, \\
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\]

\[
x_0^3 - x_0, x_0 - 1
\]
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!
Initially implemented in Sage, using Singular and PolyBoRi (for $\mathbb{F}_2$). Now, software package ("Chordal.m2") freely available 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 $B \subset \mathbb{Z}^n$, construct a graph with vertex set $\mathbb{N}^n$ in which $u, v \in \mathbb{N}^n$ are adjacent if $u - v \in \pm B$.

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

$$f_n := x_0x_1^2x_2^3 \cdots x_{n-1}^n - x_0^n x_1^{n-1} \cdots x_{n-1},$$

$$I_n := \{x_ix_{i+3} - x_{i+1}x_{i+2} : 0 \leq i < n\},$$

and where the indices are taken modulo $n$.

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

<table>
<thead>
<tr>
<th>$n$</th>
<th>ChordalNet</th>
<th>Singular</th>
<th>Epsilon</th>
</tr>
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</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...)

If you want to know more:

Thanks for your attention!
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