# 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.

The Numerical Solution of Systems of Polynomials Arising in Engineering and Science



$$
\begin{aligned}
& S+E \underset{k-1}{\stackrel{k+1}{\rightleftarrows}} E S \underset{k-2}{\stackrel{k+2}{\rightleftarrows}} P+E \\
& \frac{d[S]}{d t}=-k_{1}[E][S]+k_{-1}[E S] \\
& \frac{d[E]}{d t}=-k_{1}[E][S]+\left(k_{-1}+k_{2}\right)[E S]-k_{-2}[E][P] \\
& \frac{d[E S]}{d t}=k_{1}[E][S]-\left(k_{-1}+k_{2}\right)[E S]+k_{-2}[E][P] \\
& \frac{d[P]}{d t}=k_{2}[E S]-k_{-2}[E][P]
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\end{gathered}
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Today: MS111/MS126 - Structured Polynomial Equations and Applications

## Polynomial systems and graphs

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

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f_{i}\left(x_{0}, \ldots, x_{n-1}\right)=0, \quad i=1, \ldots, m
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Example:
$I=\left\langle x_{0}^{2} x_{1} x_{2}+2 x_{1}+1, \quad x_{1}^{2}+x_{2}, \quad x_{1}+x_{2}, \quad x_{2} x_{3}\right\rangle$


## Questions

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"Abstracted" the polynomial system to a (hyper)graph.

- 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 $I$, the set

$$
X_{l}:=\left\{x_{l}\right\} \cup\left\{x_{m}: x_{m} \text { is adjacent to } x_{l}, x_{l}>x_{m}\right\}
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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")


Reverse Cuthill-McKee


## 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 $G$.

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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.


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Informally, treewidth quantitatively measures how "tree-like" a graph is.


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

## Bad news? (I)

Recall the subset sum problem, with data $A=\left\{a_{1}, \ldots, a_{n}\right\} \subset \mathbb{Z}$. Is there a subset of $A$ that adds up to 0 ?

Letting $s_{i}$ be the partial sums, we can write a polynomial system:

$$
\begin{aligned}
& 0=s_{0} \\
& 0=\left(s_{i}-s_{i-1}\right)\left(s_{i}-s_{i-1}-a_{i}\right) \\
& 0=s_{n}
\end{aligned}
$$

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

$$
\text { (so) - } \mathrm{S}_{1} \text { - } \mathrm{S}_{2}-\cdots-\mathrm{S}_{n}
$$

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

## Bad news? (II)

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For polynomials, however, Groebner bases can destroy chordality.
Ex: Consider

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whose associated graph is the path $x_{0}$ - $x_{2}$ - $x_{1}$.

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

## How to resolve this (apparent) contradiction?

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

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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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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


## Example 1: Coloring a cycle

Let $C_{n}=(V, E)$ be the cycle graph and consider the ideal I given by the equations

$$
\begin{aligned}
x_{i}^{3}-1 & =0, & & i \in V \\
x_{i}^{2}+x_{i} x_{j}+x_{j}^{2} & =0, & & i j \in E
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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

$$
\begin{aligned}
& x_{0} x_{2} x_{4} x_{6}+x_{0} x_{2} x_{4} x_{7}+x_{0} x_{2} x_{4} x_{8}+x_{0} x_{2} x_{5} x_{6}+x_{0} x_{2} x_{5} x_{7}+x_{0} x_{2} x_{5} x_{8}+x_{0} x_{2} x_{6} x_{8}+x_{0} x_{2} x_{7} x_{8}+x_{0} x_{2} x_{8}^{2}+x_{0} x_{3} x_{4} x_{6}+x_{0} x_{3} x_{4} x_{7} \\
& +x_{0} x_{3} x_{4} x_{8}+x_{0} x_{3} x_{5} x_{6}+x_{0} x_{3} x_{5} x_{7}+x_{0} x_{3} x_{5} x_{8}+x_{0} x_{3} x_{6} x_{8}+x_{0} x_{3} x_{7} x_{8}+x_{0} x_{3} x_{8}^{2}+x_{0} x_{4} x_{6} x_{8}+x_{0} x_{4} x_{7} x_{8}+x_{0} x_{4} x_{8}^{2}+x_{0} x_{5} x_{6} x_{8} \\
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\end{aligned}
$$

## 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.


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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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- Efficient encoding of components in paths/subtrees.
- 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, ...
- 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 $\ell$ 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:

- each node $F$ is given a $\operatorname{rank}(F) \in\{0, \ldots, n-1\}$, s.t. $F \subset \mathbb{K}\left[X_{\operatorname{rank}(F)}\right]$.
- for any arc $\left(F_{\ell}, F_{p}\right)$ we have that $x_{p}$ is the parent of $x_{\ell}$ in the elimination tree of $G$, where $\ell=\operatorname{rank}\left(F_{\ell}\right), p=\operatorname{rank}\left(F_{p}\right)$.

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

## Chordal networks (Example)



## Computing chordal networks (Example)

$$
I=\left\langle x_{2}-x_{3}, x_{1}-x_{2}, x_{1}^{2}-x_{1}, x_{0} x_{2}-x_{2}, x_{0}^{3}-x_{0}\right\rangle
$$

The output of the algorithm will be


This represents the decomposition of $I$ into the triangular sets

$$
\begin{gathered}
\left(x_{3}, x_{2}, x_{1}-x_{2}, x_{0}^{3}-x_{0}\right), \\
\left(x_{3}, x_{2}-1, x_{1}-x_{2}, x_{0}-1\right) \\
\left(x_{3}-1, x_{2}-1, x_{1}-x_{2}, x_{0}-1\right)
\end{gathered}
$$

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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 $\mathbb{F}_{2}$ ).

- 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


## I - 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

$$
\begin{aligned}
& f_{n}:=x_{0} x_{1}^{2} x_{2}^{3} \cdots x_{n-1}^{n}-x_{0}^{n} x_{1}^{n-1} \cdots x_{n-1}, \\
& I_{n}:=\left\{x_{i} x_{i+3}-x_{i+1} x_{i+2}: 0 \leq i<n\right\},
\end{aligned}
$$

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 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ChordalNet | 0.7 | 3.0 | 8.5 | 14.3 | 21.8 | 29.8 | 37.7 | 48.2 | 62.3 | 70.6 |
| 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 | - | - |

## II - Algebraic statistics (Evans et al.)

Consider the binomial ideal $I^{n, n_{2}}$ that models a 2D dimensional generalization of the birth-death Markov process. We fix $n_{2}=1$.

We can compute all irreducible components of the ideal faster than specialized packages (e.g., Macaulay2's "Binomials")

| $n$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| \#components | 3 | 11 | 40 | 139 | 466 | 1528 | 4953 |
| time | ChordalNet | $0: 00: 00$ | $0: 00: 01$ | $0: 00: 04$ | $0: 00: 13$ | $0: 02: 01$ | $0: 37: 35$ |
|  | Binomials | $0: 00: 00$ | $0: 00: 00$ | $0: 00: 01$ | $0: 00: 12$ | $0: 03: 00$ | $4: 15: 36$ |

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|  | Binomials | $0: 00: 00$ | $0: 00: 00$ | $0: 00: 01$ | $0: 00: 12$ | $0: 03: 00$ | $4: 15: 36$ | - |

Our methods are particularly efficient for computing the highest dimensional components.

Highest 5 dimensions
Highest 7 dimensions

| $n$ | 20 | 40 | 60 | 80 | 100 | 10 | 20 | 30 | 40 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| \#comps <br> time | 404 | $0: 01: 07$ | $0: 04: 54$ | $0: 15: 12$ | $0: 41: 52$ | $1: 34: 05$ | $0: 05: 02$ | $0: 41: 41$ | $3: 03: 29$ |

## 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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- 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. arXiv:1604.02618.


## Thanks for your attention!

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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, to appear. 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. arXiv:1604.02618.

Thanks for your attention!
(and please come to MS111/MS126!)

