## Graph structure in polynomial systems: chordal networks

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Based on joint work with **Diego Cifuentes** (MIT)

SIAM Annual Meeting - July 2016

### 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.





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

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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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Example:

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





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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?

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(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

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

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")



#### Chordality, treewidth, and a meta-theorem

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

Graph structure in polynomial systems

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)

$$s_0 - s_1 - s_2 - \cdots - s_n$$

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

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For polynomials, however, Groebner bases can destroy chordality.

Ex: Consider

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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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- 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

$$\begin{aligned} x_i^3-1 &= 0, \qquad \quad i \in V \\ x_i^2+x_ix_j+x_i^2 &= 0, \qquad \quad ij \in E \end{aligned}$$



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

$$\begin{split} & x_{0}x_{2}x_{4}x_{6} + x_{0}x_{2}x_{4}x_{7} + x_{0}x_{2}x_{4}x_{8} + x_{0}x_{2}x_{5}x_{6} + x_{0}x_{2}x_{5}x_{7} + x_{0}x_{2}x_{5}x_{8} + x_{0}x_{2}x_{6}x_{8} + x_{0}x_{2}x_{7}x_{8} + x_{0}x_{2}x_{7}x_{8}^{2} + x_{0}x_{3}x_{4}x_{6} + x_{0}x_{3}x_{4}x_{7} \\ & +x_{0}x_{3}x_{4}x_{8} + x_{0}x_{3}x_{5}x_{6} + x_{0}x_{3}x_{5}x_{7} + x_{0}x_{3}x_{5}x_{8} + x_{0}x_{3}x_{6}x_{8} + x_{0}x_{3}x_{7}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{7}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{7}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{6}x_{8} + x_{0}x_{3}x_{7}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{7}x_{8} + x_{0}x_{3}x_{7}^{2}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{6}^{2}x_{8} + x_{0}x_{3}x_{7}^{2}x_{8} + x_{0}x_{3}x_{7}^{2}x_{8} + x_{1}x_{2}x_{5}x_{8} + x_{1}x_{2}x_{5}x_{8} + x_{1}x_{2}x_{5}x_{8} + x_{1}x_{2}x_{5}x_{8} + x_{1}x_{2}x_{5}x_{8} + x_{1}x_{2}x_{5}x_{8} + x_{1}x_{3}x_{5}x_{7} + x_{1}x_{3}x_{5}x_{7} + x_{1}x_{3}x_{5}x_{8} + x_{1}x_{3}x_{6}x_{8} + x_{1}x_{3}x_{7}x_{8} \\ + x_{1}x_{3}x_{6}^{2}x_{8} + x_{1}x_{4}x_{6}x_{8} + x_{1}x_{4}x_{7}x_{8} + x_{1}x_{4}x_{6}^{2}x_{8} + x_{1}x_{5}x_{7}x_{8} + x_{1}x_{5}x_{7}^{2}x_{8} + x_{1}x_{5}x_{7}^{2}x_{8} + x_{1}x_{5}x_{7}^{2}x_{8} + x_{1}x_{5}x_{7}^{2}x_{8} + x_{1}x_{5}x_{7}x_{8}^{2} + x_{1}x_{7}x_{8}^{2} + x_{1}x_{7}x_{8}^{2} + x_{1}x_{7}x_{8} + x_{1}x_{4}x_{7}x_{8} + x_{2}x_{4}x_{7}^{2}x_{8} + x_{2}x_{7}x_{8}^{2} + x_{2}x_{7}$$

### 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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  - Efficient encoding of components in paths/subtrees.
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  - 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  $x_{n-1}$ .





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 rank $(F) \in \{0, \ldots, n-1\}$ , s.t.  $F \subset \mathbb{K}[X_{\mathsf{rank}(F)}]$ .
- 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  $\ell = \operatorname{rank}(F_{\ell}), p = \operatorname{rank}(F_p)$ .

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

# 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

$$egin{aligned} &(x_3,x_2,x_1-x_2,x_0^3-x_0),\ &(x_3,x_2-1,x_1-x_2,x_0-1),\ &(x_3-1,x_2-1,x_1-x_2,x_0-1). \end{aligned}$$

Cifuentes, Parrilo (MIT)

Graph structure in polynomial systems











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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!

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

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

and where the indices are taken modulo n.

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

п	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
Epsilon	0.0	0.0	0.2	2.0	1036.2 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")

п		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	12:22:19
	Binomials	0:00:00	0:00:00	0:00:01	0:00:12	0:03:00	4:15:36	-

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

Highest 5 dimensions							Highest 7 dimensions			
п	20	40	60	80	100	10	20	30	40	
#comps time	404 0:01:07	684 0:04:54	964 0:15:12	1244 0:41:52	1524 1:34:05	2442 0:05:02	5372 0:41:41	8702 3:03:29	12432 9:53:09	

## 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:

- 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!

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