Sparse Triangular Decomposition Based on Chordal Graphs

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11:20 — 12:10	**Chenqi Mou** On the chordality of polynomial sets in triangular decomposition in top-down style slides abstract

Backgrounds

$\mathbb{K}$: a field, $x_1, \ldots, x_n$: the variables

Polynomial system solving

Find all the solutions in $\tilde{\mathbb{K}}^n$ of

$$F_1(x_1, \ldots, x_n) = \cdots = F_s(x_1, \ldots, x_n) = 0,$$

where $\tilde{\mathbb{K}}$ is some field extension of $\mathbb{K}$.

Example

Cyclic-n system in $\mathbb{Q}[x_1, \ldots, x_n]$

$$\begin{cases} x_1 + x_2 + \cdots + x_n = 0, \\ x_1x_2 + x_2x_3 + \cdots + x_nx_1 = 0, \\ \qquad \cdots\cdots \\ x_1x_2\cdots x_n - 1 = 0. \end{cases}$$

Polynomial system solving: triangular decomposition

$x_1 < \cdots < x_n$, triangular set in $\mathbb{R}[x_1, \ldots, x_n]$

$T_1(x_1, \ldots, x_{s_1})$ ⟶ real root isolation

$T_2(x_1, \ldots, x_{s_1}, \ldots, x_{s_2})$ ⟶ substitution

$T_3(x_1, \ldots, x_{s_1}, \ldots, x_{s_2}, \ldots, x_{s_3})$

$\vdots$

$T_r(x_1, \ldots, x_{s_1}, \ldots, x_{s_2}, \ldots, x_{s_3}, \ldots, \ldots, x_{s_r})$

Triangular decomposition

Polynomial set $\mathcal{F} \subset \mathbb{R}[x_1, \ldots, x_n]$

$\Downarrow$

Triangular sets $\mathcal{T}_1, \ldots, \mathcal{T}_t$ s.t. $\mathsf{Z}(\mathcal{F}) = \bigcup_{i=1}^{t} \mathsf{Z}(\mathcal{T}_i / \mathrm{ini}(\mathcal{T}_i))$

- ⇝ Solving $\mathcal{F} = 0 \Longrightarrow$ solving all $\mathcal{T}_i = 0$
- ⇝ Polynomial generalization of Gaussian elimination

Triangular decomposition: back to the example

Example

Cyclic-n system in $\mathbb{Q}[x_1, \ldots, x_n]$

$$\begin{cases} x_1 + x_2 + \cdots + x_n = 0, \\ x_1x_2 + x_2x_3 + \cdots + x_nx_1 = 0, \\ \qquad \cdots\cdots \\ x_1x_2\cdots x_n - 1 = 0. \end{cases}$$

Triangular decomposition for $n = 3$

$$\mathcal{T}_1 = [x_1 - 1, {x_2}^2 + x_2 + 1, x_3 + x_2 + 1],$$
$$\mathcal{T}_2 = [x_1^2 + x_1 + 1, x_2 - 1, x_3 + x_1 + 1],$$
$$\mathcal{T}_3 = [x_1^2 + x_1 + 1, x_2 + x_1 + 1, x_3 - 1].$$

Polynomial system solving: variable ordering

Polynomial system solving

Find all the solutions in $\tilde{\mathbb{K}}^n$ of

$$F_1(x_1, \ldots, x_n) = \cdots = F_m(x_1, \ldots, x_n) = 0,$$

where $\tilde{\mathbb{K}}$ is some field extension of $\mathbb{K}$.

Denote $\mathcal{F} = \{F_1, \ldots, F_n\}$

- Gröbner bases: $x_1 < \cdots < x_n$ + LEX $\Longrightarrow$ Compute the LEX Gröbner basis $\mathcal{G}$ of $\langle \mathcal{F} \rangle$
- Triangular sets: $x_1 < \cdots < x_n$ $\Longrightarrow$ Compute triangular sets $\mathcal{T}_1, \ldots, \mathcal{T}_r$

But why $x_1 < \cdots < x_n$?

Find a "good" variable ordering by using the graph structure of $\mathcal{F}$

Chordal graph

Chordal graph: definition

$G = (V, E)$ *chordal* $\Longleftrightarrow$ for any cycle C contained in G of four or more vertices, there is an edge $e \in E \setminus C$ connects two vertices in C.

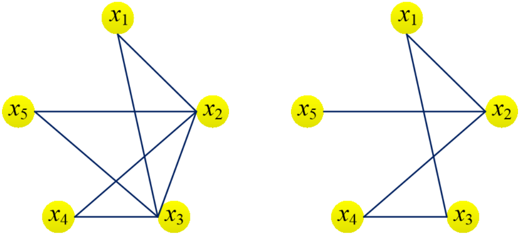


Figure: Chordal VS non-chordal graphs

- The connecting edge: chord.
- A chordal graph: triangulated graph.

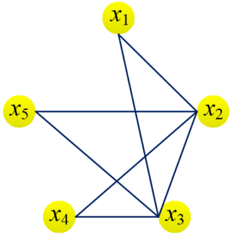
Chordal graph

Equivalent condition via perfect elimination ordering

$G = (V, E)$ a graph with $V = \{x_1, \dots, x_n\}$:
An ordering $x_{i_1} < x_{i_2} < \cdots < x_{i_n}$ of the vertices is called a *perfect elimination ordering* of G if for each $j = i_1, \dots, i_n$, the restriction of G on

$$X_j = \{x_j\} \cup \{x_k : x_k < x_j \text{ and } (x_k, x_j) \in E\}$$

is a clique. A graph G is said to be *chordal* if there exists a perfect elimination ordering of it.



Inspired by the pioneering works of

D. Cifuentes P.A. Parrilo (from MIT)

on triangular sets and chordal graphs

[Cifuentes and Parrilo 2017]: chordal networks of polynomial systems

- Connections between triangular sets and chordal graphs
- Algorithms for computing triangular sets due to Wang become more efficient when the input polynomial set is chordal ($\Longrightarrow$ Why?)

Associated graphs of polynomial sets

$F \in \mathbb{K}[x_1, \ldots, x_n]$ a polynomial: the (variable) *support* of F, $\operatorname{supp}(F)$, is the set of variables in $x_1, \ldots, x_n$ which effectively appear in F

- $\operatorname{supp}(\mathcal{F}) := \cup_{F \in \mathcal{F}} \operatorname{supp}(F)$ for $\mathcal{F} \subset \mathbb{K}[x_1, \ldots, x_n]$

Associated graphs

$\mathcal{F} \subset \mathbb{K}[x_1, \ldots, x_n]$, *associated graph* $G(\mathcal{F})$ of $\mathcal{F}$ is an undirected graph:

(a) vertices of $G(\mathcal{F})$: the variables in $\operatorname{supp}(\mathcal{F})$

(b) edge (x_i, x_j) in $G(\mathcal{F})$: if there exists one polynomial $F \in \mathcal{F}$ with $x_i, x_j \in \operatorname{supp}(F)$

Chordal polynomial set

A polynomial set $\mathcal{F} \subset \mathbb{K}[x_1, \ldots, x_n]$ is said to be *chordal* if $G(\mathcal{F})$ is chordal.

Associated graphs of polynomial sets

$$\mathbb{K}[x_1, \ldots, x_5]$$

$$\mathcal{P} = \{x_2 + x_1, x_3 + x_1, x_4^2 + x_2, x_4^3 + x_3, x_5 + x_2, x_5 + x_3 + x_2\}$$

$$\mathcal{Q} = \{x_2 + x_1, x_3 + x_1, x_3, x_4^2 + x_2, x_4^3 + x_3, x_5 + x_2\}$$

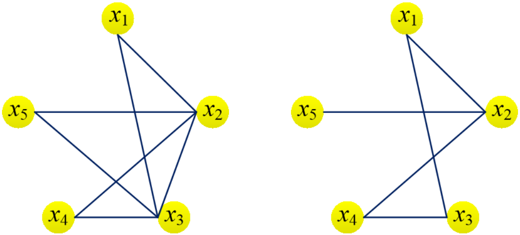
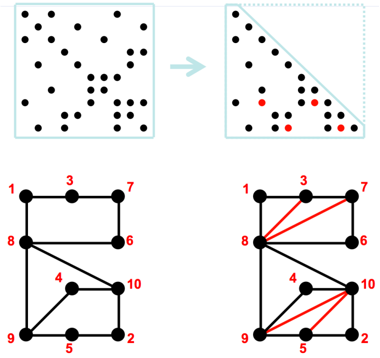


Figure: Associated graphs $G(\mathcal{P})$ (chordal) and $G(\mathcal{Q})$ (not chordal)

Chordal graphs in Gaussian elimination

New fill-ins in Cholesky factorization of a matrix $A = LL^t$ (credits to J. Gilbert)



G(A)

G(L)
[chordal]

Matrices with chordal graphs: no new fill-ins (subgraphs) $\Longrightarrow$ sparse Gaussian elimination [Parter 61, Rose 70, Gilbert 94]

Triangular decomposition in top-down style

The variables are handled in a strictly decreasing order: $x_n, x_{n-1}, \ldots, x_1$

- widely used strategy [Wang 1993, 1998, 2000], [Chai, Gao, Yuan 2008]
- the closest to Gaussian elimination
- algorithms due to Wang are mostly in top-down style (!!)

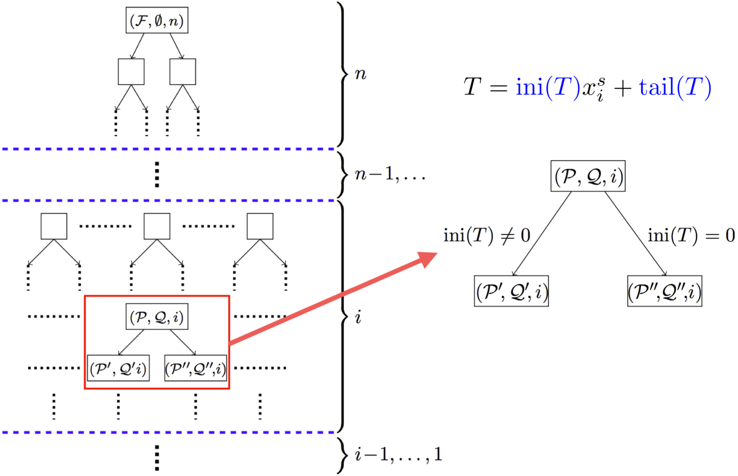
Matrix in echelon form			Triangular set		
x_1	x_2	x_3	x_1	x_2	x_3
1	$*$	$*$	$*$	0	0
0	1	$*$	$*$	$*$	0
0	0	1	$*$	$*$	$*$
Gaussian elimination			Top-down triangular decomposition		

Problems

1. Chordal graphs in Gaussian elimination $\Longrightarrow$ Chordal graphs in triangular decomposition in top-down style: polynomial generalization (algebraic [Mou, Bai 2018], [Mou, Lai 2019])
   - Changes of graph structures of the polynomials in triangular decomposition
   - relationships (like inclusion) between associated graphs of computed triangular sets and the input polynomial set
2. Sparse Gaussian elimination $\Longrightarrow$ sparse triangular decomposition in top-down style: polynomial generalization [Mou, Bai, Lai 2019]

Wang's method: binary decomposition tree

[Wang 93]: Wang's method, simply-structured, top-down style



$$\mathcal{P}' := \mathcal{P} \setminus \mathcal{P}^{(i)} \cup \{T\} \cup \{\mathrm{prem}(P, T) : P \in \mathcal{P}\}, \quad \mathcal{Q}' := \mathcal{Q} \cup \{\mathrm{ini}(T)\},$$

$$\mathcal{P}'' := \mathcal{P} \setminus \{T\} \cup \{\mathrm{ini}(T), \mathrm{tail}(T)\}, \quad \mathcal{Q}'' := \mathcal{Q},$$

Wang's method: left child

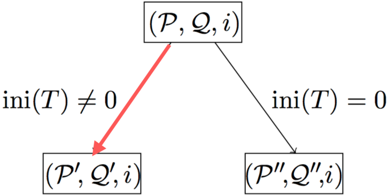
Proposition: Wang's method applied to $\mathcal{F} \subset \mathbb{K}[x_1, \ldots, x_n]$, chordal

$\mathcal{F} \subset \mathbb{K}[x_1, \ldots, x_n]$ chordal, $x_1 < \cdots < x_n$ perfect elimination ordering:

$(\mathcal{P}, \mathcal{Q}, i)$ arbitrary node in the binary decomposition tree such that $G(\mathcal{P}) \subset G(\mathcal{F})$, $T \in \mathcal{P}$ with minimal degree in x_i. Denote

$$\mathcal{P}' = \mathcal{P} \setminus \mathcal{P}^{(i)} \cup \{T\} \cup \{\text{prem}(P, T) : \; P \in \mathcal{P}^{(i)}\}.$$

Then $G(\mathcal{P}') \subset G(\mathcal{F})$.



$G(\mathcal{P}') \subset G(\mathcal{F})$ under the conditions $G(\mathcal{F})$ is chordal and $G(\mathcal{P}) \subset G(\mathcal{F})$

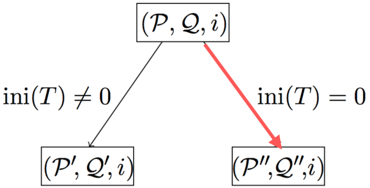
Wang's method: right child

Proposition

$(\mathcal{P}, \mathcal{Q}, i)$ arbitrary node in the binary decomposition tree, $T \in \mathcal{P}^{(i)}$ with minimal degree in x_i. Denote

$$\mathcal{P}'' = \mathcal{P} \setminus \{T\} \cup \{\mathrm{ini}(T), \mathrm{tail}(T)\}.$$

Then $G(\mathcal{P}'') \subset G(P)$.
$\rightsquigarrow$In particular, $\mathrm{supp}(\mathrm{tail}(T)) = \mathrm{supp}(T) \Longrightarrow G(\mathcal{P}'') = G(\mathcal{P})$.



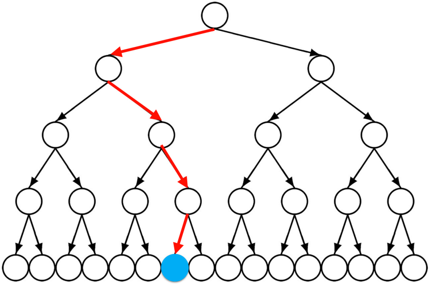
$G(\mathcal{P}'') \subset G(\mathcal{P})$ under no conditions

Wang's method: any node

Theorem: Wang's method applied to $\mathcal{F} \subset \mathbb{K}[x_1, \ldots, x_n]$, chordal

$\mathcal{F} \subset \mathbb{K}[x_1, \ldots, x_n]$ chordal, $x_1 < \cdots < x_n$ perfect elimination ordering:

For any node $(\mathcal{P}, \mathcal{Q}, i)$ in the binary decomposition tree, $G(\mathcal{P}) \subset G(\mathcal{F})$



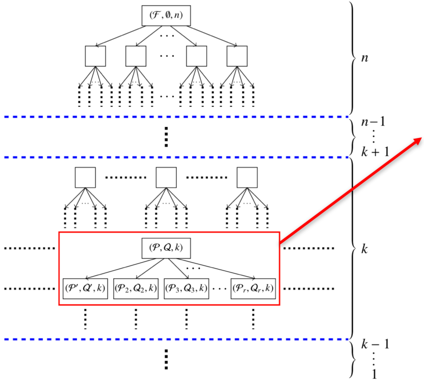
Corollary: Wang's method applied to $\mathcal{F} \subset \mathbb{K}[x_1, \ldots, x_n]$, chordal

$\mathcal{F} \subset \mathbb{K}[x_1, \ldots, x_n]$ chordal, $x_1 < \cdots < x_n$ perfect elimination ordering:

For any triangular set $\mathcal{T}$ computed by Wang's method, $G(\mathcal{T}) \subset G(\mathcal{F})$

Subresultant-based algorithm for triangular decomposition

[Wang 00]: splitting based on subresultant regular subchains



$$\mathcal{P}' := \mathcal{P} \setminus \{T_2\} \cup \{\mathrm{ini}(T_2), \mathrm{tail}(T_2)\},$$
$$\mathcal{Q}' := \mathcal{Q},$$
$$\mathcal{P}_i := \begin{cases} \mathcal{P} \setminus \{T_1, T_2\} \cup \{H_i, \mathrm{ini}(H_{i+1}), \ldots, \mathrm{ini}(H_r)\}, & i = 2, \ldots, r-1, \\ \mathcal{P} \setminus \{T_1, T_2\} \cup \{H_r\}, & i = r, \end{cases}$$
$$\mathcal{Q}_i := \mathcal{Q} \cup \{\mathrm{ini}(T_2)\} \cup \{\mathrm{ini}(H_i)\}, \quad i = 2, \ldots, r.$$

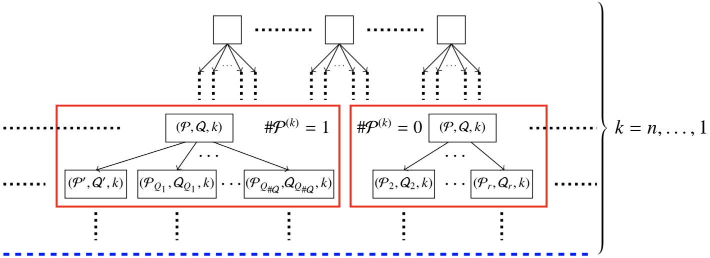
Dynamic multi-branch decomposition tree

The same results hold for this algorithm too.

Subresultant-based algorithm for regular decomposition

Regular decomposition

- the most frequently used triangular decomposition [Kalkbrener 93], [Yang, Zhang 94], [Wang 00], [Chen, Moreno Maza 12]
- [Wang 00]: top-down style, splitting based on subresultant regular subchains



Additional layer added to the dynamic multi-branch decomposition tree

The same results hold for this algorithm too.

From the viewpoint of variable orderings

Given a chordal and "sparse" polynomial set $\mathcal{F} \subset \mathbb{K}[\boldsymbol{x}]$, under the condition that the variable ordering is a perfect elimination ordering of $G(\mathcal{F})$, the "sparsity" of polynomial sets and computed triangular sets in triangular decomposition in top-down style are bounded by that of $G(\mathcal{F})$.

- Theoretical explanations to [Cifuents and Parrilo 2017]: Computationally faster when the perfect elimination orderings are used in triangular decomposition due to Dongming Wang
- When $G(\mathcal{F})$ is not chordal, a chordal completion can be performed: $\overline{G}(F)$ chordal and $\overline{G}(F) \supset G(\mathcal{F})$ [Bodlaender and Koster 2008]

Variable sparsity of polynomial sets

Sparsity in Gröbner bases

- sparse Gröbner bases [Faugère, Spaenlehauer, Svartz 2014]
- sparse FGLM algorithms [Faugère, Mou 2011, 2017]

$\Longrightarrow$ term sparsity for the theory of Gröbner bases

Variable sparsity (for the theory of triangular sets)

$G(\mathcal{F}) = (V, E)$ associated graph of $\mathcal{F} = \{F_1, \ldots, F_r\} \subset \mathbb{K}[x_1, \ldots, x_n]$.
Define the *variable sparsity* $s_v(\mathcal{F})$ of $\mathcal{F}$ as

$$s_v(\mathcal{F}) = |E| / \binom{2}{|V|},$$

denominator: edge number of a complete graph of $|V|$ vertices

Correlatively sparsity $\Longrightarrow$ sparse Sum-Of-Square [Waki et.al. 06], [Zheng et.al. 18]

Sparse triangular decomposition

A refined algorithm for regular decomposition

Input: a polynomial set $\mathcal{F} \subset \mathbb{K}[\boldsymbol{x}]$
Output: a variable ordering $\overline{\boldsymbol{x}}$ and a regular decomposition Φ of $\mathcal{F}$ with respect to $\overline{\boldsymbol{x}}$

1. Compute the variable sparsity s_v of $\mathcal{F}$
2. If s_v is smaller than some sparsity threshold s_0 ($\mathcal{F}$ is sparse), then
   1. If $G(\mathcal{F})$ is chordal, then compute its perfect elimination ordering $\overline{\boldsymbol{x}}$ [1]
   2. Else compute its chordal completion $\overline{G}(\mathcal{F})$ [2] and a perfect elimination ordering $\overline{\boldsymbol{x}}$ of $\overline{G}(\mathcal{F})$
3. Compute the regular decomposition of $\mathcal{F}$ with respect to $\overline{\boldsymbol{x}}$ with a top-down algorithm [3]

[1] [Rose, Tarjan, and Lueker 1976]
[2] [Bodlaender and Koster 2008]
[3] Say, [Wang 2000]

Sparse triangular decomposition

A sparse polynomial system arising from the lattice reachability problem
[Cifuentes and Parrilo 2017], [Diaconis, Eisenbud, Sturmfels 1998]

$$\mathcal{F}_i := \{x_k x_{k+3} - x_{k+1}x_{k+2} : k = 1, 2, \dots, i\}, \quad i \in \mathbb{Z}_{>0}$$

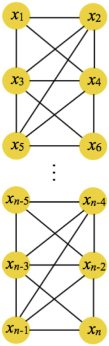


Figure: Associated graph of $\mathcal{F}_i$

Sparse triangular decomposition

- t_p: timings for a perfect elimination ordering
- t_r: timings for a random variable ordering

Table: Regular decomposition with RegSer in Epsilon: top-down

n	s_v	t_p	t_r					$\bar{t}_r$	$\bar{t}_r/t_p$
10	0.53	0.19	0.14	0.21	0.22	0.11	0.21	0.18	0.95
20	0.28	1.44	4.24	4.45	3.15	4.41	4.65	4.18	2.90
25	0.23	4.25	50.62	20.29	15.55	25.01	35.10	29.31	6.90
30	0.19	11.94	177.37	185.94	130.54	142.97	103.42	148.05	12.40
35	0.17	42.33	560.56	291.35	633.43	320.98	938.45	548.95	12.97
40	0.15	161.11	1883.64	3618.04	4289.13	4013.99	2996.37	3360.23	20.86

Application in biology

square + sparse polynomial sets? steady states of autonomous differential biological systems

$\Longrightarrow$ Good model for many biological systems: biochemical networks [Allen 94], [Gatermann, Huber 02], [Ferrell, Tsai, Yang 11], [Garfinkel, Shevtsov, Guo 17]

- square ones:

Synthesis of one enzyme in bacterial cells [Bock 81]

$$
\begin{aligned}
&\mathrm{d}x_1/\mathrm{d}t = p_1x_3 - (p_2+p_3)x_1, && \mathrm{d}x_2/\mathrm{d}t = p_{15}x_3 - p_4x_2,\\
&\mathrm{d}x_3/\mathrm{d}t = (p_2+p_3)x_1 - (p_1+p_{15})x_3 + p_4x_2, && \mathrm{d}x_4/\mathrm{d}t = p_{12}x_7x_6 - p_7x_4,\\
&\mathrm{d}x_5/\mathrm{d}t = p_6x_7 - p_8x_5, && \mathrm{d}x_6/\mathrm{d}t = p_3x_1 - p_5x_6 - p_{12}x_6x_7,\\
&\mathrm{d}x_7/\mathrm{d}t = -p_{12}x_6x_7 + p_7x_4 - p_6x_7 + p_8x_5, && \mathrm{d}x_8/\mathrm{d}t = p_{14}x_{12} - p_{13}x_8x_9,\\
&\mathrm{d}x_9/\mathrm{d}t = p_8x_5 - p_9x_9 - p_{13}x_8x_9, && \mathrm{d}x_{10}/\mathrm{d}t = p_{11}x_{11},\\
&\mathrm{d}x_{11}/\mathrm{d}t = p_{10}x_{12} - p_{11}x_{11}, && \mathrm{d}x_{12}/\mathrm{d}t = p_{13}x_8x_9 + p_{11}x_{11} - (p_{10}+p_{14})x_{12}.
\end{aligned}
$$

- $p_1, \ldots, p_{15}$: constants

- easily tens of or even hundreds of variables
- the couplings of their variables are quite loose, e.g. in chemical reaction networks [Allen 94, Gatermann Huber 02]

n-dimensional autonomous differential systems

$$\begin{cases} \dfrac{\mathrm{d}x_1}{\mathrm{d}t} = \dfrac{P_1(u_1,\ldots,u_m,x_1,\ldots,x_n)}{Q_1(u_1,\ldots,u_m,x_1,\ldots,x_n)}, \\ \quad\vdots \\ \dfrac{\mathrm{d}x_n}{\mathrm{d}t} = \dfrac{P_n(u_1,\ldots,u_m,x_1,\ldots,x_n)}{Q_n(u_1,\ldots,u_m,x_1,\ldots,x_n)}, \end{cases}$$

- $x_1,\ldots,x_n$: variables dependent on $t \Longrightarrow$ denote $\boldsymbol{x} = (x_1,\ldots,x_n)$
- $u_1,\ldots,u_m$: parameters independent on $t \Longrightarrow$ denote $\boldsymbol{u} = (u_1,\ldots,u_m)$
- $P_1,\ldots,P_n,Q_1,\ldots,Q_n \in \mathbb{R}[\boldsymbol{u},\boldsymbol{x}]$: polynomials over the real field $\mathbb{R}$

Steady states

For an arbitrary value $\overline{\boldsymbol{u}} \in \mathbb{R}^m$ of the parameters $\boldsymbol{u}$, a point $\overline{\boldsymbol{x}} = (\overline{x}_1,\ldots,\overline{x}_n) \in \mathbb{R}^n$ is said to be a steady state or equilibrium of the above system if $P_1(\overline{\boldsymbol{u}},\overline{\boldsymbol{x}}) = \cdots = P_n(\overline{\boldsymbol{u}},\overline{\boldsymbol{x}}) = 0$ and $Q_1(\overline{\boldsymbol{u}},\overline{\boldsymbol{x}}) \neq 0,\cdots,Q_n(\overline{\boldsymbol{u}},\overline{\boldsymbol{x}}) \neq 0$.

Sparse triangular decomposition for biological systems

Biological systems (large + sparse) — Equilibria Computation ⇒ Polynomial system solving

Symbolic method (free of errors) — Sparse triangular decomposition [Mou, Bai, Lai 21]

↑ Control the system sparsity

Graph theory — Chordal graph + chordal completion [Przytycka 06], [Cifuentes, Parrilo 16], [Mou, Bai 18]

Questions

1. Are biological dynamic systems sparse (w.r.t. variables)?
2. What influence will chordal completion have on the variable sparsity?
3. Applied to computation of equilibria, is sparse triangular decomposition more efficient versus ordinary one?

1. Large biological dynamic systems are sparse

Find from ODEbase database appropriate biological systems for sparse triangular decomposition: 141 systems
(autonomous differential systems over $\mathbb{Q}$, sparse, free of parameters, no variables in denominators)

- Those of ≤ 30 variables: 76$\%$ associated graphs are chordal, and 35$\%$ of them are of variable sparsity ≤ 0.4.
- Those of ≥ 30 variables: 8.3$\%$ associated graphs are chordal, and 92$\%$ of them are of variable sparsity ≤ 0.4.

Variable sparsity of polynomial sets of ≥ 30 variables

Model	n	Chor	s_v	Model	n	Chor	s_v	Model	n	Chor	s_v	Model	n	Chor	s_v
014	86	0	0.746	333	54	0	0.395	478	33	0	0.301	584	35	1	0.005
105	39	0	0.336	334	74	0	0.376	491	57	0	0.244	594	33	0	0.693
205	194	0	0.114	335	34	0	0.303	492	52	0	0.293	635	80	0	0.219
220	58	0	0.132	362	34	0	0.323	501	35	0	0.398	636	78	0	0.231
270	33	0	0.138	407	47	0	0.157	504	75	0	0.110	667	103	0	0.229
332	78	0	0.355	416	32	1	0.117	559	90	0	0.207	705	43	0	0.143

2. Influence of chordal completion on variable sparsity

Try four existing algorithms for minimal chordal completion: Lex-M [Rose, Tarjan, Lueker 76], MCS-M [Berry et. al. 04], SMS [Parra & Scheffler 97], and CMT [Mezzini & Moscarini 10]

Variable sparsity of polynomial sets ≥ 30 variables after chordal completion

Model	n	s_v	s'_{v1}	s'_{v2}	s'_{v3}	s'_{v4}	Inc	Model	n	s_v	s'_{v1}	s'_{v2}	s'_{v3}	s'_{v4}	Inc
014	86	0.746	0.879	0.879	0.868	0.972	16.37%	478	33	0.301	0.320	0.320	0.320	0.608	6.29%
105	39	0.336	0.363	0.363	0.355	0.394	5.62%	491	57	0.244	0.385	0.347	0.326	0.873	33.59%
205	194	0.114	0.270	0.270	0.238	—	108.61%	492	52	0.293	0.465	0.454	0.437	0.898	48.84%
220	58	0.132	0.180	0.167	0.166	0.624	25.11%	501	35	0.398	0.403	0.403	0.403	0.627	1.27%
270	33	0.138	0.159	0.159	0.159	0.489	15.07%	504	75	0.110	0.138	0.138	0.138	0.712	25.25%
332	78	0.355	0.568	0.568	0.509	0.654	43.47%	559	90	0.207	0.209	0.209	0.209	0.255	0.84%
333	54	0.395	0.562	0.562	0.512	0.653	29.56%	594	33	0.693	0.703	0.703	0.703	0.735	1.37%
334	74	0.376	0.626	0.626	0.556	0.719	47.98%	635	80	0.219	0.224	0.221	0.222	0.641	0.72%
335	34	0.303	0.332	0.328	0.328	0.535	8.24%	636	78	0.231	0.236	0.232	0.233	0.688	0.62%
362	34	0.323	0.335	0.335	0.337	0.508	3.87%	667	103	0.229	0.357	0.357	0.367	0.867	56.03%
407	47	0.157	0.240	0.191	0.186	0.673	18.24%	705	43	0.143	0.159	0.159	0.156	0.175	9.30%

- Considering the variable sparsity and computational time, we recommend the MCS-M algorithm for chordal completion of biological system.
- Chordal completion has a remarkable influence on the variable sparsity: 41% systems have increase ratios greater than 20% in the variable sparsity $\Rightarrow$ 71% systems are still sparse after chordal completion (variable sparsity <0.4).

3. Sparse triangular decomposition VS ordinary one

- Choose those biological systems with variable sparsity < 0.6
- Sparse triangular decomposition with 3 perfect elimination orderings VS ordinary one with 3 random variable orderings

Computation time for sparse and ordinary regular decomposition

Model	n	s'_v	t_{p1}	t_{p2}	t_{p3}	t_{r1}	t_{r2}	t_{r3}	$\overline{t_p}$	$\overline{t_r}$	Speedup
160	25	0.200	2.793	7.420	119.269	10.462	24.936	288.332	43.161	107.910	2.50
205	194	0.238	—	—	—	—	—	—			
220	58	0.166	37.263	125.788	435.904	240.095	477.932	602.467	199.652	440.165	2.20
332	78	0.509	189.764	541.506	986.204	673.333	1201.804	1540.605	572.491	1138.581	1.99
333	54	0.512	26.389	36.978	41.446	46.035	99.974	153.971	34.938	99.993	2.86
334	74	0.556	238.222	430.431	1073.222	687.416	757.550	1219.345	580.625	888.104	1.53
335	34	0.328	7.139	10.467	18.798	19.210	30.354	33.955	12.135	27.840	2.29
362	34	0.335	11.269	26.596	64.181	69.546	70.239	71.055	34.015	70.280	2.07
407	47	0.186	—	—	—	—	—	—			
478	33	0.320	2.047	3.737	5.49	8.947	9.934	19.355	3.758	12.745	3.39
501	35	0.403	4.561	7.483	12.954	—	—	—	8.333		
504	75	0.138	61.849	90.391	224.201	157.079	323.271	440.134	125.480	306.828	2.45
599	30	0.538	—	—	—	—	—	—			
635	80	0.221	—	—	—	—	—	—			
636	78	0.232	—	—	—	—	—	—			
667	103	0.357	—	—	—	—	—	—			
705	43	0.156	—	—	—	—	—	—			

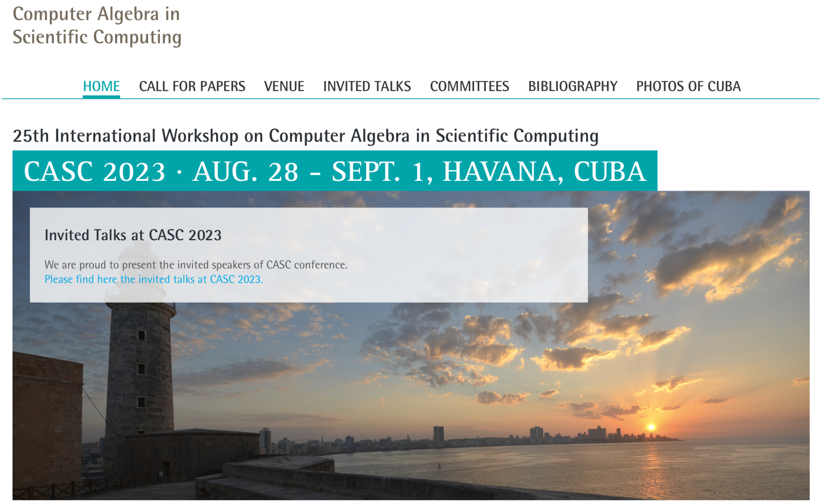
- Sparse regular decomposition is superior in computational performances than the ordinary one, with the average speed-up ratios between 1.53 to 3.39.

Conclusions

1. Chordal graphs in Gaussian elimination $\Longrightarrow$ Chordal graphs in triangular decomposition in top-down style: polynomial generalization
2. Sparse Gaussian elimination $\Longrightarrow$ sparse triangular decomposition in top-down style: polynomial generalization
3. Biological dynamic systems are sparse w.r.t. variables $\Longrightarrow$ sparse triangular decomposition works well

Thanks!

Welcome to CASC 2023



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