Solving Large Scale Semidefinite Problems by Decomposition

with application to

Topology Optimization with Vibration Constraints

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Dimensions in (linear) Semidefinite Optimization

$$\min_{x\in\mathbb{R}^n} c^\top x$$

subject to

$$\sum_{i=1}^{n} x_i A_i^{(k)} - B^{(k)} \succeq 0\,, \quad k = 1, \ldots, p$$

where

$$x \in \mathbb{R}^n, \quad A_i^{(k)},\ B^{(k)} \in \mathbb{R}^{m\times m}$$

Majority of SDP software

BAD . . . n large, m large   many variables, big matrix

OK . . . n small, m large   rare

GOOD . . . n large, m small   many variables, small matrix

GOOD . . . n large, m small, p large   many small matrix constraints

Solving (very) large scale SDP?

Given the known restrictions of interior point solvers, how can we solve very large scale SDP problems?

- Use iterative solvers
  SDPT3, PENSDP, Jacek Gondzio's recent work
- Use a different algorithm
  Bundle algorithm (Helmberg), Burer-Monteiro SDPA, ADMM (Wolkowicz), Augmented Lagrangian (Rendl, Malick, Toh-Sun,...)
- Reformulate **BAD** problems as **GOOD** problems

PENSDP with an iterative solver

$$\min_{x\in\mathbb{R}^n} c^\top x \quad \text{s.t.} \quad \sum_{i=1}^{n} x_i A_i - B \succeq 0\,, \quad A_i, B \in \mathbb{R}^{m\times m}$$

Problems with large n, small m (Kim Toh)
We have to solve repeatedly a dense $n \times n$ linear system.

problem	n	m	direct CPU	iterative CPU	CG/it
ham_8_3_4	16129	256	17701	30	1
ham_9_5_6	53761	512	mem	330	1
theta10	12470	500	12165	227	10
theta104	87845	500	mem	11953	25
theta12	17979	600	27565	254	8
theta123	90020	600	mem	10538	23
theta162	127600	800	mem	13197	13
sanr200-0.7	6 033	200	1146	30	12

mem. . . insufficient memory

PENSDP with hybrid strategy

Use PCG till it works, then switch to Cholesky and return to PCG, using the Ch-factor as a preconditioner.

Collection of chemical problems by M. Fukuda . . .

Average Dimacs error $\approx 1.0e - 7$

problem	n	Cg-it	Chol-it	Nwt-it	CPU-hy	CPU-ch
NH2-.r14	1,743	921	4	69	526	4033
NH3+.r16	2,964	1529	3	72	2427	26634
NH4+.r18	4,239	1607	3	77	8931	> 100000
AlH.r20	7,230	2283	2	102	21720	???

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where

$$x \in \mathbb{R}^n, \quad A_i^{(k)},\ B^{(k)} \in \mathbb{R}^{m \times m}$$

So we may want to replace

BAD . . . n large, m large, p=1

by

GOOD . . . n large, m small, p large   many small matrix constraints

Graph representation of matrix sparsity

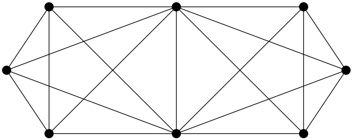
For a sparse symmetric matrix $A \in \mathbb{R}^{m\times m}$ define its (undirected, unweighted) sparsity graph $G_A(N, E)$:

$N = \{1, \dots, m\}$

$e_{ij} = E \Longleftrightarrow A_{ij} \neq 0, \quad i, j = 1, \dots n$

Some facts about the sparsity graph:

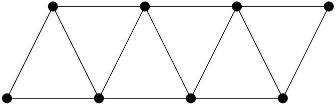
- G_A is chordal if and only if Cholesky factorization of $P^\top AP$ has zero fill-in for some perturbation P
- Cliques of G_A correspond to dense submatrices of A



$$\begin{bmatrix} \times & \times & \times & \times & \times & & & \\ \times & \times & \times & \times & \times & & 0 & \\ \times & \times & \times & \times & \times & & & \\ \times & \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times & \times \\ & & & \times & \times & \times & \times & \times \\ & 0 & & \times & \times & \times & \times & \times \\ & & & \times & \times & \times & \times & \times \end{bmatrix}$$

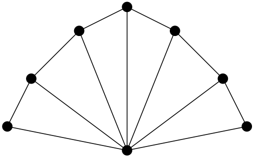
Graph representation of matrix sparsity

Another chordal sparsity graph, 5-diagonal matrix



$$\begin{bmatrix} \times & \times & \times & & & & & \\ \times & \times & \times & \times & & & 0 & \\ \times & \times & \times & \times & \times & & & \\ & \times & \times & \times & \times & \times & & \\ & & \times & \times & \times & \times & \times & \\ & & & \times & \times & \times & \times & \times \\ & 0 & & & \times & \times & \times & \times \\ & & & & & \times & \times & \times \end{bmatrix}$$

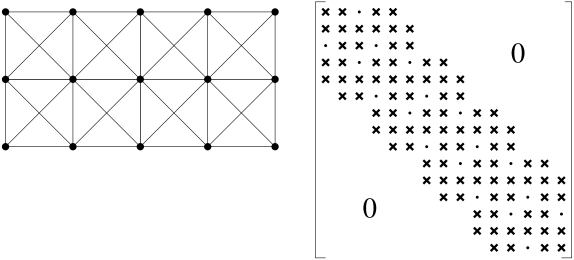
or the arrow matrix sparsity graph



$$\begin{bmatrix} \times & \times & & & & & & \times \\ \times & \times & \times & & 0 & & & \times \\ & \times & \times & \times & & & & \times \\ & & \times & \times & \times & & & \times \\ & & & \times & \times & \times & & \times \\ & 0 & & & \times & \times & \times & \times \\ & & & & & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times & \times \end{bmatrix}$$

Graph representation of matrix sparsity

A non-chordal sparsity graph



Graph representation of matrix sparsity

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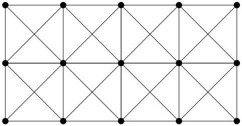
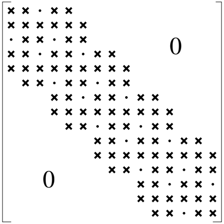
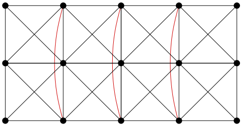
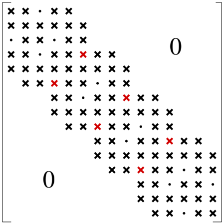




can be extended to a chordal sparsity graph





Chordal decomposition

S. Kim, M. Kojima, M. Mevissen and M. Yamashita, Exploiting Sparsity in Linear and Nonlinear Matrix Inequalities via Positive Semidefinite Matrix Completion, Mathematical Programming, 2011

Based on:

A. Griewank and Ph. Toint, On the existence of convex decompositions of partially separable functions, MPA 28, 1984

J. Agler, W. Helton, S. McCulough and L. Rodnan, Positive semidefinite matrices with a given sparsity pattern, LAA 107, 1988

See also:

L. Vandenberghe and M. Andersen, Chordal graphs and semidefinite optimization. Foundations and Trends in Optimization 1:241–433, 2015

Chordal decomposition

$G(N, E)$ – graph with $N = \{1, \dots, n\}$ and max. cliques $C_1, \dots, C_p$.

$$\mathbb{S}^n(E) = \{Y \in \mathbb{S}^n : Y_{ij} = 0 \ (i,j) \notin E \cup \{(\ell,\ell),\ \ell \in N\}$$

$$\mathbb{S}_+^{C_k} = \{Y \succeq 0 : Y_{ij} = 0 \text{ if } (i,j) \notin C_k \times C_k\}$$

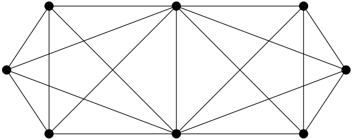
> Theorem 1: $G(N, E)$ is chordal if and only if
> for every $A \in \mathbb{S}^n(E)$, $A \succeq 0$, it holds that
> $\exists Y^k \in \mathbb{S}_+^{C_k}$ $(k = 1, \dots, p)$ s.t. $A = Y^1 + Y^2 + \dots + Y^p$.

Every psd matrix is a sum of psd matrices that are non-zero only on maximal cliques.

So constraint $A(x) \succeq 0$ replaced by:
find matrices $Y^k(x) \succeq 0$, $k = 1, \dots, p$ that sum up to A.

Graph representation of matrix sparsity

Chordal sparsity graph, overlapping blocks



$$\begin{bmatrix} \times & \times & \times & \times & \times & & & \\ \times & \times & \times & \times & \times & & 0 & \\ \times & \times & \times & \times & \times & & & \\ \times & \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times & \times \\ & & & \times & \times & \times & \times & \times \\ & 0 & & \times & \times & \times & \times & \times \\ & & & \times & \times & \times & \times & \times \end{bmatrix}$$

Chordal decomposition

Theorem 1: $G(N, E)$ is chordal if and only if
for every $A \in \mathbb{S}^n(E)$, $A \succeq 0$, it holds that
$\exists Y^k \in \mathbb{S}_+^{C_k}$ $(k = 1, \ldots, p)$ s.t. $A = Y^1 + Y^2 + \ldots + Y^p$.

Let $K = \begin{pmatrix} K_{1,1}^{(1)} & K_{1,2}^{(1)} & 0 \\ K_{2,1}^{(1)} & \boxed{K_{2,2}^{(1)} + K_{1,1}^{(2)}} & K_{1,2}^{(2)} \\ 0 & K_{2,1}^{(2)} & K_{2,2}^{(2)} \end{pmatrix}$ with $K^{(1)}, K^{(2)}$ dense.

Then $K \succeq 0 \Leftrightarrow K = Y^1 + Y^2$ such that

$$Y^1 = \begin{pmatrix} K_{1,1}^{(1)} & K_{1,2}^{(1)} & 0 \\ K_{2,1}^{(1)} & K_{2,2}^{(1)} + S & 0 \\ 0 & 0 & 0 \end{pmatrix} \succcurlyeq 0, \quad Y^2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & K_{2,2}^{(2)} - S & K_{1,2}^{(2)} \\ 0 & K_{2,1}^{(2)} & K_{2,2}^{(2)} \end{pmatrix} \succcurlyeq 0$$

Even if $K^{(1)}, K^{(2)}$ not dense, we just assume that S is dense.

Chordal decomposition

Let $A \in \mathbb{S}^n$, $n \geq 3$, with a sparsity graph $G = (N, E)$.
Let $N = \{1, 2, \ldots, n\}$ be partitioned into $p \geq 2$ overlapping sets

$$N = I_1 \cup I_2 \cup \ldots \cup I_p \,.$$

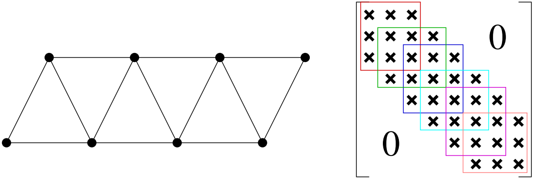
Define $I_{k,k+1} = I_k \cap I_{k+1} \neq \emptyset \,, \quad k = 1, \ldots, p-1 \,.$

Assume $A = \sum_{k=1}^{p} A_k$, with A_k only non-zero on I_k.

Corollary 1: $A \succeq 0$ if and only if
$\exists S_k \in \mathbb{S}^{I_{k,k+1}}, k = 1, \ldots, p-1$ s.t.
$A = \sum_{k=1}^{p} \widetilde{A}_k$ with $\widetilde{A}_k = A_k - S_{k-1} + S_k \quad (S_0 = S_p = [\,])$
and $\widetilde{A}_k \succeq 0$ $(k = 1, \ldots, p)$.

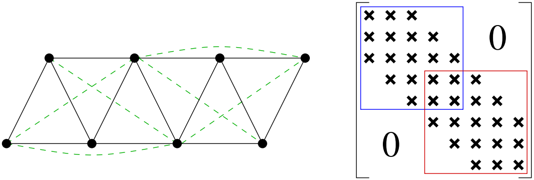
We can choose the partitioning $N = I_1 \cup I_2 \cup \ldots \cup I_p$!

Using the original theorem:



6 max. cliques of size 3, 5 additional 2×2 variables

Using the corollary:



2 “cliques” of size 5, 1 additional 2×2 variable

We can <u>choose</u> the partitioning $N = I_1 \cup I_2 \cup \ldots \cup I_p$!

When we know the sparsity structure of A, we can choose a "regular" partitioning.

Application: Topology optimization

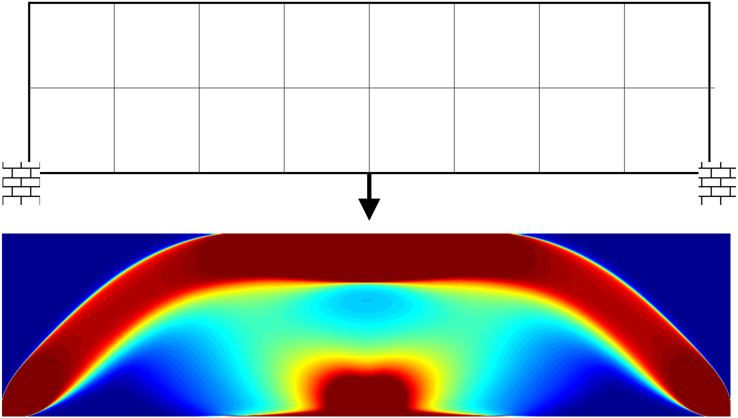
Aim:

Given an amount of material, boundary conditions and external load f, find the material distribution so that the body is as stiff as possible under f.

$E(x) = \rho(x) E_0$ with $0 \le \underline{\rho} \le \rho(x) \le \overline{\rho}$

E_0 a given (homogeneous, isotropic) material

Topology optimization, example



Pixels—finite elements

Color—value of variable ρ, constant on every element

Equilibrium

Equilibrium equation:

$$K(\rho)u = f, \qquad K(\rho) = \sum_{i=1}^{m} \rho_i K_i := \sum_{i=1}^{m} \sum_{j=1}^{G} B_{i,j} \rho_i E_0 B_{i,j}^\top$$

$$f := \sum_{i=1}^{m} f_i$$

Standard finite element discretization:

Quadrilateral elements

ρ... piece-wise constant

u... piece-wise bilinear (tri-linear)

TO primal formulation

$$\min_{\rho \in \mathbb{R}^m,\, u \in \mathbb{R}^n} f^T u$$

subject to

$$(0 \leq)\ \underline{\rho} \leq \rho_i \leq \overline{\rho}, \quad i = 1, \ldots, m$$

$$\sum_{i=1}^{m} \rho_i \leq 1$$

$$K(\rho)u = f$$

... large-scale nonlinear non-convex problem

SDP formulation of TO

The TO problem

$$\min_{\rho\in\mathbb{R}^m,\ u\in\mathbb{R}^n,\ \gamma\in\mathbb{R}} \gamma$$

subject to

$$f^T u \le \gamma, \quad K(\rho)u = f$$

$$\sum \rho_i \le 1, \quad \underline{\rho} \le \rho_i \le \overline{\rho}, \quad i = 1, \dots, m$$

can be equivalently formulated as a linear SDP:

$$\min_{\rho\in\mathbb{R}^m,\ \gamma\in\mathbb{R}} \gamma$$

subject to

$$\begin{pmatrix} \gamma & f^T \\ f & K(\rho) \end{pmatrix} \succeq 0 \qquad \text{(positive semidefinite)}$$

$$\sum \rho_i \le 1, \quad \underline{\rho} \le \rho_i \le \overline{\rho}, \quad i = 1, \dots, m.$$

Helpful when vibration/buckling constraints present

SDP formulation of TO

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SDP formulation of TO

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subject to

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Helpful when vibration/buckling constraints present

SDP formulation of TO by decomposition

Both

$$\begin{pmatrix} \gamma & f^T \\ f & \sum \rho_i K_i \end{pmatrix} \succeq 0$$

and

$$V(\hat{\lambda}; \rho) \succeq 0$$

are large matrix constraints dependent on many variables
…bad for existing SDP software

Can we replace them by several smaller constraints equivalently?

Chordal decomposition (recall)

Let $A \in \mathbb{S}^n$, $n \geq 3$, with a sparsity graph $G = (N, E)$.
Let $N = \{1, 2, \ldots, n\}$ be partitioned into $p \geq 2$ overlapping sets

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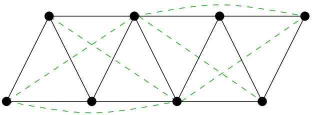
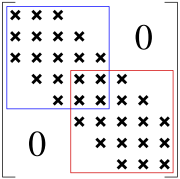
Using the corollary:





2 “cliques” of size 5, 1 additional 2×2 variable

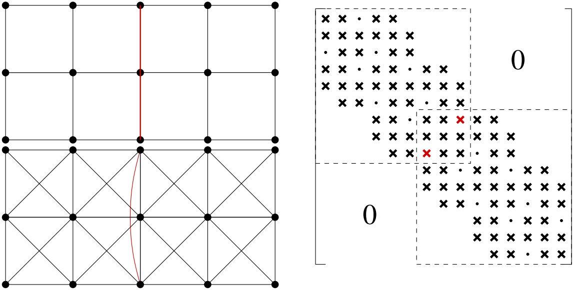
When we know the sparsity structure of A, we can choose a regular partitioning.

SDP formulation of TO by DD

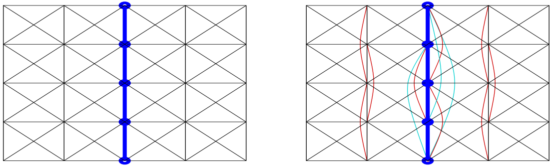
$$\begin{pmatrix} K(\rho) & f \\ f^\top & \gamma \end{pmatrix} \succeq 0 \qquad \text{and} \qquad V(\hat{\lambda};\rho) \succeq 0$$

are large matrix constraints dependent on many variables.

FE mesh, matrix $K(\rho)$ and its sparsity graph:



Chordal decomposition



$$\begin{pmatrix} K_{II}^{(1)} & K_{I\Gamma}^{(1)} & 0 & 0 \\ K_{\Gamma I}^{(1)} & K_{\Gamma\Gamma}^{(1)}+K_{\Gamma\Gamma}^{(2)} & K_{\Gamma I}^{(2)} & 0 \\ 0 & K_{I\Gamma}^{(2)} & K_{II}^{(2)} & f \\ 0 & 0 & f^\top & \gamma \end{pmatrix} = \begin{pmatrix} K_{II}^{(1)} & K_{I\Gamma}^{(1)} & 0 & 0 \\ K_{\Gamma I}^{(1)} & K_{\Gamma\Gamma}^{(1)}+S & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & K_{\Gamma\Gamma}^{(2)}-S & K_{\Gamma I}^{(2)} & 0 \\ 0 & K_{I\Gamma}^{(2)} & K_{II}^{(2)} & f \\ 0 & 0 & f^\top & \gamma \end{pmatrix}$$

Even though $K^{(1)}$ and $K^{(2)}$ are sparse, we need to assume that S is dense.

In this way, we can control the number and size of the maximal cliques and use the chordal decomposition theorem.

New result for arrow-type matrices: For the matrix inequality

$$\begin{pmatrix} K(\rho) & f \\ f^\top & \gamma \end{pmatrix} \succeq 0$$

the additional matrix variables S are rank-one; this further reduces the size of the solved SDP problem.

MK (2019): Decomposition of arrow type positive semidefinite matrices with application to topology optimization. arXiv:1911.09412

Numerical experiments

SDP codes tested: PENSDP, SeDuMi, SDPT3, Mosek

Results shown for Mosek: not the fastest for the original problem but has highest speedup

Mosek:
– version 8
– called from YALMIP
– difficult (for me) to control any options

Regular decomposition, 40x20 elements

Chordal decomposition

no of matrices	no of vars	size of matrix	no of iters	CPU total	CPU per iter	speedup total	speedup /iter
1	801	1681	69	1045	15	1	1
8	3523	243	58	31	0.53		
32	5489	73	44	9.7	0.22		
50	6376	51	46	8.8	0.19		
200	11243	19	37	6.9	0.19		
Arrow decomposition							
8	1032	243	70	28	0.40	37	38
32	1492	73	63	7.6	0.12	138	126
50	1764	51	64	7.1	0.11	147	137
200	3544	19	51	5.1	0.10	204	151
34	22997	11...260	42	301	7	3	2

Automatic decomposition using software SparseCoLO
by Kim, Kojima, Mevissen and Yamashita (2011)

Regular decomposition, 120x60 elements

Chordal decomposition

no of matr	no of vars	size of matrix	no of iters	CPU total	CPU per iter	speedup total	speedup /iter
1	7200	14641	139	1045932	7524	1	1
200	51539	99	60	236	3.9		
800	76977	33	50	129	2.6		
1800	106903	19	47	114	2.4		
Arrow decomposition							
200	12904	99	82	89	1.1	11752	6933
800	21764	33	71	37	0.52	28268	14439
1800	33424	19	65	42	0.65	24903	11645

estimated; 1045932 sec $\approx$ 6 days

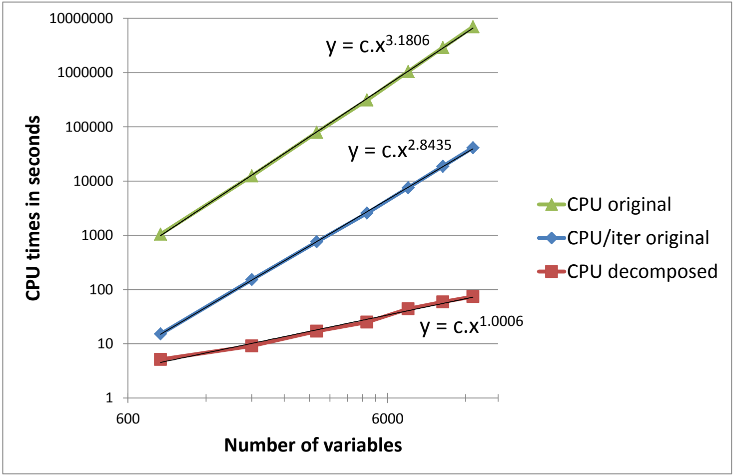
“Best” decomposition (subdomain = 4 elements)

Arrow decomposition

problem	ORIGINAL no of vars	ORIGINAL size of matrix	ORIGINAL CPU total	DECOMPOSED no of vars	DECOMPOSED size of matrix	DECOMPOSED CPU total	speedup
40×20	801	1681	1045	3544	19	5	204
60×30	1801	3721	12468	8164	19	9	1370
80×40	3201	6561	78813	14684	19	17	4636
100×50	5001	10201	312560	23104	19	25	12502
120×60	7201	14641	1045932	33424	19	42	24903
140×70	9801	19881	2900382	45664	19	59	49159
160×80	12801	25921	7003213	59764	19	74	94638
complexity $c\cdot\text{size}^q$			$q = 3.18$			$q = 1.0006$	

times estimated; 7003213 sec $\approx$ 81 days

CPU time, original versus decomposed



THE END