Polynomial optimization on finite sets.

Mauricio Velasco
Universidad Católica del Uruguay (UCU)

RECO2023
Pontificia Universidad Católica

LECTURE 2:
Sparsity in Sums of squares.

Outline

In this lecture we will discuss the proof of an exactness Theorem for the sum-of-squares hierarchy on the hypercube $\{-1, 1\}^n$. For notational simplicity, we state the result for n even.

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- The Theorem implies that $f_{\min} = f_{(\frac{n}{2}+1)}$ for every quadratic polynomial on the hypercube giving us an upper bound on the *exactness degree* for quadratic functions.
- This bound is better than the n from the previous lecture. It can be extended [Sakaue, Takeda, Kim, Ito (2017)] to f of any degree (see exercises).
- We will prove later that these upper bounds are in fact sharp.

Outline

- Recall that $\mathbb{R}[X] = \mathbb{R}[x_1, \ldots, x_n] / \left(x_j^2 - 1 : j = 1, \ldots, n \right)$ and that the square-free monomials $\chi_I := \prod_{j \in I} x_j$ form a **basis**.

Exercise

Prove that the square-free monomials $\{\chi_I : I \subseteq [n]\}$ for $I \subseteq [n]$ form an orthonormal basis of $\mathbb{R}[X]$ for the inner product

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$$\langle f, g \rangle := \frac{1}{|X|} \sum_{y \in X} f(y) g(y)$$

- A quadratic function f involves only a few of the 2^n elements of this basis

$$f = E_0 + \sum_{i=1}^{n} E_i x_i + \sum_{i<j} E_{ij} x_i x_j$$

and is therefore **sparse**.

Outline

The proofs of the (Fawzi, Parrilo, Saunderson) and (Sakaue, Takeda, Kim, Ito) Theorem leverage the sparsity of f to prove the existence of **sparse sum-of-square certificates** *for $f - \lambda$ (i.e. certificates $g = s_1^2 + \cdots + s_k^2$ where the s_i involve only a few basis elements).*

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The key tool for doing this will be the combinatorics of **chordal graphs**.

Organization:

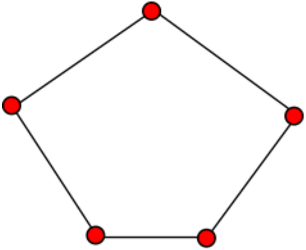
1. Preliminaries on Chordal graphs.
2. Chordality in SDP and sparsification tools for sum-of-squares.
3. Application to Sums-of-squares in the hypercube $\{-1, 1\}^4$.

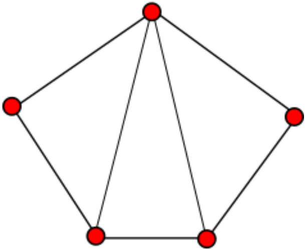
Part 1:
A primer on chordal graphs.

Chordal graphs

Definition.

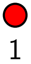
A graph G is chordal if every simple cycle in G of length at least 4 has at least one chord (i.e. an edge that "crosses" the cycle).





Theorem. (G.A. Dirac, 1961)

A graph G is chordal if and only if it is possible to totally order its vertices $v_1 < v_2 < \cdots < v_n$ so that for every $j = 1, \ldots n$ the set of neighbors of v_j which appear **before** *v_j induce a complete subgraph of G.*



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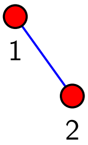

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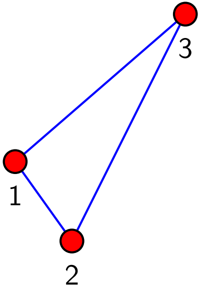

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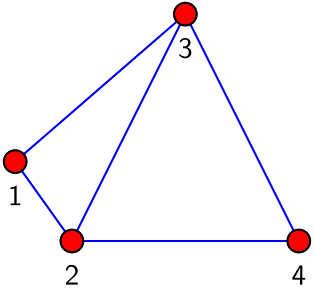

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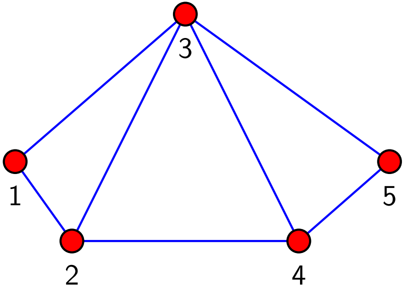

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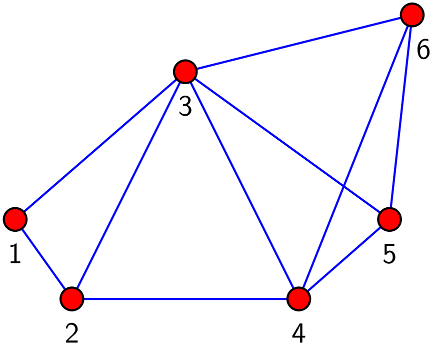

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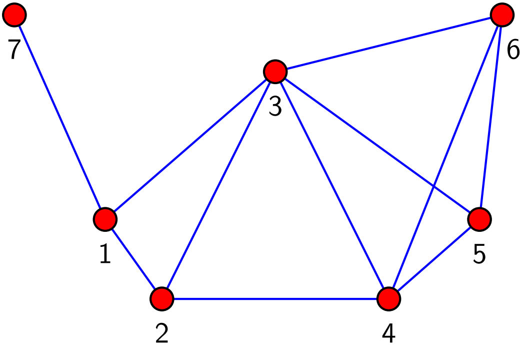
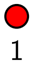


Chordal graphs

Chordal graphs are very useful objects. They appear in numerical linear algebra, semidefinite programming, algebraic geometry, etc. To a first approximation this follows from two facts:

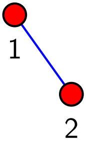
1. A perfect elimination ordering allows us to work with chordal graphs inductively very effectively. For instance several NP-hard problems admit efficient (polynomial or even linear time) solutions on chordal graphs.
2. Chordal graphs are a structured but very rich class. For example every graph is contained in some chordal graph.

Find the size $\omega(G)$ of the largest clique in G.



$\{1\}$

Find the size $\omega(G)$ of the largest clique in G.



$\{1, 2\}$

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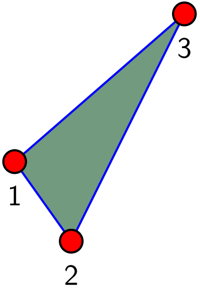

$\{1, 2, 3\}$

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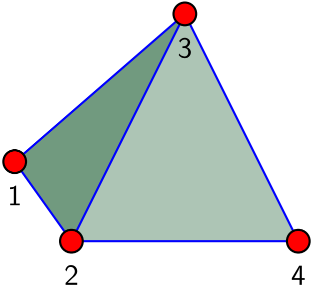

$\{1, 2, 3\}$ $\{2, 3, 4\}$

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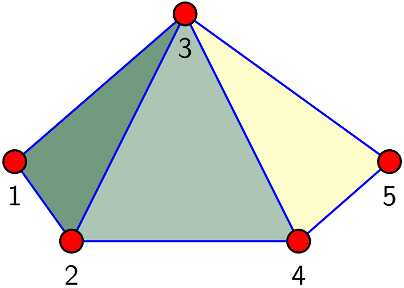

$\{1, 2, 3\}$ $\{2, 3, 4\}$ $\{3, 4, 5\}$

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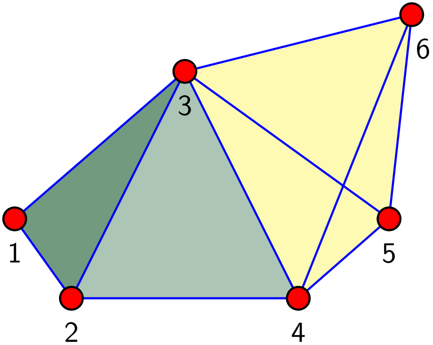
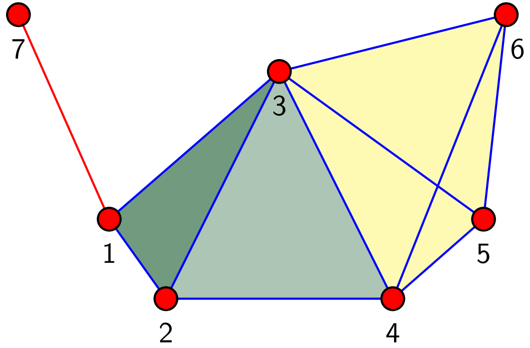


$\{1, 2, 3\}$ $\{2, 3, 4\}$ $\{3, 4, 5, 6\}$

Find the size $\omega(G)$ of the largest clique in G.



$\{1, 2, 3\}$ $\{2, 3, 4\}$ $\{3, 4, 5, 6\}$ $\{1, 7\}$

Part 2:
Chordality in SDP and sparsification tools for sums-of-squares.

Chordality in SDPs

Let A be a symmetric matrix in $\mathbb{R}^{n \times n}$.

Definition.

An (undirected, loopless) graph H with vertex set $[n]$ is an **admissible support graph** *for A if*

$$A_{ij} \neq 0 \text{ with } i \neq j \implies \{i,j\} \in E(H)$$

Example:

$$\begin{array}{c c} & \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array} & \begin{pmatrix} 2.2 & 1.1 & 0 & 1.1 \\ 1.1 & 2.2 & 1.1 & 0 \\ 0 & 1.1 & 2.2 & 1.1 \\ 1.1 & 0 & 1.1 & 2.2 \end{pmatrix} \end{array}$$

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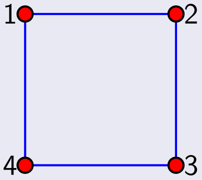

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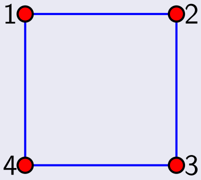

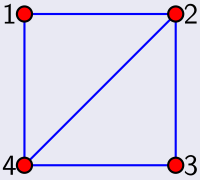

Let A be a symmetric matrix and H a support graph for A.

Theorem. (Grone and Johnson, 1984)

Assume H is a chordal graph and let $C_1, \dots, C_L \subseteq [n]$ be its collection of maximal cliques. The matrix $A \succeq 0$ if and only if there exist PSD matrices $B_1, \dots, B_L$ with $(B_j)_{s,t} = 0$ outside the edges of C_j such that

$$A = B_1 + \cdots + B_L$$

Remark.

The Lemma is very useful computationally because it transforms the large semidefinite constraint $A \succeq 0$ into several small semidefinite constraints $B_1 \succeq 0$,..., $B_L \succeq 0$.

Example:

Is the following matrix $A \succeq 0$?

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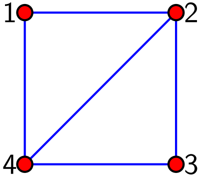

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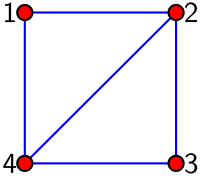

The chordal cover has cliques $\{1, 2, 4\}$ and $\{2, 3, 4\}$. so

$$A = \begin{pmatrix} a & b & 0 & f \\ b & d & 0 & e \\ 0 & 0 & 0 & 0 \\ f & e & 0 & g \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \alpha & \beta & \phi \\ 0 & \beta & \delta & \epsilon \\ 0 & \phi & \epsilon & \iota \end{pmatrix}$$

where both matrices are really 3×3 PSD.

Chordal sparsification of sums-of-squares:

Let X be finite. Assume $\chi_1, \ldots, \chi_N$ is a basis for $\mathbb{R}[X]$ and let $\vec{\chi} := (\chi_1, \ldots, \chi_N)$.

Corollary.

Assume $f = \vec{\chi}^t A \vec{\chi}$ for some $A \succeq 0$ with support H.

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Corollary.

Assume $f = \vec{\chi}^t A \vec{\chi}$ for some $A \succeq 0$ with support H. If $C_1, \ldots, C_L$ are the maximal cliques of any chordal cover of H then f admits a sum-of-squares representation

$$f = t_1 + \cdots + t_L$$

with sum-of-square summands $t_i \in \Sigma_{\langle \{\chi_j : j \in C_j\} \rangle}$

Proof.

By Grone and Johnson if $A \succeq 0$ has sparsity graph H then $A = B_1 + \cdots + B_L$ so $\vec{\chi}^t A \vec{\chi} = \vec{\chi}^t B_1 \vec{\chi} + \cdots + \vec{\chi}^t B_L \vec{\chi}$. □

Shift sparsification of sums-of-squares:

Assume X is a finite set. We can also **shift the support** as follows,

Lemma.

Suppose $h \in \mathbb{R}[X]$ satisfies $h^2 = 1$ and let $V, W \subseteq \mathbb{R}[X]$ be subspaces. If $hV \subseteq W$ then $\Sigma_V \subseteq \Sigma_W$

Proof.

For any $v \in V$ there is $w \in W$ such that $hv = w$. Squaring we get

$$w^2 = (hv)^2 = h^2 v^2 = v^2$$

summing over the v's we conclude $\Sigma_V \subseteq \Sigma_W$ □

Remark.

In particular the inclusion $\Sigma_V + \Sigma_W \subseteq \Sigma_W$ holds.

Part 3:

Application: Sparsification in the hypercube $X := \{-1, 1\}^n$.

Suppose $f \in \mathbb{R}[X]_{\leq 2}$ is nonnegative in $X = \{-1, 1\}^n$.

How to find an **initial** *sum-of-squares representation in the square-free monomial basis* $\{\chi_I : I \subseteq [n]\}$*?*

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How to find an **initial** *sum-of-squares representation in the square-free monomial basis* $\{\chi_I : I \subseteq [n]\}$*?*

- Since $f \geq 0$ we can write an **initial sum-of-squares representation** of g in the Lagrange interpolation basis $f = \sum_{y \in X} f(y) p_y^2$, that is $f = \vec{p}^t D \vec{p}$ for a nonnegative diagonal matrix D.

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- The basis $\{\chi_I : I \subseteq [n]\}$ is **orthonormal** so we can explicitly write the Lagrange interpolation functions as

$$p_z = \sum_{I \subseteq [n]} \frac{\chi_I(z)}{|G|} \chi_I \text{ for } z \in X \text{, obtaining } \vec{p} = V \vec{\chi}$$

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- Replacing the second expression in the first we obtain

$$f = \vec{\chi}^t A \vec{\chi} \text{ where } A = V^t D V \text{ is PSD.}$$

It follows that $A_{\chi_I, \chi_J} := \langle f, \chi_I \chi_J \rangle$.

Exercise

Prove that if $A_{\chi_I,\chi_J} := \langle f, \chi_I \chi_J \rangle$ *then* A *is PSD and* $f = \vec{\chi}^t A \chi$.

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Now suppose that $f = E_0 + \sum_{i=1}^{n} E_i x_i + \sum_{i<j} E_{ij} x_i x_j$. We will find a support graph for f.

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- The equality $\chi_I \chi_J = \chi_{I \triangle J}$ holds in $\mathbb{R}[X]$, where $I \triangle J$ denotes the symmetric difference $I \setminus J \cup J \setminus I$.

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$$\chi_{123}\chi_{134} = x_1 x_2 x_3 x_1 x_3 x_4 = x_2 x_4 = \chi_{123 \triangle 134}$$

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$$\chi_{123}\chi_{134} = x_1 x_2 x_3 x_1 x_3 x_4 = x_2 x_4 = \chi_{123 \triangle 134}$$

- We conclude that $A_{\chi_I,\chi_J} \neq 0$ is equivalent to

$$\langle f, \chi_I \chi_J \rangle = \langle f, \chi_{I \triangle J} \rangle \neq 0$$

which, by orthonormality of the χ_I, is equivalent to $I \Delta J$ appearing in f.

Support graph

Our initial support graph for $f \in \mathbb{R}[X]_{\leq 2}$ can be now be constructed

Definition.

Let H be the graph with vertices $\{\chi_I : I \subseteq [n]\}$ and

$$\{\chi_I, \chi_J\} \in E(H) \iff |I \triangle J| \in \{0, 1, 2\}$$

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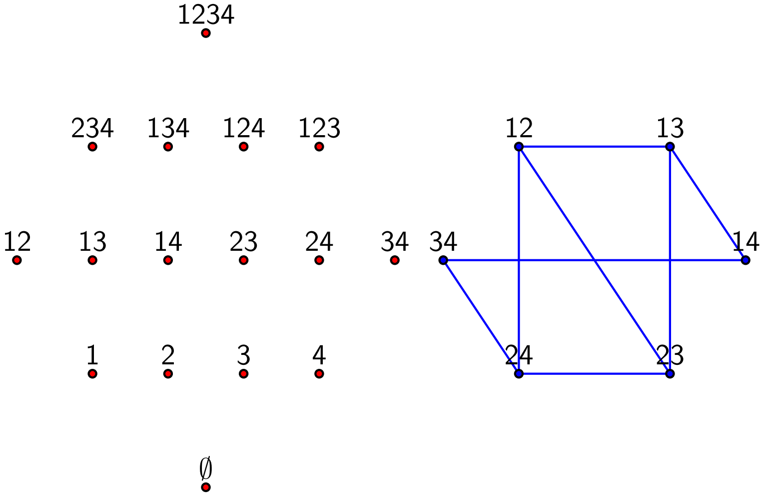
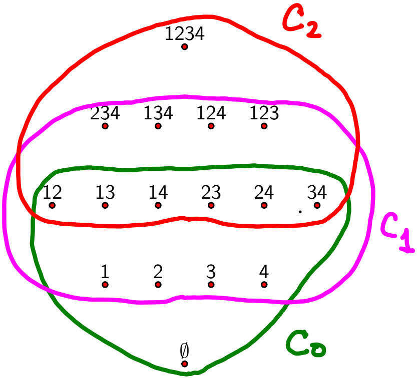
During the lecture we will focus on $n = 4$.

Support graph for $n = 4$



A chordal cover:



The cliques are C_0, C_1, C_2 and $\chi_{1234} C_2 \subseteq C_0$.

We have thus proven...

Theorem. (Fawzi, Saunderson, Parrilo for $n = 4$)

If $f \in \mathbb{R}[X]_{\leq 2}$ is nonnegative then $f = t_0 + t_1$ with $t_0 \in \Sigma_{C_0}$ and $t_1 \in \Sigma_{C_1}$. In particular f is expressible as a sum of squares of functions of degree at most $3 = n/2 + 1$.

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Exercise

Prove that if $f \in \mathbb{R}[X]_{\leq d}$ is nonnegative and n is even then f can be written as a sum of squares of elements of $\mathbb{R}[X]_{\leq \frac{n+d}{2}}$.

A wider context...

The Theorem of Grone and Johnson can be understood as saying that the cones P_Z of **nonnegative quadratic forms** and Σ_Z of **sums-of-squares of linear forms** coincide on some special projective varieties Z.

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More specifically, for a graph H let

$$Z_H = V\left(x_i x_j : \{i,j\} \notin E(H)\right) \subseteq \mathbb{R}^n$$

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Question.

How to use all these other varieties in optimization?