

Exploiting Sparsity in Sums of Squares of Polynomials

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Outline

1. Sums of squares of polynomials
2. Previous work
3. Representation of a nonnegative polynomial as a sum of squares
4. Numerical experiment
5. Concluding remarks

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Given a nonnegative polynomial $f(x)$ in $x = (x_1, x_2, \dots, x_n) \in \mathbb{R}^n$, represent $f(x)$ in terms of SOS (a sum of squares of polynomials) such that

$$f(x) = \sum_{i=1}^k (g^i(x))^2,$$

where k and polynomials $g^i(x)$ ($i = 1, 2, \dots, k$) are unknown.

Two issues

- Is such a representation possible? \Rightarrow Hilbert

$$\text{SOS} \subset \oplus\text{Pol} \text{ and } \text{SOS} \neq \oplus\text{Pol}$$

Here

SOS : the set of sums of squares of polynomials

$\oplus\text{Pol}$: the set of nonnegative polynomials

- **Computation** \Rightarrow SDP (Semidefinite Program).

- SDP relaxation of polynomial optimization problems. Lasserre '01
- SOS optimization. Parrilo '03
- Global optimization of rational functions. de Klerk ISMP2003.

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where k and polynomials $g^i(x)$ ($i = 1, 2, \dots, k$) are unknown.

How do we compute such a representation?

Step 1. Choose “a suitable common support” for unknown polynomials $g^i(x)$ ($i = 1, 2, \dots, k$).

Step 2. Convert the problem into an LMI (Linear Matrix Inequality) or an SDP (Semidefinite Program).

Step 3. Solve the LMI or the SDP.

- A suitable common support chosen in Step 1 determines the size of the LMI or the SDP to be solved in Step 3.



For numerical efficiency in Step 3, we want to choose a smaller support in Step 1.

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Notation and symbols

For $\forall x = (x_1, x_2, \dots, x_n) \in \mathbb{R}^n$ and $\forall \alpha = (\alpha_1, \alpha_2, \dots, \alpha_n) \in \mathbb{Z}_+^n$, define

$$\text{a monomial } x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_n^{\alpha_n}.$$

Then we can write a polynomial $f(x)$ in $x \in \mathbb{R}^n$ as

$$f(x) = \sum_{\alpha \in \mathcal{F}} c_\alpha x^\alpha$$

for some nonempty finite subset $\mathcal{F} \subset \mathbb{Z}_+^n$ (**a support** of $f(x)$) and $c_\alpha \in \mathbb{R}$ ($\alpha \in \mathcal{F}$).

We assume that $f(x)$ is represented as SOS such that

$$f(x) = \sum_{i=1}^k (g^i(x))^2, \quad g^i(x) = \sum_{\alpha \in \mathcal{G}} v_\alpha^i x^\alpha.$$

Here a positive number k , a common support $\mathcal{G} \subset \mathbb{Z}_+^n$ of polynomials $g^i(x)$ ($i = 1, 2, \dots, k$) and the polynomials are unknown.

Let

$$\mathcal{F}^e \equiv \{\alpha \in \mathcal{F} : \alpha_j \text{ is even } (j = 1, 2, \dots, n)\},$$
$$\mathcal{G}^0 \equiv (\text{convex hull of } \{\frac{\alpha}{2} : \alpha \in \mathcal{F}^e\}) \cap \mathbb{Z}_+^n.$$

$$f(x) = \sum_{\alpha \in \mathcal{F}} c_{\alpha} x^{\alpha} = \sum_{i=1}^k (g^i(x))^2, \quad g^i(x) = \sum_{\alpha \in \mathcal{G}} v_{\alpha}^i x^{\alpha},$$
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$$\text{Example: } f(x) = 2 - 4x_1^3x_2^4 + 2x_1^4x_2^3 + 5x_1^6x_2^8 - 2x_1^7x_2^7 + 2x_1^8x_2^6.$$

$$\left. \begin{aligned} \mathcal{F} &= \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 3 \\ 4 \end{pmatrix}, \begin{pmatrix} 4 \\ 3 \end{pmatrix}, \begin{pmatrix} 6 \\ 8 \end{pmatrix}, \begin{pmatrix} 7 \\ 7 \end{pmatrix}, \begin{pmatrix} 8 \\ 6 \end{pmatrix} \right\} \\ \mathcal{F}^e &= \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 6 \\ 8 \end{pmatrix}, \begin{pmatrix} 8 \\ 6 \end{pmatrix} \right\} \\ \mathcal{G}^0 &= \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 2 \\ 2 \end{pmatrix}, \begin{pmatrix} 3 \\ 3 \end{pmatrix}, \begin{pmatrix} 3 \\ 4 \end{pmatrix}, \begin{pmatrix} 4 \\ 3 \end{pmatrix} \right\} \end{aligned} \right\}$$

In this example, we can represent $f(x)$ as a sum of squares of polynomials with the support \mathcal{G}^0 ;

$$f(x) = \sum_{\alpha \in \mathcal{F}} c_{\alpha} x^{\alpha} = \sum_{i=1}^k (g^i(x))^2, \quad g^i(x) = \sum_{\alpha \in \mathcal{G}^0} v_{\alpha}^i x^{\alpha}$$

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Theorem 1 of Reznick '78.

$$v_{\alpha}^i = 0 \quad (i = 1, 2, \dots, k) \text{ if } \alpha \notin \mathcal{G}^0.$$

- Therefore we can take \mathcal{G}^0 for a common support of unknown polynomials $g^i(x)$ ($i = 1, 2, \dots, k$);

$$f(x) = \sum_{\alpha \in \mathcal{F}} c_{\alpha} x^{\alpha} = \sum_{i=1}^k (g^i(x))^2, \quad g^i(x) = \sum_{\alpha \in \mathcal{G}^0} v_{\alpha}^i x^{\alpha}$$

- Computation of \mathcal{G}^0 — — — discussed later.
- How can we reduce \mathcal{G}^0 further?

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$$\mathcal{G}^0 \equiv (\text{convex hull of } \{\frac{\alpha}{2} : \alpha \in \mathcal{F}^e\}) \cap \mathbb{Z}_+^n \supset \mathcal{G}.$$

Theorem 1. (Choi-Lam-Reznick '95) Suppose that

$$\beta \in \mathcal{G}, \quad 2\beta \notin \mathcal{F}^e \quad \text{and} \quad 2\beta \notin (\mathcal{G} + \mathcal{G} \setminus \{\beta\}) \quad \text{--- (1)}$$

Then $v_\beta^i = 0, \forall i \in \{1, 2, \dots, k\}$ and $f(x) = \sum_{i=1}^k \left(\sum_{\alpha \in \mathcal{G} \setminus \{\beta\}} v_\alpha^i x^\alpha \right)^2$.

Idea of Proof: We see from (*) that

$$\begin{aligned} \sum_{\alpha \in \mathcal{F}} c_\alpha x^\alpha &= \sum_{i=1}^k \left(\sum_{\alpha \in \mathcal{G}} v_\alpha^i x^\alpha \right)^2 = \sum_{i=1}^k \left(v_\beta^i x^\beta + \sum_{\alpha \in \mathcal{G} \setminus \{\beta\}} v_\alpha^i x^\alpha \right)^2 \\ &= \left(\sum_{i=1}^k (v_\beta^i)^2 \right) x^{2\beta} + \sum_{i=1}^k \left(\sum_{\alpha \in \mathcal{G}} \sum_{\gamma \in \mathcal{G} \setminus \{\beta\}} \tilde{v}_\alpha^i v_\gamma^i x^{\alpha+\gamma} \right). \end{aligned}$$

Here $\tilde{v}_\alpha^i = 2v_\alpha^i$ if $\alpha = \beta$ and $\tilde{v}_\alpha^i = v_\alpha^i$ otherwise.

$$f(x) = \sum_{\alpha \in \mathcal{F}} c_{\alpha} x^{\alpha} = \sum_{i=1}^k (g^i(x))^2, \quad g^i(x) = \sum_{\alpha \in \mathcal{G}} v_{\alpha}^i x^{\alpha} \quad \text{--- (*)}$$

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Example: $f(x) = 2 - 4x_1^3x_2^4 + 2x_1^4x_2^3 + 5x_1^6x_2^8 - 2x_1^7x_2^7 + 2x_1^8x_2^6$.

$$\mathcal{F}^e = \left\{ \begin{array}{l} \left(\begin{array}{c} 0 \\ 0 \end{array} \right), \left(\begin{array}{c} 6 \\ 8 \end{array} \right), \left(\begin{array}{c} 8 \\ 6 \end{array} \right) \end{array} \right\},$$

$$\mathcal{G}^0 = \left\{ \begin{array}{l} \left(\begin{array}{c} 0 \\ 0 \end{array} \right), \left(\begin{array}{c} 1 \\ 1 \end{array} \right), \left(\begin{array}{c} 2 \\ 2 \end{array} \right), \left(\begin{array}{c} 3 \\ 3 \end{array} \right), \left(\begin{array}{c} 3 \\ 4 \end{array} \right), \left(\begin{array}{c} 4 \\ 3 \end{array} \right) \end{array} \right\}$$

Let $\beta = \left(\begin{array}{c} 3 \\ 3 \end{array} \right)$. Then $2\beta = \left(\begin{array}{c} 6 \\ 6 \end{array} \right) \notin \mathcal{F}^e$ and $2\beta \notin (\mathcal{G}^0 + \mathcal{G}^0 \setminus \{\beta\})$.

Hence we can eliminate $\left(\begin{array}{c} 3 \\ 3 \end{array} \right)$.

$$f(x) = \sum_{\alpha \in \mathcal{F}} c_\alpha x^\alpha = \sum_{i=1}^k (g^i(x))^2, \quad g^i(x) = \sum_{\alpha \in \mathcal{G}} v_\alpha^i x^\alpha \quad \text{--- (*)}$$

$$\mathcal{F}^e \equiv \{\alpha \in \mathcal{F} : \alpha_j \text{ is even } (j = 1, 2, \dots, n)\}$$

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$$\beta \in \mathcal{G}, \quad 2\beta \notin \mathcal{F}^e \quad \text{and} \quad 2\beta \notin (\mathcal{G} + \mathcal{G} \setminus \{\beta\}) \quad \text{--- (1)}$$

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Example: $f(x) = 2 - 4x_1^3x_2^4 + 2x_1^4x_2^3 + 5x_1^6x_2^8 - 2x_1^7x_2^7 + 2x_1^8x_2^6$.

$$\left. \begin{aligned} \mathcal{F}^e &= \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 6 \\ 8 \end{pmatrix}, \begin{pmatrix} 8 \\ 6 \end{pmatrix} \right\}, \\ \mathcal{G}^1 &= \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 2 \\ 2 \end{pmatrix}, \begin{pmatrix} 3 \\ 3 \end{pmatrix}, \begin{pmatrix} 3 \\ 4 \end{pmatrix}, \begin{pmatrix} 4 \\ 3 \end{pmatrix} \right\} \end{aligned} \right\}$$

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Let $2\beta = \left(\begin{array}{c} 2 \\ 2 \end{array} \right)$. Then $2\beta = \left(\begin{array}{c} 4 \\ 4 \end{array} \right) \notin \mathcal{F}^e$ and $2\beta \notin (\mathcal{G}^1 + \mathcal{G}^1 \setminus \{\beta\})$.

Hence we can eliminate $\left(\begin{array}{c} 2 \\ 2 \end{array} \right)$.

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$$\mathcal{F}^e \equiv \{\alpha \in \mathcal{F} : \alpha_j \text{ is even } (j = 1, 2, \dots, n)\}$$

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Example: $f(x) = 2 - 4x_1^3x_2^4 + 2x_1^4x_2^3 + 5x_1^6x_2^8 - 2x_1^7x_2^7 + 2x_1^8x_2^6$.

$$\mathcal{F}^e = \left\{ \begin{array}{l} \left(\begin{array}{l} 0 \\ 0 \end{array} \right), \left(\begin{array}{l} 6 \\ 8 \end{array} \right), \left(\begin{array}{l} 8 \\ 6 \end{array} \right) \\ \left(\begin{array}{l} 0 \\ 0 \end{array} \right), \left(\begin{array}{l} 1 \\ 1 \end{array} \right), \left(\begin{array}{l} 2 \\ 2 \end{array} \right), \left(\begin{array}{l} 3 \\ 3 \end{array} \right), \left(\begin{array}{l} 3 \\ 4 \end{array} \right), \left(\begin{array}{l} 4 \\ 3 \end{array} \right) \end{array} \right\}$$

$$f(x) = \sum_{\alpha \in \mathcal{F}} c_\alpha x^\alpha = \sum_{i=1}^k (g^i(x))^2, \quad g^i(x) = \sum_{\alpha \in \mathcal{G}} v_\alpha^i x^\alpha \quad \text{--- (*)}$$

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Then $v_\beta^i = 0, \forall i \in \{1, 2, \dots, k\}$ and $f(x) = \sum_{i=1}^k \left(\sum_{\alpha \in \mathcal{G} \setminus \{\beta\}} v_\alpha^i x^\alpha \right)^2$.

Example: $f(x) = 2 - 4x_1^3x_2^4 + 2x_1^4x_2^3 + 5x_1^6x_2^8 - 2x_1^7x_2^7 + 2x_1^8x_2^6$.

$$\left. \begin{aligned} \mathcal{F}^e &= \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 6 \\ 8 \end{pmatrix}, \begin{pmatrix} 8 \\ 6 \end{pmatrix} \right\}, \\ \mathcal{G}^2 &= \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 2 \\ 2 \end{pmatrix}, \begin{pmatrix} 3 \\ 3 \end{pmatrix}, \begin{pmatrix} 3 \\ 4 \end{pmatrix}, \begin{pmatrix} 4 \\ 3 \end{pmatrix} \right\} \end{aligned} \right\}$$

Similarly we can eliminate $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

$$f(x) = \sum_{\alpha \in \mathcal{F}} c_\alpha x^\alpha = \sum_{i=1}^k (g^i(x))^2, \quad g^i(x) = \sum_{\alpha \in \mathcal{G}} v_\alpha^i x^\alpha \quad \text{--- (*)}$$

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$$\mathcal{G}^* = \left\{ \begin{array}{l} \left(\begin{array}{c} 0 \\ 0 \end{array} \right), \left(\begin{array}{c} 1 \\ 1 \end{array} \right), \left(\begin{array}{c} 2 \\ 2 \end{array} \right), \left(\begin{array}{c} 3 \\ 3 \end{array} \right), \left(\begin{array}{c} 3 \\ 4 \end{array} \right), \left(\begin{array}{c} 4 \\ 3 \end{array} \right) \end{array} \right\}$$

Now we can not reduce \mathcal{G}^* by applying Theorem 1, and we obtain “the minimal support” in this case.

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\implies Find a 3×3 $V \succeq O$ such that

$$f(x) = \left(x^{(0 \ 0)}, x^{(3 \ 4)}, x^{(4 \ 3)} \right) V \left(x^{(0 \ 0)}, x^{(3 \ 4)}, x^{(4 \ 3)} \right)^T \quad \text{for } \forall x \in \mathbb{R}^2$$

\implies Find a 3×3 $V \succeq O$ such that

$$2 = V_{11}, \quad -4 = V_{12} + V_{21}, \quad 2 = V_{13} + V_{31}, \quad 5 = V_{22}, \quad \dots$$

$$f(x) = \sum_{\alpha \in \mathcal{F}} c_\alpha x^\alpha = \sum_{i=1}^k (g^i(x))^2, \quad g^i(x) = \sum_{\alpha \in \mathcal{G}} v_\alpha^i x^\alpha \quad \text{--- (*)}$$

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Then $v_\beta^i = 0, \forall i \in \{1, 2, \dots, k\}$ and $f(x) = \sum_{i=1}^k \left(\sum_{\alpha \in \mathcal{G} \setminus \{\beta\}} v_\alpha^i x^\alpha \right)^2$.

Define the class Γ of suitable supports of $g^i(x)$ recursively by

1. $\mathcal{G}^0 \in \Gamma$.

2. If $\mathcal{G} \in \Gamma$ and (1) holds then $\Gamma = \{\mathcal{G} \setminus \{\beta\}\} \cup \Gamma$.

Theorem 2 (Main result)

(a) Γ is closed under intersection; if $\mathcal{G}, \mathcal{G}' \in \Gamma$ then $\mathcal{G} \cap \mathcal{G}' \in \Gamma$.

(b) The smallest element $\mathcal{G}^* \in \Gamma$ exists; $\mathcal{G}^* \subset \mathcal{G}$ for $\forall \mathcal{G} \in \Gamma$.

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$$f(x) = \sum_{\alpha \in \mathcal{F}} c_{\alpha} x^{\alpha} = \sum_{i=1}^k (g^i(x))^2, \quad g^i(x) = \sum_{\alpha \in \mathcal{G}} v_{\alpha}^i x^{\alpha}$$

$$\mathcal{F}^e = \{\alpha \in \mathcal{F} : \alpha_j \text{ is even } (j = 1, 2, \dots, n)\}$$

$$\mathcal{G}^0 = (\text{convex hull of } \{\frac{\alpha}{2} : \alpha \in \mathcal{F}^e\}) \cap \mathbb{Z}_+^n \supset \mathcal{G}.$$

The class Γ of suitable supports for $g^i(x)$: Let $\mathcal{G}_0 \in \Gamma$. If “ $\mathcal{G} \in \Gamma$, $2\beta \notin \mathcal{F}^e$ and $2\beta \notin (\mathcal{G} + \mathcal{G} \setminus \{\beta\})$.” — (1) holds then $\mathcal{G} \setminus \{\beta\} \in \Gamma$.

Phase 1: Computation of \mathcal{G}^0

Phase 2: Let $\mathcal{G} = \mathcal{G}^0$. While (1) holds do $\mathcal{G} = \mathcal{G} \setminus \{\beta\}$. Then we obtain a minimal element of Γ , which coincides with the smallest element \mathcal{G}^* .

- Both Phases 1 and 2 are interesting combinatorial enumeration.
- Phase 1
 - (a) Convex hull representation of a polytope — our case
 - (b) Inequality (or facet) representation of a polytope
 - (1) Use cdd(Fukuda) to get (b) from (a). Apply LattE(Loera) to (b).
 - (2) Apply a method (Barvinok-Pommersheim '99) directly to (a).
 - (3) A new practical method?
- Simple methods for Phases 1 and 2 in our numerical experiment.

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Test problems: $f(x) = \sum_{i=1}^k (x^{\alpha^i} + x^{\beta^i})^2$, where $\alpha^i, \beta^i \in \mathbb{Z}_+^n$: random.

An example: $n = 5, k = 8, \#\mathcal{F}^e = 16$:

$$\mathcal{F}^e = \{ (0\ 6\ 4\ 0\ 0), (4\ 4\ 0\ 0\ 4), (6\ 2\ 2\ 0\ 4), (0\ 8\ 0\ 4\ 4), \\ (2\ 6\ 2\ 6\ 0), (6\ 0\ 4\ 4\ 4), (2\ 2\ 8\ 0\ 6), (10\ 4\ 4\ 0\ 0), \\ (4\ 8\ 2\ 4\ 2), (0\ 4\ 4\ 8\ 4), (4\ 0\ 4\ 2\ 10), (10\ 6\ 0\ 2\ 4), \\ (4\ 2\ 6\ 2\ 8), (8\ 6\ 6\ 2\ 2), (8\ 6\ 4\ 2\ 6), (8\ 10\ 12\ 4\ 10) \}$$

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Numerical results 4 randomly generated problems with $n = 5$

$k = 3, \#\mathcal{F}^e = 6$			$k = 4, \#\mathcal{F}^e = 8$			$k = 8, \#\mathcal{F}^e = 16$		
#facet	$\#\mathcal{G}^0$	$\#\mathcal{G}^*$	#facet	$\#\mathcal{G}^0$	$\#\mathcal{G}^*$	#facet	$\#\mathcal{G}^0$	$\#\mathcal{G}^*$
6	6	6	16	16	10	94	116	25
6	6	6	20	12	8	98	152	37
12	11	7	30	14	11	124	116	23
6	7	6	18	13	8	76	164	92

#facet = the number of facets of (convex hull of $\{\frac{\alpha}{2} : \alpha \in \mathcal{F}^e\}$)

$$f(x) = \sum_{\alpha \in \mathcal{F}} c_{\alpha} x^{\alpha} = \sum_{i=1}^k (g^i(x))^2, \quad g^i(x) = \sum_{\alpha \in \mathcal{G}} v_{\alpha}^i x^{\alpha}$$

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Numerical results 4 randomly generated problems with $n = 10$

$k = 10, \#\mathcal{F}^e = 20$			$k = 12, \#\mathcal{F}^e = 24$			$k = 15, \#\mathcal{F}^e = 30$		
#facet	$\#\mathcal{G}^0$	$\#\mathcal{G}^*$	#facet	$\#\mathcal{G}^0$	$\#\mathcal{G}^*$	#facet	$\#\mathcal{G}^0$	$\#\mathcal{G}^*$
2330	186	20	6049	856	25	17760	248	31
2190	93	20	5981	193	24	17368	97	32
1906	175	20	5357	456	26	15688	192	32
2081	81	21	5748	295	25	14786	118	30

#facet = the number of facets of (convex hull of $\{\frac{\alpha}{2} : \alpha \in \mathcal{F}^e\}$)

$$f(x) = \sum_{\alpha \in \mathcal{F}} c_\alpha x^\alpha = \sum_{i=1}^k (g^i(x))^2, \quad g^i(x) = \sum_{\alpha \in \mathcal{G}} v_\alpha^i x^\alpha$$

$$\mathcal{F}^e = \{\alpha \in \mathcal{F} : \alpha_j \text{ is even } (j = 1, 2, \dots, n)\}$$

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Phase 2: Let $\mathcal{G} = \mathcal{G}^0$. While (1) holds do $\mathcal{G} = \mathcal{G} \setminus \{\beta\}$. Then we obtain a minimal element of Γ , which coincides with the smallest element \mathcal{G}^* .

6. Concluding remarks

- (a) The computation of \mathcal{G}^0 is necessary in representation of sums of squares of polynomials. This is a hard combinatorial optimization problem.
- (b) The smallest element $\mathcal{G}^* \in \Gamma$ gives numerical efficiency to representation of sums of squares of polynomials. But the efficiency depends on the structure and the sparsity of \mathcal{F}^e .