AN ALGORITHM FOR SUMS OF SQUARES OF REAL POLYNOMIALS

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Introduction

We present an algorithm to determine if a real polynomial is a sum of squares (of polynomials), and to find an explicit representation if it is a sum of squares. This algorithm uses the fact that a sum of squares representation of a real polynomial corresponds to a real, symmetric, positive semi-definite matrix whose entries satisfy certain linear equations.

Sums of squares and Gram matrices

We fix n and use the following notation in $R := \mathbb{R}[x_1, \dots, x_n]$: For $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}_0^n$, let x^α denote $x_1^{\alpha_1} \cdot \ldots \cdot x_n^{\alpha_n}$. For $m \in \mathbb{N}_0$, set $\Lambda_m := \{(\alpha_1, \dots, \alpha_n) \in \mathbb{N}_0^n \mid \alpha_1 + \dots + \alpha_n \leq m\}$. Then $f \in R$ of degree m can be written $f = \sum_{\alpha \in \Lambda_m} a_\alpha x^\alpha$. We say f is **sos** if f is a sum of squares of elements in R.

Suppose f is sos, say f is a sum of t squares in R, then f must have even degree, say $2m$. Thus $f = \sum_{i=1}^t h_i^2$, where each h_i has degree $\leq m$. Suppose $|\Lambda_m| = k$, then we order the elements of Λ_m in some way: $\Lambda_m = \{\beta_1, \dots, \beta_k\}$. Set $\bar{x} := (x^{\beta_1}, \dots, x^{\beta_k})$ and let A be the $k \times t$ matrix with ith column the coefficients of h_i. Then the equation $f = \sum h_i^2$ can be written

t summands

$$f = \bar{x} \cdot (AA^T) \cdot \bar{x}^T.$$

k monomials

The symmetric $k \times k$ matrix $B := AA^T$ is sometimes called a **Gram matrix** of f (associated to the h_i's). Note that B is psd (= "positive semi-definite"), i.e., $\bar{y} \cdot B \cdot \bar{y}^T \geq 0$ for all $\bar{y} = (y_1, \dots, y_k) \in \mathbb{R}^k$.

The following theorem, in a different form, can be found in [CLR]. However we include the theorem and its proof for the convenience of the reader.

Theorem 1. *Suppose $f \in R$ is of degree $2m$ and $\bar{x}$ is as above. Then f is a sum of squares in R iff there exists a real, symmetric, psd matrix B such that* see

$$f = \bar{x} \cdot B \cdot \bar{x}^T.$$

Horn - Johnson !!!

Given such a matrix B of rank t, then we can can construct polynomials $h_1, \dots, h_t$ such that $f = \sum h_i^2$ and B is a Gram matrix of f associated to the h_i's.

Proof. If $f = \sum h_i^2$ is sos, then as above we take $B = A \cdot A^T$, where A is the matrix whose columns are the coefficients of the h_i's.

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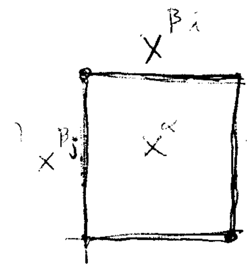
Rank B = # sumands.

Suppose there exists a real, symmetric, psd matrix B such that $f = \bar{x} \cdot B \cdot \bar{x}^T$ and rank $B = t$. Since B is real symmetric of rank t, there exists a real matrix V and a real diagonal matrix $D = \text{diag}(d_1, \dots, d_t, 0, \dots, 0)$ such that $B = V \cdot D \cdot V^T$ and $d_i \neq 0$ for all i. Since B is psd we have $d_i > 0$ for all i. Then

$$(*) \qquad f = \bar{x} \cdot V \cdot D \cdot V^T \cdot \bar{x}^T.$$



Suppose $V = (v_{i,j})$, then for $i = 1, \dots, t$, set $h_i := \sqrt{d_i} \sum_{j=1}^{k} v_{j,i} x^{\beta_i} \in R$. It follows from $(*)$ that $f = h_1^2 + \cdots + h_t^2$. □

Thus to find a representation of f as a sum of squares, we need only find a matrix B which satisfies the theorem. Further, if we can show that no such B exists, then we know that f is not a sum of squares in R. Note that if $f = \sum a_\alpha x^\alpha$ and $B = (b_{i,j})$ is a $k \times k$ symmetric matrix then by "term inspection", $f = \bar{x} \cdot B \cdot \bar{x}^T$ iff for all $\alpha \in \Lambda_{2m}$,

$$(**) \qquad \sum_{\beta_i + \beta_j = \alpha} b_{i,j} = a_\alpha.$$

The algorithm

Given $f \in R$ of degree $2m$.

1. Let $B = (b_{i,j})$ be a symmetric matrix with variable entries. Solve the linear system that arises from $f = \bar{x} \cdot B \cdot \bar{x}^T$, i.e., solve the linear system defined by equations of the form $(**)$ above, with one equation for each $\alpha \in \Lambda_{2m}$. Note that each variable $b_{i,j}$ appears in only one equation, hence the solution is found by setting all but one variable in each row equal to a parameter and solving for the remaining variable. Then the solution is given by $B = B_0 + \lambda_1 B_1 + \cdots + \lambda_l B_l$, where each B_i is a real symmetric $k \times k$ matrix and $\lambda_1, \dots, \lambda_l$ are the parameters. In this case $l = k(k+1)/2 - |\Lambda_{2m}|$.

$t\lambda_i + (1-t)\lambda_j$

Remark. In general, the size of the matrix B grows rapidly as the number of variables and the degree of the polynomial increases, since $k = |\Lambda_m| = \binom{n+m}{n}$. However for a particular polynomial we can sometimes decrease the size of the Gram matrix by eliminating unnecessary elements of Λ_m. For example, suppose $\alpha \in \Lambda_{2m}$, $\alpha = 2\beta$, and α cannot be written in any other way as a sum of elements in Λ_m. Then if the coefficient of α in f is 0, we know x^β cannot occur in any h_i, cf. [CL, §2] and [CLR, 3.7].

But there are other characterization !!!!!!

2. We want to find values for the λ_r's that make $B = B_0 + \lambda_1 B_1 + \cdots + \lambda_l B_l$ psd. As is well known, B is psd iff all eigenvalues are non-negative. Let $F(y) = y^k + b_{k-1} y^{k-1} + \cdots + b_0$ be the characteristic polynomial of B. Note that each $b_i \in \mathbb{R}[\lambda_1, \dots, \lambda_l]$. By Descarte's rule of signs, which is exact for a polynomial with only real roots, $F(y)$ has only non-negative roots iff $(-1)^{(i+k)} b_i \geq 0$ for all $i = 0, \dots, k-1$. Hence we consider the semi-algebraic set

Symbolic computation

$$S := \{(\lambda_1, \dots, \lambda_l) \in \mathbb{R}^l \mid (-1)^{(i+k)} b_i(\lambda_1, \dots, \lambda_l) \geq 0\}.$$

Is the Semialgebraic set S connected.

Then f is sos iff S is nonempty, and a point in S corresponds to a matrix satisfying the conditions of Theorem 1.

Remark. There are several different algorithms for determining whether or not a semi-algebraic set is empty, for example using quantifier elimination. Unfortunately, none of these algorithms are practical apart from "small" examples. For more on this topic, see e.g. [BCR], [C], [GV], [R].

3. Given a matrix $B = (b_{i,j})$ which satisfies the conditions of Theorem 1, then we use the procedure in the proof of the theorem to find a representation of f as a sum of squares.

Example 1. Let $f = x^2y^2 + x^2 + y^2 + 1$, then f is visibly a sum of squares. We want to find all possible representations of f as a sum of squares. Note that by the remark above, if $f = \sum h_i^2$ then the only monomials that can occur in the h_i's are $xy, x, y, 1$. So set $\beta_1 = (1,1)$, $\beta_2 = (1,0)$, $\beta_3 = (0,1)$, and $\beta_4 = (0,0)$. Then the linear system in step 1 of the algorithm is

$$\begin{aligned} &b_{1,1} = 1,\ 2b_{1,2} = 0,\ 2b_{1,3} = 0,\ 2b_{1,4} + 2b_{2,3} = 0 \\ &b_{2,2} = 1,\ 2b_{2,4} = 0 \\ &b_{3,3} = 1,\ 2b_{3,4} = 0 \\ &b_{4,4} = 1 \end{aligned}$$

Thus the general form of a Gram matrix for f is

$$B = \begin{array}{c} \begin{array}{cccc} b_{11} & \quad & \quad & b_{14} \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & \lambda \\ 0 & 1 & -\lambda & 0 \\ 0 & -\lambda & 1 & 0 \\ \lambda & 0 & 0 & 1 \end{bmatrix} \\ \begin{array}{cccc} b_{41} & \quad & \quad & b_{44} \end{array} \end{array}.$$

The characteristic polynomial of B is ← symmetric functions on the eigenvalues,

$$y^4 - 4y^3 + (6 - 2\lambda^2)y^2 + (4\lambda^2 - 4)y + (\lambda^4 - 2\lambda^2 + 1),$$

thus B is psd iff $-1 \le \lambda \le 1$. Note that rank $B = 2$ if $\lambda = \pm 1$, otherwise rank $B = 4$. Hence f can be written as a sum of 2 or 4 squares.

We have $B = V \cdot D \cdot V^T$, where $D = \operatorname{diag}(1, 1, 1-\lambda^2, 1-\lambda^2)$ and $V = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -\lambda & 1 & 0 \\ \lambda & 0 & 0 & 1 \end{bmatrix}$. This yields

$$f = (xy + \lambda)^2 + (x - \lambda y)^2 + (\sqrt{1-\lambda^2}\,y)^2 + (\sqrt{1-\lambda^2})^2.$$

Note that $\lambda = 0$ yields the original representation of f as a sum of 4 squares.

Example 2. Let $f(x,y,z) = x^4 + 2x^2y^2 + x^3z + z^4$. A Gram matrix for f would be of the form

$$\begin{bmatrix} 1 & 0 & 2 & \lambda \\ 0 & 2 & 0 & 0 \\ 2 & 0 & -2\lambda & 0 \\ \lambda & 0 & 0 & 1 \end{bmatrix}.$$

In this case, $S \subseteq \{-8 - 4\lambda + 4\lambda^3 \geq 0, -8 - 4\lambda \geq 0\} = \emptyset$. Hence f is not sos.

Example 3. Let $f(x,y,z) = x^6 + 4x^3y^2z + y^6 + 2y^4z^2 + y^2z^4 + 4z^6$. In this case the only exponents that can occur in the h_i's are $\{(3,0,0), (0,3,0), (0,2,1), (0,1,2), (0,0,3)\}$. We get

$$B = \begin{bmatrix} 1 & 0 & 2 & 0 & 0 \\ 0 & 1 & 0 & r & s \\ 2 & 0 & 2-2r & -s & t \\ 0 & r & -s & 1-2t & 0 \\ 0 & s & t & 0 & 4 \end{bmatrix}$$

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as the general form of a Gram matrix.

The corresponding semi-algebraic set is $S = \{-2r-2t+9 \geq 0, -r^2+4rt-14r-2s^2-t^2-16t+25 \geq 0, 2r^3-7r^2+2rs^2+24rt-30r+2s^2t-10s^2+2t^3-3t^2-34t+19 \geq 0, 10r^3+r^2t^2-10r^2-2rs^2t+4rs^2+36rt-26r+s^4+6s^2t-10s^2+4t^3-3t^2-4t-6 \geq 0, 8r^3+r^2t^2+8r^2+-2rs^2t+2rs^2+16rt-8r+s^4-4s^2t-2s^2+2t^3-t^2+16t-8 \geq 0\}$. If we set $s = t = 0$, we see $(-1,0,0) \in S$, and setting $s = 0$ and $r = -2$ we see $(-2,0,-3/2) \in S$. In particular, S is nonempty and so f is a sum of squares.

Using $(-1,0,0)$,

for second polynomial

$(-1,0,0)$
$(-2,0,-3/2)$
$-\frac{1}{2}$ $(-1, 0, -\frac{3}{4})$
$= (-\frac{3}{2}, 0, -\frac{3}{4})$

$$B = \begin{bmatrix} 1 & 0 & 2 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 2 & 0 & 4 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 4 \end{bmatrix}.$$

$-\frac{9}{4} + \frac{9}{4} + 21 - \frac{9}{16} + 12 + 25 \geq 0$ ✓

Note that rank $B = 3$, so this gives f as a sum of 3 squares. In this case we get

$$f = (x^3 + 2y^2z)^2 + (y^3 - yz^2)^2 + (2z^3)^2.$$

Using $(-2,0,-3/2)$,

$$B = \begin{bmatrix} 1 & 0 & 2 & 0 & 0 \\ 0 & 1 & 0 & -2 & 0 \\ 2 & 0 & 6 & 0 & -3/2 \\ 0 & -2 & 0 & 4 & 0 \\ 0 & 0 & -3/2 & 0 & 4 \end{bmatrix}.$$

Note rank $B = 4$. Proceeding as before we get

$$f = (x^3 + 2y^2z)^2 + (y^3 - 2yz^2)^2 + (\sqrt{2}y^2z - 3\sqrt{2}/4z^3)^2 + (\sqrt{23/8}z^3)^2.$$

Remark. Let $(K, \leq)$ be any ordered field with real closure R, and suppose $f \in K[x_1, \ldots, x_n]$. Then we can easily extend the algorithm to decide whether or not f is a sum of squares in $R[x_1, \ldots, x_n]$.

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