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An algorithm for sums of squares of real polynomials

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Abstract

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. © 1998 Elsevier Science B.V. All rights reserved.

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1. 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.

2. 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 $\Lambda_m := \{(\alpha_1,\dots,\alpha_n) \in \mathbb{N}_0^n \mid \alpha_1 + \cdots + \alpha_n \leq m\}$. 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.

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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: $\Lambda_m = \{\beta_1, \ldots, \beta_k\}$. Set $\bar{x} := (x^{\beta_1}, \ldots, x^{\beta_k})$ 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

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

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

The following theorem, in a different form, can be found in [4]. 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*

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

Given such a matrix B of rank t, then we can construct polynomials $h_1, \ldots, h_t$ 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 $B = A \cdot A^{\mathrm{T}}$, where A is the matrix whose columns are the coefficients of the h_i's.

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

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

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

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", $f = \bar{x} \cdot B \cdot \bar{x}^{\mathrm{T}}$ iff for all $\alpha \in \Lambda_{2m}$,

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

3. 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 $f = \bar{x} \cdot B \cdot \bar{x}^{\mathrm{T}}$, 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 $\lambda_1, \ldots, \lambda_l$ are the parameters. In this case $l = k(k+1)/2 - |\Lambda_{2m}|$.

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. [3, Section 2] and [4, 3.7].

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 nonnegative. Let $F(y) = y^k + b_{k-1}y^{k-1} + \cdots + b_0$ be the characteristic polynomial of B. Note that each $b_i \in \mathbb{R}[\lambda_1, \ldots, \lambda_l]$. By Descarte's rule of signs, which is exact for a polynomial with only real roots, $F(y)$ has only nonnegative roots iff $(-1)^{(i+k)} b_i \geq 0$ for all $i = 0, \ldots, k-1$. Hence, we consider the semialgebraic set

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

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. [1, 2, 5, 6].

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

$$b_{1,1} = 1, \quad 2b_{1,2} = 0, \quad 2b_{1,3} = 0, \quad 2b_{1,4} + 2b_{2,3} = 0,$$
$$b_{2,2} = 1, \quad 2b_{2,4} = 0,$$
$$b_{3,3} = 1, \quad 2b_{3,4} = 0,$$
$$b_{4,4} = 1.$$

Thus, the general form of a Gram matrix for f is

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

The characteristic polynomial of B is

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

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 $B = V \cdot D \cdot V^{\mathrm{T}}$, where $D = \mathrm{diag}(1, 1, 1 - \lambda^2, 1 - \lambda^2)$ 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, $S \subseteq \{-8 - 4\lambda + 4\lambda^3 \ge 0, -8 - 4\lambda \ge 0\} = \emptyset$. 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

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

as the general form of a Gram matrix.

The corresponding semialgebraic set is $S = \{-2r - 2t + 9 \ge 0,\ -r^2 + 4rt - 14r - 2s^2 - t^2 - 16t + 25 \ge 0,\ 2r^3 - 7r^2 + 2rs^2 + 24rt - 30r + 2s^2t - 10s^2 + 2t^3 - 3t^2 - 34t + 19 \ge 0,$

$10r^3 + r^2t^2 - 10r^2 - 2rs^2t + 4rs^2 + 36rt - 26r + s^4 + 6s^2t - 10s^2 + 4t^3 - 3t^2 - 4t - 6 \geq 0,\ 8r^3 + r^2t^2 + 8r^2 + -2rs^2t + 2rs^2 + 16rt - 8r + s^4 - 4s^2t - 2s^2 + 2t^3 - t^2 + 16t - 8 \geq 0\}$. 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 $(-1, 0, 0)$,

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

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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