ANNALES POLONICI MATHEMATICI 102.2 (2011)

Representations of non-negative polynomials via KKT ideals

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Abstract. This paper studies the representation of a non-negative polynomial f on a non-compact semi-algebraic set K modulo its KKT (Karush–Kuhn–Tucker) ideal. Under the assumption that f satisfies the boundary Hessian conditions (BHC) at each zero of f in K, we show that f can be represented as a sum of squares (SOS) of real polynomials modulo its KKT ideal if $f \geq 0$ on K.

1. Introduction. We know that if a polynomial in one variable $f(X) \in$ $\mathbb{R}[X]$ satisfies $f(X) \geq 0$, for all $X \in \mathbb{R}$, then $f(X) = \sum_{i=1}^m g_i^2(X)$, where $g_i(X) \in \mathbb{R}[X]$, i.e., f is a sum of squares in $\mathbb{R}[X]$ (SOS for short). However, in the multi-variable case, this is false. A counterexample was given by Motzkin in 1967. If $f(X,Y) = 1 + X^4Y^2 + X^2Y^4 - 3X^2Y^2$, then f(X,Y) > 0 for all $X,Y\in\mathbb{R}$, but f is not a SOS in $\mathbb{R}[X,Y]$. To remedy that, we will consider the polynomials that are positive on K, where K is a semi-algebraic set in \mathbb{R}^n . For example, Schmüdgen's famous theorem [Schm] says that for a compact semi-algebraic set, every strictly positive polynomial belongs to the corresponding finitely generated preordering. Putinar [Pu] simplified this representation under an additional assumption by using the quadratic module instead of the preordering. However, these results of Schmüdgen and Putinar have two restrictions. Firstly, the polynomials are positive, not merely non-negative. Secondly, K must be a compact semi-algebraic set. One would like to have results for representations of nonnegative polynomials on non-compact semi-algebraic sets.

The results of this paper are similar to those of James Demmel, Jiawang Nie and Victoria Powers in [DNP]. But we use another condition of Murray Marshall in [M], that is, the boundary Hessian condition (BHC for short). Our main result is an extension of Theorem 2.1 in [M] in the same way as Theorems 3.1 and 3.2 are extensions of the corresponding results in [NDS].

DOI: 10.4064/ap102-2-1

²⁰¹⁰ Mathematics Subject Classification: 11E25, 13P25, 14P10, 90C22.

Key words and phrases: non-negative polynomials; sum of squares (SOS); optimization of polynomials; semidefinite programming (SDP).

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2. Preliminaries. In this section, we present some notions and results from algebraic geometry and real algebra needed for our discussion. The reader may consult [BCR], [CLO], and [PD] for more details.

Throughout this section, denote by $\mathbb{R}[z]$ the ring of polynomials in $z = (z_1, \ldots, z_m)$ with real coefficients. Given an ideal $I \subseteq \mathbb{R}[z]$, define its *variety* to be the set

$$V(I) = \{ z \in \mathbb{C}^m \mid p(z) = 0, \, \forall p \in I \},$$

and its real variety to be

$$V^{\mathbb{R}}(I) = V(I) \cap \mathbb{R}^m.$$

A nonempty variety $V = V(I) \subseteq \mathbb{C}^m$ is *irreducible* if there do not exist two proper subvarieties $V_1, V_2 \subset V$ such that $V = V_1 \cup V_2$. The reader should note that in this paper, "irreducible" means that the set of complex zeros cannot be written as a proper union of subvarieties defined by real polynomials.

Given any ideal I of $\mathbb{R}[z]$, its radical \sqrt{I} is defined to be the ideal

$$\sqrt{I} = \{ q \in \mathbb{R}[z] \mid q^l \in I \text{ for some } l \in \mathbb{N} \}.$$

Clearly, $I \subseteq \sqrt{I}$; I is a radical ideal if $\sqrt{I} = I$. As usual, for a variety $V \subseteq \mathbb{C}^m$, I(V) denotes the ideal in $\mathbb{C}[z]$ of polynomials vanishing on V. We will write $I^{\mathbb{R}}(V)$ for the ideal $\mathbb{R}[z] \cap I(V)$.

We need versions of the Nullstellensatz for varieties defined by polynomials in $\mathbb{R}[z]$. The following two theorems are normally stated for ideals in $\mathbb{C}[z]$; however, keeping in mind that V(I) lies in \mathbb{C}^m , they hold as stated for ideals in $\mathbb{R}[z]$.

THEOREM 2.1 ([CLO]). If I is an ideal in $\mathbb{R}[z]$ such that $V(I) = \emptyset$, then $1 \in I$.

THEOREM 2.2 ([CLO]). If I is an ideal in $\mathbb{R}[z]$, then $I^{\mathbb{R}}(V(I)) = \sqrt{I}$.

Let $g_1, \ldots, g_s \in \mathbb{R}[x_1, \ldots, x_n]$ and set

$$K = \{x \in \mathbb{R}^n \mid g_i(x) \ge 0, i = 1, \dots, s\},\$$

and

$$P = \Big\{ \sum_{e \in \{0,1\}^s} \sigma_e g_1^{e_1} \dots g_s^{e_s} \Big\},\,$$

where $e = (e_1, ..., e_s) \in \{0, 1\}^s$ and σ_e are sums of squares of polynomials in $\mathbb{R}[x_1, ..., x_n]$.

Finally, we need the following real algebra version of Theorem 2.1; see Remark 4.2.13 in [PD].

Theorem 2.3 ([PD]). Suppose K and P are defined as above. Then $K = \emptyset$ if and only if $-1 \in P$.

3. Sum of squares modulo KKT ideals. Fix $f, g_1, \ldots, g_s \in \mathbb{R}[x_1, \ldots, x_n]$, and set

$$K = \{x \in \mathbb{R}^n \mid g_i(x) \ge 0, i = 1, \dots, s\}.$$

Let f^* denote the minimum value of f on K, i.e., the solution to the optimization problem

$$(3.1) f^* = \min_{x \in K} f(x).$$

The KKT system associated to this optimization problem is

(3.2)
$$\nabla f - \sum_{j=1}^{s} \lambda_j \nabla g_j = 0,$$

(3.3)
$$g_j \ge 0, \quad \lambda_j g_j = 0, \quad j = 1, \dots, s,$$

where the variables $\lambda = [\lambda_1 \cdots \lambda_s]^T$ are called *Lagrange multipliers* and ∇f denotes the gradient of f, i.e., the vector of first-order partial derivatives of f. A point (x,λ) in $K \times \mathbb{R}^s$ is said to be a KKT point if the KKT system holds at that point.

We work in the polynomial rings $\mathbb{C}[x,\lambda] = \mathbb{C}[x_1,\ldots,x_n,\lambda_1,\ldots,\lambda_s]$ and $\mathbb{R}[x,\lambda]$. Let

$$F_i = \frac{\partial f}{\partial x_i} - \sum_{j=1}^s \lambda_j \frac{\partial g_j}{\partial x_i},$$

and define the KKT ideal I_{KKT} in $\mathbb{R}[x, \lambda]$ and the varieties associated with the KKT system as follows:

$$I_{\text{KKT}} = \langle F_1, \dots, F_n, \lambda_1 g_1, \dots, \lambda_s g_s \rangle,$$

$$V_{\text{KKT}} = \{ (x, \lambda) \in \mathbb{C}^n \times \mathbb{C}^s \mid p(x, \lambda) = 0, \ \forall p \in I_{\text{KKT}} \},$$

$$V_{\text{KKT}}^{\mathbb{R}} = \{ (x, \lambda) \in \mathbb{R}^n \times \mathbb{R}^s \mid p(x, \lambda) = 0, \ \forall p \in I_{\text{KKT}} \}.$$

Keeping in mind that we are now working in the larger polynomial ring, we use P to denote the preordering in $\mathbb{R}[x,\lambda]$ generated by g_1,\ldots,g_s . The associated KKT preordering P_{KKT} in $\mathbb{R}[x,\lambda]$ is defined as

$$P_{\text{KKT}} = P + I_{\text{KKT}}.$$

Finally, set

$$\mathcal{H} = \{(x, \lambda) \in \mathbb{R}^n \times \mathbb{R}^s \mid g_j(x) \ge 0, \ j = 1, \dots, s\}.$$

Theorem 3.1 (Demmel-Nie-Powers [DNP]). Assume I_{KKT} is radical. If f(x) is nonnegative on $V_{KKT}^{\mathbb{R}} \cap \mathcal{H}$, then f(x) belongs to P_{KKT} .

The assumption that I_{KKT} is radical is needed in Theorem 3.1, as shown by an example due to Claus Scheiderer, presented in Example 1 of [NDS]. However, when I_{KKT} is not radical, the conclusion also holds if f(x) is strictly positive on $V_{KKT}^{\mathbb{R}}$.

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THEOREM 3.2 (Demmel-Nie-Powers [DNP]). If f > 0 on $V_{\text{KKT}}^{\mathbb{R}} \cap \mathcal{H}$, then f belongs to P_{KKT} .

The main result of this paper is the following: if f satisfies the BHC at each zero of f in K (see definition in Section 4 below), and $f \geq 0$ on $V_{\text{KKT}}^{\mathbb{R}} \cap \mathcal{H}$, then $f \in P_{\text{KKT}}$. This is an extension of Theorem 2.1 in [M] in the same way as Theorems 3.1 and 3.2 are extensions of the corresponding results in [NDS].

4. Boundary Hessian conditions. We say f satisfies the BHC (boundary Hessian condition) at the point p in K if there is some $k \in \{1, \ldots, n\}$, and $v_1, \ldots, v_k \in \mathbb{N}$ with $1 \leq v_1 < \cdots < v_k \leq s$ such that g_{v_1}, \ldots, g_{v_k} are parts of a system of local parameters at p, and the standard sufficient conditions for a local minimum of $f|_L$ at p hold, where L is the subset of \mathbb{R}^n defined by $g_{v_1}(x) \geq 0, \ldots, g_{v_k}(x) \geq 0$. This means that if t_1, \ldots, t_n are local parameters at p chosen so that $t_i = g_{v_i}$ for $i \leq k$, then in the completion $\mathbb{R}[[t_1, \ldots, t_n]]$ of $\mathbb{R}[x]$ at p, f decomposes as $f = f_0 + f_1 + f_2 + \cdots$ (where f_i is homogeneous of degree i in the variables t_1, \ldots, t_n with coefficients in \mathbb{R}), $f_1 = a_1t_1 + \cdots + a_kt_k$ with $a_i > 0$, $i = 1, \ldots, k$, and the (n - k)-dimensional quadratic form $f_2(0, \ldots, 0, t_{k+1}, \ldots, t_n)$ is positive definite.

THEOREM 4.1 (Marshall [M]). If f satisfies the BHC at each zero of f in K, then $f \in P + (f^2)$, where P denotes the preordering in $\mathbb{R}[x]$ generated by g_1, \ldots, g_s .

EXAMPLE 4.2. Let $f, g_1 \in \mathbb{R}[x, y]$ be given by f(x, y) = x and $g_1(x, y) = x - y^2$. Then

$$K = \{(x, y) \in \mathbb{R}^2 \mid x - y^2 \ge 0\}.$$

Clearly, $f \ge 0$ on K, and the unique zero of f in K occurs at (0,0). Furthermore, f satisfies the BHC at (0,0). Indeed, let $t_1 = g_1 = x - y^2$ and $t_2 = y$. These form a system of local parameters at (0,0). Then $f = x = (x-y^2)+y^2$, so $f = f_1 + f_2$, where $f_1(t_1,t_2) = t_1$, and $f_2(t_1,t_2) = t_2^2$. Also, the coefficient of t_1 in f_1 is positive (it is 1), t_2 does not appear in f_1 , and the quadratic form $f_2(0,t_2) = t_2^2$ is positive definite (when viewed as a quadratic form in the single variable t_2). So, according to the definition, f satisfies the BHC at (0,0). Here f has a representation as follows:

$$f = \sigma_0 + \sigma_1 q_1 + h f^2,$$

where $\sigma_0 = y^2, \sigma_1 = 1, h = 0.$

5. Representation of nonnegative polynomials. In this section, we present our main result. It is similar to Theorem 3.1, but without the assumption that I_{KKT} is radical. It is replaced by the BHC condition.

Theorem 5.1. Suppose that

- (i) $f \geq 0$ on $V_{KKT}^{\mathbb{R}} \cap \mathcal{H}$,
- (ii) f satisfies the BHC at each zero of f in K.

Then $f \in P_{KKT}$.

Remark 5.2. The radical condition and the BHC condition are different. The following example exhibits polynomials which satisfy the radical condition, but do not satisfy the BHC condition and conversely.

Example 5.3 (Marshall [M]).

- 1. Let n=1 and s=0 (so that $K=\mathbb{R}$). Then the polynomial $f(x)=6x^2+8x^3+3x^4$ satisfies the hypothesis of Theorem 5.1, but its KKT ideal is not radical. Indeed, $\partial f/\partial x=12x(x+1)^2, \ f(x)\geq 0$ on \mathbb{R} , f has a zero at x=0, and $(\partial^2 f/\partial x^2)(0)=12>0$. However, its KKT ideal $I=\langle 12x(x+1)^2\rangle$ is not radical, because $g=x(x+1)\in \sqrt{I}$, but $g\not\in I$.
- 2. Let n=2 and s=0 (so that $K=\mathbb{R}^2$). Then the polynomial $f(x,y)=x^2$ does not satisfy the hypothesis of Theorem 5.1, but its KKT ideal is radical. Indeed, the Hessian matrix of f is not positive definite at any zero of f in K. However, its KKT ideal $I=\langle 2x\rangle$ is radical.

To prove Theorem 5.1, we need the following lemma.

LEMMA 5.4. Let W be an irreducible component of V_{KKT} and suppose $W \cap \mathbb{R}^{n+s} \neq \emptyset$. Then f(x) is constant on W.

Proof. This follows from the proof of Lemma 3.3 in [DNP]. ■

Proof of Theorem 5.1. Decompose V_{KKT} into its irreducible components and let W_0 be the union of all the components whose intersection with \mathcal{H} is empty. We note that this includes all components W with $W^{\mathbb{R}} = \emptyset$. Thus, by Lemma 5.4, f is constant on each of the remaining components. We group together all components for which f takes the same value. Then we have pairwise disjoint subsets W_1, \ldots, W_r of W such that for each i, f takes a constant value a_i on W_i , with the a_i being distinct. Further, since each contains a real point and f is non-negative on $V_{\text{KKT}}^{\mathbb{R}} \cap \mathcal{H}$, the value of f on each W_i is real and non-negative. We assume $a_1 > \cdots > a_r \geq 0$. If $a_r > 0$ then $f \in P_{\text{KKT}}$ (see Theorem 3.2). In case $a_r = 0$, fix a primary decomposition of I_{KKT} . For each $i \in \{0, 1, \ldots, r\}$, let J_i be the intersection of those primary components corresponding to the irreducible components occurring in W_i . Thus, $V(J_i) = W_i$.

Since $W_i \cap W_j = \emptyset$, we have $J_i + J_j = \mathbb{R}[x, \lambda]$ by Theorem 2.1. Therefore the Chinese Remainder Theorem (see, e.g., [E]) implies that there is an

isomorphism

$$\varphi: \mathbb{R}[x,\lambda]/I_{\text{KKT}} \to \mathbb{R}[x,\lambda]/J_0 \times \mathbb{R}[x,\lambda]/J_1 \times \cdots \times \mathbb{R}[x,\lambda]/J_r.$$

LEMMA 5.5. There is $q_0 \in P$ such that $f \equiv q_0 \mod J_0$.

Proof. By assumption, $V(J_0) \cap \mathcal{H} = \emptyset$, hence there exists $u_0 \in P$ such that $-1 \equiv u_0 \mod J_0$. This result is a special case of Theorem 8.6 in [Lam].

We write $f = f_1 - f_2$ for SOS polynomials $f_1 = (f + 1/2)^2$ and $f_2 = f^2 + 1/4$. Hence $f \equiv f_1 + u_0 f_2 \mod J_0$. Let $q_0 = f_1 + u_0 f_2 \in P$. Then $f \equiv q_0 \mod J_0$.

LEMMA 5.6. f is a sum of squares modulo J_i for all i = 1, ..., r-1.

Proof. By assumption, on each W_i , $1 \le i \le r-1$, $f = a_i > 0$, and hence the polynomial $u = f/a_i - 1$ vanishes on W_i . Then by Theorem 2.2 there exists some integer $k \ge 1$ such that $u^k \in J_i$. From the binomial identity, it follows that

$$1 + u = \left(\sum_{j=0}^{k-1} {1/2 \choose j} u^j\right)^2 + q u^k.$$

This is explained in Lemma 7.24 in [Lau]. Thus $f = a_i(u+1)$ is a sum of squares modulo J_i .

LEMMA 5.7. There is $q_r \in P$ such that $f \equiv q_r \mod J_r$.

Proof. By the assumption that f satisfies the BHC at each zero of f on K and by Theorem 4.1, there exist $g \in P$ and $h \in \mathbb{R}[x]$ such that $f = g + hf^2$, i.e., f(1 - hf) = g. Since f vanishes on W_r , $f^m \in J_r$ for some positive integer m. Let t = hf and $v = \sum_{i=0}^{m-1} t^i$. Then $t, v \in \mathbb{R}[x]$, $t^m \in J_r$, and $(1 - t)v \equiv 1 \mod J_r$. By the binomial theorem, there exist $c_i \in \mathbb{Q}$, $i = 0, 1, \ldots, m-1$, such that

$$v \equiv \left(\sum_{i=0}^{m-1} c_i t^i\right)^2 \bmod J_r.$$

This yields $q_r \in P$ satisfying

$$f \equiv f(1 - hf)v = gv \equiv q_r \bmod J_r$$
.

To finish the proof of Theorem 5.1, we need the following lemma.

LEMMA 5.8. Given $q_0, q_1, \ldots, q_r \in \mathbb{R}[x, \lambda]$, there exists $q \in P$ such that $q - q_i \in J_i$ for all $i = 0, 1, \ldots, r$.

Proof. By the Chinese Remainder Theorem there exist $e_0, e_1, \ldots, e_r \in \mathbb{R}[x,\lambda]$ such that $e_i \equiv 1 \mod J_i$ and $e_i \equiv 0 \mod J_j$ for $j \neq i$. Set $q = \sum e_i^2 q_i$.

Lemmas 5.5–5.8 imply that there is $q \in P$ such that $f \equiv q \mod I_{\text{KKT}}$, i.e., $f \in P_{\text{KKT}}$.

Remark 5.9. The assumption that f satisfies the BHC at each zero of f in K is needed in Theorem 5.1 and cannot be removed, as the following example shows.

Example 5.10. Let $K = \mathbb{R}^3$, $P_{\text{KKT}} = \sum \mathbb{R}[x]^2 + \langle \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \rangle$ and consider the polynomial

$$f(x, y, z) = x^8 + y^8 + z^8 + M(x, y, z),$$

where $M(x, y, z) = x^4y^2 + x^2y^4 + z^6 - 3x^2y^2z^2$ is the Motzkin polynomial, which is non-negative but not a sum of squares.

It is easy to see that f does not satisfy the BHC at (0,0,0), which is a zero of f in \mathbb{R}^3 . Furthermore, $f \notin P_{\text{KKT}}$. Indeed, this is shown in Example 1 of [NDS].

6. Applications in optimization. In this section, we present a result that is similar to Theorem 4.1 in [DNP]. But instead of the assumption that I_{KKT} is radical, we assume that f satisfies the BHC at each zero of $f - f^*$ in K. Throughout this section, we always assume that the minimum value f^* of f on K is attained at some KKT point.

Recall the KKT system corresponding to (3.1):

(6.1)
$$\nabla f(x) - \sum_{j=1}^{s} \lambda_j \nabla g_j(x) = 0,$$

(6.2)
$$g_j(x) \ge 0, \quad \lambda_j g_j = 0, \quad j = 1, \dots, s.$$

Let f_{KKT}^* be the global minimum value of f(x) over the KKT system defined by (6.1) and (6.2). Assume the KKT system holds at at least one global optimizer. Then we claim that $f^* = f_{\text{KKT}}^*$. First, $f^* \leq f_{\text{KKT}}^*$ follows immediately from the fact that all solutions to the KKT system are feasible. By assumption, there exists (x^*, λ^*) satisfying the above KKT system such that $f(x^*) = f^*$. Thus $f^* \geq f_{\text{KKT}}^*$ and hence they are equal.

In order to implement membership in P_{KKT} as an SDP, we need a bound on the degrees of the sums of squares involved. Thus, for $d \in \mathbb{N}$, we define the truncated KKT ideal

$$I_{d,KKT} = \Big\{ \sum_{k=1}^{n} \phi_k F_k + \sum_{j=1}^{s} \psi_j \lambda_j g_j \mid \deg(\phi_k F_k), \deg(\psi_j \lambda_j g_j) \le 2d \Big\},$$

and the truncated preorder

$$P_{d,\text{KKT}} = \left\{ \sum_{e \in \{0,1\}^s} \sigma_e g^e \mid \deg(\sigma_e g^e) \le 2d \right\} + I_{d,\text{KKT}}.$$

Then we define a sequence $\{f_d^*\}$ of SOS relaxations of the optimization

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problem (3.1) as follows:

(6.3)
$$f_d^* = \max_{\gamma \in \mathbb{R}} \gamma \quad \text{such that}$$

$$(6.4) f(x) - \gamma \in P_{d,KKT}.$$

Obviously each γ feasible in (6.4) is a lower bound of f^* . So $f_d^* \leq f^*$. When we increase d, the feasible region defined by (6.4) is increasing, and hence the sequence $\{f_d^*\}$ of lower bounds is also increasing. Thus

$$f_1^* \le f_2^* \le \dots \le f^*.$$

It can be shown that the sequence $\{f_d^*\}$ of lower bounds obtained from (6.3) and (6.4) converges to f^* in (3.1), provided that f^* is attained at one KKT point. We have the following theorem.

Theorem 6.1. Assume f(x) has a minimum $f^* := f(x^*)$ at one KKT point x^* of (3.1). Then $\lim_{d\to\infty} f_d^* = f^*$. Furthermore, if f satisfies the BHC at each zero of $f - f^*$ in K, then there exists some $d \in \mathbb{N}$ such that $f_d^* = f^*$, i.e., the SOS relaxations (6.3) and (6.4) converge in finitely many steps.

Proof. The sequence $\{f_d^*\}$ is increasing, and $f_d^* \leq f^*$ for all $d \in \mathbb{N}$, since f^* is attained by $f(x^*)$ in the KKT system (3.2) and (3.3) by assumption and the constraint (6.4) implies that $\gamma \leq f^*$. Now for arbitrary $\epsilon > 0$, let $\gamma_{\epsilon} = f^* - \epsilon$ and replace f(x) by $f(x) - \gamma_{\epsilon}$ in (3.1). The KKT system remains unchanged, and $f(x) - \gamma_{\epsilon}$ is strictly positive on $V_{\text{KKT}}^{\mathbb{R}} \cap \mathcal{H}$. By Theorem 3.2, $f(x) - \gamma_{\epsilon} \in P_{\text{KKT}}$. Since $f(x) - \gamma_{\epsilon}$ is fixed, there must exist some integer d_1 such that $f(x) - \gamma_{\epsilon} \in P_{d_1,\text{KKT}}$. Hence $f^* - \epsilon \leq f_{d_1}^* \leq f^*$. Therefore $\lim_{d \to \infty} f_d^* = f^*$.

Now assume that f satisfies the BHC at each zero of $f-f^*$ in K. Replace f(x) by $f(x)-f^*$ in (3.1). The KKT system still remains the same, and $f(x)-f^*$ is now nonnegative on $V_{\text{KKT}}^{\mathbb{R}} \cap \mathcal{H}$. Moreover, $f-f^*$ also satisfies the BHC at each zero of $f-f^*$ in K. By Theorem 5.1, $f(x)-f^* \in P_{\text{KKT}}$. So there exists some integer d_2 such that $f(x)-f^* \in P_{d_2,\text{KKT}}$, and hence $f_{d_2}^* \geq f^*$. Then $f_d^* \leq f^*$ for all d implies that $f_{d_2}^* = f^*$.

Acknowledgements. The author would like to thank Prof. Murray Marshall, Prof. Ha Huy Vui and Assoc. Prof. Pham Tien Son for many interesting and helpful discussions on this work. The author would also like to thank Prof. Charles N. Delzell for his comments.

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Received 9.3.2010 and in final form 17.7.2011