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On Orthogonal Polynomial Bases for Triangles and Tetrahedra Invariant under the Symmetric Group

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1. Introduction

We present an L_2-orthonormal polynomial basis for triangles containing 10^{th} degree polynomials in its span. The sixty-six basis functions are defined by using 35 *generating functions* $\{B_k(x,y)\}$ with the property that $B_k(x,y)$ is orthogonal to $B_k(y,x)$ unless they are equal. For tetrahedra, we describe methods for constructing a an L_2-orthonormal basis by defining generating functions $B_k(x,y,z)$ such that the action of S_3 on the arguments of B_k can provide as many as six orthogonal basis functions. Thirty-five basis functions generated by 11 B_k have been computed. These bases are particularly useful for approximating the solution of partial differential equations using the Cell Discretization Algorithm (CDA).

The CDA allows a user to partition the domain of a problem into 'cells', choose any basis on each cell, and then 'glue' the finite dimensional approximations on each cell together across cell interfaces to achieve a form of weak continuity using a method called 'moment collocation.' This method allows a user to select a basis tailored to the type of an equation or the geometry of the cells without having to worry about continuity of an approximation.

If polynomial bases are used and we have planar interfaces between cells, we can impose sufficient collocation moments so that our approximations are continuous and we duplicate the $h-p$ finite element method [**9**]. Error estimates that establish convergence of the method contain two components; the first consists of terms arising from the lack of continuity of an approximation and the second contains terms majorized by the orthogonal complement of the projection of the solution onto the approximation space. However, in all trials of the method using polynomial bases[**4, 9, 5, 7, 6, 8**], there has been no particular advantage in enforcing continuity of an approximation; continuity does eliminate the first error component, but by doing so a parameter in the second error component grows strongly, thus cancelling any apparent gain by forcing continuity. This is discussed extensively in [**9**]. Thus we obtain additional degrees of freedom that can, for example, be used to

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enforce a weak solenoidal condition for approximating the solutions to the Stokes equations [**8**].

We have implemented the algorithm for general domains in $\mathbf{R}^2$ partitioned into cells with linear internal interfaces between cells. Affine transformations are used to map any cell into a standard configuration to effect quadrature and if a basis is defined on a cell in standard configuration, we use an affine transformation to provide a basis for the affine image of the cell. For the most part we use cells that are parallelograms or triangles–affine images of a unit square or unit simplex. A ‘good’ basis for a general implementation of the algorithm is a basis that is L_2 orthonormal, particularly for time-dependent problems and the construction of a solenoidal basis [**8**]. Since affine transformations preserve orthogonality, it suffices to construct orthonormal bases for the standard square or simplex. A global orthonormal basis is then produced by a linear combination of the cell basis functions using coefficients obtained from the QR decomposition of the matrix enforcing the moment collocation constraints [**5, 7, 6**]. These arguments generalize to $\mathbf{R}^3$.

Products of Legendre polynomials provide an L_2- orthonormal basis for a square. In Section 2, for the unit 2-simplex, with vertices at (0,0), (1,0) and (0,1), we describe the method we have used to construct an orthonormal basis with polynomials of degree 10 or less in its span.

In $\mathbf{R}^3$; products of Legendre Polynomials produce an orthonormal basis for any parallelepiped. In Section 3 we describe the construction of an orthornormal basis for the standard 3-simplex. The methods we use require that we solve a set of four simultaneous quadratic equations in five variables.

The results for tetrahedra were obtained by Hui [**2**].

2. Construction of a polynomial basis for triangles.

We contrive an L_2 orthonormal basis $B_i(x,y)$ for the 2-simplex that uses a method similar to the Gram-Schmidt process to sequentially introduce sets of monomials $x^j y^k$ into the basis. The first problem is to determine how j and k should be successively chosen to produce our basis sequence.

Consider the Taylor's expansion of any $u(x,y)$ around (x_o, y_o):

$$
\begin{gathered}
u(x,y) = u(x_o,y_o) + u_x(x-x_o) + u_y(y-y_o) + \\
(1/2!)[u_{xx}(x-x_o)^2 + \mathbf{2}u_{xy}(x-x_o)(y-y_o) + u_{yy}(y-y_o)^2] \\
+(1/3!)[u_{xxx}(x-x_o)^3 + \mathbf{3}u_{xxy}(x-x_o)^2(y-y_o) + \\
\mathbf{3}u_{xyy}(x-x_o)(y-y_o)^2 + u_{yyy}(y-y_o)^3] \\
+(1/4!)[u_{xxxx}(x-x_o)^4 + \mathbf{4}u_{xxxy}(x-x_o)^3(y-y_o) + \mathbf{6}u_{xxyy}(x-x_o)^2(y-y_o)^2 \\
+\mathbf{4}u_{xyyy}(x-x_o)(y-y_o)^3 + u_{yyyy}(y-y_o)^4] + \dots
\end{gathered}
$$

With no other information available about $u(x,y)$, the terms containing the mixed partial derivatives in the expansion with coefficients containing factors 2,3,3,4,6,4, 6,4, appear to be more important than those involving $u_{xx}, u_{yy}, u_{xxx}, u_{yyy}$, and so forth.

Polynomial approximation theory suggests that we introduce monomials into the basis span according to increasing degree and, given any chosen degree, the form of the Taylor's series suggests that the monomials with equal coefficient factors, which are either a pair $\{x^i y^j, x^j y^i\}$ or of form $x^k y^k$, be added to the basis span in order of *decreasing* coefficient factors. Thus, for example, when generating a basis that spans polynomials of degree 4, we would first introduce monomial x^2y^2 into the basis set (with Maclaurin series coefficient $u_{xxyy}(0,0)\mathbf{6}/4!$), then the pair $\{x^3y, xy^3\}$(with Maclaurin series coefficients $u_{xxxy}(0,0)\mathbf{4}/4!$ and $u_{xyyy}(0,0)\mathbf{4}/4!$) and finally the pair $\{x^4, y^4\}$. Our method follows this algorithm.

This gives a justification for increasing the number of basis functions used in the approximation gradually, lessening the need for a new full degree basis at each new approximation.

We call a function $f(x,y)$ **symmetric** if $f(x,y) = f(y,x)$; recalling that the 2-simplex is to be our domain for f, the axis of symmetry is the line $y = x$.

We say function f is **skew** if $f(x,y) = -f(y,x)$. The product of two symmetric functions is symmetric; the product of two skew functions is symmetric, and the product of a symmetric function and a skew function is skew. One easily shows that the integral of a skew function over the standard simplex is zero. We combine our monomials to form expressions that are either *symmetric* or *skew* and have the same span; our sequence of generating functions is given by two sets

$$A \equiv \{1, (x+y), xy, (x^2+y^2), (x^2y+xy^2), (x^3+y^3), \dots\} \text{ and}$$

$$B \equiv \{(x-y), (x^2-y^2), (x^2y-xy^2), (x^3-y^3), \dots.\}.$$

If we integrate by parts over the standard triangle and use a recursive argument, we obtain

$$\int_0^1 \int_0^{1-x} x^p y^q \, dy dx = [p!q!]/(p+q+2)!.$$

This gives us an exact (rational) value for the $L_2(simplex)$ inner product (denoted $< \cdot, \cdot >$) of any monomials.

We use an algorithm equivalent to the Gram-Schmidt process to generate a sequence of symmetric orthogonal polynomials $\{Q_1, Q_2, \dots\}$ from generating set A and a set of skew orthogonal polynomials $\{S_1, S_2, \dots\}$ from B.

Our basis is obtained by combining these two sets using the heuristic suggested by the Maclaurin series. For example, to generate the 7^{th}(and 8^{th}) basis functions, thus introducing x^2y and xy^2 into the basis, we form

$$\alpha \pm \beta \equiv [2 < Q_5, Q_5 >]^{-1/2} Q_5 \pm [2 < S_3, S_3 >]^{-1/2} S_3.$$

Then symmetric α is orthogonal to skew β and the skew span of B; skew β is orthogonal to the symmetric span of $A; \alpha$ and β have norm $1/\sqrt{2}$, so

$$< \alpha+\beta, \alpha-\beta >= 1/2 - 1/2 = 0$$

and $\| \alpha+\beta \|^2 =< \alpha,\alpha > + < \beta,\beta >= 1 =\| \alpha-\beta \|^2$. If $B(x,y) \equiv \alpha+\beta$, then $B(y,x) = \alpha-\beta$.

When generating basis functions with a symmetric lead term, such as $1, xy, x^2y^2$ and so forth, where there is no skew partner, we use only the appropriate Q_1, Q_3, Q_7, $\dots$; there is no skew β term.

These computations were done with care, for the matrices in the linear systems employed by the Gram-Schmidt process are very ill-conditioned. Our computations were nevertheless exact, for the matrices and vectors are arrays of rational numbers, so that the solution is rational and we have written a program that does Gaussian elimination and back substitution using rational arithmetic, thus keeping control of the instability of the system. A set of 36 polynomials has been computed, producing 66 basis functions, which allow us to generate any polynomial of degree 10 or less.

FORTRAN77 code and the necessary coefficients to generate the full set of basis functions (and their first derivatives) are available from the second author.

The use of this polynomial basis for solving partial differential equations with domains partitioned into triangles requires an efficient method for doing quadrature; points and weights for Gaussian quadrature over triangles, exact for polynomials of degree 20 or less, have been obtained by Dunavant [**1**]. As in [**3**], we generate and store an array that contains the information to look up, for example, the computations $< \frac{\partial}{\partial x}B_i, \frac{\partial}{\partial y}B_j >$ for use when the partial differential equation has constant coefficients.

3. A symmetric ortho-normal basis for tetrahedra.

The Maclaurin series expansion for $f(x,y,z)$ is

$$\begin{gathered} f(\mathbf{0}) \\ +f_x x + f_y y + f_z z \\ +(1/2)[\mathbf{2}(f_{xy}xy + f_{xz}xz + f_{yz}yz) + f_{xx}x^2 + f_{yy}y^2 + f_{zz}z^2] \\ +(1/6)[\mathbf{6}f_{xyz}xyz + \mathbf{3}(f_{xxy}x^2y + \dots f_{yyx}y^2x + \dots) + f_{xxx}x^3 + \dots]+ \\ (1/24)\big[\mathbf{12}(f_{xxyz}x^2yz + \dots) + \mathbf{6}(f_{xxyy}x^2y^2 + \dots) + \mathbf{4}(f_{xxxy}x^3y + \dots)+ \\ (f_{xxxx}x^4 + \dots)\big] + \dots \end{gathered}$$

Proceeding naively as before, we assume that, for any particular degree of basis functions, we should initially introduce monomials $x^p y^q x^r$ into the basis that correspond to the larger integer multipliers: 2 then 1; 6,3 then 1; 12,6,4 then 1 and so forth. The monomials that are associated with these multipliers occur in sets of 1 (e.g. $\{xyz\}$), 3 (e.g. $\{xy, xz, zy\}$) or 6 (e.g. $\{x^2y, x^2z, y^2x, y^2z, z^2x, z^2y\}$.) To minimize the number of functions that need to be generated, ideally, our symmetric orthonormal basis would require just one *basis generating* function $B(x,y,z)$ for each of the classes; for the classes with 3 members, $\{B(x,y,z), B(y,z,x), B(z,x,y)\}$ would be an orthonormal set, also orthogonal to the basis functions generated previously; we will call such functions *3-fold basis generating functions.* For the classes with 6 members, the full group S_3 of permutations of $B(x,y,z)$:

$$\{B(x,y,z), B(y,z,x), B(z,x,y), B(y,x,z), B(x,z,y), B(z,y,x)\}$$

would constitute an orthonormal set, orthogonal to the previously generated basis functions; we will call these *6-fold basis generating functions.*

Figure 1 shows a triangular array of the homogeneous monomials of degree 5, with the numbers below each monomial representing the bold-face integer multiplier to be used in the Maclaurin expansion above. For any particular degree, monomials with the same number under them identify those that would be included in the same set as described above. Those with higher numbers would be introduced into the basis first.

Our study takes place in the subspace S of L_2(3-simplex) consisting of polynomials in x, y and z. We denote the inner product $< \cdot, \cdot >$.

Each member of the permutation group S_3 induces a linear transformation on S:

If T is the permutation (x,y,z), it acts on $\mathbf{R}^3$ as $T < x,y,z > = < y,z,x >$; $T^2 < x,y,z > = T < y,z,x > = < z,x,y >$; T^3 is the identity. T acts on a polynomial in the following fashion: $T(2x^2yz + 3xz) = T(2x^2y^1z^1 + 3x^1y^0z^1) = 2y^2zx + 3yx$.

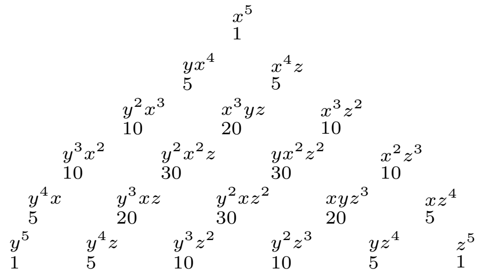

FIGURE 1. Fifth degree monomials.

Transformation $P \equiv P_{xy}$ corresponds to permutation (x, y). The basic relator is $PT = T^2P$. Since these transformations are to act on any polynomial $q(x, y, z)$, we adopt the convention that, for example, in computing $TP_{xy}q(x, y, z), P_{xy}$ acts first and then T, so the transformation $TP_{xy} = (x, y, z)(x, y) = (x, z)$ and $T^2P_{xy} = (y, z)$. We also use notation S_3 for these transformations.

We let ξ represent a generic member of $\mathbf{R}^3$; given ξ, bold face symbol $\mathbf{x}^\alpha$ represents the monomial $x^iy^jz^k$ associated with any triple of non-negative integers $[\alpha] = [i, j, k]$. For any $\mathbf{x}^\alpha$, the set of permutations of $\mathbf{x}^\alpha$ is

$$\{\mathbf{x}^\alpha, T\mathbf{x}^\alpha, T^2\mathbf{x}^\alpha, P\mathbf{x}^\alpha, TP\mathbf{x}^\alpha, T^2P\mathbf{x}^\alpha\},$$

where there will be duplicates if the set has only 3 or 1 member. We let T act on 'powers' $[\alpha] = [i, j, k]$ by defining $T[\alpha] = T[i, j, k] \equiv [k, i, j]; P[i, j, k] \equiv [j, i, k]$. Then $T\mathbf{x}^\alpha = \mathbf{x}^{T\alpha}, T^2\mathbf{x}^\alpha = \mathbf{x}^{TT\alpha}$ and so forth.

In figure 1, monomials belonging in the same set (those with the same number below them) correspond to all permutations of such a triple $[i, j, k]$. If $i = j = k$, there is only one monomial; if two of $\{i, j, k\}$ are the same, there are three monomials in the set; if $\{i, j, k\}$ are all different, there are six.

The integral of monomial $x^py^qz^r$ over the standard 3-simplex can be shown to be $[p!q!r!]/[(p + q + r + 3)!]$ using recursive methods similar to those described above [**2**]. The value of this integral is invariant under the action of S_3 on the monomials. This symmetry means that the integral depends only on *set* $\{p, q, r\}$. This observation, together with bilinearity of the inner product, can be used to prove the following lemma:

LEMMA 1. *For any polynomials G and $H \in S$,*

1. *for any $R \in S_3, < RG, RH >=< G, H >$;*
2. *for any $R \in S_3, < RG, H >=< G, R^{-1}H >$;*
3. $< G, TH >=< T^2G, H >=< TG, T^2H >$.

Results 2 and 3 follow readily from 1; 2 shows that the members of S_3 act as unitary operators on S.

Our first basis member is the normalized constant function $B_1 \equiv \sqrt{6}$. When only one basis function is produced, we call these *one-fold generators.* The images under S_3 of the next three basis-generating functions are to contain $\{x, y, z\}$, then $\{xy, yz, xz\}$ and finally $\{x^2, y^2, z^2\}$ in their span.

We give some necessary conditions for recursively defining basis-generating functions B_{r+1} that produce three basis members under the action of T, as is the case here. Assume appropriate functions $B_k(\xi)$ have already been constructed, $k = 1, \ldots, r$.

LEMMA 2. *Suppose* $[\alpha] = [i_1, i_2, i_3]$ *has exactly two of* $\{i_1, i_2, i_3\}$ *equal. The next function* G *is expressed as*

$$G(\xi) = H(\mathbf{x}^\alpha) + \sum_{k=1}^{r} \sum_{i=0}^{n(k)} \sum_{j=0}^{m(k)} a_{k,i,j} T^i P^j B_k(\xi) \tag{1}$$

where $n(k) \leq 2; m(k) \leq 1$. *When* $B_k(\xi)$ *is a 3-fold basis generating function,* $n(k) = 2$ *and* $m(k) = 0$. *Function* $H(\mathbf{x}^\alpha) \equiv b_0\mathbf{x}^\alpha + b_1 T\mathbf{x}^\alpha + b_2 T^2\mathbf{x}^\alpha$. *Suppose*

(I) $G, TG,$ *and* T^2G *are orthogonal to the previous basis functions;*
(II) G, TG *and* T^2G *are pairwise orthogonal and*
(III) *set* $\{PG, PTG, PT^2G\} = \{G, TG, T^2G\}$.

Then, without loss of generality, the following assumptions can be made about $G, [\alpha], \{b_i\}$ *and* $\{a_{k,i,j}\}$:

(a) $PG = G; PH = H$.
(b) $[\alpha] = [i_1, i_1, i_3]$; *the first two powers are equal and* $b_1 = b_2$.
(c) *(I) holds if and only if* $a_{k,i,j} = -< H, T^i P^j B_k >$. *Thus the* $a_{k,i,j}$ *are linear combinations of* b_0 *and* b_1.
(d) *In view of (a), arguing recursively, without loss of generality, we can assume that all three-fold basis generators* B_k *satisfy* $PB_k = B_k$. *Then*

$$\text{if } n(k) = 2 \text{ and } m(k) = 0, a_{k,1,0} = a_{k,2,0}.$$

$$\text{If } n(k) = 2 \text{ and } m(k) = 1, a_{k,0,1} = a_{k,0,0}; a_{k,1,1} = a_{k,2,0} \text{ and}$$

$$a_{k,2,1} = a_{k,1,0}.$$

(e) *If the substitutions in (c) and (d) are made, (I), (II) and (III) hold if and only if* $< G, TH >= 0$.

PROOF. (a) From (III) it follows that exactly one of $\{G, TG, T^2G\}$ must be fixed under P. For example, suppose $PG = T^2G$. Then TG is fixed under P, for $PTG = T^2PG = T^2T^2G = TG$. Now

$$TG(\xi) = TH(\mathbf{x}^\alpha) + \sum_{k=1}^{r} \sum_{i=0}^{n(k)} \sum_{j=0}^{m(k)} a_{k,i,j} T^{i+1} P^j B_k(\xi)$$

$$= H(\mathbf{x}^{T\alpha}) + \sum_{k=1}^{r} \sum_{i=0}^{n(k)} \sum_{j=0}^{m(k)} a_{k,i,j} T^{i+1} P^j B_k(\xi).$$

By re-labelling the $a_{k,i,j}$ and defining $[\beta] \equiv T[\alpha]$, this has the same form as (1); call it $\tilde{G}$. We are assuming that $PTG = TG$; thus $P\tilde{G} = \tilde{G}$. Then $PH(\mathbf{x}^\beta) = H(\mathbf{x}^\beta)$ follows immediately. Redefine $\tilde{G}$ to be G.

(b) Expanding $H(\mathbf{x}^\beta) = PH(\mathbf{x}^\beta)$ we get $H(\mathbf{x}^\beta) = b_0\mathbf{x}^\beta + b_1 T\mathbf{x}^\beta + b_2 T^2\mathbf{x}^\beta$

$$= b_0\mathbf{x}^\beta + b_1\mathbf{x}^{T\beta} + b_2\mathbf{x}^{TT\beta} = PH(\mathbf{x}^\beta) \equiv b_0 P\mathbf{x}^\beta + b_1 \mathrm{PT}\mathbf{x}^\beta + b_2 PT^2\mathbf{x}^\beta$$

$$= b_0\mathbf{x}^{P\beta} + b_1\mathbf{x}^{PT\beta} + b_2\mathbf{x}^{PTT\beta}.$$

Recalling that $[\beta] = [i_1, i_2, i_3]$ has exactly two of i_1, i_2, i_3 equal, one of $[\beta], T[\beta]$ and $T^2[\beta]$ has these two equal integers in the first two positions and hence this triple is invariant under P. For example, suppose that $PT[\beta] =$

$T[\beta]$. Then $PT^2[\beta] = PTPT[\beta] = [\beta]$ and $P[\beta] = T^2[\beta]$; the assumption that $PH = H$ then requires that $b_0 = b_2$. If we let $[\gamma] \equiv T[\beta]$ and express $H(\mathbf{x}^\gamma)$ as $b_1\mathbf{x}^{T\beta} + b_2T\mathbf{x}^{T\beta} + b_0T^2\mathbf{x}^{T\beta} = b_1\mathbf{x}^\gamma + b_2T\mathbf{x}^\gamma + b_0T^2\mathbf{x}^\gamma$ we get the correct representation by relabelling the b_i's.

(c) This follows if we take the inner product of $T^iP^jB_k$ with (1).

(d) When $m(k) = 0$, the assumption that $PB_k = B_k$ and $PG = G$ readily give the first result. When $m(k) = 1$, we have, for example, $-a_{k,1,1} = < H, TPB_k >=< T^2H, PB_k >=< PT^2H, B_k >=< TPH, B_k >= < TH, B_k >=< H, T^2B_k >= -a_{k,2,0}$.

(e) Since $< G, TG >=< TG, T^2G >=< T^2G, G >$, pairwise orthogonality follows if we can establish that just one of these is zero. If the substitutions in (c) are made, G will be orthogonal to all $T^iP^jB_k$ for any choice of H, hence orthogonal to the sums in the representation (1) for G. Thus $< G, TG >=< G, TH >$. The representations in (d) give us (III).

□

This lemma shows that all we need to do to establish the existence of a suitable G is to find some $H(\mathbf{x}^\alpha)$ of form $b_0\mathbf{x}^\alpha + b_1(T\mathbf{x}^\alpha + T^2\mathbf{x}^\alpha)$ so that, when the substitutions in (c) are made, which are linear in $\{b_0, b_1\}$, the expression $< G, TH >= 0$ has a real solution. This is a quadratic equation in $\{b_0, b_1\}$. If we first seek only this orthogonality, there really is only one degree of freedom here; we can set b_0 or $b_1 = 1$ so that the requirement that $< G, TH >= 0$ yields a quadratic equation in one variable. Any real root gives a suitable G with the orthogonality properties; it's final definition is found by normalizing so that $< G, G >= 1$.

The first four basis generators we have computed are

$$B_1 = \sqrt{6};$$

$$B_2 = \sqrt{30}(2(x+y) - 1);$$

$$B_3 = \sqrt{7/6}(78xy + 6z(x+y) - 2z - 14(x+y) + 3);$$

$$B_4 = \sqrt{182 + 56\sqrt{10}}\Big((6\sqrt{10}-20)z^2 + \sqrt{10}(x^2+y^2) + (2\sqrt{10}-1)xy + (6\sqrt{10}-17)z(x+y) + (3 - 2\sqrt{10})(x+y) + (19 - 6\sqrt{10})z + (\sqrt{10} - 5/2)\Big).$$

One-fold basis generators, like the one with lead term xyz, are easily computed. These are to be invariant under S_3; for any k, all $a_{k,i,j}$ will be equal. For example, $B_5 = \sqrt{2}(504xyz - 63(xy + yz + xz) + 9(x + y + z) - 3/2)$.

B_6 is the first 6-fold generating function. The lead term is a linear sum of $\{yz^2, zx^2, xy^2, xz^2, yx^2, zy^2\}$. It will have representation

$$G(\xi) = H(\mathbf{x}^\alpha) + \sum_{k=1}^{r}\sum_{i=0}^{n(k)}\sum_{j=0}^{m(k)} a_{k,i,j}T^iP^jB_k(\xi)$$

as before, except this time all three integers in $[\alpha]$ are different; $[\alpha] = [0, 1, 2]$ in this case, and

$$H(\mathbf{x}^\alpha) = b_0\mathbf{x}^\alpha + b_1T\mathbf{x}^\alpha + b_2T^2\mathbf{x}^\alpha + b_3P\mathbf{x}^\alpha + b_4\mathrm{TP}\mathbf{x}^\alpha + b_5T^2P\mathbf{x}^\alpha.$$

We wish to find values for $a_{k,i,j}$ and b_p such that

$$Q \equiv \{G, TG, T^2G, PG, TPG, T^2PG\}$$

is a set of pairwise orthogonal functions, orthogonal to the previous basis functions.

First note that for the functions in Q to be orthogonal to basis functions $T^iP^jB_k(\xi)$ it suffices to show that they are orthogonal to B_k, since Q is to be invariant under S_3 and the adjoints of operators in S_3 are in S_3.

Next, since the previous basis functions are assumed to be orthonormal, for any B_k, we can make the following reductions with the help of lemma 2.1. The orthogonality requirements are

$$0 =< G, B_k >=< H, B_k > +a_{k,0,0}$$

$$0 =< TG, B_k >=< G, T^2B_k >=< H, T^2B_k > +a_{k,2,0}$$

$$0 =< T^2G, B_k >=< G, TB_k >=< H, TB_k > +a_{k,1,0}$$

$$0 =< PG, B_k >=< G, PB_k >=< H, PB_k > +a_{k,0,1}$$

$$0 =< TPG, B_k >=< G, PT^2B_k >=< G, TPB_k >=< H, TPB_k > +a_{k,1,1}$$

$$0 =< T^2PG, B_k >=< G, PTB_k >=< G, T^2PB_k >=< H, T^2PB_k > +a_{k,2,1}.$$

For three-fold generators, where $PB_k = B_k$, the last three requirements are omitted; the associated $a_{k,i,1}$ are zero. In this way we express the $a_{k,i,j}$ as linear combinations of the $\{b_i\}$.

Finally, we need $\{b_i\}$ so that Q is a pairwise orthogonal set. Again, using adjoints, the fifteen requirements reduce to the following four.

$0 =< G, TG >=< G, T^2G >=< TG, T^2G >=< PG, TPG >=< PG, T^2PG >$
$=< TPG, T^2PG >$ (Type 1)
$0 =< G, PG >=< TG, TPG >=< T^2G, T^2PG >$ (Type 2)
$0 =< G, TPG >=< TG, T^2PG >=< T^2G, PG >$ (Type 3)
$0 =< G, T^2PG >=< TG, PG >=< T^2G, TPG >$ (Type 4).

If the substitutions for the $a_{k,i,j}$ are made, the members of Q are orthogonal to the previous basis functions, and the four equations above give us four simultaneous quadratic equations in the variables

$$\{b_0, b_1, b_2, b_3, b_4, b_5\}.$$

For example, for B_6, where all $a_{k,i,1} = 0$ with $k < 6$ and we let $a_{k,i}$ denote $a_{k,i,0}$, the four types above are equivalent to the following, where when $k = 1$ or 5, there is only a single term in the sum.

Type 1.
$0 =< G, TG >=< G, TH >=< H, TH > -\sum_{k=1}^{5}(a_{k,0}a_{k,1}+a_{k,0}a_{k,2}+a_{k,1}a_{k,2})$
Type 2.
$0 =< G, PG >=< G, PH >=< H, PH > -\sum_{k=1}^{5}(a_{k,0}^2 + 2a_{k,1}a_{k,2})$
Type 3.
$0 =< G, TPG >=< G, TPH >=< H, TPH > -\sum_{k=1}^{5}(a_{k,2}^2 + 2a_{k,0}a_{k,1})$
Type 4.
$0 =< G, T^2PG >=< G, T^2PH >=< H, T^2PH > -\sum_{k=1}^{5}(a_{k,1}^2 + 2a_{k,0}a_{k,2})$.

The normalization requirement is $1 =< G, G >=< G, H >$. $< G, G >$ is a non-negative homogeneous quadratic form; thus $< G, G >= 1$ places us on the (compact) 5-dimensional surface of an ellipsoid in $\mathbf{R}^6$. We initially confine our attention to fulfilling the orthogonality requirements, so, for example, we can let $b_0 = 1$; we must then find simultaneous roots for 4 quadratic forms in five variables. We use a variant of Newton's method that has proved to be quite effective in obtaining roots rapidly [**2**].

A number of questions remain.

1. We have computed 11 basis-generating functions so far, which produce the 35 basis functions necessary to have polynomials of the fourth degree or less in their span. More are needed for practical use of this basis. Is there some way of proving that there always exists a solution to the simultaneous quadratics?
2. Assuming that (as is the case in our experiments) there is a one-parameter family of solutions, what criteria should we use for selecting any particular one? We sought solutions $\mathbf{b}$ such that each b_i was about the same magnitude, but with many changes of sign. For example, should we rather choose some solution $\mathbf{b}$ such that just one b_i has a large magnitude?
3. The coefficients become quite large; for example, in B_{11}, with 24 distinct coefficients, the smallest is about 31, the largest about 4890, with 15 greater than 1000. We used double precision Gaussian Quadrature to evaluate all the inner products in the solution algorithm and terminated the algorithm when $\mathbf{b}$ was found so that, for each $i, \mid f_i(\mathbf{b}) \mid < 10^{-17}$, but tests of orthogonality of the normalized basis functions were beginning to have significant errors, as appears to be the case with such generalizations of the Gram-Schmidt process. The inner products of the monomials are rational; is there a way to exploit this as was done with the basis functions for triangles?

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