1995

On an orthonormal basis for tetrahedra invariant under S_3

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DOI: <https://doi.org/10.31979/etd.xn4d-x4zm>

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**ON AN ORTHONORMAL BASIS FOR TETRAHEDRA
INVARIANT UNDER S_3**

A Thesis

Presented to

**The Faculty of the Department of Mathematics
San Jose State University**

In Partial Fulfillment

**of the Requirements for the Degree
Master of Science**

By

Gary Man-Kwong Hui

August, 1995

UMI Number: 1375701

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ABSTRACT

ON AN ORTHONORMAL BASIS FOR TETRAHEDRA INVARIANT UNDER S_3

by Gary Man-Kwong Hui

This thesis presents a method for constructing an orthonormal polynomial basis for tetrahedra. This basis may be used to solve Neumann problems on tetrahedra or more general problems using the cell discretization algorithm.

This thesis shows how to convert elliptic boundary-value problems to variational boundary-value problems. This thesis discusses how these can be solved by the Galerkin method to illustrate the need for a basis. The mathematical foundations for the basis construction and methods for finding such a basis are given. This thesis describes an iterative method for solving four simultaneous quadratic equations with five unknowns which was needed to obtain the basis.

ACKNOWLEDGMENTS

I would like to thank Dr. Leslie Foster who let me use his FORTRAN compiler for my computational work in my thesis and also helped me through a part of my thesis in the summer of 1993.

I would also like to thank the secretaries in the Mathematics Department at San Jose State University: Marilyn, DeAnna, and Pauline, who generously allowed me to use the Xerox machine and other office supplies to complete this thesis.

By far my greatest debt is to my thesis advisor, Dr. Howard Swann. He encouraged me to write this thesis and patiently guided me through the whole thesis for two and a half years -- problems after problems, day after day.

Finally, I would like to thank my parents for all that they have done for me through the years and also my girlfriend, Christine Wong, who gave me the support to finish this thesis.

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Introduction

Classification of Second-Order Partial Differential Equations

Suppose that Ω is a bounded region in the xy -plane with boundary Γ . Consider the quasilinear equation

$$a_{11}u_{xx} + 2a_{12}u_{xy} + a_{22}u_{yy} = f(x, y, u, u_x, u_y) \quad (1)$$

where a_{11} , a_{12} and a_{22} are twice continuously differentiable functions of x and y and f is any continuous function of its arguments. We classify such Partial Differential Equations (PDEs) into one of three types - elliptic, parabolic, or hyperbolic - and each type of PDE displays characteristics quite distinct from the others. This classification is stated as follows:

- Case 1. If $a_{12}^2 - a_{11}a_{22} > 0$ for all points (x,y) in Ω , then equation (1) is called a hyperbolic PDE;
- Case 2. If $a_{12}^2 - a_{11}a_{22} = 0$ for all points (x,y) in Ω , then equation (1) is called a parabolic PDE;
- Case 3. If $a_{12}^2 - a_{11}a_{22} < 0$ for all points (x,y) in Ω , then equation (1) is called an elliptic PDE [11].

For the purpose of this thesis, we will focus our attention on linear elliptic PDEs of form

$$a_{11}u_{xx} + 2a_{12}u_{xy} + a_{22}u_{yy} + a_1u_x + a_2u_y + a_0u = f$$

where the a_{ij} , a_1 , a_2 , a_0 , and f are functions of x and y .

Three problems for elliptic equations arise depending on the boundary conditions prescribed on Ω .

- (i) The first boundary value problem, or Dirichlet problem, requires that a solution u of equation (1) take on prescribed values, $u = f(x,y)$, on the boundary Γ

of Ω ;

- (ii) The second boundary value problem, or Neumann problem, requires that

$$\left. \frac{\partial u}{\partial \mathbf{n}} \right|_{\Gamma} = g(x, y). \text{ Here } \frac{\partial}{\partial \mathbf{n}} \text{ refers to a form of differentiation along the normal}$$

to Γ directed away from the interior of Ω depending on the coefficients of the equations. If $\underline{n} = (n_1, n_2)$ is the unit outward normal to Γ , then

$$\frac{\partial u}{\partial \mathbf{n}} \equiv (a_{11} \frac{\partial u}{\partial x_1} + a_{12} \frac{\partial u}{\partial x_2})n_1 + (a_{12} \frac{\partial u}{\partial x_1} + a_{22} \frac{\partial u}{\partial x_2})n_2;$$

- (iii) The third boundary value problem, or Robin problem, is a linear combination

of a Dirichlet and a Neumann condition with $\alpha(x, y)u + \beta(x, y)\frac{\partial u}{\partial \mathbf{n}} = \gamma(x, y)$ on

Γ , where $\alpha(x, y) > 0$, $\beta(x, y) > 0$ for $(x, y) \in \Gamma$ [11].

Outline of the thesis:

In chapter 1 we give a more detailed description of Elliptic PDEs that have either Dirichlet or Neumann boundary conditions. Then we are going to broaden the concept of a boundary-value problem by introducing what is known as a variational boundary-value problem. In chapter 2 we present two approximation methods, the Galerkin method and the Rayleigh-Ritz method, based on the variational formulation. In chapter 3 we introduce our polynomial basis construction for tetrahedra, which in turn can be used to solve the Neumann problem. However, using the Cell Discretization Algorithm, this basis can be used for general partitions of domains in R^3 into parallelepipeds and tetrahedra [10]. In chapter 4 we give the analysis for our basis construction and describe the actual computations for functions needed to span the set of polynomials of order four or less. In appendix A we list the 11 generating functions needed to produce this basis.

CHAPTER 1

Elliptic Partial Differential Equations

Section 1.1: Description of Elliptic Partial Differential Equations

Consider the general second order linear equation

$$Bu = f ,$$

where

$$Bu \equiv - \sum_{i,j=1}^2 b_{ij} D_i D_j u + \sum_{i=1}^2 b_i D_i u + b_0 u \quad (1)$$

and $D_i u$ denotes differentiation with respect to x_i .

Let A be a second order linear operator of form

$$Au \equiv - \sum_{i,j=1}^2 D_i (a_{ij} D_j u) + \sum_{i=1}^2 a_i D_i u + a_0 u \quad (2)$$

where $a_{ij} = a_{ji}$ and $D_i D_j u = D_j D_i u$. We can convert (1) into the form (2), using the following argument .

$$\begin{aligned} Bu &\equiv - \sum_{i,j=1}^2 b_{ij} D_i D_j u + \sum_{i=1}^2 b_i D_i u + b_0 u \\ &= -b_{11} D_1 D_1 u - b_{12} D_1 D_2 u - b_{21} D_2 D_1 u - b_{22} D_2 D_2 u + b_1 D_1 u + b_2 D_2 u + b_0 u \\ &= -b_{11} D_1 D_1 u - (b_{12} + b_{21}) D_1 D_2 u - b_{22} D_2 D_2 u + b_1 D_1 u + b_2 D_2 u + b_0 u \\ &= -b_{11} D_1 D_1 u - \frac{(b_{12} + b_{21})}{2} D_1 D_2 u - \frac{(b_{12} + b_{21})}{2} D_1 D_2 u - b_{22} D_2 D_2 u + \\ &\quad b_1 D_1 u + b_2 D_2 u + b_0 u. \end{aligned}$$

From the product rule , $D_i (\alpha_{ij} D_j u) = \alpha_{ij} D_i D_j u + D_j u D_i \alpha_{ij}$. We can now write

$$Bu = -D_1 (b_{11} D_1 u) + D_1 b_{11} D_1 u - D_1 \left[\frac{(b_{12} + b_{21})}{2} D_2 u \right] + D_1 \left[\frac{(b_{12} + b_{21})}{2} \right] D_2 u$$

$$\begin{aligned}
& -D_2\left[\frac{(b_{12}+b_{21})}{2}D_1u\right]+D_2\left[\frac{(b_{12}+b_{21})}{2}\right]D_1u-D_2(b_{22}D_2u)+D_2b_{22}D_2u \\
& +b_1D_1u+b_2D_2u+b_0u \\
& =-D_1(b_{11}D_1u)-D_1\left[\frac{(b_{12}+b_{21})}{2}D_2u\right]-D_2\left[\frac{(b_{12}+b_{21})}{2}D_1u\right]-D_2(b_{22}D_2u) \\
& +\left\{D_1b_{11}+D_2\left[\frac{(b_{12}+b_{21})}{2}\right]+b_1\right\}D_1u+\left\{D_1\left[\frac{(b_{12}+b_{21})}{2}\right]+D_2b_{22}+b_2\right\}D_2u \\
& +b_0u.
\end{aligned}$$

If we now define $a_{11} = b_{11}$, $a_{22} = b_{22}$ and $a_{12} \equiv \frac{(b_{12}+b_{21})}{2} \equiv a_{21}$, then we obtain

$$\begin{aligned}
Bu & = -D_1(a_{11}D_1u) - D_1(a_{12}D_2u) - D_2(a_{21}D_1u) - D_2(a_{22}D_2u) \\
& +a_1D_1u+a_2D_2u+a_0u
\end{aligned}$$

where $a_1 = D_1b_{11} + D_2\left[\frac{(b_{12}+b_{21})}{2}\right] + b_1$, $a_2 = D_1\left[\frac{(b_{12}+b_{21})}{2}\right] + D_2b_{22} + b_2$ and $a_0 = b_0$. Thus,

$$Bu = -\sum_{i,j=1}^2 D_i(a_{ij}D_ju) + \sum_{i=1}^2 a_i D_iu + a_0u \equiv Au. \quad \blacksquare \quad (3)$$

For the purpose of this thesis, we only focus our attention on self-adjoint problems,

where we consider (3) without its first order terms, $\sum_{i=1}^2 a_i D_iu$.

The task is to find $u(x_1, x_2)$ that satisfies

$$Au = f$$

over a suitable domain Ω , an open bounded set in $\mathbb{R}^2$, with boundary Γ , where A is an elliptic self-adjoint partial differential operator of form

$$Au = -\sum_{i,j=1}^2 D_i(a_{ij}(x)D_ju) + a_0(x)u,$$

where $x \in \Omega \subset \mathbb{R}^2$ and u satisfies prescribed boundary conditions. The function f and the coefficients $a_{ij}(x)$ and $a_0(x)$ are given functions of x on Ω .

We discuss only two types of boundary conditions: the Dirichlet, the Neumann, or a mixture of the two. We do not consider the Robin type here. Dirichlet and Neumann boundary conditions are described previously. The mixed boundary condition is where the boundary $\Gamma = \Gamma_1 \cup \Gamma_2$ and has Dirichlet and Neumann conditions on portions of the boundary:

$$u|_{\Gamma_1} = g_1(x_1, x_2) \quad \text{and} \quad \frac{\partial u}{\partial n}\bigg|_{\Gamma_2} = g_2(x_1, x_2).$$

To summarize, we consider (in this discussion of two dimensional problems) an equation of form $Au = f$; or

$$-\left[\frac{\partial}{\partial x_1} \left(a_{11} \frac{\partial u}{\partial x_1} + a_{12} \frac{\partial u}{\partial x_2} \right) + \frac{\partial}{\partial x_2} \left(a_{21} \frac{\partial u}{\partial x_1} + a_{22} \frac{\partial u}{\partial x_2} \right) \right] + a_0 u = f, \quad (4)$$

together with appropriate boundary conditions. We assume that $a_{12} = a_{21}$ and $a_{12}^2 - a_{11}a_{22} < 0$.

A typical example is the equation

$$-\Delta u + a_0 u - f = 0$$

defined over some domain Ω with boundary conditions:

$$u|_{\Gamma_1} = g_1 \quad \text{and} \quad \frac{\partial u}{\partial n}\bigg|_{\Gamma_2} = g_2. \quad (5)$$

Section 1.2: Variational boundary-value problems

In this section, we proceed by using example (5) in section 1.1 instead of the general partial differential equation (4). We first convert the problem of solving (5) to an equivalent variational boundary-value problem by means of Green's Theorem. A variational boundary-value problem is a problem of the following form:

Find a function u that belongs to a Hilbert space V , and satisfies the equation

$$B(u,v) = l(v)$$

for all functions v in a subspace of V . Here B is a bilinear form and l is a linear functional:

$$B : V \times V \rightarrow \mathbb{R} \text{ and } l : V \rightarrow \mathbb{R} \text{ [9].}$$

Green's Theorem

Let Ω be a domain in the xy -plane and let Γ be a piecewise smooth simple closed curve oriented counterclockwise in Ω . Let $P(x_1, x_2)$ and $Q(x_1, x_2)$ be functions defined and continuous, having continuous first partial derivatives in Ω . Then

$$\iint_{\Omega} \left(\frac{\partial Q}{\partial x_1} - \frac{\partial P}{\partial x_2} \right) dx_1 dx_2 = \oint_{\Gamma} (P dx_1 + Q dx_2) \text{ [7].}$$

Consider the functional expression

$$\iint_{\Omega} \left[-\Delta u + a_0 u \right] v \, dx_1 dx_2. \tag{6}$$

Rewriting (6) in its partial derivative notation, we get

$$\begin{aligned} & \iint_{\Omega} \left[- \left(\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} \right) + a_0 u \right] v \, dx_1 dx_2 \quad \text{or} \\ & \iint_{\Omega} \left[- \frac{\partial}{\partial x_1} \left(\frac{\partial u}{\partial x_1} \right) v - \frac{\partial}{\partial x_2} \left(\frac{\partial u}{\partial x_2} \right) v + a_0 uv \right] dx_1 dx_2. \end{aligned}$$

By the product rule, $\frac{\partial}{\partial x}(\alpha\beta) = \frac{\partial\alpha}{\partial x}\beta + \alpha\frac{\partial\beta}{\partial x}$, so $\frac{\partial\alpha}{\partial x}\beta = -\alpha\frac{\partial\beta}{\partial x} + \frac{\partial}{\partial x}(\alpha\beta)$.

Suppose we let $\alpha = \frac{\partial u}{\partial x_1}$ and $\beta = v$. Then (6) is

$$\iint_{\Omega} \left\{ \left[-\left(\frac{\partial u}{\partial x_1} \frac{\partial v}{\partial x_1} + \frac{\partial}{\partial x_1} \left(\frac{\partial u}{\partial x_1} v \right) \right) - \left(\frac{\partial u}{\partial x_2} \frac{\partial v}{\partial x_2} + \frac{\partial}{\partial x_2} \left(\frac{\partial u}{\partial x_2} v \right) \right) \right] + a_0 uv \right\} dx_1 dx_2$$

or

$$\iint_{\Omega} \left[\frac{\partial u}{\partial x_1} \frac{\partial v}{\partial x_1} - \frac{\partial}{\partial x_1} \left(\frac{\partial u}{\partial x_1} v \right) + \frac{\partial u}{\partial x_2} \frac{\partial v}{\partial x_2} - \frac{\partial}{\partial x_2} \left(\frac{\partial u}{\partial x_2} v \right) + a_0 uv \right] dx_1 dx_2.$$

Now the integral above can be re-grouped to two separate integrals as

$$\begin{aligned} & \iint_{\Omega} \left[\frac{\partial u}{\partial x_1} \frac{\partial v}{\partial x_1} + \frac{\partial u}{\partial x_2} \frac{\partial v}{\partial x_2} + a_0 uv \right] dx_1 dx_2 \\ & - \iint_{\Omega} \left[\frac{\partial}{\partial x_1} \left(\frac{\partial u}{\partial x_1} v \right) - \frac{\partial}{\partial x_2} \left(\frac{\partial u}{\partial x_2} v \right) \right] dx_1 dx_2. \end{aligned} \quad (7)$$

The second integral term in (7) can be written as

$$- \iint_{\Omega} \left[\frac{\partial}{\partial x_1} (Q) - \frac{\partial}{\partial x_2} (P) \right] dx_1 dx_2 \quad (8)$$

where $Q = \frac{\partial u}{\partial x_1} v$ and $P = -\frac{\partial u}{\partial x_2} v$.

Using Green's Theorem, (8) is

$$\begin{aligned} & - \oint_{\Gamma} [P dx_1 + Q dx_2] \text{ or} \\ & - \oint_{\Gamma} \left[-\frac{\partial u}{\partial x_2} v dx_1 + \frac{\partial u}{\partial x_1} v dx_2 \right]. \end{aligned} \quad (9)$$

If the curve Γ is parametrically written as $(x_1(t), x_2(t))$, then (9) is

$$- \oint_{\Gamma} \left[-\frac{\partial u}{\partial x_2} v x_1'(t) dt + \frac{\partial u}{\partial x_1} v x_2'(t) dt \right] \text{ or}$$

$$\begin{aligned}
& -\oint_{\Gamma} \left[\frac{\partial u}{\partial x_1} v x'_2(t) dt + \frac{\partial u}{\partial x_2} v (-x'_1(t)) dt \right] \quad \text{or, in vector notation,} \\
& -\oint_{\Gamma} v \left\langle \frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2} \right\rangle \frac{\langle x'_2(t), -x'_1(t) \rangle}{\sqrt{x'_2(t)^2 + x'_1(t)^2}} \sqrt{x'_2(t)^2 + x'_1(t)^2} dt. \quad (10)
\end{aligned}$$

The unit tangent vector to Γ in the counter-clockwise direction is $\frac{\langle x'_1(t), x'_2(t) \rangle}{\sqrt{x'_1(t)^2 + x'_2(t)^2}}$, so

the outward unit normal vector is $\frac{\langle x'_2(t), -x'_1(t) \rangle}{\sqrt{x'_2(t)^2 + x'_1(t)^2}}$. For our example,

$$\frac{\partial u}{\partial n} \equiv \left\langle \frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2} \right\rangle \cdot \frac{\langle x'_2(t), -x'_1(t) \rangle}{\sqrt{x'_2(t)^2 + x'_1(t)^2}} \quad \text{and} \quad ds \equiv \sqrt{x'_2(t)^2 + x'_1(t)^2} dt.$$

So, (10) can be written as

$$-\oint_{\Gamma} v \frac{\partial u}{\partial n} ds.$$

Thus, for any smooth v , (6) is

$$\iint_{\Omega} \left[\frac{\partial u}{\partial x_1} \frac{\partial v}{\partial x_1} + \frac{\partial u}{\partial x_2} \frac{\partial v}{\partial x_2} + a_0 uv \right] dx_1 dx_2 - \oint_{\Gamma} v \frac{\partial u}{\partial n} ds.$$

If u is the solution, then $-\Delta u + a_0 u - f = 0$. This implies that

$$\iint_{\Omega} [-\Delta u + a_0 u - f] v dx_1 dx_2 = \iint_{\Omega} [0] v dx_1 dx_2 = 0.$$

So

$$\begin{aligned}
0 &= \iint_{\Omega} [-\Delta u + a_0 u - f] v dx_1 dx_2 \\
&= \iint_{\Omega} [-\Delta u + a_0 u] v dx_1 dx_2 - \iint_{\Omega} f v dx_1 dx_2 \\
&= \iint_{\Omega} \left[\frac{\partial u}{\partial x_1} \frac{\partial v}{\partial x_1} + \frac{\partial u}{\partial x_2} \frac{\partial v}{\partial x_2} + a_0 uv \right] dx_1 dx_2 - \oint_{\Gamma} v \frac{\partial u}{\partial n} ds - \iint_{\Omega} f v dx_1 dx_2. \quad (11)
\end{aligned}$$

Finally, (11) can be written as

$$\iint_{\Omega} \left[\frac{\partial u}{\partial x_1} \frac{\partial v}{\partial x_1} + \frac{\partial u}{\partial x_2} \frac{\partial v}{\partial x_2} + a_0 uv \right] dx_1 dx_2 - \oint_{\Gamma} v \frac{\partial u}{\partial n} ds = \iint_{\Omega} f v dx_1 dx_2. \quad (12)$$

We now apply the boundary conditions on (12) where Γ_1 is the portion of the boundary curve with a Dirichlet condition, and Γ_2 is the portion with the Neumann condition, i.e.

$$u|_{\Gamma_1} = g_1 \quad \text{and} \quad \frac{\partial u}{\partial n} \Big|_{\Gamma_2} = g_2.$$

We thus have an equivalent variational boundary-value problem. Namely, find u such that

$$\iint_{\Omega} \left[\frac{\partial u}{\partial x_1} \frac{\partial v}{\partial x_1} + \frac{\partial u}{\partial x_2} \frac{\partial v}{\partial x_2} + a_0 uv \right] dx_1 dx_2 - \oint_{\Gamma_1} v \frac{\partial u}{\partial n} ds - \oint_{\Gamma_2} v \frac{\partial u}{\partial n} ds = \iint_{\Omega} f v dx_1 dx_2 \quad (13)$$

with

$$u|_{\Gamma_1} = g_1 \quad \text{and} \quad \frac{\partial u}{\partial n} \Big|_{\Gamma_2} = g_2, \quad \text{for any smooth } v \text{ [9].}$$

Define $a(u, v)$ to be the bilinear form $\iint_{\Omega} \left[\frac{\partial u}{\partial x_1} \frac{\partial v}{\partial x_1} + \frac{\partial u}{\partial x_2} \frac{\partial v}{\partial x_2} + a_0 uv \right] dx_1 dx_2$ and

$$(f, v) \equiv \iint_{\Omega} f v dx_1 dx_2.$$

If $v|_{\Gamma_1} = 0$, then (13) can be written as

$$a(u, v) - (f, v) - \oint_{\Gamma_2} g_2 v ds = 0. \quad (14)$$

Thus, if u is a twice-differentiable solution to (5), then (14) is to be satisfied by all v such that $v|_{\Gamma_1} = 0$.

The following theorem is a converse of the result above.

Theorem.

Let $H_{\Gamma_1}^1(\Omega)$ be the space of test functions that are one-time continuously differentiable on Ω and vanish on the boundary segment Γ_1 . Suppose that $u \in C^2(\Omega)$ with $u|_{\Gamma_1} = g_1$ and $f \in C(\Omega)$. If $a(u, v) - (f, v) - \oint_{\Gamma_2} g_2 v \, ds = 0$ for all $v \in H_{\Gamma_1}^1(\Omega)$, then u is a solution of (5).

Proof:

Suppose that $a(u, v) - (f, v) - \oint_{\Gamma_2} g_2 v \, ds = 0$ for all $v \in H_{\Gamma_1}^1(\Omega)$. Let

$$Lu \equiv -\frac{\partial^2 u}{\partial x_1^2} - \frac{\partial^2 u}{\partial x_2^2} + a_0 u. \text{ Recall that}$$

$$(Lu, v) \equiv \iint_{\Omega} \left[-\left(\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} \right) + a_0 u \right] v \, dx_1 dx_2.$$

We have shown that the integral

$$\iint_{\Omega} \left[-\left(\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} \right) + a_0 u \right] v \, dx_1 dx_2$$

can be written as

$$\iint_{\Omega} \left[\frac{\partial u}{\partial x_1} \frac{\partial v}{\partial x_1} + \frac{\partial u}{\partial x_2} \frac{\partial v}{\partial x_2} + a_0 uv \right] dx_1 dx_2 - \oint_{\Gamma} v \frac{\partial u}{\partial n} \, ds.$$

This implies that

$$(Lu, v) = a(u, v) - \oint_{\Gamma} v \frac{\partial u}{\partial n} \, ds$$

or,

$$a(u, v) = (Lu, v) + \oint_{\Gamma} v \frac{\partial u}{\partial n} \, ds$$

$$= (Lu, v) + \oint_{\Gamma_1} v \frac{\partial u}{\partial n} ds + \oint_{\Gamma_2} v \frac{\partial u}{\partial n} ds.$$

Substituting $a(u, v)$ in (14), we obtain

$$\iint_{\Omega} Lu \cdot v \, dx_1 dx_2 + \oint_{\Gamma_1} v \frac{\partial u}{\partial n} ds + \oint_{\Gamma_2} v \frac{\partial u}{\partial n} ds - \iint_{\Omega} fv \, dx_1 dx_2 - \oint_{\Gamma_2} g_2 v \, ds = 0.$$

Since $v \in H_{\Gamma_1}^1$, $v|_{\Gamma_1} = 0$. So, we have

$$\iint_{\Omega} Lu \cdot v \, dx_1 dx_2 + \oint_{\Gamma_2} v \frac{\partial u}{\partial n} ds - \iint_{\Omega} fv \, dx_1 dx_2 - \oint_{\Gamma_2} g_2 v \, ds = 0.$$

Rearranging terms, we get

$$\iint_{\Omega} Lu \cdot v \, dx_1 dx_2 - \iint_{\Omega} fv \, dx_1 dx_2 = - \oint_{\Gamma_2} v \frac{\partial u}{\partial n} ds + \oint_{\Gamma_2} g_2 v \, ds$$

or,

$$\iint_{\Omega} (Lu - f)v \, dx_1 dx_2 = \oint_{\Gamma_2} (g_2 - \frac{\partial u}{\partial n})v \, ds \quad \text{for all } v \in H_{\Gamma_1}^1. \quad (15)$$

We first show that $(Lu - f) = 0$. Suppose that $(Lu - f) \neq 0$ at some point $(x_{1_0}, x_{2_0}) \equiv z_0$ in open domain Ω .

Case 1. Suppose $(Lu - f)(z_0) > 0$.

Since we have assumed $u \in C^2(\Omega)$ and $f \in C(\Omega)$, this implies that $(Lu - f)$ is continuous at $z_0 \in \Omega$. So for some $\varepsilon > 0$, there exists an ε -ball $B(z_0, \varepsilon) \subset \Omega$ such that $(Lu - f)(x_1, x_2) > 0$ for all points $(x_1, x_2) \in B(z_0, \varepsilon)$. We can construct a function $v \in H_{\Gamma_1}^1$ such that $v > 0$ in $B(z_0, \varepsilon)$ and $v \equiv 0$ outside of $B(z_0, \varepsilon)$. By construction, v is zero on Γ_2 . So, the right-hand side of (15) will be zero. Thus, we have

$$\iint_{\Omega} (Lu - f)v \, dx_1 dx_2 = \iint_{B((x,y), \varepsilon)} (Lu - f)v \, dx_1 dx_2 = 0.$$

This is a contradiction since both continuous v and $(Lu - f)$ are positive on $B(z_0, \varepsilon)$.

Hence, there cannot exist any point $z_0 \in \Omega$ where $(Lu - f) > 0$.

Case 2. Suppose $(Lu - f)(z_0) < 0$.

A similar contradiction argument holds if $(Lu - f) < 0$ at some point $z_0 \in \Omega$.

Hence, $(Lu - f) = 0$ in Ω .

From the above argument, (15) now becomes

$$0 = \oint_{\Gamma_2} \left(g_2 - \frac{\partial u}{\partial n}\right) v \, ds \quad \text{for all } v \in H_{\Gamma_1}^1.$$

Since we have assumed that Γ_2 is smooth, if there exists some point

$(x_1(t_0), x_2(t_0)) \equiv z(t_0) \in \Gamma_2$ such that the continuous function $(g_2 - \frac{\partial u}{\partial n})(x_1(t), x_2(t))$ is positive when $t = t_0$, then for some $\varepsilon > 0$ there exists an ε -ball $B(t_0, \varepsilon)$ where $(g_2 - \frac{\partial u}{\partial n})(x_1(t), x_2(t)) > 0$ for all $t \in B(t_0, \varepsilon)$. We can construct a function $v \in H_{\Gamma_1}^1$ such that $v(x_1(t), x_2(t)) > 0$ for $t \in B(t_0, \varepsilon)$ and $v(x_1(t), x_2(t)) \equiv 0$ for t outside of $B(t_0, \varepsilon)$.

Then again we would have

$$\begin{aligned} 0 &= \oint_{\Gamma_2} \left(g_2 - \frac{\partial u}{\partial n}\right) v \, ds \\ &= \oint_{\Gamma_2} \left[\left(g_2 - \frac{\partial u}{\partial n}\right)(x_1(t), x_2(t)) \right] v(x_1(t), x_2(t)) \sqrt{x_2'(t)^2 + x_1'(t)^2} \, dt \\ &= \int_{t_0 - \varepsilon}^{t_0 + \varepsilon} \left[\left(g_2 - \frac{\partial u}{\partial n}\right)(x_1(t), x_2(t)) \right] v(x_1(t), x_2(t)) \sqrt{x_2'(t)^2 + x_1'(t)^2} \, dt. \end{aligned}$$

This is a contradiction since all terms in the integral are positive. Hence

$(g_2 - \frac{\partial u}{\partial n}) \leq 0$ on Γ_2 . A similar contradiction argument holds if $(g_2 - \frac{\partial u}{\partial n}) < 0$ at some

point $(x_1(t_0), x_2(t_0)) \in \Gamma_2$. Hence $\frac{\partial u}{\partial n} = g_2$ on Γ_2 . ■

Therefore, finding a twice-differentiable solution for (5) in section 1.1 is equivalent to finding the solution for (13).

For the purpose of this thesis, we do not consider the Dirichlet condition here. Assume $\Gamma_1 = \emptyset$. We focus our attention only on the homogeneous Neumann condition. i.e.,

$$\Gamma_1 = \emptyset \quad \text{and} \quad \left. \frac{\partial u}{\partial n} \right|_{\Gamma_2} = 0 .$$

Thus, we seek a solution u to

$$\iint_{\Omega} \left[\frac{\partial u}{\partial x_1} \frac{\partial v}{\partial x_1} + \frac{\partial u}{\partial x_2} \frac{\partial v}{\partial x_2} + a_0 uv \right] dx_1 dx_2 = \iint_{\Omega} f v \, dx_1 dx_2 \quad (16)$$

for all $v \in H^1_{\Gamma_1} \equiv H^1(\Omega)$ when $\Gamma_1 = \emptyset$.

CHAPTER 2

Approximate methods of solution

In chapter 1, we defined elliptic boundary-value problems and showed how one may convert an elliptic boundary-value problem to an equivalent variational boundary-value problem. The stage has now been reached where we can ask: how does one actually obtain a solution to such a problem? Unfortunately, the answer is rather disappointing. It is quite impossible to obtain exact solutions to most boundary-value problems in either the conventional or variational formulations except for a very few simple PDEs and types of domains. Thus, we seek approximate solutions. Here things are more encouraging. There are many good methods for finding approximate solutions. For the purpose of this thesis, we choose to present the Galerkin method and the Rayleigh-Ritz method, which are based on the variational formulation.

Section 2.1: The Galerkin Method

The basic idea behind the Galerkin method is a simple one. Consider the variational boundary-value problem of finding $u \in V$ that satisfies

$$B(u,v) = l(v) \quad \text{for all } v \in W, \text{ some subspace of } V \quad (1)$$

where V is a Hilbert space [2,4,8,9]. We treat only the homogeneous Neumann problem, where $V = W$. The difficulty in trying to solve (1) lies with the fact that V is a very large space. So, instead of posing the problem in V , we pick N linearly independent functions $\phi_1, \phi_2, \dots, \phi_N$ in V and define the space V_N to be the finite-dimensional subspace of V spanned by the functions ϕ_i . That is,

$$V_N \subset V, \quad \text{span}\{\phi_i\}_{i=1}^N = V_N.$$

So $v \in V_N$ is represented by $v_N = \sum_{j=1}^N b_j \phi_j$ where the coefficients b_j are arbitrary.

In the limit, as $N \rightarrow \infty$, we would like to choose $\{\phi_i\}$ to be "complete", so that V_N will approach V .

Having defined the space V_N we now pose problem (1) in V_N instead of in V . That is, we try to find a function $u_N \in V_N$ that satisfies

$$B(u_N, v_N) = l(v_N) \quad \text{for all } v_N \in V_N. \quad (2)$$

This is the essence of the Galerkin method.

Since $u_N \in V_N$, $v_N \in V_N$ and $\text{span}\{\phi_i\}_{i=1}^N = V_N$, this implies that both u_N and v_N must be linear combinations of the basis functions of V_N . So

$$u_N = \sum_{i=1}^N a_i \phi_i \quad \text{and} \quad v_N = \sum_{j=1}^N b_j \phi_j, \quad (3)$$

where the coefficients b_j are arbitrary. We substitute (3) in (2) to obtain

$$B\left(\sum_{i=1}^N a_i \phi_i, \sum_{j=1}^N b_j \phi_j\right) = l\left(\sum_{j=1}^N b_j \phi_j\right).$$

We now use the fact that B is bilinear and l is linear to obtain

$$\sum_{i=1}^N \sum_{j=1}^N a_i b_j B(\phi_i, \phi_j) = \sum_{j=1}^N l(\phi_j) b_j$$

or,

$$\sum_{i=1}^N \sum_{j=1}^N a_i b_j B(\phi_i, \phi_j) - \sum_{j=1}^N l(\phi_j) b_j = 0$$

or,

$$\sum_{j=1}^N b_j \left[\sum_{i=1}^N B(\phi_i, \phi_j) a_i - l(\phi_j) \right] = 0$$

or , more concisely,

$$\sum_{j=1}^N b_j \left[\sum_{i=1}^N K_{ij} a_i - F_j \right] = 0 , \quad (4)$$

where $K_{ij} = B(\phi_i, \phi_j)$ and $F_j = l(\phi_j)$.

Note that K_{ij} is an $N \times N$ matrix and F_j is an N -tuple (vector) and both can be evaluated in practice since the ϕ_i are known functions and the forms of B and l are also known.

Since the coefficients b_j are arbitrary, it follows that (4) will only hold if the term in brackets is zero. Thus, we have reduced the problem to solving the set of simultaneous linear equations

$$\sum_{i=1}^N K_{ij} a_i = F_j , \quad j=1, 2, \dots, N.$$

Once these equations are solved, the approximate solution u_N can be found from the first of equations (3).

An example from Ordinary Differential Equations is the following.

Consider the boundary-value problem of finding $y(x)$ such that

$$-y'' + y = x \text{ where } x \in [-1, 1] \text{ and } y'(-1) = y'(1) = 0.$$

We find the approximate solution of this boundary-value problem by using the Galerkin method with two different ϕ_i (bases) to illustrate how the Galerkin method works.

The corresponding variational boundary-value problem is: find $y \in V$ such that

$$\int_{-1}^1 [y'v' + yv] dx = \int_{-1}^1 xv dx \quad \text{for all } v \in V,$$

where $V = C^1[-1,1]$. The boundary conditions $y'(-1) = y'(1) = 0$ are the homogeneous Neumann boundary value problem requirements in a one-dimensional problem. We consider V_N to be the subspace of V spanned by two different bases.

The first example uses Legendre Polynomials [5] as a basis.

$$\begin{aligned}\phi_1(x) &= P_0(x) = 1; & \phi'_1(x) &= 0; \\ \phi_2(x) &= P_1(x) = x; & \phi'_2(x) &= 1; \\ \phi_3(x) &= P_2(x) = \frac{1}{2}(3x^2 - 1); & \phi'_3(x) &= 3x; \\ \phi_4(x) &= P_3(x) = \frac{1}{2}(5x^3 - 3x); & \phi'_4(x) &= \frac{15}{2}x^2 - \frac{3}{2}; \\ \vdots & & \vdots & \\ \vdots & & \vdots & \\ \vdots & & \vdots & \end{aligned}$$

We then have

$$K_{ij} = B(\phi_i, \phi_j) = \int_{-1}^1 [\phi'_i \phi'_j + \phi_i \phi_j] dx$$

and

$$F_j = l(\phi_j) = \int_{-1}^1 x \phi_j dx.$$

Suppose that we take $N=2$. Then we obtain the set of simultaneous equations

$$\sum_{i=1}^2 K_{ij} a_i = F_j \quad \text{for } j=1 \text{ and } 2,$$

where

$$K_{11} = \int_{-1}^1 [\phi'_1 \phi'_1 + \phi_1 \phi_1] dx = \int_{-1}^1 1 dx = 2;$$

$$K_{21} = \int_{-1}^1 [\phi'_2 \phi'_1 + \phi_2 \phi_1] dx = \int_{-1}^1 x dx = 0;$$

$$K_{12} = \int_{-1}^1 [\phi'_1 \phi'_2 + \phi_1 \phi_2] dx = \int_{-1}^1 x dx = 0;$$

$$K_{22} = \int_{-1}^1 [\phi_2' \phi_2' + \phi_2 \phi_2] dx = \int_{-1}^1 (1+x^2) dx = \frac{8}{3};$$

$$F_1 = \int_{-1}^1 x \phi_1 dx = \int_{-1}^1 x dx = 0;$$

$$F_2 = \int_{-1}^1 x \phi_2 dx = \int_{-1}^1 x^2 dx = \frac{2}{3}.$$

Write this as a matrix equation:

$$2a_1 + 0a_2 = 0;$$

$$0a_1 + \frac{8}{3}a_2 = \frac{2}{3}.$$

It has solution $a_1 = 0$ and $a_2 = \frac{1}{4}$.

Thus, the approximate solution with $N=2$ is

$$y(x) = \frac{1}{4}x.$$

The exact solution to this problem is

$$y(x) = \left(\frac{e}{1+e^2} \right) [e^{-x} - e^x] + x.$$

This is compared with the approximate solution in Figure 2.1.1 .

Figure 2.1.1

Numerical(.) vs Exact(+) for $-y'' + y = x$ by using Legendre Poly. / $N = 2$

Suppose that we take $N=4$. Then we obtain the set of simultaneous equations

$$\sum_{i=1}^4 K_{ij} a_i = F_j \quad \text{for } j=1,2,3,4 .$$

Then the K_{ij} are

$$K_{11} = 2 , K_{21} = 0 , K_{31} = 0 , K_{41} = 0 ;$$

$$K_{12} = 0 , K_{22} = \frac{8}{3} , K_{32} = 0 , K_{42} = 2 ;$$

$$K_{13} = 0 , K_{23} = 0 , K_{33} = \frac{32}{5} , K_{43} = 0 ;$$

$$K_{14} = 0 , K_{24} = 2 , K_{34} = 0 , K_{44} = \frac{86}{7} ;$$

$$F_1 = 0 , F_2 = \frac{2}{3} , F_3 = 0 , F_4 = 0 .$$

The linear system is

$$2a_1 + 0a_2 + 0a_3 + 0a_4 = 0 ;$$

$$0a_1 + \frac{8}{3}a_2 + 0a_3 + 2a_4 = \frac{2}{3} ;$$

$$0a_1 + 0a_2 + \frac{32}{5}a_3 + 0a_4 = 0 ;$$

$$0a_1 + 2a_2 + 0a_3 + \frac{86}{7}a_4 = 0 ;$$

$$\text{or, } \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & \frac{8}{3} & 0 & 2 \\ 0 & 0 & \frac{32}{5} & 0 \\ 0 & 2 & 0 & \frac{86}{7} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{2}{3} \\ 0 \\ 0 \end{pmatrix}, \text{ with solution } \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{43}{151} \\ 0 \\ -\frac{7}{151} \end{pmatrix} .$$

Thus, the approximate solution for $N=4$ is

$$\begin{aligned} y(x) &= \frac{43}{151}x - \frac{7}{151} \left[\frac{1}{2}(5x^3 - 3x) \right] \\ &= -\frac{35}{302}x^3 + \frac{107}{302}x . \end{aligned}$$

The exact solution is compared with the approximate solution in Figure 2.1.2 .

Figure 2.1.2

Numerical(.) vs Exact(+) for $-y''+y = x$ by using Legendre Poly. / $N = 4$

Using Legendre Polynomials as a basis with $N=4$, the maximum error is computed to be ≈ 0.0066 .

According to the theory, the derivative of the approximate solution is supposed to converge to that of the exact solution. Here, the derivative of the approximate solution is compared with the derivative of the exact solution in Figure 2.1.3.

Figure 2.1.3

y' of Numerical(.) vs y' of Exact(+) by using Legendre Poly. / $N = 4$

The second example uses Fourier Cosine Series as a basis.

$$\begin{aligned}
 \phi_1(x) &= \cos\left[\frac{\pi}{2}(x+1)\right] ; & \phi'_1(x) &= -\frac{\pi}{2} \sin\left[\frac{\pi}{2}(x+1)\right]; \\
 \phi_2(x) &= \cos[\pi(x+1)] ; & \phi'_2(x) &= -\pi \sin[\pi(x+1)]; \\
 \phi_3(x) &= \cos\left[\frac{3\pi}{2}(x+1)\right] ; & \phi'_3(x) &= -\frac{3\pi}{2} \sin\left[\frac{3\pi}{2}(x+1)\right]; \\
 \phi_4(x) &= \cos[2\pi(x+1)] ; & \phi'_4(x) &= -2\pi \sin[2\pi(x+1)]; \\
 & \vdots & & \vdots \\
 & \vdots & & \vdots \\
 & \vdots & & \vdots
 \end{aligned}$$

We then have

$$K_{ij} = B(\phi_i, \phi_j) = \int_{-1}^1 [\phi'_i \phi'_j + \phi_i \phi_j] dx$$

and

$$F_j = I(\phi_j) = \int_{-1}^1 x \phi_j dx .$$

Let $t = \frac{x+1}{2}$, then $dt = \frac{1}{2} dx$. The integrals

$$\int_{-1}^1 \cos\left[n\pi\left(\frac{x+1}{2}\right)\right] \cos\left[m\pi\left(\frac{x+1}{2}\right)\right] dx = 2 \int_0^1 \cos(n\pi t) \cos(m\pi t) dt = \begin{cases} 0, & n \neq m \\ 1, & n = m \end{cases}$$

$$\int_{-1}^1 \sin\left[n\pi\left(\frac{x+1}{2}\right)\right] \sin\left[m\pi\left(\frac{x+1}{2}\right)\right] dx = 2 \int_0^1 \sin(n\pi t) \sin(m\pi t) dt = \begin{cases} 0, & n \neq m \\ 1, & n = m \end{cases}$$

and

$$\int_{-1}^1 \sin\left[n\pi\left(\frac{x+1}{2}\right)\right] \cos\left[m\pi\left(\frac{x+1}{2}\right)\right] dx = 2 \int_0^1 \sin(n\pi t) \cos(m\pi t) dt = 0 .$$

Suppose that we take $N=2$. Then we obtain the set of simultaneous equations

$$\sum_{i=1}^2 K_{ij} a_i = F_j \quad \text{for } j=1 \text{ and } 2 ,$$

where

$$K_{11} = \int_{-1}^1 [\phi_1' \phi_1' + \phi_1 \phi_1] dx = \frac{\pi^2}{4} + 1;$$

$$K_{21} = \int_{-1}^1 [\phi_2' \phi_1' + \phi_2 \phi_1] dx = 0;$$

$$K_{12} = \int_{-1}^1 [\phi_1' \phi_2' + \phi_1 \phi_2] dx = 0;$$

$$K_{22} = \int_{-1}^1 [\phi_2' \phi_2' + \phi_2 \phi_2] dx = \pi^2 + 1;$$

$$F_1 = \int_{-1}^1 x \phi_1 dx = -\frac{8}{\pi^2};$$

$$F_2 = \int_{-1}^1 x \phi_2 dx = 0.$$

The linear system is

$$\begin{pmatrix} \frac{\pi^2}{4} + 1 & 0 \\ 0 & \pi^2 + 1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} -\frac{8}{\pi^2} \\ 0 \end{pmatrix}, \text{ with solution } \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} -\frac{32}{\pi^2(\pi^2+4)} \\ 0 \end{pmatrix}.$$

Thus, the approximate solution with N=2 is

$$y(x) = -\frac{32}{\pi^2(\pi^2+4)} \cos[\pi(\frac{x+1}{2})].$$

The exact solution to this problem is

$$y(x) = \left(\frac{e}{1+e^2} \right) [e^{-x} - e^x] + x.$$

The exact solution is compared with the approximate solution in Figure 2.1.4 .

Figure 2.1.4

Numerical(.) vs Exact(+) for $-y''+y = x$ by using Fourier Series / $N = 2$

Suppose that we take $N=4$. Then we obtain the set of simultaneous equations

$$\sum_{i=1}^4 K_{ij}a_i = F_j \quad \text{for } j=1,2,3,4 ,$$

where

$$K_{11} = \frac{\pi^2}{4} + 1, K_{21} = 0, K_{31} = 0, K_{41} = 0;$$

$$K_{12} = 0, K_{22} = \pi^2 + 1, K_{32} = 0, K_{42} = 0;$$

$$K_{13} = 0, K_{23} = 0, K_{33} = \frac{9\pi^2}{4} + 1, K_{43} = 0;$$

$$K_{14} = 0, K_{24} = 0, K_{34} = 0, K_{44} = 4\pi^2 + 1;$$

$$F_1 = -\frac{8}{\pi^2}, F_2 = 0, F_3 = -\frac{8}{9\pi^2}, F_4 = 0 .$$

The linear system is

$$\begin{pmatrix} \frac{\pi^2}{4} + 1 & 0 & 0 & 0 \\ 0 & \pi^2 + 1 & 0 & 0 \\ 0 & 0 & \frac{9\pi^2}{4} + 1 & 0 \\ 0 & 0 & 0 & 4\pi^2 + 1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = \begin{pmatrix} -\frac{8}{\pi^2} \\ 0 \\ -\frac{8}{9\pi^2} \\ 0 \end{pmatrix},$$

which has solution

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = \begin{pmatrix} -\frac{8}{\pi^2(\pi^2+4)} \\ 0 \\ -\frac{8}{9\pi^2(9\pi^2+4)} \\ 0 \end{pmatrix}.$$

The approximate solution for N=4 is

$$y(x) = -\frac{32}{\pi^2(\pi^2+4)} \cos\left[\pi\left(\frac{x+1}{2}\right)\right] - \frac{32}{9\pi^2(9\pi^2+4)} \cos\left[3\pi\left(\frac{x+1}{2}\right)\right].$$

The exact solution is compared with the approximate solution in Figure 2.1.5 .

Figure 2.1.5

Numerical(.) vs Exact(+) for $-y''+y = x$ by using Fourier Series / N = 4

Using Fourier Cosine Series as a basis with N=4, the maximum error is computed to be ≈ 0.0058 .

Here, once again, the derivative of the approximate solution is compared with the derivative of the exact solution in Figure 2.1.6 .

Figure 2.1.6

y' of Numerical (.) vs y' of Exact(+) by using Fourier Series / $N = 4$

Section 2.2: Rayleigh-Ritz Method

In section 1.2, we discussed how an elliptic boundary-value problem of form

$$Au = f$$

defined over some domain Ω with boundary conditions

$$u|_{\Gamma_1} = g_1 \quad \text{and} \quad \frac{\partial u}{\partial n}\bigg|_{\Gamma_2} = g_2 \quad (5)$$

can be converted to an alternative form of a variational boundary-value problem. The variational boundary-value problem is to find

$$u \in V, \text{ which satisfies } B(u, v) = l(v) \text{ for all } v \in V. \quad (6)$$

Suppose the bilinear form in (6) is symmetric, that is,

$$B(u, v) = B(v, u) \quad \text{for all } u, v \in V.$$

We show below that the variational boundary-value problem is equivalent to a minimization problem in which we are required to find a function $u \in V$ which makes the value of a functional $J: V \rightarrow \mathbb{R}$ a minimum, that is,

$$J(u) \leq J(v) \quad \text{for all } v \in V, \quad (7)$$

where J is defined by

$$J(v) = \frac{1}{2} B(v, v) - l(v). \quad (8)$$

The method is called the Rayleigh-Ritz method [2,4,9], and it is very closely linked to the Galerkin method. It takes the minimization problem (7) as its starting-point, and just like the Galerkin method, this problem is posed in a finite-dimensional subspace. That is, we consider the problem of finding $u_N \in V_N$ such that

$$J(u_N) \leq J(v_N) \quad \text{for all } v_N \in V_N,$$

where V_N is a finite-dimensional subspace of V . If $\{\phi_k\}_{k=1}^N$ is a basis for V_N , then substitution of $v_N = \sum_{k=1}^N c_k \phi_k$ in the expression for J yields the function

$$\Phi(c_k) \equiv J(\sum_{k=1}^N c_k \phi_k),$$

which is a function of the N variables $c_1, c_2, \dots, c_N$. In order to minimize $J(v_N)$, therefore, we require that

$$\frac{\partial \Phi}{\partial c_k} = 0, \quad \text{for } k = 1, 2, \dots, N, \quad (9)$$

which yields a set of N simultaneous equations in the N variables $c_1, \dots, c_N$. Solution of these equations yields the components c_k of u_N . In particular, if J is defined by (8) then

$$\Phi(c_k) = \frac{1}{2} B\left(\sum_{i=1}^N c_i \phi_i, \sum_{j=1}^N c_j \phi_j\right) - l\left(\sum_{m=1}^N c_m \phi_m\right)$$

or,

$$\Phi(c_k) = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N B(\phi_i, \phi_j) c_i c_j - \sum_{m=1}^N F_m c_m \quad (10)$$

where $K_{ij} = B(\phi_i, \phi_j)$ and $F_m = l(\phi_m)$.

We now apply (9) on (10) to obtain the set of linear equations

$$\sum_{r=1}^N K_{rs} c_r = F_s, \quad s = 1, \dots, N$$

which is precisely the same as the linear system obtained by the Galerkin method. Here, though, K_{rs} is symmetric since $B(\cdot, \cdot)$ is symmetric.

In both the Galerkin method and the Rayleigh-Ritz method, if the set of basis functions $\{\phi_i\}_{i=1}^N$ is chosen in such a way that they are orthogonal with respect to the $L_2(\Omega)$ inner product, then the system of equations in both methods often simplify considerably. The purpose of this thesis is to construct a set of orthonormal functions on a standard simplex in R^3 so that one can take advantage of such simplifications.

CHAPTER 3

A basis for the tetrahedra

Section 3.1: Introduction

Our basis construction begins with the study of domains made up of parallelepipeds and tetrahedra in any orientation in $\mathbb{R}^3$.

We define two standard shapes, a standard cube and a standard simplex, as in Figure 3.1.1.

Figure 3.1.1

Standard cube (left) and Standard simplex (right)

Let $\underline{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$ represent the x , y , and z coordinates of any point in either of these

standard shapes. For any parallelepiped, we can choose any corner ; suppose that

$\underline{y}^i = \begin{bmatrix} i \\ y_1 \\ y_2 \\ y_3 \end{bmatrix}$ are defined to be the vertices at or adjacent to this corner of a parallelepiped for $i=1,2,3$ and 4; $\underline{y}^1$ is the corner and the $\underline{y}^i$ are the adjacent vertices; see Figure 3.1.2 .

Figure 3.1.2
Parallelepiped

Then the transformation $T : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ defined by

$$T(\underline{x}) = \underline{y}^1 + M\underline{x},$$

where M is a 3×3 matrix defined by

$$M = [(\underline{y}^2 - \underline{y}^1), (\underline{y}^3 - \underline{y}^1), (\underline{y}^4 - \underline{y}^1)],$$

will map the standard cube onto the parallelepiped taking $\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$ onto $\underline{y}^1$, $\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ onto $\underline{y}^2$,

$\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$ onto $\underline{y}^3$ and $\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$ onto $\underline{y}^4$. The mapping T is an affine transformation. see Figure 3.1.3 .

Figure 3.1.3

Standard cube (left) and Parallelepiped (right)

In a similar manner, suppose that $\underline{y}^i = \begin{bmatrix} y_1^i \\ y_2^i \\ y_3^i \end{bmatrix}$ are defined to be the vertices of any tetrahedron for $i=1,2,3$ and 4; see Figure 3.1.4 .

Figure 3.1.4

Tetrahedron

Then the transformation $T : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ defined by

$$T(\underline{x}) = \underline{y}^1 + M\underline{x} ,$$

where M is a 3×3 matrix defined by

$$M = [(\underline{y}^2 - \underline{y}^1), (\underline{y}^3 - \underline{y}^1), (\underline{y}^4 - \underline{y}^1)] ,$$

will map the standard simplex onto the tetrahedron , taking $\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$ onto $\underline{y}^1$, $\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ onto $\underline{y}^2$,

$\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$ onto $\underline{y}^3$, and $\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$ onto $\underline{y}^4$. The mapping T is again an affine transformation; see Figure

3.1.5 .

Figure 3.1.5

Standard simplex (left) and Tetrahedron (right)

For the purpose of this thesis, we focus our attention on tetrahedra.

Integrals over tetrahedra are approximated by using Gauss quadrature. Gaussian quadrature is done as follows: Special points s^r are known together with real numbers w^r so that the sum

$$\sum_r P(s^r) w^r = \int_0^1 P(s) ds$$

is exact for polynomial $P(s)$ of a suitable degree or less. We use 12 Gauss points, enabling us to exactly integrate polynomials of order 23 or less [10].

Pairs (s^p, s^q) of points have been computed, together with appropriate weights $w^{p,q}$ to give exact quadrature over the standard 2-simplex (triangle) for polynomials of degree 20 or less [10].

These methods of quadrature can be combined to give exact quadrature over the 3-simplex (standard tetrahedron) for polynomials of degree 20 or less. We use our Gaussian quadrature over the triangle and one-dimensional Gaussian quadrature as follows:

The integral of a polynomial $P(x,y,z)$ over the 3-simplex is

$$\int_0^1 \int_0^{1-x} \int_0^{1-x-y} P(x, y, z) dz dy dx .$$

The inner most integral can be done using one-dimensional Gaussian quadrature; the result is then a polynomial $q(x,y)$ which is at most one degree higher than that of P . The evaluation can then be completed by applying our Gaussian quadrature on triangles to the 2-simplex.

Suppose $f(\underline{y})$ is a polynomial in $\underline{y}$ where $\underline{y}$ is in any tetrahedron. Let T be an affine transformation mapping the standard simplex X onto Y . Then $f(T(\underline{x}))$ will also be a polynomial in $\underline{x}$ of the same order. If Q is the standard simplex and $T(Q)$ is the tetrahedron Y , change of variable in integration yields

$$\iiint_{T(Q)} f(\underline{y}) d\underline{y} = |\det(M)| \sum_p \sum_q \sum_r f(T(s^p, s^q, s^r)) w^{p,q,r},$$

where (s^p, s^q, s^r) are Gauss points in the 3-simplex and $w^{p,q,r}$ are the appropriate weights. Thus, Gaussian quadrature can be done on any tetrahedron.

We wish to construct a good set of basis functions for any tetrahedron. With our use of Gaussian quadrature to perform the integration, it is natural to select a polynomial basis. For computational reasons, it is desirable to find a set of polynomials $\{P(n, x, y, z)\}$, where $n=1,2,3 \dots$ that are ortho-normal in $L_2[3 - \text{simplex}]$ in the sense that the inner product

$$\int_0^1 \int_0^{1-x} \int_0^{1-x-y} P(n, x, y, z) P(m, x, y, z) dz dy dx = \begin{cases} 1 & \text{if } n = m \\ 0 & \text{if } n \neq m \end{cases}.$$

Section 3.2: A basis for the standard 3-simplex : Introduction

We seek an ortho-normal polynomial basis $\{P(n, x, y, z) \text{ with } n = 1, 2, \dots\}$ that spans the Hilbert space $L_2[3\text{-simplex}]$. We consider the question of how to introduce the basis functions of various orders.

Consider the Maclaurin Series expansion for a function $f(x, y, z)$ with all partial derivatives evaluated at $\langle 0, 0, 0 \rangle \equiv 0$. Then, the function $f(x, y, z)$ can be written as follows:

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

With no other information available about $f(x, y, z)$, assume that the partial derivatives of any particular order are about the same size. Then the terms involving the mixed partials in the expansion (with factors 2, 6, 3, ..., 12, ..., 6, ..., 4, ..., etc. in the coefficients) appear to be more important than those involving $f_{xx}, f_{yy}, f_{zz}, f_{xxx}, \dots, f_{xxxx}, \dots$, and so forth. For example, in the 3rd order terms, it would seem appropriate to first introduce xyz into the basis, then $\{x^2y, x^2z, y^2x, y^2z, z^2x, z^2y\}$ with equal importance and finally $\{x^3, y^3, z^3\}$ with equal importance.

Then we should be able to increase the number of basis functions used in the approximation arbitrarily, lessening the need for a new full order basis at each new approximation. These reasons remain valid under affine transformation. Thus, we assume that for any particular order of basis, we should initially introduce monomials $x^i y^j z^k$ 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. $\{x^2y, x^2z, y^2x, y^2z, z^2x, z^2y\}$.)

As an aid to study the problem, consider a triangular array of homogeneous monomials of each order with the numbers below each monomial representing the integer multiplier to be used in the Maclaurin expansion above. For any particular order, monomials with the same number under them identify those that would be included in the same set of monomials as described above. If we were to stack these triangles according to decreasing size, we would get the following triangular arrays (which we might call Pascal's Tetrahedron); see Figure 3.2.1 .

Order 0.

1

Order 1.

$$\begin{array}{c} x \\ 1 \\ y \quad \quad z \\ 1 \quad \quad 1 \end{array}$$

Order 2.

$$\begin{array}{ccccc} & & x^2 & & \\ & & 1 & & \\ & xy & & xz & \\ & 2 & & 2 & \\ y^2 & & yz & & z^2 \\ 1 & & 2 & & 1 \end{array}$$

Order 3.

$$\begin{array}{ccccccc}
 & & & x^3 & & & \\
 & & & 1 & & & \\
 & & yx^2 & & x^2z & & \\
 & & 3 & & 3 & & \\
 & y^2x & & xyz & & xz^2 & \\
 & 3 & & 6 & & 3 & \\
 y^3 & & y^2z & & yz^2 & & z^3 \\
 1 & & 3 & & 3 & & 1
 \end{array}$$

Order 4.

$$\begin{array}{ccccccccc}
 & & & & x^4 & & & & \\
 & & & & 1 & & & & \\
 & & & yx^3 & & x^3z & & & \\
 & & & 4 & & 4 & & & \\
 & & y^2x^2 & & x^2yz & & x^2z^2 & & \\
 & & 6 & & 12 & & 6 & & \\
 & y^3x & & y^2xz & & xyz^2 & & xz^3 & \\
 & 4 & & 12 & & 12 & & 4 & \\
 y^4 & & y^3z & & y^2z^2 & & yz^3 & & z^4 \\
 1 & & 4 & & 6 & & 4 & & 1
 \end{array}$$

Order 5.

$$\begin{array}{ccccccccccc}
 & & & & & x^5 & & & & & \\
 & & & & & 1 & & & & & \\
 & & & & yx^4 & & x^4z & & & & \\
 & & & & 5 & & 5 & & & & \\
 & & & y^2x^3 & & x^3yz & & x^3z^2 & & & \\
 & & & 10 & & 20 & & 10 & & & \\
 & & y^3x^2 & & y^2x^2z & & yx^2z^2 & & x^2z^3 & & \\
 & & 10 & & 30 & & 30 & & 10 & & \\
 & y^4x & & y^3xz & & y^2xz^2 & & xyz^3 & & xz^4 & \\
 & 5 & & 20 & & 30 & & 20 & & 5 & \\
 y^5 & & y^4z & & y^3z^2 & & y^2z^3 & & yz^4 & & z^5 \\
 1 & & 5 & & 10 & & 10 & & 5 & & 1
 \end{array}$$

.... and so forth

Figure 3.2.1

Pascal's Tetrahedron

We wish to minimize the number of functions that need to be generated. We construct an ortho-normal basis that requires just one function $B(x,y,z)$ for each of the classes described above. The group of permutations S_3 [3] acting on the arguments of these functions produces all the other basis functions.

Thus, for the classes with 3 members, $\{ B(x,y,z), B(y,z,x), B(z,x,y) \}$ is an ortho-normal set, also orthogonal to the basis functions generated previously. For the classes with 6 members, $\{ B(x,y,z), B(y,z,x), B(z,x,y), B(y,x,z), B(x,z,y), B(z,y,x) \}$, the result of the action of the full group S_3 of permutations on $B(x,y,z)$, produces an ortho-normal set, also orthogonal to the previously generated functions.

Two questions: First, given n , how many monomials of order n are there ? Second, given n , how many generating functions are needed so that the span of the set produced under the action of S_3 together with the lower order basis functions contains the monomials of order n ?

For example, order 3 has a total of 10 monomials that fall into 3 classes as mentioned above, namely, sets of 1 ($\{xyz\}$), 3 ($\{x^3, y^3, z^3\}$), and 6 ($\{x^2y, x^2z, y^2x, y^2z, z^2x, z^2y\}$). Under the action of S_3 , the symmetric group of permutations, we will need only 3 generating functions:

1. One generating function B_α , so that , together with the lower order basis functions , the monomial xyz is in its span.
2. Another generating function B_β , so that , B_β and the other two functions produced by permutating its arguments under S_3 , (together with lower order basis functions) contain x^3, y^3 and z^3 in their span.
3. Another generating function B_η , so that , B_η and the other 5 functions produced by permutating its arguments under S_3 , (together with lower order basis functions) contain $x^2y, x^2z, y^2x, y^2z, z^2x$, and z^2y in their span.

We can count the number of basis functions by counting the independent monomials that have the same span. Consider the monomials $x^{i_1}y^{i_2}z^{i_3}$ of order n . Finding the total number of monomials is equivalent to finding the number of ordered triples of nonnegative integer solutions of $i_1 + i_2 + i_3 = n$ that satisfy $0 \leq i_k \leq n$ for $k=1,2,3$. The solutions of the above question can be computed by the following theorem.

Theorem

The number of ordered k -tuples with unlimited repetition of non-negative integers summing to n is exactly $C(n+k-1, n)$ where $C(p, q)$ is the number of combinations of p objects taken q at a time [6].

Proof:

The number k -tuples with unlimited repetition is also equal to the number of sequences of length $n+k-1$, consisting of n symbols " $*$ " where n is the total number of objects, and $k-1$ symbols " $|$ " where k is the number of different types of objects. Suppose $n = 6$ and we have 3 types of objects; 2 of type 1, 3 of type 2, and 1 of type 3 (note: $2+3+1=6$). We represent this partition by string $** | *** | *$. More general partitions of k types with a total of n objects can also be represented by such strings as:

type 1	type 2	type 3	...	type k
**	***	*	...	**

The number of sequences of this kind can be computed by the following procedure:

1. Choosing n $*$ -positions in $C(n+k-1, n)$ ways.
2. Choose the $k-1$ $|$ -positions in $C(k-1, k-1)$ ways.

Thus, the total number of ways is $C(n+k-1, n) \cdot C(k-1, k-1) = C(n+k-1, n)$. ■

So, if $A = \{a_1, a_2, \dots, a_m\}$ consists of all nonnegative integer triples that are solutions of $i_1 + i_2 + i_3 = n$. Then

$$|A| = |C(n+3-1, n)| = |C(n+2, n)| = \left| \frac{(n+2)!}{2!n!} \right| = \left| \frac{(n+2)(n+1)}{2} \right|.$$

For example, the total number of monomials for $n=5$ is $\left| \frac{(5+2)(5+1)}{2} \right| = 21$. There are 21 monomials of order 5.

The second problem is to count how many generating functions are needed so that these functions, their images under the action of S_3 , and the lower order basis functions contain all these monomials in their span.

First, consider order 4 ($n=4$). Let the triples (i_1, i_2, i_3) be the powers of x , y , and z respectively. If we write out all possible ordered triples (i_1, i_2, i_3) summing to 4, we obtain the following grouped according to initial digit.

0,0,4		1,0,3		2,0,2		3,0,1		4,0,0
0,1,3		1,1,2		2,1,1		3,1,0		
0,2,2		1,2,1		2,2,0				
0,3,1		1,3,0						
0,4,0								
group 1	3	group 2	1	group 3		group 4		group 5

In order to generate the triples displayed in group 1, we need 3 generating functions to do so under the action of S_3 , one to generate the triples $\{(0,0,4), (0,4,0)\}$, one to generate the triples $\{(0,1,3), (0,3,1)\}$, and one to generate the triple $\{(0,2,2)\}$. To generate the triples with the arrangement in group 2, we need only 1 generating function to produce $\{(1,1,2), (1,2,1)\}$ because any triple with 0 as an entry has already been produced as a permutation of the triples in group 1. For example, triples $\{(1,0,3), (1,3,0)\}$ are images of $\{(0,1,3), (0,3,1)\}$ under S_3 . By the same argument, to generate the triples with the

arrangement in groups 3,4, and 5 we do not need any new generating functions because the triples that contain the 0's or 1's have already been generated by the previous generating functions in group 1 and 2. Thus, we need only introduce 4 generating functions (and their images under S_3) to the basis to generate the 4th order monomials.

Next, consider order 5 ($n=5$). The triples are organized as follows:

In order to generate the triples in group 1, we need 3 generating functions to do so under the actions of S_3 , one to generate the triples $\{(0,0,5),(0,5,0)\}$, one to generate the triples $\{(0,1,4),(0,4,1)\}$, and one to generate the triples $\{(0,2,3),(0,3,2)\}$. To generate the triples with the arrangement in group 2, we need only 2 generating functions, one for the triples $\{(1,1,3),(1,3,1)\}$ and one for the triple $\{(1,2,2)\}$, because any triple with 0 in it is a permutation on a triple in group 1. The triples in groups 3,4,5, and 6 are permutations of those in groups 1 and 2. Referring back to monomials, this analysis shows that we need introduce only 5 monomials so that their image under S_3 consists of all 5th order monomials.

Now, if we are to write out the numbers of generating functions required for any particular order by the above argument, we obtain Table 3.2.1 as follows:

Table 3.2.1

The numbers of generating functions required for any order n

<u>order</u>	<u>group 1</u>	<u>group 2</u>	<u>group 3</u>	...	
{ n = 0 n = 1 n = 2	1				
	1				
	2				
{ n = 3 n = 4 n = 5	2	+	1		
	3	+	1		
	3	+	2		
{ n = 6 n = 7 n = 8	4	+	2	+	1
	4	+	3	+	1
	5	+	3	+	2
		.			
		.			
		.			

As we can see from Table 3.2.1 above, any two consecutive orders, from an even to an odd order, contain the same numbers of generating functions in group 1. For any two consecutive orders, from an odd to an even order, the even order always has one more generating function than that of the odd order for the first group. Since group 1 contains a total of $(n+1)$ triples, we need an integer function $\left\lceil \frac{n+1}{2} \right\rceil$ for $n=0,1,2,\dots$ in order to accommodate this behavior. Similar type of argument holds for group 2,3,... . Thus, we can generalize to order n as follows: see Figure 3.2.2 .

Figure 3.2.2

Generalization for the numbers of generating functions required for any order n

So, in order to generate the triples with the arrangement in group 1, we need $\left\lceil \frac{n+1}{2} \right\rceil$ generating functions. Since any triples that contains 0 are permutations of the generating

functions in group 1, we need only $\left\lceil \frac{n-2}{2} \right\rceil$ generating functions for group 2. Likewise, any triples that contains 0's or 1's are permutations of the previous generating functions in group 1 and group 2; we need only $\left\lceil \frac{n-5}{2} \right\rceil$ generating functions for group 3 and so on.

From the pattern of the number of generating functions for each group above, it can be shown that the counting function $\left\lceil \frac{(n+1)-3(i)}{2} \right\rceil$ for $i = 0, 1, 2, \dots$ is the desired function by the following argument.

Group 1 contains a total of $(n+1)$ triples. Group 2 contains 3 triples less than Group 1 because Group 2 only has n triples to start with and the triple at the top and the triple at the bottom contain 0's. Therefore, Group 2 has only $(n+1)-3$ triples. Group 3 contains 6 triples less than Group 2 because Group 3 only has $(n-1)$ triples to start with and the two triples at the top and the two triples at the bottom contain 0's or 1's. Therefore, Group 3 has only $(n+1)-6$ triples. The same pattern holds for Groups 4, 5, ... and so on. The number of generating functions required to generate all triples for order n can be obtained by the following function $P_3(n)$, the number of partitions of n into 3 parts or less,

$$P_3(n) = \sum_{i=0}^{g(n)} \left\lceil \frac{(n+1)-3(i)}{2} \right\rceil,$$

where $g(n)$ is discussed below.

The only remaining question is that what should be the upper index function $g(n)$ in order to terminate the sum. Note from Table 1 above, the sum contains only 1 term for $n=0, 1$, and 2, contains 2 terms for $n=3, 4$, and 5, contains 3 terms for $n=6, 7$, and 8, and etc. Function $g(n) \equiv \left\lceil \frac{n-2}{3} \right\rceil$ gives an appropriate upper index to terminate the sum. Thus, the number of generating functions required to generate all triples for order n can be computed by the following counting function $P_3(n)$:

$$P_3(n) = \sum_{i=0}^{\lceil \frac{n-2}{3} \rceil} \left\lceil \frac{(n+1)-3(i)}{2} \right\rceil.$$

Consider function $f(x) = \frac{1}{1-x} - \frac{1}{1-x^2} + \frac{1}{1-x^3}$. Dr. Edward Schmeichel noted that the number of generating functions is precisely the coefficient of x^n of the function $f(x)$ above, expressed as an infinite series. We express this in partial fraction form as

$$\frac{1}{1-x} - \frac{1}{1-x^2} + \frac{1}{1-x^3} = \frac{A}{(1-x)} + \frac{B}{(1-x)^2} + \frac{C}{(1-x)^3} + \frac{D}{(1+x)} + \frac{E}{(\omega-x)} + \frac{F}{(\bar{\omega}-x)},$$

where ω is $e^{i\pi/3}$, as suggested by the number theory seminar at S.J.S.U. Expressing these as infinite series, the coefficient of x^n is

$$[A + (n+1)B + \frac{(n+1)(n+2)}{2}C + (-1)^n D + (\bar{\omega})^{n+1}E + (\omega)^{n+1}F].$$

Then the coefficients of A,B,C,D, and E are computed to give the following formula:

$$P_3(n) = \frac{47}{72} + \frac{n}{2} + \frac{(-1)^n}{8} + \frac{n^2}{12} + \frac{2}{9} \begin{cases} 1 & \text{if } n = 0 \pmod{3} \\ -\frac{1}{2} & \text{otherwise} \end{cases}$$

where $P_3(n)$ is a counting function for the number of generating functions needed for any particular order n [6].

Here, let $N_m(n)$ = number of monomials of order n , $\sum_{k=0}^n N_m(k)$ = total number of basis functions needed so that polynomials of order n or less are in their span, and

$\sum_{k=0}^n P_3(k)$ = number of generating functions such that, under S_3 , we have a basis for polynomials of order n or less. We show a table of order 0 up to 15 of

$P_3(n)$, $N_m(n)$, $\sum_{k=0}^n N_m(k)$, and $\sum_{k=0}^n P_3(k)$ as follows:

Table 3.3.2
Results of order 0 up to 15

<u>order</u>	$P_3(n)$	$N_m(n)$	$\sum_{k=0}^n N_m(k)$	$\sum_{k=0}^n P_3(k)$
$n = 0$	1	1	1	1
$n = 1$	1	3	4	2
$n = 2$	2	6	10	4
$n = 3$	3	10	20	7
$n = 4$	4	15	35	11
$n = 5$	5	21	56	16
$n = 6$	7	28	84	23
$n = 7$	8	36	120	31
$n = 8$	10	45	165	41
$n = 9$	12	55	220	53
$n = 10$	14	66	286	67
$n = 11$	16	78	364	83
$n = 12$	19	91	455	102
$n = 13$	21	105	560	123
$n = 14$	24	120	680	147
$n = 15$	27	136	816	174

Thus, for example, when $n = 5$, we need generate only 16 functions to obtain the 56 functions necessary to contain all fifth degree polynomials in their span; see Table 3.3.2 .

Section 3.3: A basis for the standard 3-simplex : Theory

Each member of the permutation group S_3 induces a linear transformation on the space $R[x,y,z]$ of polynomials in x , y , and z .

We let T be the permutation (x,y,z) ; T acts on the monomial $x^i y^j z^k$ by

$$T : x^i y^j z^k \rightarrow y^i z^j x^k .$$

Then $T^2(x^i y^j z^k) = T(y^i z^j x^k) = z^i x^j y^k$ and $T^3(x^i y^j z^k) = (x^i y^j z^k)$ is the identity. We extend T linearly to polynomials. For example, T acts on polynomial $2x^2 yz + 3xz$ in the following way:

$$\begin{aligned} T(2x^2 yz + 3xz) &= T(2x^2 y^1 z^1 + 3x^1 y^0 z^1) = 2T(x^2 y^1 z^1) + 3T(x^1 y^0 z^1) \\ &= 2y^2 z^1 x^1 + 3y^1 z^0 x^1 \\ &= 2y^2 zx + 3yx . \end{aligned}$$

Transformation P_{xy} corresponds to permutation (x,y) ; P_{yz} corresponds to permutation (y,z) and P_{zx} corresponds to permutation (z,x) . Note that $TP_{xy} = P_{zx}$, $T^2 P_{xy} = P_{yz}$. These are the same relations as in S_3 , so we also use S_3 to denote this group of transformations. We give the multiplication table (Figure 3.3.1) below for S_3 : $T^3 = I = \text{identity}$.

•	I	T^1	T^2	P^1	$T^1 P^1$	$T^2 P^1$
I	I	T^1	T^2	P^1	$T^1 P^1$	$T^2 P^1$
T^1	T^1	T^2	I	$T^1 P^1$	$T^2 P^1$	P^1
T^2	T^2	I	T^1	$T^2 P^1$	P^1	$T^1 P^1$
P^1	P^1	$T^2 P^1$	$T^1 P^1$	I	T^2	T^1
$T^1 P^1$	$T^1 P^1$	P^1	$T^2 P^1$	T^1	I	T^2
$T^2 P^1$	$T^2 P^1$	$T^1 P^1$	P^1	T^2	T^1	I

Figure 3.3.1

Multiplication table for S_3

Bold face x represents a typical monomial $x^i y^j z^k$ associated with any triple of non-negative integers $\langle i, j, k \rangle$. Given any x , with $P \equiv P_{xy}$, the set of permutations of x can be given by $\{x, Tx, T^2x, Px, TPx, T^2Px\}$, where there will be duplicates if the set has only 3 or 1 member (see Figure 3.2.1).

For any particular order in 'Pascal's Tetrahedron' above, monomials belonging in the same set (those with the same number below them) correspond to all permutations of such a triple $\langle i, j, k \rangle$. 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. In the Maclaurin expansion for any $f(x, y, z)$, the coefficient accompanying any $x^i y^j z^k$ is

$\frac{1}{i!j!k!} \cdot \frac{\partial^{i+j+k} f}{\partial x^i \partial y^j \partial z^k}(0)$; these are combined due to equality of mixed partials to obtain

$\frac{(i+j+k)!}{i!j!k!}$ duplicates; these are the numbers under the monomials in 'Pascal's Tetrahedron' above.

The integral of monomials $x^p y^q z^r$ over the standard 3-simplex,

$$\int_0^1 \int_0^{1-x} \int_0^{1-x-y} x^p y^q z^r dz dy dx,$$

is $\frac{p!q!r!}{(p+q+r+3)!}$. We show this by using integration by parts and a recursive argument.

$$\begin{aligned} & \int_0^1 \int_0^{1-x} \int_0^{1-x-y} x^p y^q z^r dz dy dx \\ &= \int_0^1 \int_0^{1-x} x^p y^q \left[\int_0^{1-x-y} z^r dz \right] dy dx \\ &= \frac{1}{r+1} \int_0^1 \int_0^{1-x} x^p y^q (1-x-y)^{r+1} dy dx \\ &= \frac{1}{r+1} \int_0^1 x^p \left[\int_0^{1-x} y^q (1-x-y)^{r+1} dy \right] dx. \end{aligned}$$

To evaluate the inner integral, let $u = y^p$ and $dv = (1 - x - y)^{r+1} dy$, integration by parts we obtain

$$= \frac{q}{(r+1)(r+2)} \int_0^1 x^p \left[\int_0^{1-x} y^{q-1} (1-x-y)^{r+2} dy \right] dx.$$

Using integration by parts again, we obtain

$$= \frac{q(q-1)}{(r+1)(r+2)(r+3)} \int_0^1 x^p \left[\int_0^{1-x} y^{q-2} (1-x-y)^{r+3} dy \right] dx.$$

Notice a recursive relationship for the integral with respect to y above as we use integration by parts over and over again. This recursiveness terminates if the power of y is 0. Namely,

$$\begin{aligned} &= \frac{q(q-1)\cdots 1}{(r+1)(r+2)(r+3)\cdots(r+q+1)} \int_0^1 x^p \left[\int_0^{1-x} y^{q-q} (1-x-y)^{r+q+1} dy \right] dx \\ &= \frac{q(q-1)\cdots 1}{(r+1)(r+2)(r+3)\cdots(r+q+1)(r+q+2)} \int_0^1 x^p (1-x)^{r+q+2} dx. \end{aligned}$$

For the integral with respect to x , let $u = x^p$ and $dv = (1-x)^{r+q+2} dx$, integration by parts we obtain

$$= \frac{[q(q-1)\cdots 1] p}{(r+1)(r+2)(r+3)\cdots(r+q+1)(r+q+2)(r+q+3)} \int_0^1 x^{p-1} (1-x)^{r+q+3} dx.$$

Similarly, using integration by parts for the integral with respect to x , we obtain the recursiveness once again. This terminates if the power of x is 0. Namely,

$$\begin{aligned} &= \frac{[q(q-1)\cdots 1] p(p-1)\cdots 1}{(r+1)(r+2)(r+3)\cdots(r+q+1)(r+q+2)(r+q+3)(r+q+4)\cdots(r+q+p+2)} \int_0^1 x^{p-p} (1-x)^{r+q+p+2} dx \\ &= \frac{[q(q-1)\cdots 1] [p(p-1)\cdots 1]}{(r+1)(r+2)(r+3)\cdots(r+q+1)(r+q+2)(r+q+3)(r+q+4)\cdots(r+q+p+2)(r+q+p+3)} \\ &= \frac{r! [q(q-1)\cdots 1] [p(p-1)\cdots 1]}{r!(r+1)(r+2)(r+3)\cdots(r+q+1)(r+q+2)(r+q+3)(r+q+4)\cdots(r+q+p+2)(r+q+p+3)} \\ &= \frac{p! q! r!}{(p+q+r+3)!}. \end{aligned}$$

This symmetry means that the integral depends only on $\{p,q,r\}$; any permutation of the monomial produces the same integral. This observation can be used to prove the following lemma, expressed in terms of the $L_2(\text{simplex})$ inner product $\langle \bullet, \bullet \rangle$.

Lemma 3.3.1 For any polynomials G and $H \in R[x,y,z]$:

1. For any $R \in S_3$, $\langle RG, RH \rangle = \langle G, H \rangle$.
2. For any $R \in S_3$, $\langle RG, H \rangle = \langle G, R^{-1}H \rangle$.
3. $\langle G, TG \rangle = \langle G, T^2G \rangle = \langle TG, T^2G \rangle$.
4. For any $R \in S_3$, if 1 is the polynomial identically 1, then $\langle RG, 1 \rangle = \langle G, 1 \rangle$ when G is any monomial.

Proof

(1):

For any polynomials G and $H \in R[x,y,z]$, if $R \in S_3$, then $\langle RG, RH \rangle = \langle G, H \rangle$.

By bilinearity of the inner product, it suffices to prove the result for monomials G and H . Let $G = x^{p_1} y^{q_1} z^{r_1}$ and $H = x^{p_2} y^{q_2} z^{r_2}$. Since $R \in S_3$, this implies that $R \in \{T, T^2, T^3, P, TP, T^2P\}$. Suppose that $R=T$. This implies that

$$RG = TG = T(x^{p_1} y^{q_1} z^{r_1}) = y^{p_1} z^{q_1} x^{r_1} \text{ and}$$

$$RH = TH = T(x^{p_2} y^{q_2} z^{r_2}) = y^{p_2} z^{q_2} x^{r_2}.$$

Thus,

$$\begin{aligned} \langle G, H \rangle &= \int_0^1 \int_0^{1-x} \int_0^{1-x-y} (x^{p_1} y^{q_1} z^{r_1}) (x^{p_2} y^{q_2} z^{r_2}) dz dy dx \\ &= \int_0^1 \int_0^{1-x} \int_0^{1-x-y} (x^{p_1+p_2} y^{q_1+q_2} z^{r_1+r_2}) dz dy dx \\ &= \frac{(p_1+p_2)!(q_1+q_2)!(r_1+r_2)!}{[(p_1+p_2)+(q_1+q_2)+(r_1+r_2)+3]!} \end{aligned}$$

and

$$\begin{aligned}
\langle RG, RH \rangle &= \int_0^1 \int_0^{1-x} \int_0^{1-x-y} (y^{p_1} z^{q_1} x^{r_1}) (y^{p_2} z^{q_2} x^{r_2}) dz dy dx \\
&= \int_0^1 \int_0^{1-x} \int_0^{1-x-y} (y^{p_1+p_2} z^{q_1+q_2} x^{r_1+r_2}) dz dy dx \\
&= \frac{(r_1+r_2)!(p_1+p_2)!(q_1+q_2)!}{[(r_1+r_2)+(p_1+p_2)+(q_1+q_2)+3]!} .
\end{aligned}$$

Therefore, $\langle RG, RH \rangle = \langle G, H \rangle$.

Similar argument holds for $R = T^2$, $R = T^3$, $R = P$, $R = TP$, and $R = T^2P$ because all we are doing is permutating the x , y , and z around and the order of p , q , and r in $\frac{p!q!r!}{(p+q+r+3)!}$ is irrelevant.

(2):

$$\text{By (1), } \langle RG, H \rangle = \langle R^{-1}RG, R^{-1}H \rangle = \langle G, R^{-1}H \rangle.$$

(3):

$$\begin{aligned}
\text{By (1), } \langle G, TG \rangle &= \langle T^2G, T^2TG \rangle = \langle T^2G, G \rangle = \langle G, T^2G \rangle; \\
\langle G, TG \rangle &= \langle TG, TTG \rangle = \langle TG, T^2G \rangle; \\
\langle G, T^2G \rangle &= \langle T^2G, T^2T^2G \rangle = \langle T^2G, TG \rangle = \langle TG, T^2G \rangle.
\end{aligned}$$

(4):

$$\text{By (1), } \langle RG, 1 \rangle = \langle R^{-1}RG, R^{-1}1 \rangle = \langle G, 1 \rangle. \quad \blacksquare$$

CHAPTER 4

Basis Construction

Section 4.1: Basis Construction

With Lemma 3.3.1 established in section 3.3, we begin to construct an ortho-normal basis. Since the volume of the standard 3-simplex is $\frac{1}{3!} = \frac{1}{6}$, we have, for the constant basis function,

$$B_1(x, y, z) = \sqrt{6}.$$

We construct B_2 , which together with TB_2 , T^2B_2 and B_1 will contain $\{x, y, z\}$ in its span. Set $x = x^1y^0z^0 = x$;

$$Tx = y^1z^0x^0 = y;$$

$$T^2x = z^1x^0y^0 = z.$$

We first seek b_1, b_2 and d such that if

$$G(x) = x + b_1Tx + b_2T^2x + dB_1,$$

then $\{G(x), G(T(x)), G(T^2(x)), B_1\} = \{G(x), TG(x), T^2G(x), B_1\}$ are pairwise orthogonal.

Set $H(x) = x + b_1Tx + b_2T^2x$. Then $G(x) = H(x) + dB_1$. The first requirement is that $G(x)$, $TG(x)$, and $T^2G(x)$ be orthogonal to B_1 . So, we need

$$0 = \langle H(x) + dB_1, B_1 \rangle = \langle H(x), B_1 \rangle + d;$$

$$0 = \langle TH(x) + dB_1, B_1 \rangle = \langle TH(x), B_1 \rangle + d;$$

$$0 = \langle T^2H(x) + dB_1, B_1 \rangle = \langle T^2H(x), B_1 \rangle + d.$$

Since $B_1 = \sqrt{6}$ is a constant, by lemma 3.3.1(4), these are all the same equation because

$$\langle TH(x), B_1 \rangle + d = \langle H(x), B_1 \rangle + d \quad \text{and}$$

$$\langle T^2H(x), B_1 \rangle + d = \langle H(x), B_1 \rangle + d.$$

Thus, we need only set $d = -\langle H(x), B_1 \rangle$ once $H(x)$ is determined.

Next we need $G(x)$ to be orthogonal to $TG(x)$, and $T^2G(x)$. i.e.

- (i) $0 = \langle H(\mathbf{x}) + dB_1, TH(\mathbf{x}) + dB_1 \rangle;$
- (ii) $0 = \langle H(\mathbf{x}) + dB_1, T^2H(\mathbf{x}) + dB_1 \rangle;$
- (iii) $0 = \langle TH(\mathbf{x}) + dB_1, T^2H(\mathbf{x}) + dB_1 \rangle.$

Upon substituting for d and using lemma 3.3.1, we find that these three requirements are met by just the one equation

$$\langle H(\mathbf{x}), TH(\mathbf{x}) \rangle = \langle H(\mathbf{x}), B_1 \rangle^2.$$

For example, expand (i) to get

$$\begin{aligned} \text{(i)} \quad & \langle H(\mathbf{x}) + dB_1, TH(\mathbf{x}) + dB_1 \rangle \\ &= \langle H(\mathbf{x}), TH(\mathbf{x}) \rangle + d\langle B_1, TH(\mathbf{x}) \rangle + d\langle H(\mathbf{x}), B_1 \rangle + d^2 \\ &= \langle H(\mathbf{x}), TH(\mathbf{x}) \rangle + d\langle B_1, H(\mathbf{x}) \rangle + d\langle H(\mathbf{x}), B_1 \rangle + d^2 \\ &= \langle H(\mathbf{x}), TH(\mathbf{x}) \rangle + 2d\langle H(\mathbf{x}), B_1 \rangle + d^2. \end{aligned}$$

If $\langle H(\mathbf{x}), TH(\mathbf{x}) \rangle = \langle H(\mathbf{x}), B_1 \rangle^2$, then we have

$$\begin{aligned} \langle H(\mathbf{x}), TH(\mathbf{x}) \rangle + 2d\langle H(\mathbf{x}), B_1 \rangle + d^2 &= \langle H(\mathbf{x}), B_1 \rangle^2 + 2d\langle H(\mathbf{x}), B_1 \rangle + d^2 \\ &= (\langle H(\mathbf{x}), B_1 \rangle + d)^2. \end{aligned}$$

Since we will set $d = -\langle H(\mathbf{x}), B_1 \rangle$, $(\langle H(\mathbf{x}), B_1 \rangle + d)^2 = 0$.

Similar argument holds for (ii) and (iii). Thus, if $\langle H(\mathbf{x}), TH(\mathbf{x}) \rangle = \langle H(\mathbf{x}), B_1 \rangle^2$, we can satisfy all 3 cases above.

The equation $\langle H(\mathbf{x}), TH(\mathbf{x}) \rangle = \langle H(\mathbf{x}), B_1 \rangle^2$ is a quadratic expression in unknowns b_1 and b_2 , thus, in fact, there is a one-parameter class of solutions, any one of which would produce a suitable $B_2(x, y, z)$. However, note that here we seek only to have B_2, TB_2 and T^2B_2 be an orthonormal set. When we consider the problem of constructing B_6 with a linear combination of $\{x^2y, x^2z, y^2x, y^2z, z^2x, z^2y\} +$ (a linear combination of previous basis functions) , we would like B_6 to provide six orthonormal basis functions generated under the action of S_3 . Then the set of basis functions generated by B_6 would be invariant under the full action of S_3 . So if we also require that

$\{B_2, TB_2, T^2B_2\}$ be invariant under S_3 , the extra degree of freedom is eliminated as follows:

Un-normalized B_2 and its images under T and T^2 are

$$B_2(x, y, z) = x + b_1y + b_2z + dB_1;$$

$$TB_2(x, y, z) = y + b_1z + b_2x + dB_1;$$

$$T^2B_2(x, y, z) = z + b_1x + b_2y + dB_1 .$$

These are already an invariant set under T and T^2 . For these to also be an invariant set under P_{xy} , they would have to constitute the same set as

$$PB_2(x, y, z) = y + b_1x + b_2z + dB_1;$$

$$PTB_2(x, y, z) = x + b_1z + b_2y + dB_1;$$

$$PT^2B_2(x, y, z) = z + b_1y + b_2x + dB_1 .$$

If we set $b_1 = 1$, then $PB_2 = B_2$, $PTB_2 = T^2B_2$, and $PT^2B_2 = TB_2$. With this substitution, the set is invariant under $P_{xz} = TP_{xy}$ and $P_{yz} = T^2P_{xy}$.

So, setting $b_1 = 1$, we then solve the equation

$$\langle H(x), TH(x) \rangle = \langle H(x), B_1 \rangle^2,$$

which is a quadratic expression in b_2 . One root is $b_2 = 0$ and we use this value. We require that $d = -\langle H(x), B_1 \rangle$; we obtain $d = -\frac{\sqrt{6}}{12}$. The un-normalized B_2 is $B_2 = k(2x + 2y - 1)$ with normalizer k . Finally, to normalize B_2 so that $\langle B_2, B_2 \rangle = 1$, we need $k = \sqrt{30}$. Thus,

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

To construct B_3 , let $x = x^0y^1z^1 = yz$;

$$Tx = y^0z^1x^1 = xz;$$

$$T^2x = z^0x^1y^1 = xy .$$

We seek b_1, b_2, a_0, a_1, a_2 and d such that if

$$G(x) = x + b_1Tx + b_2T^2x + a_0B_2 + a_1TB_2 + a_2T^2B_2 + dB_1 ,$$

then $G(\mathbf{x}), TG(\mathbf{x}), T^2G(\mathbf{x}), B_2, TB_2, T^2B_2$, and B_1 are pairwise orthogonal. Set $H(\mathbf{x}) = \mathbf{x} + b_1T\mathbf{x} + b_2T^2\mathbf{x}$ and $\tilde{B}_2 = a_0B_2 + a_1TB_2 + a_2T^2B_2$. Then $G(\mathbf{x}) = H(\mathbf{x}) + \tilde{B}_2 + dB_1$. The first requirement is that $G(\mathbf{x}), TG(\mathbf{x})$, and $T^2G(\mathbf{x})$ be orthogonal to B_1 . So, we need

$$\begin{aligned} 0 &= \langle H(\mathbf{x}) + \tilde{B}_2 + dB_1, B_1 \rangle = \langle H(\mathbf{x}), B_1 \rangle + d; \\ 0 &= \langle TH(\mathbf{x}) + T\tilde{B}_2 + dB_1, B_1 \rangle = \langle TH(\mathbf{x}), B_1 \rangle + d; \\ 0 &= \langle T^2H(\mathbf{x}) + T^2\tilde{B}_2 + dB_1, B_1 \rangle = \langle T^2H(\mathbf{x}), B_1 \rangle + d, \end{aligned}$$

where we use the fact that $\langle T^i\tilde{B}_2, B_1 \rangle = 0$ for $i = 0, 1, 2$.

Since $B_1 = \sqrt{6}$ is a constant, by lemma 3.3.1(4), these are once again all the same equation because

$$\begin{aligned} \langle TH(\mathbf{x}), B_1 \rangle + d &= \langle H(\mathbf{x}), B_1 \rangle + d \quad \text{and} \\ \langle T^2H(\mathbf{x}), B_1 \rangle + d &= \langle H(\mathbf{x}), B_1 \rangle + d. \end{aligned}$$

Thus, we need only set $d = -\langle H(\mathbf{x}), B_1 \rangle$ once $H(\mathbf{x})$ is determined.

Next we need $G(\mathbf{x}), TG(\mathbf{x})$, and $T^2G(\mathbf{x})$ to be orthogonal to T^iB_2 for $i = 0, 1, 2$. So, we need

$$\begin{aligned} \text{(i)} \quad 0 &= \langle H(\mathbf{x}) + \tilde{B}_2 + dB_1, T^iB_2 \rangle = \langle H(\mathbf{x}), T^iB_2 \rangle + a_i; \\ \text{(ii)} \quad 0 &= \langle TH(\mathbf{x}) + T\tilde{B}_2 + dB_1, T^iB_2 \rangle = \langle TH(\mathbf{x}), T^iB_2 \rangle + a_{[i-1(\bmod 3)]}; \\ \text{(iii)} \quad 0 &= \langle T^2H(\mathbf{x}) + T^2\tilde{B}_2 + dB_1, T^iB_2 \rangle = \langle T^2H(\mathbf{x}), T^iB_2 \rangle + a_{[i-2(\bmod 3)]}. \end{aligned}$$

Using lemma 3.3.1, we show that these 9 equations reduce to the following three

$$\begin{aligned} \text{(iv)} \quad 0 &= \langle H(\mathbf{x}) + \tilde{B}_2 + dB_1, B_2 \rangle = \langle H(\mathbf{x}), B_2 \rangle + a_0; \\ \text{(v)} \quad 0 &= \langle TH(\mathbf{x}) + T\tilde{B}_2 + dB_1, B_2 \rangle = \langle TH(\mathbf{x}), B_2 \rangle + a_2; \\ \text{(vi)} \quad 0 &= \langle T^2H(\mathbf{x}) + T^2\tilde{B}_2 + dB_1, B_2 \rangle = \langle T^2H(\mathbf{x}), B_2 \rangle + a_1. \end{aligned}$$

For example, expanding (i) we get

$$\begin{aligned} \text{(i)} \quad 0 &= \langle H(\mathbf{x}) + \tilde{B}_2 + dB_1, T^iB_2 \rangle \\ &= \langle H(\mathbf{x}), T^iB_2 \rangle + a_i \quad \text{for } i = 0, 1, 2. \end{aligned}$$

By using the unitary properties of T ($T^{-1} = T^*$), we get equations

$$\begin{aligned} 0 &= \langle H(\mathbf{x}), B_2(\mathbf{y}) \rangle + a_0; \\ 0 &= \langle H(\mathbf{x}), TB_2(\mathbf{y}) \rangle + a_1 = \langle T^2 H(\mathbf{x}), B_2(\mathbf{y}) \rangle + a_1; \\ 0 &= \langle H(\mathbf{x}), T^2 B_2(\mathbf{y}) \rangle + a_2 = \langle TH(\mathbf{x}), B_2(\mathbf{y}) \rangle + a_2. \end{aligned}$$

But these are just (iv), (vi), and (v).

A similar argument holds for (ii) and (iii). Thus, a_0, a_1 , and a_2 are uniquely determined once $H(\mathbf{x})$ is known: they will be affine functions of form $a_i = \beta_0^i + \beta_1^i b_1 + \beta_2^i b_2$.

There remains the problem of finding b_1 and b_2 such that $\{G(\mathbf{x}), TG(\mathbf{x}), T^2 G(\mathbf{x})\}$ are pairwise orthogonal. By lemma 3.3.1(3),

$$\langle G(\mathbf{x}), TG(\mathbf{x}) \rangle = \langle G(\mathbf{x}), T^2 G(\mathbf{x}) \rangle = \langle TG(\mathbf{x}), T^2 G(\mathbf{x}) \rangle.$$

Recall that with the substitution above for a_i and d , the members of set $\{G(\mathbf{x}), TG(\mathbf{x}), T^2 G(\mathbf{x})\}$ are orthogonal to the span of $\{B_2, TB_2, T^2 B_2, B_1\}$. Hence it suffices to establish that $\langle G(\mathbf{x}), TG(\mathbf{x}) \rangle = \langle G(\mathbf{x}), TH(\mathbf{x}) \rangle = 0$. Now with the substitution above and lemma 3.2.1(2), we obtain

$$\begin{aligned} \langle G(\mathbf{x}), TH(\mathbf{x}) \rangle &= \langle H(\mathbf{x}) + a_0 B_2 + a_1 TB_2 + a_2 T^2 B_2 + dB_1, TH(\mathbf{x}) \rangle \\ &= \langle H(\mathbf{x}), TH(\mathbf{x}) \rangle + a_0 \langle B_2, TH(\mathbf{x}) \rangle + a_1 \langle TB_2, TH(\mathbf{x}) \rangle + \\ &\quad a_2 \langle T^2 B_2, TH(\mathbf{x}) \rangle + d \langle B_1, TH(\mathbf{x}) \rangle \\ &= \langle H(\mathbf{x}), TH(\mathbf{x}) \rangle - a_0 a_2 - a_1 a_0 - a_2 a_1 - d^2. \end{aligned}$$

Thus, setting $0 = \langle H(\mathbf{x}), TH(\mathbf{x}) \rangle - a_0 a_2 - a_1 a_0 - a_2 a_1 - d^2$, we get a quadratic expression in b_1 and b_2 , and thus a one-parameter class of formulae for B_3 . We require the set $\{B_3, TB_3, T^2 B_3\}$ to be invariant under T and T^2 . We also want the set $\{B_3, TB_3, T^2 B_3\}$ be invariant under the full action of S_3 . It suffices to consider $P \equiv P_{xy}$ since $P_{xz} = TP_{xy}$ and $P_{yz} = T^2 P_{xy}$. First, $\{H(\mathbf{x}), TH(\mathbf{x}), T^2 H(\mathbf{x})\}$ would have to be

invariant under P . i.e. $\{H, TH, T^2H\} = \{PH, PTH, PT^2H\}$. There are several choices, but with any choice, one of H, TH, T^2H must be invariant under P . To see that this is the case, suppose that $PH = T^2H$. Then $PTH = T^2PH = T^2T^2H = TH$; TH is invariant under P . Or else if $PH = TH$, then $PT^2H = TPH = TTH = T^2H$; T^2H is invariant under P . Since we have yet to define H , without loss of generality, assume it is the basis function invariant under P . Thus, the following conditions must meet:

$$H(x) = PH(x), \quad \text{which implies that } yz + b_1xz + b_2xy = xz + b_1yz + b_2xy;$$

$$TH(x) = PT^2H(x), \quad \text{which implies that } xz + b_1xy + b_2yz = xy + b_1xz + b_2yz;$$

$$T^2H(x) = PTH(x), \quad \text{which implies that } xy + b_1yz + b_2xz = yz + b_1xy + b_2xz.$$

From this we see that we would need $b_1 = 1$. Recalling that $PB_2 = B_2$, $PTB_2 = T^2B_2$, and $PT^2B_2 = TB_2$, we next ask if the resulting B_3 , TB_3 and T^2B_3 would be an invariant set under P . These are

$$\begin{aligned} \{ B_3 &= H + a_0B_2 + a_1TB_2 + a_2T^2B_2 + dB_1, \\ TB_3 &= TH + a_0TB_2 + a_1T^2B_2 + a_2B_2 + dB_1, \\ T^2B_3 &= T^2H + a_0T^2B_2 + a_1B_2 + a_2TB_2 + dB_1 \}. \end{aligned}$$

The image of this set under P is the following:

$$\begin{aligned} \{ PB_3 &= PH + a_0PB_2 + a_1PTB_2 + a_2PT^2B_2 + dPB_1 \\ &= H + a_0B_2 + a_1T^2B_2 + a_2TB_2 + dB_1, \\ PTB_3 &= PTH + a_0PTB_2 + a_1PT^2B_2 + a_2PB_2 + dPB_1 \\ &= T^2H + a_0T^2B_2 + a_1TB_2 + a_2B_2 + dB_1, \\ PT^2B_3 &= PT^2H + a_0PT^2B_2 + a_1PB_2 + a_2PTB_2 + dPB_1 \\ &= TH + a_0TB_2 + a_1B_2 + a_2T^2B_2 + dB_1 \}. \end{aligned}$$

For these to be the same sets, we would have to have $a_1 = a_2$. Since $b_1 = 1$, setting $b = b_2$ and making appropriate substitutions for the a_i , we can then solve the equation

$$0 = \langle H(x), TH(x) \rangle - a_0a_2 - a_1a_0 - a_2a_1 - d^2,$$

a quadratic expression of b . Upon simplifying the equation above, we obtain the quadratic equation

$$0 = 504b^2 - 6384b - 2184.$$

So, the roots are $b = 13$ or $b = -\frac{1}{3}$. We take the first value of $b = 13$, and the unnormalized B_3 is

$$B_3 = k(xy + \frac{1}{13}yz + \frac{1}{13}zx - \frac{7}{39}x - \frac{7}{39}y - \frac{1}{39}z + \frac{1}{26})$$

with normalizer k . Finally, to normalize B_3 so that $\langle B_3, B_3 \rangle = 1$, we find that $k = 13\sqrt{42}$.

Thus,

$$B_3 = \sqrt{\frac{7}{6}}(78xy + 6yz + 6zx - 14x - 14y - 2z + 3).$$

The following lemma shows that the reduction above always takes place.

Lemma 4.1.1a : A monomial $x = x^i y^j z^k$ produces precisely 3 images under S_3 if and only if exactly two of i, j , and k are equal. Without loss of generality, we set $x = x^i y^j z^j$ as in the discussion of B_3 and form

$$H(x) = b_0 x + b_1 T x + b_2 T^2 x;$$

$$TH(x) = b_0 T x + b_1 T^2 x + b_2 x;$$

$$T^2 H(x) = b_0 T^2 x + b_1 x + b_2 T x.$$

This set is invariant under $P = P_{xy}$ (and hence all of S_3) if and only if two of the b_i are equal for $i = 0, 1, 2$. If we require $PH = H$, then $b_0 = b_1$.

Proof:

$$\text{Given monomial } x = x^i y^j z^k;$$

$$Tx = y^i z^j x^k;$$

$$T^2 x = z^i x^j y^k.$$

So, the images under P are, $Px = y^i x^j z^k$;

$$PTx = x^i z^j y^k;$$

$$PT^2x = z^i y^j x^k.$$

If $i \neq j$, then either $j = k$ or $i = k$. If $i \neq k$, then either $j = k$ or $i = j$. If $j \neq k$, then $i = j$ or $i = k$. Therefore, exactly two of i, j , and k are equal.

By relabelling i, j , and k if necessary, choose x to be the member of $(x^i y^j z^k, y^i z^j x^k, z^i x^j y^k)$ such that the exponents of y and z are the same. Thus, if $j = k$, then set $x = x^i y^j z^k$. If $i = j \neq k$, then set $x = y^i z^j x^k$ or if $i = k \neq j$, then set $x = z^i x^j y^k$.

We need the set

$$\begin{aligned} \{ H(x) = b_0 x + b_1 Tx + b_2 T^2 x, \\ TH(x) = b_0 Tx + b_1 T^2 x + b_2 x, \\ T^2 H(x) = b_0 T^2 x + b_1 x + b_2 Tx \} \end{aligned} \quad = \quad \begin{aligned} \{ PH(x) = b_0 Px + b_1 PTx + b_2 PT^2 x, \\ PTH(x) = b_0 PTx + b_1 PT^2 x + b_2 Px, \\ PT^2 H(x) = b_0 PT^2 x + b_1 Px + b_2 PTx \}. \end{aligned}$$

Since we assume $x = x^i y^j z^j$, $Tx = y^i z^j x^j$, $T^2 x = z^i x^j y^j$, $Px = y^i x^j z^j$, $PTx = x^i z^j y^j$, and $PT^2 x = z^i y^j x^j$. So, we need

$$\begin{aligned} \{ H(x) = b_0 x + b_1 Tx + b_2 T^2 x, \\ TH(x) = b_0 Tx + b_1 T^2 x + b_2 x, \\ T^2 H(x) = b_0 T^2 x + b_1 x + b_2 Tx \} \end{aligned} \quad = \quad \begin{aligned} \{ PH(x) = b_0 Tx + b_1 x + b_2 T^2 x, \\ PTH(x) = b_0 x + b_1 T^2 x + b_2 Tx, \\ PT^2 H(x) = b_0 T^2 x + b_1 Tx + b_2 x \}. \end{aligned}$$

For these to be the same sets, we have three choices. First, if $b_0 = b_1$, then $PH=H$, $PTH = T^2 H$, and $PT^2 H = TH$. Second, if $b_0 = b_2$, then $PH = T^2 H$, $PTH = TH$, and $PT^2 H = H$. Third, if $b_1 = b_2$, then $PH = TH$, $PTH = H$, and $PT^2 H = H$. Thus, if $x = x^i y^j z^j$ and we set $b_0 = b_1$, then we have the desired symmetry $PH=H$, $PTH = T^2 H$, and $PT^2 H = TH$. ■

We seek to extend H (in lemma 4.1.1a) to form G by adding a linear sum of the previous basis functions, so that $\{G, TG, T^2G\}$ is an orthonormal set, orthogonal to the previous basis function.

Assume that we wish to compute B_{j+1} . The previous basis functions occur either in singleton set $\{B_k\}$, where all powers of $x = x^i y^j z^k$ are the same, or triples $\{B_k, TB_k, T^2B_k\}$, where exactly two of the powers of $x = x^i y^j z^k$ are the same, or 6-fold $\{B_k, TB_k, T^2B_k, PB_k, TPB_k, T^2PB_k\}$, where all powers of $x = x^i y^j z^k$ are distinct. For the singleton sets or triples, we assume that we have constructed our basis such that $PB_k = B_k$, $PTB_k = T^2B_k$, and $PT^2B_k = TB_k$. Let $n(k) = 0$ for the singleton sets and $n(k) = 2$ for the triples. Then we can write (un-normalized) G as

$$G = H + \sum_{k=1}^i \sum_{i=0}^{n(k)} a_{k,i} T^i B_k + S(k),$$

where $S(k) \equiv$ sum over 6 – fold sets .

Lemma 4.1.1b : Let $x = x^i y^j z^k$ where exactly two of i, j , and k are equal and $H(x) = b_0 x + b_1 T x + b_2 T^2 x$. If we take $j = k$ (Lemma 4.1.1a) and H is chosen so that $PH = H$, $PTH = T^2 H$, and $PT^2 H = TH$ and G has the form above, then if $n(k) = 2$, and $PG = G$, then $a_{k,1} = a_{k,2}$.

Proof:

Given $G = H + \sum_{k=1}^i \sum_{i=0}^{n(k)} a_{k,i} T^i B_k + S(k)$. We require that the set $\{G, TG, T^2G\}$ to

be invariant under P with $PG = G$, $PTG = T^2G$, and $PT^2G = TG$. For $PG = G$, we require that

$$G = H + \sum_{k=1}^i \sum_{i=0}^{n(k)} a_{k,i} T^i B_k + S(k) = H + \sum_{k=1}^i a_{k,0} B_k + a_{k,1} T B_k + a_{k,2} T^2 B_k + S(k)$$

be equal to

$$\begin{aligned} PG &= PH + \sum_{k=1}^i \sum_{i=0}^{n(k)} a_{k,i} P T^i B_k + PS(k) \\ &= PH + \sum_{k=1}^i a_{k,0} P B_k + a_{k,1} P T B_k + a_{k,2} P T^2 B_k + PS(k) \\ &= H + \sum_{k=1}^i a_{k,0} B_k + a_{k,1} T^2 B_k + a_{k,2} T B_k + PS(k). \end{aligned}$$

Thus, $a_{k,1} = a_{k,2}$. Similar argument holds for $PTG = T^2G$ and $PT^2G = TG$. ■

To construct B_4 , set $x = x^2 y^0 z^0 = x^2$;

$$Tx = y^2 z^0 x^0 = y^2;$$

$$T^2 x = z^2 x^0 y^0 = z^2.$$

We seek $b_1, b_2, a_{3,0}, a_{3,1}, a_{3,2}, a_{2,0}, a_{2,1}, a_{2,2}$ and d such that if

$$G(x) = x + b_1 Tx + b_2 T^2 x + a_{3,0} B_3 + a_{3,1} T B_3 + a_{3,2} T^2 B_3 + a_{2,0} B_2 + a_{2,1} T B_2 + a_{2,2} T^2 B_2 + dB_1,$$

then $\{G, TG, T^2G, B_3, TB_3, T^2B_3, B_2, TB_2, T^2B_2, B_1\}$ are pairwise orthogonal.

Set $H(x) = x + b_1 Tx + b_2 T^2 x$. By Lemma 4.1.1a, we must set $b_1 = 1$; let $b_2 = b$. Thus,

$$H(x) = x + Tx + bT^2 x;$$

$$\tilde{B}_3 = a_{3,0} B_3 + a_{3,1} T B_3 + a_{3,2} T^2 B_3;$$

$$\tilde{B}_2 = a_{2,0} B_2 + a_{2,1} T B_2 + a_{2,2} T^2 B_2.$$

Then $G(x) = H(x) + \tilde{B}_3 + \tilde{B}_2 + dB_1$. The first requirement is that

$G(x)$, $TG(x)$, and $T^2G(x)$ be orthogonal to B_1 . As before, we need only set

$$d = -\langle H(\mathbf{x}), B_1 \rangle.$$

Next we need $\{G, TG, T^2G\}$ to be orthogonal to $T^i B_k$ for $k = 2, 3$ and $i = 0, 1, 2$. So, we need

$$(i) \ 0 = \langle H(\mathbf{x}) + \tilde{B}_3 + \tilde{B}_2 + dB_1, T^i B_k \rangle = \langle H(\mathbf{x}), T^i B_k \rangle + a_{k,i};$$

$$(ii) \ 0 = \langle TH(\mathbf{x}) + T\tilde{B}_3 + T\tilde{B}_2 + dB_1, T^i B_k \rangle = \langle TH(\mathbf{x}), T^i B_k \rangle + a_{k,[i-1(\bmod 3)]};$$

$$(iii) \ 0 = \langle T^2H(\mathbf{x}) + T^2\tilde{B}_3 + T^2\tilde{B}_2 + dB_1, T^i B_k \rangle = \langle T^2H(\mathbf{x}), T^i B_k \rangle + a_{k,[i-2(\bmod 3)]}.$$

Using lemma 3.3.1, as in the case of constructing B_3 , for $k = 2, 3$, these equations reduce to the following

$$(iv) \ 0 = \langle H(\mathbf{x}) + \tilde{B}_3 + \tilde{B}_2 + dB_1, B_k \rangle = \langle H(\mathbf{x}), B_k \rangle + a_{k,0};$$

$$(v) \ 0 = \langle TH(\mathbf{x}) + T\tilde{B}_3 + T\tilde{B}_2 + dB_1, B_k \rangle = \langle TH(\mathbf{x}), B_k \rangle + a_{k,2};$$

$$(vi) \ 0 = \langle T^2H(\mathbf{x}) + T^2\tilde{B}_3 + T^2\tilde{B}_2 + dB_1, B_k \rangle = \langle T^2H(\mathbf{x}), B_k \rangle + a_{k,1}.$$

Thus, $a_{2,i}$ and $a_{3,i}$ for $i = 0, 1, 2$ are uniquely determined once $H(\mathbf{x})$ is known where $H(\mathbf{x})$ depends only on parameter b . So we can consider $a_{k,i}$ to be functions of form $\alpha_{k,i} + \beta_{k,i}b$ for suitable constants $\alpha_{k,i}$ and $\beta_{k,i}$.

There remains the problem of finding b such that G, TG , and T^2G are pairwise orthogonal. An argument similar to the case of constructing B_3 show that it suffices to establish that $\langle G(\mathbf{x}), TG(\mathbf{x}) \rangle = \langle G(\mathbf{x}), TH(\mathbf{x}) \rangle = 0$. Now with the substitutions for a_i and d above and lemmas 3.2.1(2) and 4.1.1(b), we obtain

$$\begin{aligned} \langle G(\mathbf{x}), TH(\mathbf{x}) \rangle &= \langle H(\mathbf{x}) + a_{3,0}B_3 + a_{3,1}TB_3 + a_{3,2}T^2B_3 + a_{2,0}B_2 + a_{2,1}TB_2 + \\ &\quad a_{2,2}T^2B_2 + dB_1, TH(\mathbf{x}) \rangle \\ &= \langle H(\mathbf{x}), TH(\mathbf{x}) \rangle + a_{3,0}\langle B_3, TH(\mathbf{x}) \rangle + a_{3,1}\langle TB_3, TH(\mathbf{x}) \rangle + \\ &\quad a_{3,2}\langle T^2B_3, TH(\mathbf{x}) \rangle + a_{2,0}\langle B_2, TH(\mathbf{x}) \rangle + a_{2,1}\langle TB_2, TH(\mathbf{x}) \rangle + \\ &\quad a_{2,2}\langle T^2B_2, TH(\mathbf{x}) \rangle + d\langle B_1, TH(\mathbf{x}) \rangle \\ &= \langle H(\mathbf{x}), TH(\mathbf{x}) \rangle - a_{3,0}a_{3,2} - a_{3,1}a_{3,0} - a_{3,2}a_{3,1} - a_{2,0}a_{2,2} - \\ &\quad a_{2,1}a_{2,0} - a_{2,2}a_{2,1} - d^2 \end{aligned}$$

$$= \langle H(x), TH(x) \rangle - 2a_{3,0}a_{3,1} - a_{3,1}^2 - 2a_{2,0}a_{2,1} - a_{2,1}^2 - d^2.$$

Thus, setting $0 = \langle H(x), TH(x) \rangle - 2a_{3,0}a_{3,1} - a_{3,1}^2 - 2a_{2,0}a_{2,1} - a_{2,1}^2 - d^2$ gives a quadratic expression in b and making appropriate substitutions for $a_{k,i}$, we can then solve the quadratic

$$0 = \langle H(x), TH(x) \rangle - 2a_{3,0}a_{3,1} - a_{3,1}^2 - 2a_{2,0}a_{2,1} - a_{2,1}^2 - d^2$$

for b . Upon simplifying the equation above, we obtain the quadratic equation

$$0 = b^2 - 12b - 4.$$

So, the roots are $b = (6 + 2\sqrt{10})$ or $b = (6 - 2\sqrt{10})$. We take the second value of $b = (6 - 2\sqrt{10})$ (chosen for its closeness to 1), and B_4 is computed.

To construct B_5 , we set $x = x^1 y^1 z^1 = xyz$;

$$Tx = y^1 z^1 x^1 = xyz;$$

$$T^2 x = z^1 x^1 y^1 = xyz.$$

Since $x = Tx = T^2 x$, we only need a singleton leading term for B_5 . We seek $a_{4,0}$, $a_{4,1}$, $a_{4,2}$, $a_{3,0}$, $a_{3,1}$, $a_{3,2}$, $a_{2,0}$, $a_{2,1}$, $a_{2,2}$ and d such that if

$$G(x) = x + a_{4,0}B_4 + a_{4,1}TB_4 + a_{4,2}T^2B_4 + a_{3,0}B_3 + a_{3,1}TB_3 + a_{3,2}T^2B_3 + a_{2,0}B_2 + a_{2,1}TB_2 + a_{2,2}T^2B_2 + dB_1,$$

then the members of $\{G, B_4, TB_4, T^2B_4, B_3, TB_3, T^2B_3, B_2, TB_2, T^2B_2, B_1\}$ are pairwise orthogonal. We require $G = TG = T^2G$.

Set $H(x) = x$;

$$\tilde{B}_4 = a_{4,0}B_4 + a_{4,1}TB_4 + a_{4,2}T^2B_4;$$

$$\tilde{B}_3 = a_{3,0}B_3 + a_{3,1}TB_3 + a_{3,2}T^2B_3;$$

$$\tilde{B}_2 = a_{2,0}B_2 + a_{2,1}TB_2 + a_{2,2}T^2B_2.$$

Thus, $G(\mathbf{x}) = H(\mathbf{x}) + \tilde{B}_4 + \tilde{B}_3 + \tilde{B}_2 + dB_1$. The first requirement is that $G(\mathbf{x})$ is orthogonal to B_1 . As before, we need only set

$$d = -\langle H(\mathbf{x}), B_1 \rangle.$$

Next we need G to be orthogonal to $T^i B_k$ for $k = 2, 3, 4$ and $i = 0, 1, 2$. So, we need

$$0 = \langle H(\mathbf{x}) + \tilde{B}_4 + \tilde{B}_3 + \tilde{B}_2 + dB_1, T^i B_k \rangle = \langle H(\mathbf{x}), T^i B_k \rangle + a_{k,i}.$$

Using lemma 3.3.1 as before and $H = TH = T^2H$, these equations reduce to the following

$$(i) \quad 0 = \langle H(\mathbf{x}), B_k \rangle + a_{k,0};$$

$$(ii) \quad 0 = \langle H(\mathbf{x}), TB_k \rangle + a_{k,1} = \langle T^2H(\mathbf{x}), B_k \rangle + a_{k,1} = \langle H(\mathbf{x}), B_k \rangle + a_{k,1};$$

$$(iii) \quad 0 = \langle H(\mathbf{x}), T^2B_k \rangle + a_{k,2} = \langle TH(\mathbf{x}), B_k \rangle + a_{k,2} = \langle H(\mathbf{x}), B_k \rangle + a_{k,2}.$$

We obtain the symmetry $a_{k,0} = a_{k,1} = a_{k,2}$ for $k = 2, 3, 4$. Thus, $a_{4,i}$, $a_{3,i}$ and $a_{2,i}$ for $i = 0, 1, 2$ are uniquely determined by the above expressions. Thus, B_5 is easily computed.

We wish to make B_6 out of $\{x^2y, y^2z, z^2x, y^2x, z^2y, x^2z\}$. This is the first test to see if complete symmetry can be achieved. Recall that $P \equiv P_{xy}$. Un-normalized B_6 has form

$$G = H + \sum_{k=1}^5 \sum_{i=0}^{n(k)} a_{k,i} T^i B_k$$

where H is defined as follows: Let $\mathbf{x} = x^2y^1z^0 = x^2y$; then

$$H \equiv \mathbf{x} + b_1 T\mathbf{x} + b_2 T^2\mathbf{x} + b_3 P\mathbf{x} + b_4 TP\mathbf{x} + b_5 T^2P\mathbf{x}$$

where $T\mathbf{x} = y^2z^1x^0 = y^2z$, $T^2\mathbf{x} = z^2x^1y^0 = z^2x$, $P\mathbf{x} = y^2x^1z^0 = y^2x$, $TP\mathbf{x} = z^2y^1x^0 = z^2y$, and $T^2P\mathbf{x} = x^2z^1y^0 = x^2z$.

We wish to find values for $a_{k,i}$ and b_j 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 Q to be orthogonal to basis functions that comprise triples $\{B_k, TB_k, T^2B_k\}$, it suffices to show that Q is orthogonal to B_k , since Q is invariant under S_3 and the adjoints of operators in S_3 are in S_3 .

Next, since the previous basis functions are orthonormal, for any B_k , we can make the following reductions with the help of lemma 3.3.1 and the fact that $PB_k = B_k$, $PTB_k = T^2B_k$, and $PT^2B_k = TB_k$. We require

- (i) $0 = \langle G, B_k \rangle = \langle H, B_k \rangle + a_{k,0};$
- (ii) $0 = \langle TG, B_k \rangle = \langle G, T^2B_k \rangle = \langle H, T^2B_k \rangle + a_{k,2} = \langle TH, B_k \rangle + a_{k,2};$
- (iii) $0 = \langle T^2G, B_k \rangle = \langle G, TB_k \rangle = \langle H, TB_k \rangle + a_{k,1} = \langle T^2H, B_k \rangle + a_{k,1};$
- (iv) $0 = \langle PG, B_k \rangle = \langle G, PB_k \rangle = \langle G, B_k \rangle = \langle H, B_k \rangle + a_{k,0};$
- (v) $0 = \langle TPG, B_k \rangle = \langle G, PT^2B_k \rangle = \langle G, TB_k \rangle = \langle H, TB_k \rangle + a_{k,1}$
 $= \langle T^2H, B_k \rangle + a_{k,1};$
- (vi) $0 = \langle T^2PG, B_k \rangle = \langle G, PTB_k \rangle = \langle G, T^2B_k \rangle = \langle H, T^2B_k \rangle + a_{k,2}$
 $= \langle H, T^2B_k \rangle + a_{k,2}.$

Since the last three requirements (iv)-(vi) replicate the first three (i)-(iii), the requirements can met by satisfying the first three equations, and $\{a_{k,i}\}$ is uniquely determined once H is known.

Finally, we need $\{b_i\}$ so that Q is a pairwise orthogonal set. Again, using adjoints, the fifteen requirements can be reduced to the following four types, since $PTP = T^2$ and $PT^2P = T$:

$$\text{Type 1: } 0 = \langle G, TG \rangle = \langle G, T^2G \rangle = \langle TG, T^2G \rangle = \langle PG, TPG \rangle = \langle PG, T^2PG \rangle = \langle TPG, T^2PG \rangle;$$

$$\text{Type 2: } 0 = \langle G, PG \rangle = \langle TG, TPG \rangle = \langle T^2G, T^2PG \rangle;$$

$$\text{Type 3: } 0 = \langle G, TPG \rangle = \langle TG, T^2PG \rangle = \langle T^2G, PG \rangle;$$

$$\text{Type 4: } 0 = \langle G, T^2PG \rangle = \langle TG, PG \rangle = \langle T^2G, TPG \rangle.$$

If the substitutions for the $a_{k,i}$ are made, the members of Q are orthogonal to the previous basis functions, and the four types above can be shown to be equivalent to the following, where when $k = 1$ or 5 , there is only a single term in the sum.

$$\text{Type 1: } 0 = \langle G, TG \rangle = \langle G, TH \rangle = \langle H, TH \rangle - \sum_{k=1}^5 (a_{k,0}a_{k,1} + a_{k,0}a_{k,2} + a_{k,1}a_{k,2});$$

$$\text{Type 2: } 0 = \langle G, PG \rangle = \langle G, PH \rangle = \langle H, PH \rangle - \sum_{k=1}^5 (a_{k,0}^2 + 2a_{k,1}a_{k,2});$$

$$\text{Type 3: } 0 = \langle G, TPG \rangle = \langle G, TPH \rangle = \langle H, TPH \rangle - \sum_{k=1}^5 (a_{k,2}^2 + 2a_{k,0}a_{k,1});$$

$$\text{Type 4: } 0 = \langle G, T^2PG \rangle = \langle G, T^2PH \rangle = \langle H, T^2PH \rangle - \sum_{k=1}^5 (a_{k,1}^2 + 2a_{k,0}a_{k,2}).$$

With the substitutions for $a_{k,i}$, these four are quadratic requirements $f_i(\underline{b}) = 0$ in the five unknowns $b_1, \dots, b_5$, again suggesting that there may be an extra degree of freedom in a solution (if there is one.)

Here, we develop an iterative method to compute simultaneous zeros $b_1, \dots, b_5$ for the four quadratic equations above. To illustrate the method in a simpler manner, we first show an example in $\mathbb{R}^2$.

Given two functions $f_1(x, y) = x^2 - \frac{y^2}{2} - 1$ and $f_2(x, y) = x^2 + y^2 - 4$, we wish to find the intersection for $f_1(x, y) = 0$ and $f_2(x, y) = 0$ on the xy -plane. Choose an arbitrary initial point (x_0, y_0) , say $(x_0, y_0) = (5, 3)$. We first take the gradient of $f_1(x, y)$ and $f_2(x, y)$ at $(5, 3)$ to obtain the gradient vectors $\nabla f_1(5, 3)$ and $\nabla f_2(5, 3)$ as follows:

$$\nabla f_1(x, y) = (2x, -y); \text{ at } (5, 3), \nabla f_1(5, 3) = (10, -3);$$

$$\nabla f_2(x, y) = (2x, 2y); \text{ at } (5, 3), \nabla f_2(5, 3) = (10, 6).$$

Then we move along the vector $\nabla f_1(5,3)$ from $(x_0, y_0) = (5,3)$ to the locus of $f_1(x, y) = 0$. This line $(x(\lambda_1), y(\lambda_1)) \equiv (5,3) + \lambda_1(f_{1,x}, f_{1,y})$ is the direction of steepest ascent / descent of surface $z_1 = f_1(x, y)$. Similarly, move along the vector $\nabla f_2(5,3)$ from $(5,3)$ to the locus of $f_2(x, y) = 0$; is along line $(x(\lambda_2), y(\lambda_2)) \equiv (5,3) + \lambda_2(f_{2,x}, f_{2,y})$.

Thus, we solve for λ_1 and λ_2 of $f_1(x(\lambda_1), y(\lambda_1)) = 0$ and $f_2(x(\lambda_2), y(\lambda_2)) = 0$ which are the following quadratic equations in λ_1 and λ_2 respectively:

$$\begin{aligned} f_1(5 + \lambda_1 f_{1,x}, 3 + \lambda_1 f_{1,y}) &= f_1(5 + 10\lambda_1, 3 - 3\lambda_1) \\ &= (5 + 10\lambda_1)^2 - \frac{(3 - 3\lambda_1)^2}{2} - 1 \\ &= 191\lambda_1^2 + 218\lambda_1 + 39 \stackrel{\text{set}}{=} 0. \end{aligned}$$

We obtain $\lambda_1 = -0.2221$ or -0.9192 to four significant digits. We choose the values for λ_i 's with smallest absolute values to be closest to the starting point $(x_0, y_0) = (5,3)$.

Taking $\lambda_1 = -0.2221$, we have a point

$$(x_1^1, y_1^1) = (5,3) + (-0.2221)(10, -3) = (2.7790, 3.6663)$$

on the locus of $f_1(x, y) = 0$.

$$\begin{aligned} \text{Similarly, } f_2(5 + \lambda_2 f_{2,x}, 3 + \lambda_2 f_{2,y}) &= f_2(5 + 10\lambda_2, 3 + 6\lambda_2) \\ &= (5 + 10\lambda_2)^2 + (3 + 6\lambda_2)^2 - 4 \\ &= 136\lambda_2^2 + 136\lambda_2 + 30 \stackrel{\text{set}}{=} 0. \end{aligned}$$

We obtain $\lambda_2 = -0.3285$ or -0.6714 in four significant digits. Taking $\lambda_2 = -0.3285$, we have a point

$$(x_1^2, y_1^2) = (5,3) + (-0.3285)(10, 6) = (1.7150, 1.0290)$$

on the locus of $f_2(x, y) = 0$.

Now we find the intersection of the line perpendicular to $\nabla f_1(x_1^1, y_1^1)$ through (x_1^1, y_1^1) and the line perpendicular to $\nabla f_2(x_1^2, y_1^2)$ through (x_1^2, y_1^2) . We call this intersection point our new point (x_1, y_1) . Thus, we find the intersection of the line through (x_1^1, y_1^1)

tangent to locus $f_1(x, y) = 0$ and the line through (x_1^2, y_1^2) tangent to locus $f_2(x, y) = 0$.

So, the point of intersection (x, y) of the tangent lines satisfies

$$[f_{1,x}(x_1^1, y_1^1)] \cdot (x - x_1^1) + [f_{1,y}(x_1^1, y_1^1)] \cdot (y - y_1^1) = 0 \quad \text{and}$$

$$[f_{2,x}(x_1^2, y_1^2)] \cdot (x - x_1^2) + [f_{2,y}(x_1^2, y_1^2)] \cdot (y - y_1^2) = 0;$$

see Figure 4.1.1 .

Figure 4.1.1

Iterative method

This linear system is

$$\begin{pmatrix} f_{1,x}(x_1^1, y_1^1) & f_{1,y}(x_1^1, y_1^1) \\ f_{2,x}(x_1^2, y_1^2) & f_{2,y}(x_1^2, y_1^2) \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} [f_{1,x}(x_1^1, y_1^1)]x_1^1 + [f_{1,y}(x_1^1, y_1^1)]y_1^1 \\ [f_{2,x}(x_1^2, y_1^2)]x_1^2 + [f_{2,y}(x_1^2, y_1^2)]y_1^2 \end{pmatrix}.$$

Thus, we obtain

$$\begin{pmatrix} 5.5580 & -3.6663 \\ 3.4300 & 2.0580 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 2.0089 \\ 8.0001 \end{pmatrix}$$

which has solution $(x, y) \equiv (x_1, y_1) = (1.3931, 1.5654)$. We repeat the same procedure beginning at (x_1, y_1) to obtain (x_2, y_2) and so on.

The exact solution to this problem is $x = \sqrt{2}$ and $y = \sqrt{2}$. Using a computer program with double precision to carry this procedure, we obtain the solution $(x, y) \equiv (x_4, y_4)$ accurate to 12 decimal places within 4 iterations as follows:

$$(x_0, y_0) = (5, 3)$$

$$(x_1, y_1) = (1.392893053281894, 1.565812841093710)$$

$$(x_2, y_2) = (1.415170338669979, 1.417922421105357)$$

$$(x_3, y_3) = (1.414213347970639, 1.414215109556979)$$

$$(x_4, y_4) = (1.414213562373200, 1.414213562373539).$$

We generalize the iterative method to R^5 as follows: We seek values $b_1, \dots, b_5$ such that $f_i(\underline{b}) = 0$ for $i = 1, \dots, 4$.

Choose an arbitrary initial point $\underline{b}_0$. We first take the gradient of $f_i(\underline{b})$ at $\underline{b}_0$. We use the vector notation

$$\nabla f_i(\underline{b}_0) = \left(\frac{\partial f_i}{\partial b_1}, \frac{\partial f_i}{\partial b_2}, \frac{\partial f_i}{\partial b_3}, \frac{\partial f_i}{\partial b_4}, \frac{\partial f_i}{\partial b_5} \right) \Big|_{\underline{b}_0}$$

for this gradient. To compute each of the $\frac{\partial f_i}{\partial b_j} \Big|_{\underline{b}_0}$ for $i = 1, \dots, 4$ and $j = 1, \dots, 5$ explicitly

can be very complicated. However, we use the central-difference approximation to obtain

$\frac{\partial f_i}{\partial b_j} \Big|_{\underline{b}_0}$. The central-difference approximation [1] of $f'(x)$ at x_0 is

$$f'(x_0) = \frac{f(x_0 + \Delta) - f(x_0 - \Delta)}{2\Delta} + \frac{2f'''(x_0 + \theta\Delta)\Delta x^2}{6}.$$

For quadratic functions f , f''' and any higher order derivatives are zero. So, we can compute $f'(x)$ at x_0 by

$$f'(x_0) = \frac{f(x_0 + \Delta) - f(x_0 - \Delta)}{2\Delta}.$$

In our case,

$$\left. \frac{\partial f_i}{\partial b_j} \right|_{\underline{b}_0} = \frac{f^i(\underline{b}_0 + \Delta_j) - f^i(\underline{b}_0 - \Delta_j)}{2\Delta_j},$$

where $\Delta_j = \Delta(0, 0, \dots, 1, \dots, 0)$ with 1 in the j th position. Then we seek for values of λ_i for $i = 1, \dots, 4$ (as in $\mathbb{R}^2$) to move along vectors $\nabla f_i(\underline{b}_0)$ to each of the loci $f_i(\underline{b}) = 0$ along the lines $\underline{b}(\lambda_i) \equiv \underline{b}_0 + \lambda_i \nabla f_i(\underline{b}_0)$ respectively. Once we find the values for λ_i , we obtain points $\underline{b}_1^i$ on each of the loci $f_i(\underline{b}) = 0$ and we express $\underline{b}_1^i$ as

$$\underline{b}_1^i = \underline{b}_0 + \lambda_i \nabla f_i(\underline{b}_0). \quad (1)$$

We now use the points $\underline{b}_1^i$ to obtain 4 tangent planes at loci $f_i(\underline{b}) = 0$ for $i = 1, \dots, 4$.

Next, we find the intersection point of these 4 tangent planes which is the closest to the initial point $\underline{b}_0$. We call this intersection point our new point $\underline{b}_1$. We express this new point as

$$\underline{b}_1 = \underline{b}_0 + \sum_{j=1}^4 \mu_j \nabla f_j(\underline{b}_1^j). \quad (2)$$

Since $\underline{b}_1$ is an intersection point on all 4 tangent planes and $\underline{b}_1^i$ is a point on the i th tangent plane, we know that $\underline{b}_1 - \underline{b}_1^i$ are vectors in the i th tangent plane. Thus, for $i = 1, \dots, 4$, we get

$$(\underline{b}_1 - \underline{b}_1^i) \cdot \nabla f_i(\underline{b}_1^i) = 0. \quad (3)$$

We expand expression (3) to obtain

$$\underline{b}_1 \cdot \nabla f_i \underline{b}_1^i = \underline{b}_1^i \cdot \nabla f_i \underline{b}_1^i. \quad (4)$$

Now substitute (2) into (4), we have

$$[\underline{b}_0 + \sum_{j=1}^4 \mu_j \nabla f_j(\underline{b}_1^j)] \bullet \nabla f_i \underline{b}_1^i = \underline{b}_1^i \bullet \nabla f_i \underline{b}_1^i$$

or,

$$\underline{b}_0 \bullet \nabla f_i \underline{b}_1^i + \sum_{j=1}^4 \mu_j \nabla f_j(\underline{b}_1^j) \bullet \nabla f_i \underline{b}_1^i = \underline{b}_1^i \bullet \nabla f_i \underline{b}_1^i$$

or,

$$\sum_{j=1}^4 \mu_j \nabla f_j(\underline{b}_1^j) \bullet \nabla f_i \underline{b}_1^i = \underline{b}_1^i \bullet \nabla f_i \underline{b}_1^i - \underline{b}_0 \bullet \nabla f_i \underline{b}_1^i$$

or,

$$\sum_{j=1}^4 \mu_j \nabla f_j(\underline{b}_1^j) \bullet \nabla f_i \underline{b}_1^i = (\underline{b}_1^i - \underline{b}_0) \bullet \nabla f_i \underline{b}_1^i . \quad (5)$$

Substituting (1) into the expression $(\underline{b}_1^i - \underline{b}_0)$ in (5), we get

$$\sum_{j=1}^4 \mu_j \nabla f_j(\underline{b}_1^j) \bullet \nabla f_i \underline{b}_1^i = \lambda_i \nabla f_i(\underline{b}_0) \bullet \nabla f_i \underline{b}_1^i . \quad (6)$$

For $i = 1, \dots, 4$, equation (6) is a system of 4 equations with 4 unknowns μ_1, μ_2, μ_3 , and μ_4 . We rewrite (6) in a matrix form as

$$\begin{bmatrix} \nabla f_1(\underline{b}_1^1) \bullet \nabla f_1(\underline{b}_1^1) \\ \nabla f_1(\underline{b}_1^1) \bullet \nabla f_2(\underline{b}_1^2) \\ \nabla f_1(\underline{b}_1^1) \bullet \nabla f_3(\underline{b}_1^3) \\ \nabla f_1(\underline{b}_1^1) \bullet \nabla f_4(\underline{b}_1^4) \end{bmatrix} \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \mu_4 \end{pmatrix} = \begin{bmatrix} \lambda_1 \nabla f_1(\underline{b}_0) \bullet \nabla f_1(\underline{b}_1^1) \\ \lambda_2 \nabla f_2(\underline{b}_0) \bullet \nabla f_2(\underline{b}_1^2) \\ \lambda_3 \nabla f_3(\underline{b}_0) \bullet \nabla f_3(\underline{b}_1^3) \\ \lambda_4 \nabla f_4(\underline{b}_0) \bullet \nabla f_4(\underline{b}_1^4) \end{bmatrix}. \quad (7)$$

Thus we have a linear system $A\mu = B$ where all of the entries in matrix A and B can be computed. Once we have μ_1, μ_2, μ_3 , and μ_4 , we then have a new point $\underline{b}_1$ as

$$\underline{b}_1 = \underline{b}_0 + \sum_{j=1}^4 \mu_j \nabla f_j(\underline{b}_1^j) .$$

We iterate this until we obtain $\underline{b}_n$ such that $(\sum_{i=1}^4 [f_i(\underline{b}_n)]^2) \times 10^{16} < 10^{-18}$. Once we obtain $\underline{b}_n$, B_6 , our first basis function that contains a 6-fold symmetry, is computed.

So, does our iterative method work in R^5 as well as in the case in R^2 and how many iterations does it take to obtain the desired accuracy? We provide the following a sample run of computing B_{10} , the second basis function that contains a 6-fold symmetry which is considerably more complicated than B_6 . We choose $\underline{b}_0 = (1, -1, 1, -1, 1)$. Then we obtain the following 4 iterations:

Sample run to obtain roots $b(i)$ to simultaneous quadratics $f(i) = 0$:

Initial $b(i)$: 1.000 -1.000 1.000 -1.000 1.000

$f(1)=$ -0.2003190381670919E-06
 $f(2)=$ -0.3904442171914204E-06
 $f(3)=$ 0.2099577432518773E-06
 $f(4)=$ 0.6576791182214334E-07

$b(1)=$ 0.1750827185054384E+01
 $b(2)=$ -0.2742526219378425E+01
 $b(3)=$ 0.7569340662087711E+00
 $b(4)=$ 0.1882328049054546E+01
 $b(5)=$ -0.7780765795713513E+00

1

f(1)= 0.5749663327235142E-08
f(2)= -0.7013663610723172E-07
f(3)= 0.2414519175965519E-07
f(4)= -0.6901084471401791E-09

b(1)= 0.1862913586642787E+01
b(2)= -0.1848431907582706E+01
b(3)= 0.1391451376385444E+01
b(4)= 0.1643595945338747E+01
b(5)= 0.4808018438203114E+00

2

f(1)= -0.1024500812256326E-08
f(2)= -0.7751841866164306E-09
f(3)= 0.8778736616766800E-09
f(4)= -0.2104961969214957E-08

b(1)= 0.1944943698152658E+01
b(2)= -0.1784010320310387E+01
b(3)= 0.1403256723975137E+01
b(4)= 0.1503536346205464E+01
b(5)= 0.6360567587304976E+00

3

f(1)= 0.6143988855004945E-12
f(2)= 0.1638602583698204E-11
f(3)= 0.1774663749287697E-11
f(4)= -0.6288820104862619E-12

b(1)= 0.1946402856393202E+01
b(2)= -0.1776632242005079E+01
b(3)= 0.1400082623275721E+01
b(4)= 0.1506937290706204E+01
b(5)= 0.6437853155459894E+00

4

$$\begin{aligned}f(1) &= 0.4878909776184769\text{E-}18 \\f(2) &= 0.6505213034913026\text{E-}18 \\f(3) &= 0.4336808689942017\text{E-}18 \\f(4) &= 0.1599198204416119\text{E-}17\end{aligned}$$

$$\begin{aligned}b(1) &= 0.1946400053015636\text{E+}01 \\b(2) &= -0.1776639352772805\text{E+}01 \\b(3) &= 0.1400077474715218\text{E+}01 \\b(4) &= 0.1506939139172791\text{E+}01 \\b(5) &= 0.6437846839656678\text{E+}00.\end{aligned}$$

We obtain different solutions for each $\underline{b}_0$. We choose a solution $\underline{b}_n$ according to the following objective. Recall that we defined

$$H \equiv \mathbf{x} + b_1 T\mathbf{x} + b_2 T^2\mathbf{x} + b_3 P\mathbf{x} + b_4 TP\mathbf{x} + b_5 T^2P\mathbf{x}.$$

Since we defined the coefficient of $\mathbf{x}$ in H is 1, propose that the other coefficients b_i to be close to 1 in magnitude so that all of the terms in H have about the same weights.

We completed constructing generating functions through the 4th order, giving 11 basis functions $B_1, \dots, B_{11}$ that can generate a total of 35 basis functions under S_3 . In appendix A, we exhibit these 11 polynomial basis functions and their coefficients. In the process of constructing these polynomials, we ran into a few computational problems and reduction of accuracy, perhaps due to excessive amount of computation.

For example, using double precision, the magnitude of the value of $\langle B_2, B_4 \rangle$ is 10^{-14} which we consider to be acceptable. However, the magnitude of the value of $\langle B_2, B_{11} \rangle$ is 10^{-7} . This shows a decay in accuracy.

Assuming that we can resolve the problem of growing error, there still remain 2 major questions:

- (1) If we continue to construct more basis functions $B_{12}, B_{13}, \dots$, do the quadratic expressions that we have to solve always have real roots?

(2) In solving the four quadratic equations with five unknowns $b_1, \dots, b_5$, our approach now is to choose a solution $\underline{b}_n$ whose components are close to 1 in magnitude. What if we were to choose a solution $\underline{b}_n$ with a different approach? Will we get a basis with less error in the inner product computation? For example, choose a $\underline{b}_n$ such that only one coefficient has a large magnitude.

In order to answer these two questions, further analysis and more computation will be required for future research.

Appendix A

Constructed orthonormal polynomial basis B1-B11:

$$B1 = \text{cf}(1)$$

$$B2 = \text{cf}(2)x + \text{cf}(3)y + \text{cf}(4)z$$

$$B3 = \text{cf}(5)xy + \text{cf}(6)yz + \text{cf}(7)zx + \text{cf}(8)x^2 + \text{cf}(9)y^2 + \text{cf}(10)z^2 + \text{cf}(11)$$

$$B4 = \text{cf}(12)x^2 + \text{cf}(13)y^2 + \text{cf}(14)z^2 + \text{cf}(15)xy + \text{cf}(16)xz + \text{cf}(17)yz + \text{cf}(18)x + \text{cf}(19)y + \text{cf}(20)z + \text{cf}(21)$$

$$B5 = \text{cf}(22)xyz + \text{cf}(23)xy + \text{cf}(24)xz + \text{cf}(25)yz + \text{cf}(26)x + \text{cf}(27)y + \text{cf}(28)z + \text{cf}(29)$$

$$B6 = (xy(\text{cf}(30)x + \text{cf}(32)y + \text{cf}(40)z)) + (xz(\text{cf}(31)x + \text{cf}(34)z + \text{cf}(41)y)) + (yz(\text{cf}(33)y + \text{cf}(35)z + \text{cf}(42)x)) + \text{cf}(36)xyz + \text{cf}(37)x^2 + \text{cf}(38)y^2 + \text{cf}(39)z^2 + \text{cf}(43)x + \text{cf}(44)y + \text{cf}(45)z + \text{cf}(46)$$

$$B7 = (x^2(\text{cf}(47)x + \text{cf}(50)y + \text{cf}(51)z + \text{cf}(57))) + (y^2(\text{cf}(48)y + \text{cf}(52)x + \text{cf}(53)z + \text{cf}(58))) + (z^2(\text{cf}(49)z + \text{cf}(54)x + \text{cf}(55)y + \text{cf}(59))) + \text{cf}(56)xyz + (x(\text{cf}(60)y + \text{cf}(61)z + \text{cf}(63))) + (y(\text{cf}(62)z + \text{cf}(64))) + (\text{cf}(65)z) + \text{cf}(66)$$

$$B8 = (x^2(\text{cf}(67)yz + \text{cf}(70)y + \text{cf}(71)z + \text{cf}(77))) + (y^2(\text{cf}(68)xz + \text{cf}(72)x + \text{cf}(73)z + \text{cf}(78))) + (z^2(\text{cf}(69)xy + \text{cf}(74)x + \text{cf}(75)y + \text{cf}(79))) + \text{cf}(76)xyz + (x(\text{cf}(80)y + \text{cf}(81)z + \text{cf}(83))) + (y(\text{cf}(82)z + \text{cf}(84))) + (\text{cf}(85)z) + \text{cf}(86)$$

$$B9 = (x^2(\text{cf}(87)y^2 + \text{cf}(89)z^2 + \text{cf}(90)yz + \text{cf}(93)y + \text{cf}(94)z + \text{cf}(100))) + (y^2(\text{cf}(88)z^2 + \text{cf}(91)xz + \text{cf}(95)x + \text{cf}(96)z + \text{cf}(101))) + (z^2(\text{cf}(92)xy + \text{cf}(97)x + \text{cf}(98)y + \text{cf}(102))) + (\text{cf}(99)xyz) + (x(\text{cf}(103)y + \text{cf}(104)z + \text{cf}(106))) + (y(\text{cf}(105)z + \text{cf}(107))) + \text{cf}(108)z + \text{cf}(109)$$

$$\begin{aligned}
B10 = & (x^3(cf(110)y + cf(115)z + cf(122))) + \\
& (y^3(cf(111)z + cf(113)x + cf(123))) + \\
& (z^3(cf(112)x + cf(114)y + cf(124))) + \\
& (x^2(cf(116)y^2 + cf(119)yz + cf(125)y + cf(126)z + cf(132))) + \\
& (y^2(cf(117)z^2 + cf(120)zx + cf(127)x + cf(128)z + cf(133))) + \\
& (z^2(cf(118)x^2 + cf(121)xy + cf(129)x + cf(130)y + cf(134))) + \\
& cf(131)xyz + (x(cf(135)y + cf(136)z + cf(138))) + \\
& (y(cf(137)z + cf(139))) + cf(140)z + cf(141)
\end{aligned}$$

$$\begin{aligned}
B11 = & (x^4cf(142) + y^4cf(143) + z^4cf(144)) + (x^3(cf(145)y + cf(150)z + cf(157))) + \\
& (y^3(cf(146)z + cf(148)x + cf(158))) + (z^3(cf(147)x + cf(149)y + cf(159))) + \\
& (x^2(cf(151)y^2 + cf(154)yz + cf(160)y + cf(161)z + cf(167))) + \\
& (y^2(cf(152)z^2 + cf(155)zx + cf(162)x + cf(163)z + cf(168))) + \\
& (z^2(cf(153)x^2 + cf(156)xy + cf(164)x + cf(165)y + cf(169))) + \\
& cf(166)xyz + (x(cf(170)y + cf(171)z + cf(173))) + (y(cf(172)z + cf(174))) + \\
& cf(175)z + cf(176)
\end{aligned}$$

Coefficient file cf(i) for i = 1 to 176 for basis B1-B11:

B1: 0.2449489742783178E+01

B2: 0.1095445115010332E+02
0.1095445115010332E+02
-0.5477225575051661E+01

B3: 0.8424962907930215E+02
0.6480740698407859E+01
0.6480740698407859E+01
-0.1512172829628500E+02
-0.1512172829628500E+02
-0.2160246899469286E+01
0.3240370349203929E+01

B4: 0.5992391417200940E+02
0.5992391417200940E+02
-0.1944862515992894E+02
0.1008982228344194E+03

0.3740019136886879E+02
0.3740019136886879E+02
-0.6299901181522097E+02
-0.6299901181522097E+02
0.4990196503297000E+00
0.1254990039801122E+02

B5: 0.7127636354360336E+03
-0.8909545442950407E+02
-0.8909545442950407E+02
-0.8909545442950407E+02
0.1272792206135763E+02
0.1272792206135763E+02
0.1272792206135763E+02
-0.2121320343559561E+01

B6: 0.5676338384258064E+03
0.1234564442127483E+03
0.4542172819971128E+03
-0.3306049602475586E+02
-0.1108108418180178E+03
0.1472863839251848E+03
0.5169251748238688E+03
-0.8638628532981821E+02
-0.5264459824654215E+02
-0.4559442763393672E+01
-0.5755412070644406E+03
-0.7093844805034617E+02
-0.1217285908031968E+03
0.7085891403100351E+02
0.6484629934669887E+02
0.1506462927907833E+02
-0.8376102369821103E+01

B7: 0.3028479951938411E+03
0.3028479951938411E+03
-0.1347819854961351E+03
0.5974756131529863E+03
0.3901772012456136E+03
0.5974756131529863E+03

0.3901772012456136E+03
-0.2441962256553190E+02
-0.2441962256553190E+02
0.5137243689834529E+03
-0.4641605963928934E+03
-0.4641605963928934E+03
0.1577346393245378E+03
-0.6616911592759172E+03
-0.2470943354629615E+03
-0.2470943354629615E+03
0.1975305628793155E+03
0.1975305628793155E+03
-0.9767849026590808E+01
-0.2140518204066864E+02

B8: 0.5496643754770631E+04
0.5496643754770631E+04
0.2041899797016385E+04
-0.5496643755068393E+03
-0.5496643755073825E+03
-0.5496643755068393E+03
-0.5496643755073825E+03
-0.2041899797331987E+03
-0.2041899797331987E+03
-0.5214074922682864E+04
0.6107381951682088E+02
0.6107381951682088E+02
0.2268777554305542E+02
0.5339661070616519E+03
0.4571940191127395E+03
0.4571940191127395E+03
-0.5147730851460313E+02
-0.5147730851460313E+02
-0.4188079752134465E+02
0.5172693377466389E+01

B9: 0.7075674669569420E+03
-0.1459748127554288E+04
-0.1459748127554288E+04
-0.5748271102140304E+03
-0.5748271102140304E+03

-0.1122056297138504E+04
-0.2255442757549665E+03
0.6413819620482784E+03
-0.2255442757549665E+03
0.6413819620482784E+03
0.6961048807412159E+03
0.6961048807412159E+03
0.9086842070392228E+03
-0.2310209368569323E+02
-0.2310209368569323E+02
-0.7734498675222710E+02
0.4975944438431610E+02
-0.3477017543481466E+03
-0.3477017543481466E+03
0.1626461186393970E+02
0.1626461186363970E+02
0.4186597732172652E+02
-0.2656971466160727E+01

B10: 0.2412667738459828E+04
0.1223966270257313E+04
0.1329131277376937E+04
0.3599311319282041E+04
-0.1554405416542449E+04
-0.4090055547358414E+03
0.5804733630414911E+04
-0.3215525335466923E+03
0.9027056693263931E+03
0.4239532278337909E+04
0.6721386508096437E+04
0.2020800686011876E+04
-0.2003662183422511E+03
-0.4823277590390758E+03
0.2252741397053955E+02
-0.4917247644617672E+04
-0.4169304962580586E+03
-0.6233412290297092E+04
-0.1645087280631080E+04
-0.1759380486148640E+04
0.1325505819771913E+04
-0.5192687789152743E+04
0.3965263392555881E+03

0.6788583000370791E+03
0.1284044123531886E+02
0.2766407084668712E+04
0.7721073178107479E+03
0.3595007573235500E+03
-0.2135258233491258E+03
-0.2433892099636079E+03
-0.4929041010139955E+02
0.1807876583770241E+02

B11: 0.1473483887539281E+04
0.1473483887348471E+04
-0.7132254437278510E+03
0.3301688708048298E+04
0.2794625936499669E+04
-0.1008345971703264E+04
0.3301688707573324E+04
-0.1008345971440250E+04
0.2794625936395218E+04
0.3698220068032965E+04
0.1036140462803515E+04
0.1036140462791325E+04
0.4370075972010329E+04
0.4370075972176212E+04
0.5671050046587616E+03
-0.2967205684552609E+04
-0.2967205684669973E+04
0.1342829904356809E+04
-0.4887815461306522E+04
-0.3366627124975619E+04
-0.4887815461521109E+04
-0.3366627124910317E+04
0.4363446886799828E+03
0.4363446888962744E+03
-0.3722902779618582E+04
0.1942182985723540E+04
0.1942182986091824E+04
-0.7198976952240778E+03
0.2379190359084295E+04
0.8580018070698366E+03
0.8580018064487967E+03
-0.4585801709599821E+03

-0.4585801710299106E+03
0.4848279846344384E+02
0.3102419799579530E+02

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