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OPTIMAL CHOICE OF DIRECTIONS FOR THE RECONSTRUCTION OF AN OBJECT FROM A FINITE NUMBER OF ITS PLANE INTEGRALS

Audrey M. Tam
(Ph.D. thesis)

May 1982

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OPTIMAL CHOICE OF DIRECTIONS FOR THE RECONSTRUCTION OF AN OBJECT FROM A FINITE NUMBER OF ITS PLANE INTEGRALS[1]

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Ph.D. Thesis

May 1982

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Optimal Choice of Directions for the Reconstruction of an Object from a Finite Number of its Plane Integrals

by

Audrey M. Tam

To my parents

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Optimal Choice of Directions for the Reconstruction of an Object from a Finite Number of its Plane Integrals

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Audrey M. Tam

Abstract

The density of hydrogen nuclei in an object is a function $f(x,y,z)$ with compact support whose plane integrals can be approximated by nuclear magnetic resonance (NMR) measurements. Shepp [21] considered the problem of reconstructing f from a finite set of projections, i.e., integrals over N_s equi-spaced planes which are perpendicular to $\bar{u}_i$, for each of N directions $\bar{u}_1, \ldots, \bar{u}_N$:

$$P(t_i, \bar{u}_j) = \int_{\mathbf{R}^3} f(\bar{x})\, \delta(\bar{x}\cdot\bar{u}_j - t_i)\, d\bar{x}$$

The numerical implementation of the inversion formula

$$f(\bar{x}) = -\frac{1}{8\pi^2} \int_{\bar{u}\in\mathbf{S}^2} P''(\bar{x}\cdot\bar{u}, \bar{u})\, d\bar{u}\,,$$

$$\text{where} \quad P''(t,\bar{u}) \equiv \frac{d^2}{dt^2} P(t,\bar{u})$$

has three major steps: a second-derivative approximation and interpolation of a function of one variable, and quadrature over the unit sphere, $\mathbf{S}^2$. In this paper, we concentrate on finding quadrature formulas for functions defined on $\mathbf{S}^2$, in order to efficiently implement the inversion formula. Since, for each $\bar{x}$, the integrand $P''(\bar{x}\cdot\bar{u}, \bar{u})$ is an *even* function of $\bar{u}$, we are particularly interested in quadrature formulas for even functions. Product-space formulas, as in [15] and [21], are convenient, but inefficient.

We show how a large number of basis polynomials are automatically integrated by formulas which are invariant with respect to the group of rotations associated with one of the regular solids (tetrahedron, octahedron-cube, dodecahedron-icosahedron). Formulas of this type have been extensively investigated by Sobolev, et al., see [9], [11], [19], [23]. We describe the method of McLaren in detail and outline the method of Lebedev and Konyaev.

In an effort to simplify the procedure for finding icosahedral formulas, we eliminated one of the three degrees of freedom associated with a node by assigning the same weight to each node. The resulting system of non-linear equations can be solved by numerical methods, but good initial guesses, as well as some preliminary manipulations, are still needed.

Grünbaum [4] proposed the heuristic principle that, for large N, a good set of nodes $\bar{u}_1, \ldots, \bar{u}_N$ could be found by minimizing the potential energy due to N pairs of electrons positioned at $\pm\bar{u}_i$. Numerically minimizing this function of $2N$ variables is practically impossible for $N > 200$, however. We reduced the number of variables by a factor of 60 by requiring that the set of points consist of several icosahedral orbits. This method of finding quadrature nodes is almost "automatic", requiring no special adjustments beyond a good initial guess.

We compare the different quadrature formulas by reconstructing a three-dimensional model of a human head. The uniform-weight and equilibrium distributions perform as well as product-space methods which use twice as many directions.

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Introduction

The density of hydrogen nuclei in an object is a function $f(x,y,z)$ with compact support whose plane integrals can be approximated by nuclear magnetic resonance (NMR) measurements. Shepp [21] considered the problem of reconstructing f from a finite set of projections, i.e., integrals over N_s equi-spaced planes which are perpendicular to $\bar{u}_i$, for each of N directions $\bar{u}_1, \ldots, \bar{u}_N$:

$$P(t_i, \bar{u}_j) = \int_{\mathbf{R}^3} f(\bar{x})\, \delta(\bar{x}\cdot\bar{u}_j - t_i)\, d\bar{x}$$

In Chapter 1, we give the derivation of the inversion formula

$$f(\bar{x}) = -\frac{1}{8\pi^2} \int_{\bar{u}\in\mathbf{S}^2} P''(\bar{x}\cdot\bar{u}, \bar{u})\, d\bar{u}, \quad \text{where} \quad P''(t,\bar{u}) \equiv \frac{d^2}{dt^2} P(t,\bar{u})$$

and Shepp's basic algorithm for implementing it. The algorithm has three major features: a second-derivative approximation, linear interpolation, and quadrature over the unit sphere, $\mathbf{S}^2$. Shepp tested this algorithm by applying it to measurements taken from a three - dimensional model of a human head, which we describe in Section 1.2.

For any finite set of directions, $\bar{u}_1, \ldots, \bar{u}_N$, there exist non-zero functions $g(x,y,z)$ whose projections along $\bar{u}_1, \ldots, \bar{u}_N$ are all zero. The null-space of the finite two-dimensional Radon transform has been studied extensively by Smith, et al., see [22]. Louis [15] proposed a condition on the set of directions, $\bar{u}_1, \ldots, \bar{u}_N$, which minimizes the effect of these functions on the reconstruction. He observed that this condition could be satisfied using approximately ***half*** of the directions which Shepp used. He also pointed out that the number of plane integrals per direction, N_s, is tied to N, the number of directions. There is an optimal choice of N_s and taking more than this number of measurements actually *increases* the error in the reconstruction.

Both Shepp and Louis perform the numerical integration by discretizing the spherical coordinates parametrization of integration over $\mathbf{S}^2$,

$$\int_{\mathbf{S}^2} f(\bar{u}) = \int_0^{\pi} \sin\vartheta \, d\vartheta \int_0^{2\pi} f(\vartheta, \varphi) \, d\varphi . \qquad \text{Shepp}$$

$$\int_{\mathbf{S}^2} f(\bar{u}) = 2 \int_0^{\pi/2} \sin\vartheta \, d\vartheta \int_0^{2\pi} f(\vartheta, \varphi) \, d\varphi . \qquad \text{Louis}$$

using N_φ equi-spaced points on each of N_ϑ co-latitudes (product-space quadrature). This is not a very efficient choice of nodes, since there are a large number of nodes clustered near the poles, while the nodes nearer the equator are spaced farther apart. In addition, the contribution of each point is weighted by $\sin\vartheta$, where ϑ is its co-latitude. Hence, a point which is near a pole is weighted by a small amount, while the weight of a point near the equator is almost 1.

We decided to concentrate on the problem of finding good quadrature formulas for functions defined on $\mathbf{S}^2$. Since, for each $\bar{x}$, the integrand $P''(\bar{x} \cdot \bar{u}, \bar{u})$ is an *even* function of $\bar{u}$, we are particularly interested in quadrature formulas for even functions, e.g., formulas which exactly integrate all even polynomials in x, y and z up to some degree $2K$. There are $(K+1)(2K+1)$ independent even polynomials in x, y and z of degree less than or equal to $2K$. Thus, the nodes and coefficients of a $2K$th degree quadrature formula must simultaneously satisfy $(K+1)(2K+1)$ equations. In Chapter 2, we show how a large number of these constraints can be eliminated by restricting the search to formulas which are invariant with respect to the group of rotations associated with one of the regular solids (tetrahedron, octahedron-cube, dodecahedron-icosahedron). The remaining constraints involve only polynomials which are also invariant with respect to this rotation group.

An invariant quadrature formula has the form

$$I(f) \equiv \sum_{i=1}^{J} a_i \sum_{k=1}^{n_i} f(\overline{u}_i^{(k)}).$$

The action of the finite rotation group on a node $\overline{u}_i$ produces n_i distinct points, the *orbit* of $\overline{u}_i$. The members of this orbit have the same weight, a_i.

McLaren [19] derived several efficient low-order quadrature formulas, invariant with respect to either the octahedral group or the icosahedral group. The procedure he uses to find these formulas is relatively easy to implement, but cannot be applied to obtain formulas of order greater than 18. We demonstrate this procedure by deriving an even 91-point 18th-degree formula. (McLaren's formulas integrate both odd and even functions, and the last formula he derives has order 14.)

Lebedev [11] used a much more complicated method to produce octahedral formulas. We outline this procedure in Section 2.4. Konyaev [9] derived a 302-point 29th-degree formula by adapting this method to the icosahedral group. His formula is especially efficient, for our purposes, since he restricts his points to lie on the edges and medians of the associated icosahedron. This restriction produces icosahedral orbits which consist of 30 antipodal pairs. Thus, we could integrate even functions using only half of his set of points, i.e., we could integrate up to degree 28 using only 151 points.

Konyaev does not fully describe his method for finding this formula. It seems likely, however, that this procedure might also be limited in its range of application. Certainly, placing too many points on the edges and medians of the icosahedron will eventually produce a clustering of points and, probably, a reduction in efficiency.

Hoping to simplify the procedure for finding icosahedral formulas, we decided to sacrifice some of the efficiency of the formulas found by McLaren and Konyaev. We eliminated one of the three degrees of freedom associated with a node by assigning the same weight to each node. The resulting system of non-linear equations can be solved by numerical methods, but good initial guesses, as well as some preliminary manipulations, are still needed.

In Section 3.3, we combine two ideas to produce another method of finding nodes for uniform-weight quadrature formulas. Grünbaum [4] proposed the heuristic principle that, for large N, a good set of nodes $\bar{u}_1, \ldots, \bar{u}_N$ could be found by minimizing the potential energy due to N pairs of electrons positioned at $\pm\bar{u}_i$. Numerically minimizing this function of $2N$ variables is practically impossible for $N > 200$, however. We can reduce the number of variables by a factor of 60 if we require that the set of points consist of several icosahedral orbits. This method of finding quadrature nodes is almost "automatic", requiring no special adjustments beyond a good initial guess. Better convergence might be obtained by devising an optimization routine specifically tailored for the function

$$Q - \frac{N}{2} = 2D = 60\left[\sum_{j=2}^{60} d_{1j} + \sum_{j=62}^{120} d_{61,j} + \cdots + \sum_{j=N-58}^{N} d_{N-59,j}\right],$$

$$\text{where} \quad d_{ij} \equiv \frac{1}{|\bar{u}_i - \bar{u}_j|} + \frac{1}{|\bar{u}_i + \bar{u}_j|}$$

(The second term in d_{ij} is the potential due to the electron at $-\bar{u}_i$.)

In Chapter 4, we compare the results of simulation experiments conducted with the different quadrature formulas. The uniform-weight and equilibrium 600-point distributions perform as well as Shepp's or Louis' methods using twice as many directions. We conclude by summarizing the strengths and weaknesses of the methods we have described.

Chapter One: Methods of Shepp and Louis

1. Inversion Formula

Definition: Let $f: \mathbf{R}^3 \to \mathbf{R}$ be a continuous function with compact support. The *Radon transform of f* is the function

$$P(t,\bar{u}) = \int_{\mathbf{R}^3} f(\bar{x})\, \delta(\bar{x}\cdot\bar{u} - t)\, d\bar{x}$$

where $t \varepsilon \mathbf{R}$, $\bar{u} \varepsilon \mathbf{S}^2$ (the unit sphere), and $\bar{x} \varepsilon \mathbf{R}^3$.

Remark: The points $\bar{x}$ which satisfy $\bar{x}\cdot\bar{u} = t$ form the plane which is perpendicular to the direction $\bar{u}$, at distance t from the origin (0,0,0). $P(-t,-\bar{u}) = P(t,\bar{u})$, since $\bar{x}\cdot(-\bar{u}) = -t$.

Now define

$$m(\bar{x}) = \frac{1}{4\pi}\int_{\mathbf{S}^2} P(\bar{u}\cdot\bar{x},\bar{u})\, d\bar{u}\,.$$

We can rewrite this as

$$m(\bar{x}) = \frac{1}{2}\int_{\mathbf{R}^3} f(x',y',z')\, \frac{dx'\,dy'\,dz'}{\sqrt{(x'-x)^2 + (y'-y)^2 + (z'-z)^2}} = \frac{1}{2}(f * \frac{1}{r})(\bar{x})$$

Then $2\cdot m(\bar{x})$ can be viewed as the electrostatic potential of a field $\vec{E}$, with charge density $f(\bar{x})$ and [8, p.58]

$$f(\bar{x}) = \frac{1}{4\pi}\operatorname{div}\vec{E} = -\frac{1}{2\pi}\nabla^2 m(\bar{x})$$

Thus, if $P(t,\bar{u})$ is known for all values of t and $\bar{u}$, $f(\bar{x})$ can be uniquely recovered. (This formula, published by Radon [20] in 1917, was already known to Lorentz in 1906, see [2],[24].) Typically, however, we have only the values $P(t_i,\bar{u}_j)$, i.e., some finite number of plane integrals along each of some finite number of directions. The interpolation and numerical quadrature required to

compute $m(\bar{x})$ from this data would create a large amount of distortion, which would be compounded by the discrete Laplacian. A more convenient inversion formula can be derived by manipulating the Fourier transforms of f and P.

For each $\bar{u}$, the one-dimensional Fourier transform of $P(t,\bar{u})$, $\hat{P}(s,\bar{u})$, is the three-dimensional Fourier transform, $\tilde{f}(s\bar{u})$, of f along $\bar{u}$:

$$\int_{-\infty}^{\infty} P(t,\bar{u})e^{-ist}\,dt = \int_{\mathbf{R}^3} f(\bar{x})e^{-is\bar{x}\cdot\bar{u}}\,d\bar{x}$$

The inverse transform of $\tilde{f}$ (in spherical coordinates) gives

$$\begin{aligned} f(x,y,z) &= \mathrm{Re}\left(\frac{1}{2\pi}\right)^3 \int_0^{2\pi} d\varphi \int_0^{\pi} d\vartheta \int_0^{\infty} ds\ \tilde{f}(s,\vartheta,\varphi)s^2\sin\vartheta e^{ist} \\ &= \frac{1}{2}\left(\frac{1}{2\pi}\right)^3 \int_0^{2\pi} d\varphi \int_0^{\pi} d\vartheta \int_{-\infty}^{\infty} ds\ \tilde{f}(s,\vartheta,\varphi)s^2\sin\vartheta e^{ist}, \end{aligned} \tag{1.1.1}$$

since $\tilde{f}(-s,\vartheta,\varphi) = \overline{\tilde{f}(s,\vartheta,\varphi)}$ (f is real), while the inverse transform of $\hat{P}$ is

$$P(t,\vartheta,\varphi) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{P}(s,\vartheta,\varphi)e^{ist}\,ds.$$

Formally differentiating this twice with respect to t, we get

$$-P''(t,\vartheta,\varphi) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{P}(s,\vartheta,\varphi)s^2e^{ist}\,ds,$$

which, substituted into (1.1.1), gives

$$f(x,y,z) = -\frac{1}{8\pi^2}\int_0^{2\pi} d\varphi \int_0^{\pi} d\vartheta P''(t,\vartheta,\varphi)\sin\vartheta,$$

where $t = \bar{x}\cdot\bar{u}$ is the distance along $\bar{u}$ to the plane perpendicular to $\bar{u}$ which contains $\bar{x}$. This is just a particular parametrization of the more general formula

$$f(\bar{x}) = -\frac{1}{8\pi^2}\int_{\bar{u}\in S^2} P''(\bar{x}\cdot\bar{u},\bar{u})\,d\bar{u} \tag{1.1.2}$$

This formula can be implemented using a discrete (one-dimensional) second-derivative formula, followed by interpolation and numerical quadrature. We describe a particular implementation in Section 3.

2. Head Phantom

In actual tomography or zeugmatography [10], the error in the reconstruction can result from noise or error in the measurement of the data, as well as from the algorithm. To isolate the error which is due to a particular implementation of (1.1.2), the data is computed directly from a *phantom* -- a three-dimensional model of a human head, consisting of 17 ellipsoids:

inner and outer skull (2), densities 2. and 1.02
left and right ventricles (2), density 1.
eyes,ears,nose and mouth (6), incremental densities -1,1,1.5,-1
assorted tumors and a blood clot (7), densities 1.03 and 1.05

(This is Shepp's extension of his two-dimensional head phantom [13]. Except for the top and bottom of the skull, the three-dimensional phantom is contained in S^2. The exact data for the ellipsoids is listed in Table 1.) The equation of an ellipsoid with

center at $\vec{\xi}_0 = (x_0, y_0, z_0)$
orthonormal axes $\vec{v}_i$, i = 1,2,3
lengths of semi-axes a_i, i = 1,2,3

is

$$\sum_{i=1}^{i=3} \left[\frac{(\vec{\xi} - \vec{\xi}_0)\cdot\vec{v}_i}{a_i} \right]^2 \leq 1.$$

The area of the intersection of this ellipsoid with the plane $\vec{\xi}\cdot\vec{u} = t$ is

$$A = \pi a_1 a_2 a_3 (s^2 - \bar{t}^2) s^{-3},$$

where

$$\bar{t} = t - (\vec{\xi}_0 \cdot \vec{u})$$
$$s^2 = \alpha_1^2 a_1^2 + \alpha_2^2 a_2^2 + \alpha_3^2 a_3^2$$
$$\alpha_i = \vec{u}\cdot\vec{v}_i$$

and $A = 0$ if $s^2 - \bar{t}^2 < 0$.

Table 1

17 - ellipsoid Head Phantom

outer	0.	0.	0.	0.723	0.964	1.270	2.000	1.000
skull	0.	0.	0.	1.000	0.	0.	0.	1.000
inner	0.	-0.018	-0.019	0.701	0.925	1.224	-0.980	1.000
skull	0.	0.	0.	1.000	0.	0.	0.	1.000
right	0.220	0.	0.381	0.110	0.310	0.254	-0.020	0.951
ventricle	-0.309	0.	0.309	0.951	0.	0.	0.	1.000
left	-0.220	0.	0.381	0.160	0.410	0.381	-0.020	-0.951
ventricle	-0.309	0.	-0.309	0.951	0.	0.	0.	1.000
left	-0.080	-0.605	0.381	0.046	0.023	0.023	0.010	1.
tumor	0.	0.	0.	1.000	0.	0.	0.	1.000
center	0.	-0.605	0.381	0.023	0.023	0.046	0.010	1.
tumor	0.	0.	0.	1.	0.	0.	0.	1.
right	0.060	-0.605	0.381	0.023	0.046	0.023	0.010	1.
tumor	0.	0.	0.	1.	0.	0.	0.	1.
old "f"	0.	0.100	0.381	0.046	0.046	0.046	0.010	1.
	0.	0.	0.	1.0	0.	0.	0.	1.
old "g"	0.	-0.100	0.127	0.258	0.258	0.258	0.010	1.
	0.	0.	0.	1.0	0.	0.	0.	1.
old "e"	0.	0.350	0.381	0.210	0.250	0.230	0.010	1.
	0.	0.	0.	1.0	0.	0.	0.	1.
blood	0.560	-0.400	0.381	0.030	0.200	0.200	0.030	0.919
clot	-0.338	0.202	0.345	0.938	0.	0.190	-0.070	-0.979
left eye	0.258	0.753	0.	0.127	0.127	0.127	-1.0	1.0
	0.	0.	0.	1.0	0.	0.	0.	1.
right eye	-0.258	0.753	0.	0.127	0.127	0.127	-1.	1.
	0.	0.	0.	1.0	0.	0.	0.	1.
nose	0.	1.140	-0.196	0.127	0.340	0.170	1.500	1.
	0.	0.	0.	0.545	-0.839	0.	0.839	0.545
mouth	0.	0.	-0.762	0.458	0.610	0.508	-1.	-1.
	0.	0.	0.	1.0	0.	0.	0.	1.
left ear	0.708	-0.138	-0.191	0.064	0.318	0.318	1.	0.990
	-0.109	-0.087	0.109	0.994	0.	0.086	-0.009	0.996
right ear	-0.708	-0.138	-0.191	0.064	0.318	0.318	1.	-0.990
	-0.109	-0.087	-0.109	0.994	0.	-0.086	-0.009	0.996

Table 1 gives the center (x_0, y_0, z_0), the lengths (a_1, a_2, a_3) of the semi-axes, the incremental gray level (G), the coordinates (v_{11}, v_{12}, v_{13}), (v_{21}, v_{22}, v_{23}), (v_{31}, v_{32}, v_{33}) of the 3 orthonormal axes of each of the 17 ellipsoids corresponding to the head part indicated. "old f,g,e" refer to the tumors used in [13].

3. Reconstruction Algorithm

Let $f(x,y,z)$ be the density function of the head phantom. We assume that, for each of N directions, we have the integrals of f over N_s parallel planes at intervals of $h = \frac{2}{N_s - 1}$. I.e., we compute the plane integrals

$$P(t_i,\bar{u}_j)\ ,\ 1 \le j \le N\ ,\ t_i = (i-1)h - 1,\ 1 \le i \le N_s.$$

There are three parts to the numerical implementation of (1.1.2). Here, we describe Shepp's discretization. The other methods which we will discuss differ primarily in part (c), the quadrature formula.

(a) a second-derivative formula to get $Q(t_i,\bar{u}_j) \approx P''(t_i,\bar{u}_j)$

$$Q(t_i,\bar{u}_j) = \frac{1}{h^2}[P(t_{i+1},\bar{u}_j) - 2P(t_i,\bar{u}_j) + P(t_{i-1},\bar{u}_j)]$$

(b) an interpolation formula to get $Q(t,\bar{u}_j)$ when $t_i < t < t_{i+1}$

$$Q(t,\bar{u}_j) = Q(t_i,\bar{u}_j) + \frac{t - t_i}{h}[Q(t_{i+1},\bar{u}_j) - Q(t_i,\bar{u}_j)]$$

(c) a formula for numerical integration of functions defined on $\mathbf{S}^2$, i.e., a set of directions, $\bar{u}_1, \ldots, \bar{u}_N$, and a set of coefficients, $c_1, \ldots, c_N$, such that, for g in some class of functions,

$$\sum_{i=1}^{i=N} c_j g(\bar{u}_j) \approx \int_{\mathbf{S}^2} g(\bar{u})d\bar{u}\ .$$

Remark: Since $P(\bar{x}\cdot\bar{u},\bar{u})$ is an even function of $\bar{u}$, the plane integrals along $-\bar{u}$ provide the same information as the plane integrals along $\bar{u}$. By a set of *directions*, we mean one which contains no antipodal pairs.

Shepp's choice of directions is suggested by the spherical coordinate parametrization of (1.1.2):

$$f(\bar{x}) = -\frac{1}{8\pi^2}\int_0^{2\pi} d\varphi \int_0^{\pi} d\vartheta P''(\bar{x}\cdot\bar{u},\bar{u})\sin\vartheta,$$

where $\bar{x} = (x,y,z)$ and $\bar{u} = (\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta)$. This can be discretized as

$$\bar{f}(\bar{x}) \equiv -\frac{1}{8\pi^2}\frac{\pi}{N_\vartheta}\frac{2\pi}{N_\varphi}\sum_{j=1}^{N_\vartheta}\sum_{k=1}^{N_\varphi} \sin\vartheta_j\, Q(\bar{x}\cdot\bar{u}_{jk},\bar{u}_{jk})$$

where

$$\bar{u}_{jk} = (\sin\vartheta_j\cos\varphi_k, \sin\vartheta_j\sin\varphi_k, \cos\vartheta_j)$$
$$\vartheta_j = (j - \tfrac{1}{2})\frac{\pi}{N_\vartheta}, \quad 1 \le j \le N_\vartheta$$
$$\varphi_k = (k - 1)\frac{2\pi}{N_\varphi}, \quad 1 \le k \le N_\varphi$$

and N_ϑ, N_φ are odd integers to prevent redundancy in the set of directions.

We will refer to this type of formula as a *product - space* formula, since its nodes are the points on $\mathbf{S}^2$ whose spherical coordinates are all possible ordered pairs (ϑ_j, φ_k), for some set of $\{\vartheta_j\}$ and some set of $\{\varphi_k\}$.

Shepp tested this algorithm on the head phantom, using $N_\vartheta = N_\varphi$ and $N_s = 101$ to reconstruct the $z = .381$ plane, which passes through the centers of most of the tumors. More precisely, the values of $\bar{f}$ were computed on a 128 x 128 grid of the square [-1,1] x [-1,1]. Satisfactory reconstruction of the complete 17 - ellipsoid phantom required 99 x 99 directions. (A reconstruction was judged to be satisfactory if the three small tumors could be readily distinguished.) However, if the "high - contrast" features were removed, the resulting 11 - ellipsoid phantom could be reconstructed using only 25 x 25 directions. The high - contrast features are the eyes, ears, nose and mouth, which "cast tangents" into the plane of reconstruction.

4. Louis's Modifications

Given any finite set of directions, $\bar{u}_1, \ldots, \bar{u}_N$, there exist non-zero functions $g(x,y,z)$ such that

$$P_g(t,\bar{u}_i) = 0 \quad a.e.t \ , \ 1 \le i \le N.$$

These functions belong to the null space of the "discrete" Radon transform. Louis [15] calls them the *ghosts* associated with the set of directions $\{u_1, \ldots, u_N\}$ (not to be confused with the head "phantom" described in Section Two). The null-space of the finite two-dimensional Radon transform has been studied extensively by Smith, et al., see [22]. A density function, f, can be uniquely expressed as the sum of a ghost, g, and a non-ghost, h. I.e., h is in the orthogonal complement of the null-space of $P(t,\bar{u}_i)$. Using the plane integrals along $\bar{u}_1, \ldots, \bar{u}_N$, we can recover, at most, only the non-ghostly part of f.

Louis [15] proposed a condition on the set of directions, $\bar{u}_1, \ldots, \bar{u}_N$, which ensures the near-absence of lower frequencies in this set's ghosts. If the ghosts have negligible Fourier coefficients for frequencies $s < K$, we can hope to accurately reconstruct details of size $\frac{2}{K}$. In order to present this condition and its consequences, we will need some definitions and properties of spherical harmonics.

Definition: A polynomial, $V_n(x,y,z)$, homogeneous of degree n, is an *n-degree spherical harmonic* if $\nabla^2 V_n = 0$.

A general homogeneous polynomial of degree n has $\frac{1}{2}(n+1)(n+2)$ coefficients. $\nabla^2 V_n$ has degree $(n-2)$, or $\frac{1}{2}(n-1)n$ coefficients which must be zero if V_n is a spherical harmonic. This gives $\frac{1}{2}(n-1)n$ conditions on $\frac{1}{2}(n+1)(n+2)$ coefficients, which means that V_n is determined by only $2n + 1$ coefficients. An

orthonormal basis for the space of n-degree spherical harmonics is given by the $2n + 1$ functions [17]

$$Y_n^m(\bar{u}) = \left[\frac{2\pi}{2n+1}\frac{(n+|m|)!}{n-|m|)!}\right]^{-1/2} T_n^{|m|}(\cos\vartheta)\begin{cases}\cos m\varphi \\ \sin|m|\varphi\end{cases}$$

$$Y_n^0(\bar{u}) = \left[\frac{4\pi}{2n+1}\right]^{-1/2} P_n(\cos\vartheta)$$

where $\bar{u} = (\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta)$,

$$T_n^m(x) = (-1)^m(1-x^2)^{m/2}\frac{d^m}{dx^m}P_n(x),$$

and $P_n(x) = (2^n n!)^{-1}\frac{d^n}{dx^n}(x^2-1)^n$ are the Legendre polynomials.

The reader is cautioned that this is not the standard notation. T_n^m more commonly appears as $(-1)^m P_n^m$.

A *spherical polynomial of degree* n is a linear combination of spherical harmonics of degree $\leq n$. An arbitrary n-degree spherical polynomial has $(n+1)^2$ coefficients. An even or odd spherical polynomial of degree n has $\frac{1}{2}(n+1)(n+2)$ coefficients.

Theorem (Louis) Let $g(x,y,z)$ have support in the unit ball and suppose g is a ghost function of the set of directions $\bar{u}_1, \ldots, \bar{u}_N$. Let $K \geq 1$ be such that $\frac{1}{2}K(K+1) \leq N$. If $\bar{u}_1, \ldots, \bar{u}_N$ are not roots of any spherical polynomial of degree $\leq (K-1)$, then $\tilde{g}(s\bar{u}) \approx 0$ for $|s| < K+\frac{1}{2}$.

Proof: If $g(x,y,z)$ has support in the unit ball, then $P_g(t,\bar{u}) = 0$ for $|t| \geq 1$, and the Radon transform of g can be expanded in terms of the Gegenbauer polynomials, $C_m^{3/2}(t)$, which are orthogonal over the interval [-1,1] with respect to the

weight function $(1 - t^2)$:

$$P_g(t,\bar{u}) = (1 - t^2) \sum_{m=0}^{\infty} C_m^{3/2}(t) q_m(\bar{u}) \tag{1.4.1}$$

where the coefficients, $q_m(\bar{u})$ are

$$q_m(\bar{u}) = \frac{m + \frac{3}{2}}{(m+1)(m+2)} \int_{-1}^{1} C_m^{3/2}(t) P_g(t,\bar{u}) dt$$

The conditions of Helgason [7] and Ludwig [16] require that $q_m(\bar{u})$ be a spherical polynomial of degree m. Recall that $P(-t,-\bar{u}) = P(t,\bar{u})$ (Section 1.1), i.e., $P(t,\bar{u})$ is an even function. Then the fact that $C_m^{3/2}$ is odd if m is odd, and even if m is even, requires that the same be true of q_m. Thus, we can write q_m as

$$q_m(\bar{u}) = \sum_{\substack{l=0 \\ m+l \text{ even}}}^{l=m} \sum_{k=-l}^{k=l} d_{mlk} Y_l^k(\bar{u}) \tag{1.4.2}$$

If g is a ghost, then $P_g(t,\bar{u}_i) = 0$ for $1 \le i \le N$. From (1.4.1), $q_m(\bar{u}_i) = 0$ for all m and for $1 \le i \le N$, since the Gegenbauer polynomials $C_m^{3/2}(t)$ are linearly independent. If $\bar{u}_1, \ldots, \bar{u}_N$ are not roots of any spherical polynomial of degree $< K$, then the coefficients d_{mlk} in (1.4.2) must be 0 for all $m < K$, i.e., $q_m \equiv 0$ for $m < K$.

Remark: Let $M = \frac{1}{2}(m + 1)(m + 2)$ and denote the M spherical harmonics $\{Y_l^k\colon\ 0 \le l < m,\ m + l \text{ even}, -l \le k \le l\}$ by $Z_1, \ldots, Z_M$. Then the condition on the set of directions $\bar{u}_1, \ldots, \bar{u}_N$ is equivalent to the linear independence of the columns of the $N \times M$ matrix $\mathbf{Z} \equiv [Z_j(\bar{u}_i)]$. This is possible only if $M \le N$.

Now, with $q_m \equiv 0$ for $m < K$,

$$P_g(t,\bar{u}) = \sum_{m=K}^{\infty} C_m^{3/2}(t) q_m(\bar{u}). \tag{1.4.3}$$

The Fourier transform of g is the one-dimensional Fourier transform of $P_g(t,\bar{u})$:

$$\hat{g}(s\bar{u}) = \hat{P_g}(s,\bar{u}) = \sum_{m=K}^{\infty} [(1-t^2)\, C_m^{3/2}(t)]^{\wedge}\,(s)\, q_m(\bar{u}).$$

Since $C_m^{3/2}(t) = P'_{m+1}(t)$, where $P_m(t)$ is the mth Legendre polynomial,

$$(1-t^2)\, C_m^{3/2}(t) \;=\; \frac{(m+1)(m+2)}{2m+3}[P_m(t) - P_{m+2}(t)]$$

From a table of Fourier transforms [18],

$$\begin{aligned}[P_m(t) - P_{m+2}(t)]^{\wedge}\,(s) \;&=\; (-i)^m \left(\frac{2\pi}{s}\right)^{1/2} \cdot [J_{m+\frac{1}{2}}(s) - J_{m+\frac{5}{2}}(s)] \\ &=\; (-i)^m \sqrt{2\pi}\, s^{-3/2}\, 2(m+\frac{3}{2}) \cdot J_{m+\frac{3}{2}}(s),\end{aligned}$$

where $J_\nu(s)$ is the Bessel function of the first kind. Substituting this into (1.4.3) gives

$$\tilde{g}(s\bar{u}) \;=\; \sum_{m=K}^{\infty} k_m\, s^{-3/2} J_{m+\frac{3}{2}}(s)\, q_m(\bar{u}) \tag{1.4.4}$$

where

$$k_m \;=\; (-i)^m \sqrt{2\pi}\,(m+1)(m+2)$$

Louis asserts that, since $J_\nu(s) \approx 0$ for $|s| < \nu - 1$, $\tilde{g}(s\bar{u})$ is "small" for $|s| < K + \frac{1}{2}$. We were unable to reconstruct a proof of this statement, although we have no reason to doubt its validity. Using the bound [25, p. 255],

$$J_\nu(\nu x) \;\le\; e^{-\nu\lambda(x)} \cdot (1-x^2)^{-1/4} \cdot (2\pi\nu)^{-1/2} \tag{1.4.5}$$

for ν large and $0 < x \le 1$, and with

$$\lambda(x) \;=\; \ln \frac{1+\sqrt{1-x^2}}{x} - \sqrt{1-x^2},$$

we could only prove the weaker statement:

$$\tilde{g}(s\bar{u}) \to 0 \text{ uniformly as } \nu \to \infty \text{ if } x = \frac{s}{\nu} < 1 - \varepsilon, \text{ for } \varepsilon > 0.$$

The main obstacle is the fact that $\lambda(x) \approx 0$ for x close to 1. Rewriting (1.4.4), we get

$$\tilde{g}(s\bar{u}) = \sqrt{2\pi}\, s^{-3/2} \sum_{m=K}^{\infty} (-i)^m \left(m + \frac{3}{2}\right) J_{m+\frac{3}{2}}(s) \int_{-1}^{1} C_m^{3/2}(t)\, P(t,\bar{u})\, dt\,.$$

Taking absolute values and replacing $J_\nu(\nu x)$ by the expression in (1.4.5) gives us

$$|\tilde{g}(\nu x\bar{u})| \le (x^6 - x^8)^{-1/4} \sum_{\nu=K+3/2}^{\infty} \frac{e^{-\nu\lambda(x)}}{\nu} \cdot \left| \int_{-1}^{1} C_m^{3/2}(t)\, P(t,\bar{u})\, dt \right|.$$

We bound $C_m^{3/2}$ by its maximum value, $\frac{1}{2}(m+1)(m+2)$ and denote the integral of $P(t,\bar{u})$ by I. Writing $m+1$ as $\nu - \frac{1}{2}$, and $m+2$ as $\nu + \frac{1}{2}$, we obtain

$$|\tilde{g}(\nu x\bar{u})| \le \frac{I}{2}(x^6 - x^8)^{-1/4} \sum_{\nu=K+3/2}^{\infty} e^{-\nu\lambda(x)} \left(\nu - \frac{1}{4\nu}\right)$$

Now, if $x < 1-\varepsilon$, then $\lambda(x) > 0$, and $e^{-\nu\lambda(x)} < \frac{3!}{(\nu\lambda(x))^3}$. This gives us

$$|\tilde{g}(\nu x\bar{u})| \le \frac{I}{2}(x^6 - x^8)^{-1/4} \frac{6}{\lambda^3(x)} \sum_{\nu=K+3/2}^{\infty} \frac{1}{\nu^2} - \frac{1}{\nu^4}$$

The summation is less than $\dfrac{1}{K + \frac{1}{2}}$ and

$$(x^6 - x^8)^{-1/4} < \begin{cases} \dfrac{3}{2x} & 0 < x \le \dfrac{\sqrt{3}}{2} \\[2ex] \dfrac{1}{4(1-x)} & \dfrac{\sqrt{3}}{2} \le x < 1-\varepsilon \end{cases}$$

Thus, K can always be chosen to make this bound less than some ε'.

Choice of Directions

The set of directions which Shepp used in his algorithm (Section 3) fall on the longitudes

$$\varphi = (k - 1)\frac{2\pi}{N_\varphi}, \quad 1 \le k \le N_\varphi$$

and are therefore roots of the spherical harmonic, $Y_n^{-n}(\bar{u})$, where $n = N_\varphi$. If g is a ghost function of this set of directions, its Fourier transform,

$$\tilde{g}(s\bar{u}) = \sum_{m=0}^{\infty} k_m s^{-3/2} J_{m+\frac{3}{2}}(s)\, q_m(\bar{u})$$

has $q_m \equiv 0$ for $m < N_\varphi - 1$, provided that $\bar{u}_1, \ldots, \bar{u}_N$ are not roots of any lower degree polynomial. But this can be accomplished using only $\frac{1}{2}N_\varphi(N_\varphi + 1)$ directions, instead of the N_φ^2 directions which are generated by Shepp's choice of $N_\vartheta = N_\varphi$. In fact, a slight modification of Shepp's set of directions gives the $\frac{1}{2}N_\varphi(N_\varphi + 1)$ directions

$$\bar{u}_{jk} = (\sin\vartheta_j \cos\varphi_k, \sin\vartheta_j \sin\varphi_k, \cos\vartheta_j)$$
$$\vartheta_j = (j - \tfrac{1}{2})\frac{\pi}{N_\vartheta + 1}, \quad 1 \le j \le \tfrac{1}{2}(N_\vartheta + 1)$$
$$\varphi_k = (k - 1)\frac{2\pi}{N_\varphi}, \quad 1 \le k \le N_\varphi \text{ (as before)}$$

Louis [15] performed simulation experiments using this set of directions to reconstruct the head phantom described in Section 3. However, the eyes, ears, nose and mouth were not included in the calculation of the projections $P(t_i, \bar{u}_{jk})$ in order to obtain reasonably good reconstructions from relatively small sets of data.

Louis computed $\bar{f}$ at 128 equi-spaced points on each of the lines $y = .23$ and $y = -.605$ of the plane $z = .381$, comparing

$$(a)\ \ N_\varphi = 25,\ N_\vartheta = 13,\ N = N_\varphi \cdot N_\vartheta = 325,\ N_s = 51$$

and

$$(b)\ \ N_\varphi = 35,\ N_\vartheta = 18,\ N = N_\varphi \cdot N_\vartheta = 630,\ N_s = 71$$

with

$$(c)\ \ N_\varphi = 25,\ N_\vartheta = 25,\ N = N_\varphi \cdot N_\vartheta = 625,\ N_s = 101$$

He concluded that (a) achieved roughly the same resolution as (c), i.e., the significant details of the phantom were visible, and that (b) did better than (c).

Optimal Lateral Sampling

It is important to note that Louis varied a parameter that Shepp left fixed. Recall that Shepp took as his data the values of $P_f(t_i, \bar{u}_j)$ for N directions $\bar{u}$ and N_s equi-spaced values of t. He used $N_s = 101$ in his simulations, regardless of the value of N_φ, remarking that, to achieve higher resolution, a larger number of plane integrals per direction would be needed. Louis, however, reasoned that the Shannon sampling theorem implies a relationship between the set of directions and N_s. If the Fourier transform of an object is "known" (i.e., not affected by ghosts) inside a ball of radius $K + \frac{1}{2}$, its Nyquist frequency is $\frac{1}{2K+1}$. For the set of directions which Louis used, $K = N_\varphi$. Hence,

$$N_s = 2N_\varphi + 1.$$

This seems to be a (locally) optimal choice of N_s -- for example, increasing the value of N_s in (a) to 75 or 101 actually *increases* the L^2 error in the reconstruction. This fact is surprising since a larger number of measurements (on the same interval) should give a better approximation to the function, $P_f(t, \bar{u})$, hence, to $P''_f(t, \bar{u})$. Louis's explanation for this phenomenon is that the low - order quadrature formula cannot handle the high - frequency parts of the more

accurate approximation to the second derivative.

Shepp's Method with Optimal Lateral Sampling

It seemed likely that Shepp's set of directions would produce better results if a smaller N_s were used. In particular, these directions also eliminate the effects of ghosts inside the ball of radius $N_\varphi + \frac{1}{2}$. By Louis's argument, therefore, the best results should be obtained by using $N_s \approx 2N_\varphi + 1$. However, when we re-tested this set of directions, allowing N_s to vary, we found that the optimal N_s was *not* the inverse of its *own* Nyquist frequency. Instead, the lowest L^2 errors resulted from using

$$N_s \approx 2K + 1, \quad \frac{K(K+1)}{2} \le N \le \frac{(K+1)(K+2)}{2}, \quad K \text{ odd}. \tag{1.4.4}$$

With this value for N_s, Shepp's directions produced a lower L^2 error than a comparable number of Louis's directions (see Table 9, Sec. 4.1).

$K - 1$, with K defined as in (1.4.4), is the "expected" order of a fixed-node N-point quadrature formula for even functions defined on the sphere. This type of formula has one free parameter for each node -- its weight, α_i -- and so we expect to be able to satisfy N constraints. In particular, if this quadrature integrates well the first $\frac{1}{2}K(K+1)$ even spherical harmonics, i.e., those of even degree $\le K-1$, then its order is $K-1$. Note that, for Louis's method, $K = N_\varphi$.

5. Order of Product-Space Quadratures

Any function in $L^2(\mathbf{S}^2)$ can be expanded in a series of spherical harmonics. Just as a one-dimensional quadrature formula is exact for polynomials in x up to some degree p, we can look for quadrature formulas

$$I(f) \equiv \sum_{i=1}^{N} a_i f(\bar{u}_i) \approx \int_{\mathbf{S}^2} f(\bar{u})\, d\bar{u} \tag{1.5.1}$$

which exactly integrate all spherical harmonics up to some degree p. With three variables, however, such a formula must satisfy $(p+1)^2$ equations (or $\frac{1}{2}(p+1)(p+2)$ equations, if only even functions must be integrated):

$$\sum_{i=1}^{N} a_i = 4\pi$$

$$\sum_{i=1}^{N} a_i\, Y_m^n(\bar{u}_i) = 0, \quad -m \le n \le m, \quad 1 \le m \le p \quad (m \text{ even})$$

where $\{Y_m^{-m}, \ldots, Y_m^m\}$ is the orthonormal basis (defined in Section 1.4) for $\mathbf{Y}_m$, the space of m-degree spherical harmonics.

A quadrature formula (1.5.1) is exact for all spherical polynomials of degree $\le p$ if and only if

$$E_m \equiv \sum_{i,j=1}^{N} a_i a_j P_m(\bar{u}_i, \bar{u}_j) = 0 \tag{1.5.2}$$

for Legendre polynomials of degree $m \le p$, $m \ne 0$. This property is a result of the addition theorem for spherical harmonics:

$$P_m(\bar{u} \cdot \bar{v}) = \frac{4\pi}{2m+1} \sum_{n=-m}^{m} Y_m^n(\bar{u})\, Y_m^n(\bar{v}), \quad m \ne 0.$$

Substituting this into (1.5.2), we see that

$$\sum_{i,j=1}^{N} a_i a_j P_m(\bar{u}_i, \bar{u}_j) = \frac{4\pi}{2m+1} |[I(Y_m^n)]|^2.$$

where

$$[I(Y_m^n)] \equiv \begin{bmatrix} I(Y_m^{-m}) \\ \vdots \\ I(Y_m^m) \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} a_i \, Y_m^{-m}(\bar{u}_i) \\ \vdots \\ \sum_{i=1}^{N} a_i \, Y_m^m(\bar{u}_i) \end{bmatrix}.$$

Thus, (1.5.2) is true if and only if the quadrature formula, $\{a_i, \bar{u}_i\}$, exactly integrates all spherical harmonics of degree $m \le p$, $m \ne 0$.

The quadrature formulas used by both Shepp and Louis integrate a function of two variables by ***repeated 1 - dimensional quadrature***. Shepp discretizes

$$\int_0^{\pi} \sin\vartheta \, d\vartheta \int_0^{2\pi} f(\vartheta, \varphi) \, d\varphi .$$

Louis restricts his nodes to the upper hemisphere, discretizing

$$2 \int_0^{\pi/2} \sin\vartheta \, d\vartheta \int_0^{2\pi} f(\vartheta, \varphi) \, d\varphi .$$

Both methods use nodes of the form

$$\begin{aligned} \bar{u}_{ij} &\equiv (\vartheta_i, \varphi_j) \\ \vartheta_i &= (i - \tfrac{1}{2}) \frac{\pi}{M_\vartheta}, \qquad 1 \le i \le N_\vartheta \\ \varphi_j &= (j - 1) \frac{2\pi}{N_\varphi}, \qquad 1 \le j \le N_\varphi \end{aligned}$$

I.e., the nodes lie on N_φ equi-spaced meridians and N_ϑ co-latitudes equi-spaced between $\frac{\pi}{2M_\vartheta}$ and $(2N_\vartheta - 1) \frac{\pi}{2M_\vartheta}$.

The order of a product - space quadrature formula depends on the relationship

between N_ϑ and M_ϑ. To illustrate, we list the values of E_m $0 \le m \le 52$, m even, for 4 cases:

(1) $N_\varphi = 25$, $M_\vartheta = 26$, $N_\vartheta = 13$ (Louis)
(2) $N_\varphi = 29$, $M_\vartheta = 22$, $N_\vartheta = 11$
(3) $N_\varphi = M_\vartheta = N_\vartheta = 25$ (Shepp)
(4) $N_\varphi = 49$, $M_\vartheta = 12$, $N_\vartheta = 6$

E_m for $2 \le m \le 52$, m even				
m	$N_\varphi = 25$, $M_\vartheta = 26$, $N_\vartheta = 13$, $N = 325$	$N_\varphi = 29$, $M_\vartheta = 22$, $N_\vartheta = 11$, $N = 319$	$N_\varphi = 25$, $M_\vartheta = 25$, $N_\vartheta = 25$, $N = 625$	$N_\varphi = 49$, $M_\vartheta = 12$, $N_\vartheta = 6$, $N = 294$
2	.00006	.00012	.00007	.00134
4	.00006	.00012	.00007	.00146
6	.00006	.00012	.00007	.00168
8	.00006	.00013	.00008	.00205
10	.00007	.00014	.00008	.00267
12	.00007	.00015	.00009	.00379
14	.00008	.00017	.00009	.00598
16	.00008	.00019	.00010	.01100
18	.00009	.00022	.00011	.02568
20	.00010	.00026	.00013	.09443
22	.00012	.00032	.00015	1.39288
24	.00014	.00040	.00017	5.07027
26	2.56597	.00052	.00021	.00022
28	.23065	.00071	.00026	.00028
30	.74713	2.13813	.00033	.00037
32	.10851	.18290	.00043	.00051
34	.39315	.68696	.00059	.00076
36	.05094	.08435	.00086	.00119
38	.25622	.41725	.00133	.00208
40	.02178	.07494	.00226	.00419
42	.19676	1.05408	.00444	.01061
44	.00885	2.78538	.01092	.04204
46	.18814	.37886	.04200	.66383
48	.04090	.06760	.64431	2.57347
50	1.60807	.87432	3.21987	1.46635
52	2.75052	.14210	.33782	.00882

E_m measures the error in approximating the integrals

$$\int_{S^2} Y_m^n(\vartheta, \varphi) = \int_0^{2\pi} \begin{Bmatrix} \cos \\ \sin \end{Bmatrix} n\varphi \, d\varphi \int_0^{\pi} T_m^n(\cos\vartheta) \sin\vartheta \, d\vartheta \,, \qquad -m \le n \le m$$

By performing each quadrature separately, we determined that, for N_φ odd, the one - dimensional quadrature over φ is exact for $n \le N_\varphi - 1$, n even:

$$\frac{\pi}{M_\vartheta} \sum_{j=1}^{N_\varphi} \begin{Bmatrix} \cos \\ \sin \end{Bmatrix} n\varphi_j \;=\; \int_0^{2\pi} \begin{Bmatrix} \cos \\ \sin \end{Bmatrix} n\varphi \, d\varphi ,$$

and the one - dimensional quadrature over ϑ is exact for $n \neq 0$:

$$\frac{M_\vartheta}{N_\vartheta} \cdot \frac{2\pi}{N_\varphi} \sum_{i=1}^{N_\vartheta} \sin\vartheta_i \, T_m^n(\cos\vartheta_i) \;=\; \int_0^{\pi} \sin\vartheta \, T_m^n(\cos\vartheta) \, d\vartheta .$$

Thus, for $m \le N_\varphi - 1$, E_m is exactly the quadrature of the mth Legendre polynomial:

$$E_m \;=\; \frac{4\pi}{2m+1} \left\{ \frac{M_\vartheta}{N_\vartheta} \, 2\pi \cdot \frac{2\pi}{N_\varphi} \sum_{i=1}^{N_\vartheta} \sin\vartheta_i \, P_m(\cos\vartheta_j) \right\}^2 .$$

Now, examining the list of values of E_m, we see that E_m is small for $m \ll 2M_\vartheta$, increases sharply near $m = 2M_\vartheta$, and then repeats this pattern. Thus, the E_m values for Louis's method, with $N_\varphi \approx M_\vartheta$, are small for $m \le N_\varphi - 1$, and then are dominated by the error in the φ - quadrature. The E_m values for Shepp's method, on the other hand, increase gradually, with a large error at $m = 2M_\vartheta = 2N_\varphi$. Using nodes in the lower hemisphere as well as the upper hemisphere, with the ϑ - levels distributed symmetrically about the equator, effectively halves the φ - increment, from $\frac{\pi}{M_\vartheta}$ to $\frac{2\pi}{2N_\varphi}$. The large error at $m = 2M_\vartheta = 2N_\varphi$, then, is the combined "large error" of both of the one - dimensional quadratures.

The second of our 4 cases appears to be an optimal choice of N_φ and M_ϑ: $M_\vartheta \approx \frac{2}{3} N_\varphi$. The error in the φ - quadrature takes over just before the error in the $P_m(\cos\vartheta)$ - quadrature begins to increase significantly. This quadrature

formula has a higher order than Louis's method, although it uses fewer points. Or, if the order of quadrature is specified, an "optimal" formula would use $\frac{1}{3}$ fewer points than Louis's.

Chapter Two: Invariant Quadrature Formulas

1. Automatic Integration (Group representation theory)

The efficiency of a quadrature formula can be described by the number $\frac{q}{3N}$, where N is the number of quadrature nodes, and q is the total number of spherical harmonics for which the formula is exact. An efficiency of 1 indicates that each of the $3N$ free parameters -- the weights and coordinates of the nodes -- is being used to eliminate one of the constraints. A product - space quadrature formula has only one free parameter for each node, i.e., its weight. Thus, its efficiency is about $\frac{1}{3}$. Sobolev [24] proposed the idea of Gauss - type quadrature formulas, invariant with respect to some (finite) rotation group. These formulas automatically integrate all but a few of the spherical harmonics of a given degree. The weights and positions of the nodes are then found by solving the system of constraints which remains. These quadrature formulas are difficult to derive, but their efficiency is close to 1, since each node has three free parameters. Another advantage of these quadratures is the more uniform distribution of their nodes. In this section, we present the theoretical basis for these formulas. Similar discussions can be found in [24] and [19].

There are five regular solids: tetrahedron, cube, octahedron, dodecahedron and icosahedron. The tetrahedron is self-dual, the cube is dual to the octahedron, and the dodecahedron is dual to the icosahedron, i.e., the centers of the faces of one are the vertices of the other.

If the orientation of a regular solid is fixed, there is a finite group of rota-

tions in $\mathbf{R}^3$ which move vertices to vertices and thus preserve that orientation. The axes of these rotations are the lines which connect opposing vertices, opposing centers of faces, and opposing midpoints of edges. The permissible angles of rotation depend upon the number of faces which share a vertex and the number of sides of a face (rotations about midpoints of edges must be 180 degrees). This group of rotations acting on a point of the unit sphere which does not lie on an axis of rotation generates an orbit of n points widely distributed over the surface of the sphere, where n is the order of the group. Quadrature formulas whose nodes consist of several of these orbits are invariant with respect to the group of rotations and, as we will show, "automatically" integrate exactly a large class of spherical polynomials.

Let G be the group of rotations of the sphere associated with a fixed regular solid. The vertices, centroids and edges of this solid -- $\{V_i\},\{C_i\},\{E_i\}$ -- are the *special invariant sets* of G. If a point $\bar{u}$ on the sphere is not in one of the special sets, the *general invariant set* $\{\rho\bar{u}\colon \rho\varepsilon G\}$ contains n points. (If $\bar{u}$ lies on a median or an edge of a face, these n points are actually $\frac{n}{2}$ antipodal pairs.)

A quadrature formula which uses J invariant sets of G has the form

$$\sum_{i=1}^{J} a_i \sum_{k=1}^{n_i} f\,(\bar{u}_i^{(k)}), \tag{2.1.2}$$

i.e., every point in the invariant set $\{\bar{u}_i^{(k)}\colon 1 \le k \le n_i\}$ is assigned the same weight a_i, $i = 1,\ldots,J$. We will call the points $\bar{u}_i$, $1 \le i \le J$, the *base nodes* of this quadrature formula. Then, the system of equations (2.1.1) becomes

$$\begin{aligned} \sum_{i=1}^{J} a_i n_i &= 4\pi \\ \sum_{i=1}^{J} a_i \sum_{k=1}^{n_i} Y_m^n(\bar{u}_i^{(k)}) &= 0, \quad ,-m \le n \le m\,, \quad 1 \le m \le p\,. \end{aligned} \tag{2.1.3}$$

We will use some basic properties of group representations to show that most of these equations are automatically satisfied. Details of these properties can be found in [5].

An element ρ of the group G acts on the vector space $\mathbf{Y}_m$ by transforming a spherical harmonic $h \varepsilon \mathbf{Y}_m$ into the function ρh, satisfying

$$(\rho h)(\bar{u}) = h(\rho^{-1}\bar{u}), \quad \text{for all } \bar{u} \varepsilon \mathbf{S}^2.$$

$\mathbf{Y}_m$ is invariant under the action of the full rotation group, so it is invariant under the action of G. I.e., the function ρY_m^n is a linear combination of the basis functions $\{Y_m^{-m}, \ldots, Y_m^m\}$. Thus there is a $(2m + 1)$ - dimensional representation, M, of the action of G on $\mathbf{Y}_m$. For every $\rho \varepsilon G$, $M(\rho)$ is the $(2m + 1)$ x $(2m + 1)$ matrix satisfying

$$M(\rho) \cdot \begin{bmatrix} Y_m^{-m} \\ \vdots \\ Y_m^m \end{bmatrix} = \begin{bmatrix} \rho Y_m^{-m} \\ \vdots \\ \rho Y_m^m \end{bmatrix}.$$

There is an orthonormal basis $\{Z_1, \ldots, Z_{2m+1}\}$ of $\mathbf{Y}_m$ which brings M into reduced form:

$$M = M_1 \oplus \cdots \oplus M_r,$$
$$dim\ M_1 \oplus \cdots \oplus dim\ M_r = 2m + 1.$$

Then $\mathbf{Y}_m = \mathbf{Y}_{m1} \oplus \cdots \oplus \mathbf{Y}_{mr}$, where $dim\ \mathbf{Y}_{mk} = dim\ M_k$, $\mathbf{Y}_{mk}$ is invariant under the irreducible representation M_k, and $\mathbf{Y}_{mk}$ is spanned by some subset of $\{Z_1, \ldots, Z_{2m+1}\}$.

Let $D^{(1)}, \ldots, D^{(s)}$ be all of the distinct irreducible unitary representations of G, with $dim\ D^{(\alpha)} = n_\alpha$. Each M_k is one of these $D^{(\alpha)}$'s, although the list --

$M_1, \ldots, M_r$ -- might not include all of the $D^{(\alpha)}$'s. Fix some ordering of the elements of G, $\rho_1 = \mathbf{I}, \rho_2, \ldots, \rho_n$, and let $\{a(ij)\}$ be the $(n_\alpha)^2$ n-vectors whose kth components are the ij-elements of $D^{(\alpha)}(\rho_k)$:

$$a(ij) = \begin{bmatrix} [\,D^{(\alpha)}(\rho_1)\,]_{ij} \\ \vdots \\ [\,D^{(\alpha)}(\rho_n)\,]_{ij} \end{bmatrix} \qquad 1 \le i,j \le n_\alpha .$$

Let $b(ij)$ be the $(n_\beta)^2$ n-vectors obtained in this way from the representation $D^{(\beta)}$. Then, from the orthogonality relation for irreducible unitary representations,

$$\sum_{\rho \varepsilon G} [D^{(\alpha)}(\rho)]_{ij} \cdot [D^{(\beta)}(\rho)]_{kl} = \frac{n}{n_\alpha} \delta_{\alpha\beta}\, \delta_{ik}\, \delta_{jl} ,$$

we know that *vectors corresponding to different irreducible representations are orthogonal.*

Now for a fixed $\bar{u} \varepsilon \mathbf{S}^2$, define the projection π: $\mathbf{Y}_m \to \mathbf{R}^n$,

$$\pi(f) \equiv \begin{bmatrix} f(\bar{u}) \\ f(\rho_2^{-1}\bar{u}) \\ \vdots \\ f(\rho_n^{-1}\bar{u}) \end{bmatrix} = \begin{bmatrix} f(\bar{u}) \\ \rho_2 f(\bar{u}) \\ \vdots \\ \rho_n f(\bar{u}) \end{bmatrix} .$$

Suppose that $M_k = D^{(\alpha)}$, and denote by $\{Z_1^{(k)}, \ldots, Z_{n_\alpha}^{(k)}\}$ the subset of $\{Z_1, \ldots, Z_{2m+1}\}$ which spans $\mathbf{Y}_{mk}$. Since $\mathbf{Y}_{mk}$ transforms according to the irreducible representation M_k,

$$\rho Z_i^{(k)} = \sum_{j=1}^{n_\alpha} [\,D^{(\alpha)}(\rho)\,]_{ij}\, Z_j^{(k)} .$$

This is just the ρ-element of the vector equation

$$\pi(Z_i^{(k)}) = \sum_{j=1}^{n_\alpha} Z_j^{(k)}(\bar{u}) \cdot a(ij),$$

and we see that $\pi(\mathbf{Y}_{mk})$ *is spanned by the vectors* $\{a(ij)\}$. Thus, if $\mathbf{Y}_{mj}$ and $\mathbf{Y}_{mk}$ transform according to different irreducible representations, $M_j \neq M_k$, then $\pi(\mathbf{Y}_{mj})$ *is orthogonal to* $\pi(\mathbf{Y}_{mk})$.

$D^{(1)}$ is usually taken to be the identical representation, consisting of the 1 x 1 matrix with entry 1, denoted here by the symbol 1. If $D^{(1)}$ appears μ times in the list -- $M_1, \ldots, M_r$ -- then there are μ basis functions which are themselves invariant under the action of G, i.e., $\rho Z_i = Z_i$ for all $\rho \varepsilon G$. We may assume that any such basis functions are $Z_1 \equiv \mathbf{Y}_{m1}, \ldots, Z_\mu \equiv \mathbf{Y}_{m\mu}$ and $M_1 = \cdots = M_\mu = 1$. Define

$$H_m \equiv \mathbf{Y}_{m1} \oplus \cdots \oplus \mathbf{Y}_{m\mu} \quad \text{and} \quad K_m \equiv \mathbf{Y}_{m(\mu+1)} \oplus \cdots \oplus \mathbf{Y}_{mr}.$$

Then $\mathbf{Y}_m = H_m \oplus K_m$ and, if $f \varepsilon H_m$, then $\pi(f)$ is a multiple of the vector $E \equiv (1,1,\ldots,1)^T$, since

$$f(\rho\bar{u}) = f(\bar{u}) \quad \text{for all } \rho \varepsilon G.$$

Any function $g \varepsilon K_m$ transforms according to some other irreducible representation(s), so $\pi(g)$ is in the orthogonal complement of E. Thus,

$$\sum_{\rho \varepsilon G} g(\rho\bar{u}) = 0.$$

Since the choice of $\bar{u} \varepsilon \mathbf{S}^2$ was arbitrary, *any function in* K_m *is automatically integrated by any invariant quadrature formula.*

If $\mu = 0$, then $\mathbf{Y}_m = K_m$ and

$$\sum_{i=1}^{J} a_i \sum_{k=1}^{n_i} f(\bar{u}_i^{(k)}) = 0$$

for all $f \varepsilon \mathbf{Y}_m$ and for any choice of nodes and weights. Thus, only the following equations impose constraints on the $\{a_i\}$ and $\{\bar{u}_i\}$:

$$\sum_{i=1}^{J} a_i n_i Z_j(\bar{u}_i) = \begin{cases} 4\pi & j = 1 \\ 0 & j = 2, \ldots, C_p, \end{cases}$$

where $C_p = \sum_{m=0}^{p} \mu(m)$ and $\{Z_1, \ldots, Z_{C_p}\}$ is a basis for $H_0 \oplus \cdots \oplus H_p$. ($Z_1$ is the constant function 1, since $H_0 = \mathbf{Y}_0$ = constant functions.) This set of equations may include some for spherical harmonics of odd degree. Since we are only interested in integrating *even* polynomials, we discard these and are left with

$$\sum_{i=1}^{J} a_i n_i Z_j(\bar{u}_i) = \begin{cases} 4\pi & j = 1 \\ 0 & j = 2, \ldots, E_p, \end{cases} \tag{2.1.3}$$

where $E_p = \sum_{m=0}^{p/2} \mu(2m)$ and $\{Z_1, \ldots, Z_{E_p}\}$ is a basis for $H_0 \oplus H_2 \oplus \cdots \oplus H_p$.

$\mu(m) = dim\ H_m$ can be calculated from the characters of the representation M:

$$\mu(m) = \frac{1}{n} \sum_{\rho \varepsilon G} \chi_M(\rho), \qquad \chi_M(\rho) \equiv \operatorname{tr} M(\rho).$$

This is a consequence of the orthogonality relation for the characters of irreducible unitary representations:

$$\sum_{\rho \varepsilon G} \chi_\alpha(\rho) \chi_\beta(\rho) = n \cdot \delta_{\alpha\beta}.$$

Since $M = M_1 \oplus \cdots \oplus M_r$,

$$\chi_M(\rho) = \operatorname{tr} M(\rho) = \sum_{i=1}^{r} \chi_i(\rho) = \mu\chi_1(\rho) + \sum_{i=\mu+1}^{r} \chi_i(\rho),$$

where $\chi_i(\rho) = \operatorname{tr} M_i(\rho)$, $\chi_1(\rho) = \operatorname{tr} 1 = 1$. Then

$$\sum_{\rho \varepsilon G} \chi_M(\rho) = \sum_{\rho \varepsilon G} \chi_M(\rho) \chi_1(\rho) = \sum_{\rho \varepsilon G} \sum_{i=1}^{r} \chi_i(\rho) \chi_1(\rho) = n \cdot \mu.$$

The characters of M have been calculated in [6] (for example). Briefly, since the trace of $M(\rho)$ is just the sum of its eigenvalues, and any rotation through an angle ψ (about any axis) has eigenvalues $e^{ij\psi}$, $-m \le j \le m$,

$$\chi_M(\text{axis},\psi) = \sum_{j=-m}^{m} e^{ij\psi} = \frac{\sin(m+\frac{1}{2})\psi}{\sin\frac{1}{2}\psi}.$$

Thus, the number of m-degree spherical harmonics which are invariant with respect to the group of rotations, G, associated with a particular regular solid is given by

$$\mu(m) = \frac{1}{n}\sum_{\psi_k} n_k \frac{\sin(m+\frac{1}{2})\psi_k}{\sin\frac{1}{2}\psi_k},$$

where the ψ_k are the permissible angles of rotation for that solid, and there are n_k rotations through the angle ψ_k in the group G.

Table 2 lists the values of ψ_k and n_k for the tetrahedral, octahedral and icosahedral rotation groups. The tetrahedral group, with order 12, is isomorphic to A_4, the alternating group on 4 elements. The octahedral group, with order 24, is isomorphic to S_4, the symmetric group on 4 elements. The icosahedral group, with order 60, is isomorphic to S_5, the symmetric group on 5 elements. [12]

Table 2

	Tetrahedral				Octahedral					Icosahedral				
ψ_k	0	π	$\frac{2\pi}{3}$	$-\frac{2\pi}{3}$	0	$\frac{\pi}{2}$	$\pm\frac{2\pi}{3}$	π	π	0	π	$\frac{2\pi}{3}$	$\frac{2\pi}{5}$	$\frac{4\pi}{5}$
n_k	1	3	4	4	1	6	8	3	6	1	15	20	12	12

Using this information, we can compute the values of $\mu(m)$ for the rotation groups associated with the tetrahedron, the octahedron - cube, and the

icosahedron - dodecahedron. Notice that the right - hand side of

$$\mu(m) - \frac{2m+1}{n} = \frac{1}{n}\sum_{\psi_k \neq 0} n_k \frac{\sin(m+\frac{1}{2})\psi_k}{\sin\frac{1}{2}\psi_k}$$

is periodic in m with period $\frac{n}{2}$, this being the smallest common multiple of the integers $\frac{2\pi}{\psi_k}$. Thus,

$$\mu(m+\frac{n}{2}) = \frac{n+2m+1}{n} + \frac{1}{n}\sum_{\psi_k \neq 0} n_k \frac{\sin(m+\frac{1}{2})\psi_k}{\sin\frac{1}{2}\psi_k} = 1 + \mu(m),$$

and only the first $\frac{n}{2}$ characters need to be calculated:

$$\begin{aligned}
0 \le m \le 5: \quad & \mu(m) = \begin{cases} 1 & \text{if } m = 0,3, \text{ or } 4 \\ 0 & \text{otherwise} \end{cases} && \text{(TETRA)} \\
m \ge 6: \quad & \mu(m) = \mu(m-6) + 1 \\
0 \le m \le 11: \quad & \mu(m) = \begin{cases} 1 & \text{if } m = 0,4,6,8,9, \text{ or } 10 \\ 0 & \text{otherwise} \end{cases} && \text{(OCTA)} \\
m \ge 12: \quad & \mu(m) = \mu(m-12) + 1 \\
0 \le m \le 14: \quad & \mu(m) = \begin{cases} 1 & \text{if } m = 0,6,10, \text{ or } 12 \\ 0 & \text{otherwise} \end{cases} && \text{(ICOS)} \\
15 \le m \le 29: \quad & \mu(m) = \begin{cases} 0 & \text{if } m = 17,19,23, \text{ or } 29 \\ 1 & \text{otherwise} \end{cases} \\
m \ge 30: \quad & \mu(m) = \mu(m-30) + 1
\end{aligned}$$

An invariant quadrature formula is determined by its base nodes, $\bar{u}_1, \ldots, \bar{u}_J$ and their corresponding weights, $a_1, \ldots, a_J$. The system of equations (2.1.3) has $K + 3(J-K)$ unknowns -- the weights of the K special invariant sets used, and the weights and spherical coordinates of the base nodes of the general invariant sets used. Thus, we can hope to integrate exactly the first

$K + 3(J - K) = E_p$ invariant functions. As a function of p, E_p increases more slowly for the icosahedral group than for the other two groups. For fixed J and K, therefore, an icosahedral formula would be of higher degree than an octahedral or tetrahedral formula. Since the difficulty of solving system (2.1.3) depends primarily on the number of base nodes used, we will concentrate on quadrature formulas which are invariant with respect to the icosahedral rotation group.

In the rest of this chapter, we review some of the earlier work done on invariant quadrature formulas. We describe in detail the method used by McLaren to construct his octahedral and icosahedral formulas, and demonstrate it by deriving an 18th - degree formula which does not appear in [19]. Lebedev, using a more complicated and versatile method, produced octahedral formulas, and Konyaev derived icosahedral formulas by a method based on Lebedev's.

2. McLaren's Method

McLaren's method for solving the system (2.1.3) is based on the fact (Sec. 1.5) that a quadrature formula

$$I(f) \equiv \sum_{i=1}^{N} a_i f(\bar{u}_i) = \int_{S^2} f(\bar{u})\, d\bar{u}$$

is exact for all spherical polynomials of degree $\leq p$ if and only if

$$\sum_{i,j=1}^{N} a_i a_j P_m(\bar{u}_i, \bar{u}_j) = 0 \tag{2.2.1}$$

for Legendre polynomials of degree $m \leq p$, $m \neq 0$.

Rewriting (2.2.1) to correspond to an *invariant* quadrature formula, we get

$$\sum_{i,j=1}^{J} a_i a_j \sum_{r=1}^{n_i} \sum_{s=1}^{n_j} P_m(\bar{u}_i^{(r)} \cdot \bar{u}_j^{(s)}) = 0, \quad m \leq p, \quad m \neq 0. \tag{2.2.2}$$

The left - hand side of this is, in matrix form, $a^T \Pi^{(m)} a$, where

$$\pi_{ij}^{(m)} \equiv \sum_{r=1}^{n_i} \sum_{s=1}^{n_j} P_m(\bar{u}_i^{(r)} \cdot \bar{u}_j^{(s)}), \quad 1 \leq i,j \leq J.$$

$\Pi^{(m)}$ is symmetric by construction, non-negative by the addition theorem, and has rank $\leq \mu(m)$.

Consider the case: rank $\Pi^{(m)} = \mu(m) = 1$. Then $\Pi^{(m)} = q^{(m)} \cdot q^{(m)^T}$ and $\pi_{ij}^{(m)} = q_i^{(m)} q_j^{(m)}$, for some (column) J-vector, $q^{(m)}$. In fact,

$$q_i^{(m)} = \pm\sqrt{\pi_{ii}^{(m)}},$$

since $\pi_{ii}^{(m)} = q_i^{(m)} q_i^{(m)}$. Denote the sign of $q_i^{(m)}$ by $\varepsilon_i = \pm 1$. Then

$$\pi_{ij}^{(m)} = \varepsilon_i \varepsilon_j \sqrt{\pi_{ii}^{(m)}} \sqrt{\pi_{jj}^{(m)}}.$$

Now the condition $a^T \Pi^{(m)} a = 0$ reduces to $a^T q^{(m)} = 0$, but the inner products $(\bar{u}_i^{(r)} \cdot \bar{u}_j^{(s)})$ are complicated functions to calculate. We adjust the problem once more and use the vertices $\{V_i\}$ as pivots so that only inner products of the form $(\bar{u}_i^{(r)} \cdot V_j)$ are needed. Define

$$\pi_{00}^{(m)} \equiv \sum_{i,j=1}^{12} P_m(V_i \cdot V_j)$$

and observe that

$$[0 \quad a^T] \begin{bmatrix} \varepsilon_0 \sqrt{\pi_{00}^{(m)}} \\ q^{(m)} \end{bmatrix} [\varepsilon_0 \sqrt{\pi_{00}^{(m)}} \quad q^{(m)T}] \begin{bmatrix} 0 \\ a \end{bmatrix}$$

$$= [0 \quad a^T] \begin{bmatrix} \pi_{00}^{(m)} & \pi_{01}^{(m)} & \cdots & \pi_{0J}^{(m)} \\ \pi_{10}^{(m)} & & & \\ \vdots & & \Pi^{(m)} & \\ \pi_{J0}^{(m)} & & & \end{bmatrix} \begin{bmatrix} 0 \\ a \end{bmatrix}$$

$$= a^T \Pi^{(m)} a .$$

When $\mu(m) = 1$, $\pi_{00}^{(m)} \neq 0$, so $[\pi_{00}^{(m)} \quad \cdots \quad \pi_{0J}^{(m)}]$ is not the 0 - vector. Since the rank of

$$\begin{bmatrix} \varepsilon_0 \sqrt{\pi_{00}^{(m)}} \\ q^{(m)} \end{bmatrix} [\varepsilon_0 \sqrt{\pi_{00}^{(m)}} \quad q^{(m)T}]$$

is at most 1, the other rows are either multiples of the first row, or 0. So $a^T \Pi^{(m)} a = 0$ whenever $\sum_{i=1}^{J} a_i \pi_{i0}^{(m)} = 0$, and this condition may be substituted for the corresponding equation in system (2.1.3). Referring to the list of $\mu(m)$ for

the icosahedral group, we see that if $m < 30$, $\mu(m) \leq 1$, and the constraints in (2.1.3) can be replaced by

$$\sum_{i=1}^{J} a_i n_i = 4\pi$$

$$\sum_{i=1}^{J} a_i \pi_{i0}^{(m)} = 0, \quad 1 \leq m \leq p, \quad \mu(m) = 1. \tag{2.2.3}$$

We demonstrate McLaren's solution of (2.2.3) by deriving an *even* invariant formula which is exact for degree $2m \leq 18$. Notice that, since $\pi_{00}^{(m)} = 0$ when m is odd, any constraints which correspond to odd harmonics must be satisfied by other means, for example, by requiring that any general nodes lie on a median or an edge of the solid. This produces general sets which consist of antipodal pairs. The special sets also consist of antipodal pairs, so odd harmonics automatically integrate to 0.

3. 18 - degree Invariant Formula

$\mu(2m) = 1$ for $2m = 0, 6, 10, 12, 16$ and 18, so $E_{18} = 6$. We set about to find an invariant quadrature formula which uses all three special sets ($K = 3$) and one general set ($J = K + 1 = 4$). Recall that the six unknowns are the four weights -- a_v, a_c, a_e, and $a_{\bar{u}}$ -- and the spherical coordinates of the general base node, $\bar{u}$. These must satisfy the equations

$$a_v \pi_{vv}^{(2m)} + a_c \pi_{vc}^{(2m)} + a_e \pi_{ve}^{(2m)} + a_{\bar{u}} \pi_{v\bar{u}}^{(2m)} = 0, \quad 1 \le m \le 9. \tag{2.3.1}$$

Note that only five of these nine equations are really constraints on the unknowns, since the equations for $m = 1, 2, 4$ and 7 are satisfied by *any* invariant formula. The sixth constraint involves only the weights:

$$12a_v + 20a_c + 30a_e + 60a_{\bar{u}} = 4\pi \tag{2.3.2}$$

McLaren assumes that the vertices of the icosahedron are

$$(\pm p, \pm q, 0) \qquad (0, \pm p, \pm q) \qquad (\pm q, 0, \pm p),$$

where

$$p^2 = \frac{5 + \sqrt{5}}{10} \qquad q^2 = \frac{5 - \sqrt{5}}{10}$$

The quantities $V_i \cdot V_j$, $V_i \cdot C_j$ and $V_i \cdot E_j$ are calculated in [19], giving us

$$\begin{aligned}
\pi_{vv}^{(2m)} &= 24(P_{2m}(1) + 5P_{2m}(\tfrac{1}{\sqrt{5}})) \\
\pi_{vc}^{(2m)} &= 120(P_{2m}(\lambda) + P_{2m}(\eta)), \quad \lambda^2, \eta^2 = \frac{1}{15}(5 \pm 2\sqrt{5}) \\
\pi_{ve}^{(2m)} &= 120(P_{2m}(0) + P_{2m}(\gamma) + P_{2m}(\delta)), \quad \gamma^2, \delta^2 = \frac{1}{10}(5 \pm \sqrt{5}) \\
\pi_{v\bar{u}}^{(2m)} &= 120 \sum_{i=1}^{6} P_{2m}(\sqrt{\nu_i}), \quad \pm\sqrt{\nu_i} = \pm V_i \cdot \bar{u}
\end{aligned}$$

We substitute these into (2.3.1) and divide out $120a_{\bar{u}}$ to get

$$\frac{b_v}{5}[P_{2m}(1) + 5P_{2m}(\frac{1}{\sqrt{5}})] + b_c\,[P_{2m}(\lambda) + P_{2m}(\eta)] \tag{2.3.3}$$

$$+ b_e\,[P_{2m}(\gamma) + P_{2m}(\delta) + P_{2m}(0)] + \sum_{i=1}^{6} P_{2m}(\sqrt{\nu_i}) = 0, \quad 1 \le m \le 9,$$

where $b_v = a_v / a_{\bar{u}}$, $b_c = a_c / a_{\bar{u}}$ and $b_e = a_e / a_{\bar{u}}$.

We can transform (2.3.3) into

$$\frac{b_v}{5}[1^{2m} + 5(\frac{1}{\sqrt{5}})^{2m}] + b_c[\lambda^{2m} + \eta^{2m}] + b_e[0^{2m} + \gamma^{2m} + \delta^{2m}] + \sum_{i=1}^{6} \sqrt{\nu_i}^{\,2m}$$

$$= \frac{1}{2m+1}[\frac{6b_v}{5} + 2b_c + 3b_e + 6], \quad 1 \le m \le 9. \tag{2.3.4}$$

The left - hand side is obtained by writing $(*)^{2m}$ in place of $P_{2m}(*)$ in (2.3.3), e.g., λ^{2m} in place of $P_{2m}(\lambda)$. Now each term $(*)^{2m}$ can be expanded in terms of $P_{2i}(*)$, $0 \le i \le m$ [17]. But, since (2.3.3) is true for $1 \le i \le m$, we are left with only the constant term of each expansion, $\frac{1}{2m+1}$, which gives us the right - hand side of (2.3.4).

Denote by S_m the sum $\sum_{i=1}^{6} \nu_i^m$. Each S_m is a linear function of the ratios b_v, b_c, b_e. The icosahedral coordinates of $\bar{u}$ -- $\nu_1, \ldots, \nu_6$ -- are the roots of the 6th-degree monic polynomial, $Q(\nu)$, whose coefficients, $c_1, \ldots, c_6$, are related to the symmetric functions, S_m, by Newton's formulas [3]:

$$\begin{aligned} S_1 + c_1 &= 0 \\ S_2 + c_1 S_1 + 2c_2 &= 0 \\ &\cdots \\ S_9 + c_1 S_8 + \cdots + 9c_9 &= 0 \end{aligned} \tag{2.3.5}$$

We solve these equations to obtain $c_1, \ldots, c_9$ as functions of b_v, b_c, b_e:

$$c_1 = -2 \qquad c_2 = \frac{7}{5}$$

$$c_3 = \frac{864b_v - 800b_c - 675b_e - 29700}{70875}$$

$$c_4 = -\frac{864b_v - 800b_c - 675b_e - 6075}{118125}$$

$$c_5 = \frac{49248b_v - 20000b_c - 50625b_e - 101250}{41765625}$$

$$c_6, c_7, c_8 = \text{quadratics in } b_v, b_c, b_e$$

$$c_9 = \text{cubic in } b_v, b_c, b_e$$

Since $c_7 = c_8 = c_9 = 0$, we can solve the last three equations for b_v, b_c, b_e. There are four solutions, but only one of them gives non-zero weights for all four invariant sets:

$$b_v = \frac{46646875}{53833764} \quad b_c = \frac{52966953}{53833764} \quad b_e = \frac{50266112}{53833764}$$

With these values,

$$Q(\nu) = \nu^6 - 2\nu^5 + \frac{7}{5}\nu^4 - \frac{692}{1615}\nu^3 + \frac{461}{8075}\nu^2 - \frac{53222}{17708475}\nu + \frac{529}{13041125}$$

and

$$\nu_1 \approx .89822338 \qquad \nu_4 \approx .142068429$$

$$\nu_2 \approx .45836723 \qquad \nu_5 \approx .087835698$$

$$\nu_3 \approx .39343758 \qquad \nu_6 \approx .0200677256$$

The roots of $Q(\nu)$ are real and lie between 0 and 1. $\cos^{-1}(\sqrt{\nu_1}) + \cos^{-1}(\sqrt{\nu_2}) \approx 66^\circ$, which is larger than the angle between two neighboring vertices, since $\cos^{-1}(\frac{1}{\sqrt{5}}) < 64^\circ$. Hence, ν_1 and ν_2 are icosahedral

coordinates of a general base node $\bar{u}$. In fact, $\bar{u}$ is determined up to sign by ν_1 and ν_2. Since four of the conditions on $\nu_1, \ldots, \nu_6$ are always true, regardless of the position of $\bar{u}$, $\nu_3, \ldots, \nu_6$ are the remaining icosahedral coordinates of $\bar{u}$. An additional check on the ν_i is provided by the equations which relate the icosahedral coordinates to the Cartesian coordinates of $\bar{u}$:

$$\begin{aligned} \gamma y + \delta z &= \omega_1 & \delta x + \gamma y &= \omega_4 \\ -\gamma y + \delta z &= \omega_2 & -\gamma x + \delta y &= \omega_5 \\ -\delta x + \gamma z &= \omega_3 & \gamma x + \delta y &= \omega_6 \end{aligned} \tag{2.3.6}$$

where (x,y,z) are the Cartesian coordinates of the element of the general invariant set which is closest to the vertex $(0,\gamma,\delta)$, $\gamma = \sqrt{\frac{1}{10}(5-\sqrt{5})}$, $\delta = \sqrt{\frac{1}{10}(5+\sqrt{5})}$ and $\mu_i = \sqrt{\nu_i}$.

From these equations, we see that $\nu_1 \geq \nu_2 \geq \cdots \geq \nu_6 > 0$ are icosahedral coordinates of a point on the sphere if and only if

$$\sum_{i=1}^{6} \nu_i = 2$$

and

$$\frac{\mu_1 + \mu_2}{\mu_3 + \mu_4} = \frac{\mu_3 - \mu_4}{\mu_5 - \mu_6} = \frac{\mu_5 + \mu_6}{\mu_1 - \mu_2} = \frac{\delta}{\gamma} = \frac{1+\sqrt{5}}{2}.$$

Applying this test to the roots of $Q(\nu)$, we obtain for these three quotients the values 1.618034 , 1.618033 , 1.618035 , respectively. A slight deviation from $\frac{1+\sqrt{5}}{2} = 1.618033988\ldots$ is expected, since the numerically obtained roots of $Q(\nu)$ are only approximate.

Solving (2.3.6) for (x,y,z), we get

$$x = \frac{\mu_4 - \mu_3}{2\gamma} = \frac{\mu_6 - \mu_5}{2\delta} \approx -.147138$$

$$y = \frac{\mu_5 + \mu_6}{2\gamma} = \frac{\mu_1 - \mu_2}{2\delta} \approx .257468$$

$$z = \frac{\mu_1 + \mu_2}{2\gamma} = \frac{\mu_3 + \mu_4}{2\delta} \approx .955018$$

From the sixth constraint, (2.3.2), and the values of b_v, b_c and b_e, we calculate the weights a_v, a_c, a_e and $a_{\overline{u}}$:

$$a_v = \frac{625\pi}{21294} \approx .09221$$

$$a_c = \frac{19683\pi}{590590} \approx .10470$$

$$a_e = \frac{32768\pi}{1036035} \approx .09936$$

$$a_{\overline{u}} = \frac{8972294\pi}{264879615} \approx .10642$$

We now have the nodes and weights of a quadrature formula which exactly integrates all even spherical polynomials of degree ≤ 18.

4. Method of Lebedev and Konyaev

Lebedev [11] obtained quadrature formulas up to order 29 which are invariant with respect to the octahedral group with inversion, denoted by G_8^*. Konyaev [9], using similar methods, obtained quadratures of orders 19 and 29 which are invariant with respect to the icosahedral group with inversion, G_{20}^*. We outline Lebedev's method first, using his notation.

Let Ω be the octahedron inscribed in $\mathbf{S}^2$, with vertices on the x-, y-, z-axes. Let

$$I(f) \equiv \frac{1}{4\pi}\int_{\mathbf{S}^2} f(\bar{u})p(\bar{u})d\bar{u}$$

where $\bar{u}\varepsilon\mathbf{S}^2$, $p(\bar{u}) \neq 0$ is an integrable weight function invariant with respect to G_8^* such that $I(1) = 1$, and $d\bar{u} \equiv \sin\vartheta d\vartheta d\varphi$.

Lebedev's method finds the base-nodes b_i^k, c_i^k, d_i^k, and the weights A_k, B_k, C_k, D_k of the n-degree quadrature formula

$$\begin{aligned} S_n(f) \equiv\ & A_1\sum_{i=1}^{6} f(a_i^1) + A_2\sum_{i=1}^{12} f(a_i^2) + A_3\sum_{i=1}^{8} f(a_i^3) \\ & + \sum_{k=1}^{N_1} B_k \sum_{i=1}^{24} f(b_i^k) + \sum_{k=1}^{N_2} C_k \sum_{i=1}^{24} f(c_i^k) + \sum_{k=1}^{N_3} D_k \sum_{i=1}^{48} f(d_i^k) \end{aligned}$$

where a_i^1 are the vertices, a_i^2 are the midpoints of the edges, a_i^3 are the centers of the faces, b_i^k lie on medians, c_i^k lie on edges, and d_i^k are general base-nodes. The coordinates of the special sets a_i^k are known and the coordinates of the points in the orbits of b_i^k, c_i^k, d_i^k are

b_i^k: $(\pm l_k, \pm l_k, \pm m_k)$, $(\pm l_k, \pm m_k, \pm l_k)$, $(\pm m_k, \pm l_k, \pm l_k)$,
where $l_k^2 = \dfrac{1 - m_k^2}{2}$

c_i^k: $(\pm p_k, \pm q_k, 0)$, $(\pm q_k, \pm p_k, 0)$, $(\pm p_k, 0, \pm q_k)$,
$(0, \pm p_k, \pm q_k)$, $(\pm q_k, 0, \pm p_k)$, $(0, \pm q_k, \pm p_k)$,
where $q_k^2 = 1 - p_k^2$

d_i^k: $(\pm r_k, \pm u_k, \pm w_k)$, $(\pm r_k, \pm w_k, \pm u_k)$, $(\pm u_k, \pm r_k, \pm w_k)$,
$(\pm u_k, \pm w_k, \pm r_k)$, $(\pm w_k, \pm u_k, \pm r_k)$, $(\pm w_k, \pm r_k, \pm u_k)$.

I.e., for a fixed k, b_i^k and c_i^k each have only one free parameter in their coordinates.

Any polynomial $P(x, y, z)$ which is invariant with respect to G_8^* must be a symmetric function of x^2, y^2, z^2, and so can be written as a polynomial in

$$\sigma_1 = x^2 + y^2 + z^2$$

$$\sigma_2 = x^2y^2 + x^2z^2 + y^2z^2$$

$$\text{and } \sigma_3 = x^2y^2z^2$$

Since $\sigma_1 \equiv 1$ on $\mathbf{S}^2$, the restriction to $\mathbf{S}^2$ of $P(x, y, z)$ is

$$P(x, y, z) = Q(\sigma_2, \sigma_3) = \sum_{0 \le 4i + 6j \le n} a_{ij}\, \sigma_2^i \sigma_3^j$$

Lebedev now divides into four groups the invariant polynomials of degree ≥ 6. Group A contains the four simplest polynomials, whose terms are constant multiples of σ_2, σ_3, or σ_2^2. The polynomials in Group B have terms involving $\sigma_2^i \sigma_3^j$, where $i, j \le 2$ and $i + j \le 3$. Polynomials in Group C contain $\sigma_2^i \sigma_3^j$, terms, with $j \le 2$, but no restriction on i or on $i + j$. Group D contains the polynomials with higher-order terms.

Requiring that $I(f) = S_n(f)$ for polynomials of degree $\le n$ produces four subsystems of algebraic equations. For each value of n, each subsystem must be re-worked into the form of a moment system of equations:

$$\sum_{i=1}^{p} B_i u_i^k = c_k, \qquad k = 0, 1, \ldots, 2p-1$$

where the B_i and u_i are to be found from the known values, c_k. The u_i are the roots of the monic p-degree polynomial

$$F_p(u) = u^p - f_{p-1}u^{p-1} - \cdots - f_0,$$

where the vector $(f_0, \ldots, f_{p-1})$ is the solution of the Hankel matrix equation

$$\begin{bmatrix} c_0 & c_1 & \cdots & c_{p-1} \\ c_1 & c_2 & \cdots & c_p \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ c_{p-1} & c_p & \cdots & c_{2p-2} \end{bmatrix} \begin{bmatrix} f_0 \\ f_1 \\ \cdot \\ \cdot \\ \cdot \\ f_{p-1} \end{bmatrix} = \begin{bmatrix} c_p \\ c_{p+1} \\ \cdot \\ \cdot \\ \cdot \\ c_{2p-1} \end{bmatrix}$$

Then $B_i = G_{p-1}(u_i)/F'_p(u_i)$, where $G_{p-1}(u_i) = g_0 + g_1 u + \cdots + g_{p-1}u^{p-1}$ and

$$g_{p-1} = c_0$$

$$g_{p-2} = c_1 - f_{p-1}c_0$$

$$\cdots$$

$$g_0 = c_{p-1} - f_{p-1}c_{p-2} - \cdots - f_1 c_0.$$

Konyaev uses a similar approach to obtain quadrature formulas which are invariant with respect to the icosahedral group of rotations. Using the icosahedron, **T**, whose vertices we give in Section 3.1, he assumes that his general base-nodes lie on the meridian $\varphi = 0$. These "general" nodes, however, are actually analogues of the b_i^k and c_i^k in Lebedev's formulas, since this meridian contains only edges and medians of **T**. By restricting all his base-nodes to $\varphi = 0$, he is able to simplify the invariant polynomials h and k (also given in Section

3.1) to

$$h(t) = 1 - 2t^2 - t^3$$
$$k(t) = 1 - 10t^2 - 5t^3 + 20t^4 + 12t^5$$

where

$$t = 2\sin\vartheta\cos\vartheta - \sin^2\vartheta$$

He obtains a 29-degree quadrature formula

$$S_n(f) = a\sum_{i=1}^{12} f(A_i) + b\sum_{i=1}^{30} f(B_i) + c\sum_{i=1}^{20} f(C_i) + \sum_{k=1}^{j} d_k \sum_{i=1}^{60} f(D_{ki}),$$

where the A_i are the vertices, the B_i are the midpoints of the edges, the C_i are the centers of the faces, and the D_{ki} lie on the medians or edges of **T**. The weights of the special sets and of the base-nodes D_{ki} are (rounded to 6 decimal places)

$a = .002964$	$d_1 = .004635$
$b = -.001905$	$d_2 = .003780$
$c = .003862$	$d_3 = .003546$
	$d_4 = .003778$

and the coordinates of the base-nodes D_k are

$$D_j = (\sqrt{1 - z_j^2}, 0, z_j),$$

where

$z_1 = -.611254$	$z_3 = -.978512$
$z_2 = -.909192$	$z_4 = -.935811$

This formula integrates exactly all polynomials of degree ≤ 29 using 302 nodes. These 302 nodes are actually 151 *directions*, which would integrate exactly all *even* polynomials of degree ≤ 28. For a small number of base-nodes, D_k, restricting all the quadrature nodes to lie on medians and edges allows for a relatively uniform distribution of nodes. For larger numbers of base-nodes, how-

Chapter Three: Uniform-Weight Invariant Quadratures

In Chapter Two, we described two methods for finding Gauss-type quadratures for the sphere. These formulas are very efficient, but finding the coordinates and weights of the base nodes requires intricate manipulation of the system of non-linear equations which they must satisfy. Far from the simplicity of the product-space formulas, where a new formula can be obtained by changing a single number, each of these invariant formulas is the end-product of a complete re-working of the system of non-linear constraints into a sequence of linear and simpler non-linear problems. Finally, neither McLaren's nor Konyaev's method seems capable of producing quadratures of higher order than Konyaev's 28-degree formula. In this chapter, we describe two methods for finding uniform-weight quadratures. These methods are more straightforward, but sacrifice some of the efficiency of the Gauss-type formulas.

1. Icosahedral Group of Rotations

In order to use quadrature formulas which are invariant with respect to a particular icosahedron, we must be able to generate the orbit of a given point $\bar{u} \varepsilon \mathbf{S}^2$. In this section, we describe the 60 rotations which preserve the icosahedron, **T**, whose vertices are (in spherical coordinates):

$$\vartheta = 0,$$
$$\vartheta = \cos^{-1}\frac{1}{\sqrt{5}}: \quad \varphi = 0, \frac{2\pi}{5}, \frac{4\pi}{5}, \frac{6\pi}{5}, \frac{8\pi}{5},$$
$$\vartheta = \cos^{-1}\frac{-1}{\sqrt{5}}: \quad \varphi = \frac{\pi}{5}, \frac{3\pi}{5}, \pi, \frac{7\pi}{5}, \frac{9\pi}{5},$$
$$\vartheta = \pi,$$

and associate any point on **T** with its projection onto $\mathbf{S}^2$ (i.e., $x \to \frac{x}{|x|}$). We will refer to a rotation ρ in either of two ways:

[1] $\rho(\vartheta,\varphi,\gamma)$, where ϑ and φ are the spherical coordinates of a point $\bar{u}\,\varepsilon\,\mathbf{S}^2$, the axis of the rotation is the line through (0,0,0) and $\bar{u}$, and γ is the angle of rotation about this axis.

[2] the 3 x 3 matrix representation $P(\rho) \equiv Z_\varphi Y_{-\vartheta} Z_\gamma Y_\vartheta Z_{-\varphi}$, where

$$Z_\alpha = \begin{bmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad Y_\alpha = \begin{bmatrix} \cos\alpha & 0 & -\sin\alpha \\ 0 & 1 & 0 \\ \sin\alpha & 0 & \cos\alpha \end{bmatrix}.$$

$P(\rho)$ performs the rotation ρ through the angle γ about the axis $\bar{u} = (\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta)$ by

(a) rotating $\bar{u}$ to (0,0,1): $(Y_\vartheta Z_{-\varphi})\cdot\bar{u}$

(b) rotating through γ about (0,0,1): $Z_\gamma \cdot (Y_\vartheta Z_{-\varphi}\bar{u})$

(c) rotating back to $\bar{u}$: $(Y_\vartheta Z_{-\varphi})^{-1}\cdot(Z_\gamma Y_\vartheta Z_{-\varphi}\bar{u})$

The 60 rotations which preserve **T** are the identity, **I**, and the rotations $\rho(\text{axis},\gamma)$:

axis	γ	number possible
V_i	$\pm\frac{2\pi}{5}, \pm\frac{4\pi}{5}$	6 x 4 = 24
C_i	$\pm\frac{2\pi}{3}$	10 x 2 = 20
E_i	π	15 x 1 = 15

where $\{V_i\}$ are the 12 vertices, $\{C_i\}$ are the centers of the 20 faces and $\{E_i\}$ are the midpoints of the 30 edges. (Since $\rho(-\bar{u},-\gamma) = \rho(\bar{u},\gamma)$, we count the rotations using only half of each set of axes.)

These rotations permute the five cubes which can be inscribed in **T** [12], and they form a group, G. Hence, G is isomorphic to a subgroup of S_5, the

symmetric group on five elements. Since A_5 is the only subgroup of S_5 of order 60, $G \approx A_5$. A_5 is generated by rotations ρ and τ which satisfy

$$\rho^3 = \mathbf{I} \quad \tau^5 = \mathbf{I} \quad (\rho\tau)^2 = \mathbf{I}$$

We can arbitrarily choose one of the C_i for the axis of ρ, and one of the V_i for the axis of τ. If we set $\rho = \rho(C_1, \frac{2\pi}{3})$, $\tau = \tau(V_1, \frac{2\pi}{5})$, then $\rho\tau = \mu(E_1, \pi)$, with E_1 determined by ρ and τ.

Taking $V_1 = (0,0,1)$ creates the simplest possible τ:

$$P(\tau) = Z_{\frac{2\pi}{5}} = \begin{bmatrix} \cos\frac{2\pi}{5} & -\sin\frac{2\pi}{5} & 0 \\ \sin\frac{2\pi}{5} & \cos\frac{2\pi}{5} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Five faces of **T** share the vertex V_1. One of these has as its other two vertices $(\vartheta_V, 0)$ and $(\vartheta_V, \frac{2\pi}{5})$, where $\vartheta_V \equiv \cos^{-1}\frac{1}{\sqrt{5}} \approx \frac{7\pi}{20}$. Let C_1 be the center of this face, $C_1 = (\vartheta_C, \frac{\pi}{5})$, with ϑ_C to be determined later. Then $E_1 = (\frac{\vartheta_V}{2}, 0)$, the midpoint of the edge between V_1 and $(\vartheta_V, 0)$. (See Fig. 3.1.1) Thus,

$$P(\mu) = Y^{-1}_{\vartheta_V/2}\, Z_\pi\, Y_{\vartheta_V/2} = \begin{bmatrix} -\frac{1}{\sqrt{5}} & 0 & \frac{2}{\sqrt{5}} \\ 0 & -1 & 0 \\ \frac{2}{\sqrt{5}} & 0 & \frac{1}{\sqrt{5}} \end{bmatrix}$$

Then, since $\mu = \rho\tau$,

$$P(\rho) = P(\mu)\,P^{-1}(\tau) = \begin{bmatrix} -\frac{c}{\sqrt{5}} & -\frac{s}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\ s & -c & 0 \\ \frac{2c}{\sqrt{5}} & \frac{2s}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{bmatrix}$$

where $c = \cos\frac{2\pi}{5}$, $s = \sin\frac{2\pi}{5}$. The eigenvector of $P(\rho)$ is its axis C_1:

$$C_1 = \frac{1}{\sqrt{15-3\sqrt{5}}}\begin{bmatrix} \sqrt{2} \\ \frac{(3-\sqrt{5})\sqrt{5+\sqrt{5}}}{2} \\ \frac{\sqrt{5}+1}{\sqrt{2}} \end{bmatrix}$$

So $\vartheta_C = \cos^{-1}(\frac{\sqrt{5}+1}{\sqrt{2}}) \approx .6524.$

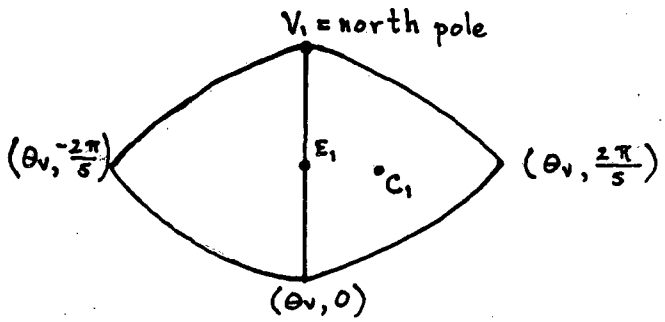


Figure 3.1.1

With these choices of ρ and τ, the elements of G are

$$\sigma_i \rho^j \tau^k, \quad i = 0,1,2,3, \quad j = 0,1,2, \quad k = 0,1,2,3,4,$$

$$\begin{aligned} \sigma_0 &= \mathrm{I} \\ \sigma_1 &= \tau^{-1}\mu\tau \\ \sigma_2 &= \nu\mu\nu, \text{ where } \nu = \tau\rho \\ \sigma_3 &= \sigma_1\sigma_2 \ (= \sigma_2\sigma_1). \end{aligned}$$

The σ_i are rotations of order 2 which preserve the tetrahedron whose vertices are

$$\begin{aligned} C_1 &= (\vartheta_C, \frac{\pi}{5}) = \text{axis of } \rho \\ C_2 &= (\pi - \vartheta'_C, -\frac{3\pi}{5}) \\ C_3 &= (\pi - \vartheta_C, 0) \\ C_4 &= (\vartheta'_C, \frac{4\pi}{5}) \end{aligned}$$

where $\cos\vartheta'_C = \frac{-1}{\sqrt{15+6\sqrt{5}}} \approx -.1876$, $\vartheta'_C \approx 1.7595$. Since the σ_i have order

2, they exchange pairs of these C_i:

$$\begin{aligned}
\sigma_1&: \quad C_1 \leftrightarrow C_2, \quad C_3 \leftrightarrow C_4 \\
\sigma_2&: \quad C_1 \leftrightarrow C_4, \quad C_2 \leftrightarrow C_3 \\
\sigma_3&: \quad C_1 \leftrightarrow C_3, \quad C_2 \leftrightarrow C_4
\end{aligned}$$

2. Exact Uniform-Weight Quadrature

T is the icosahedron described in the previous section and G is its associated group of rotations. A polynomial $f(\bar{u})$ is *invariant* with respect to G if $\rho f = f$ for all $\rho \varepsilon G$. From Section 2.1, we know that there exist invariant spherical harmonics of degrees 0, 6, 10, 12, 16, 18, etc. $Y_0 = 1$ is, of course, the 0-degree invariant harmonic. A 6th-degree polynomial which is invariant with respect to G is

$$\begin{aligned} h(x,y,z) = {} & 5x^4z^2 + 5y^4z^2 + z^6 + 10x^2y^2z^2 - 5x^2z^4 - 5y^2z^4 \\ & + 2x^5z + 10xy^4z - 20x^3y^2z \end{aligned}$$

A 10th-degree invariant polynomial is

$$\begin{aligned} k(x,y,z) = {} & (4x^2 - 6xz + z^2)(x^4 + 5y^4 + z^4 + 2x^3z - 2xz^3 \\ & - 10x^2y^2 - x^2z^2 - 30xy^2z - 25y^2z^2)(x^4 + 5y^4 + z^4 \\ & - 8x^3z + 8xz^3 - 10x^2y^2 + 14x^2z^2 - 10y^2z^2). \end{aligned}$$

Remark: $h(x,y,z) = H_6(x,y,z) + \frac{5}{21}r^6$ and $k(x,y,z) = K_{10} + r^4K_6 + \frac{125}{77}r^{10}$, where $r^2 = x^2 + y^2 + z^2$, H_6 and K_6 are 6th-degree spherical harmonics, and K_{10} is a 10th-degree spherical harmonic. (h and k are given in [9].)

All other invariant polynomials can be expressed as polynomials in h and k, i.e., as linear combinations of the functions $q_{ij} \equiv h^ik^j$. To construct a uniform-weight quadrature formula which is exact for all polynomials of degree $\leq M$, we need to find K base nodes, $\bar{u}_1, \ldots, \bar{u}_K$, each in a distinct general invariant set, such that

$$v\ q_{ij}(V) + c\ q_{ij}(C) + e\ q_{ij}(E) + 60 \sum_{m=1}^{K} q_{ij}(\bar{u}_m) = \frac{v + c + e + 60K}{4\pi} \int_{S^2} q_{ij}(\bar{u}) \tag{3.2.1}$$

for the first $2N$ q_{ij} (ordered by $\deg(q_{ij}) \equiv 6i + 10j$), where $v = 12$ or 0, $c = 20$ or 0, $e = 30$ or 0, depending on which of the special invariant sets we want to use, and M = degree of the $2K$th q_{ij}. The first 10 q_{ij} are:

$$\begin{aligned} q_{10} &= h & q_{02} &= k^2 \\ q_{01} &= k & q_{21} &= h^2k \\ q_{20} &= h^2 & q_{40} &= h^4 \\ q_{11} &= hk & q_{12} &= hk^2 \\ q_{30} &= h^3 & q_{31} &= h^3k \end{aligned}$$

The K base nodes $\bar{u}_1, \ldots, \bar{u}_K$ are determined by solving the system of equations

$$v\ q_{ij}(V) + c\ q_{ij}(C) + e\ q_{ij}(E) + 60 \sum_{m=1}^{K} \alpha_m^i \beta_m^j = \frac{v + c + e + 60K}{4\pi} \int_{S^2} q_{ij}(\bar{u}) \tag{3.2.2}$$

for $\alpha_1, \ldots, \alpha_K$ and $\beta_1, \ldots, \beta_K$, and then finding points $\bar{u}_m \varepsilon S^2$ such that

$$h(\bar{u}_m) = \alpha_m \quad \text{and} \quad k(\bar{u}_m) = \beta_m .$$

If such a $\bar{u}_m$ exists and does not belong to a special set, its orbit contains 60 points whose h and k values are α_m and β_m. If, in addition, $\bar{u}_m$ does not fall on a median or on an edge, its orbit contains no antipodal pairs and therefore provides 60 *directions*.

In the next two sections, we describe our procedure for matching a pair (α_m, β_m) to a point $\bar{u}_m \varepsilon S^2$, and our method for solving system (3.2.2).

2.1 Matching (α_m, β_m) to a point $\bar{u}_m \varepsilon S^2$

In the next section, we describe our method for solving the system of equations (3.2.2) for the values α_m and β_m. For each associated pair (α_m, β_m), we look for a point $\bar{u}_m \varepsilon S^2$ such that $h(\bar{u}_m) = \alpha_m$ and $k(\bar{u}_m) = \beta_m$. We restrict our search to a region of S^2 where h and k are single-valued functions.

In Figs. 3.2.1 and 3.2.2, we plot the level curves of h and k on the region

$$\frac{\pi}{5} \le \vartheta \le \frac{4\pi}{5}, \qquad -\frac{2\pi}{5} \le \varphi \le \frac{2\pi}{5}.$$

Since h and k are symmetric with respect to medians and edges, we can restrict our attention to one of the six sub-triangles of a face. The vertices of such a sub-triangle are a vertex, an adjacent edge's midpoint, and a centroid, so we will call this triangle VCE.

Specifically, consider the triangle (Fig. 3.2.3) with vertices

$$V = (\vartheta_V, 0) \approx (.8944, 0, .4472)$$

$$C = (\vartheta'_C, 0) \approx (.9822, 0, -.1876)$$

$$E = (\frac{\pi}{2}, \frac{\pi}{10}) \approx (.9511, .3090, 0)$$

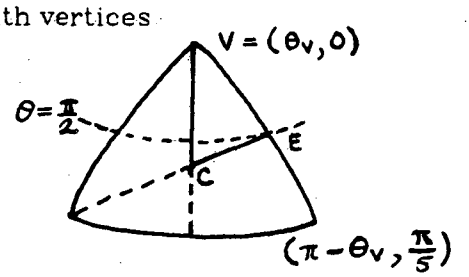


Figure 3.2.3

For each pair (α_m, β_m) in the solution of (3.2.2), we look for the spherical coordinates of a point $\bar{u}_m \varepsilon VCE$ satisfying $h(\bar{u}_m) = \alpha_m$, $k(\bar{u}_m) = \beta_m$, using IMSL subroutine ZSCNT, with starting value supplied by a search through a table of (α, β)-values for $\bar{u} = (\vartheta_j, \varphi_k)$,

$$\vartheta_j = \vartheta_V + \frac{j}{300}(\frac{\pi}{2} - \vartheta_V) \qquad j = 1, \ldots, 422$$

$$\varphi_k = \begin{cases} \frac{k}{200}\frac{\pi}{10} & k = 1, \ldots, M_\vartheta - 1 \\ \varphi_{\max}(\vartheta) & k = M_\vartheta \end{cases}$$

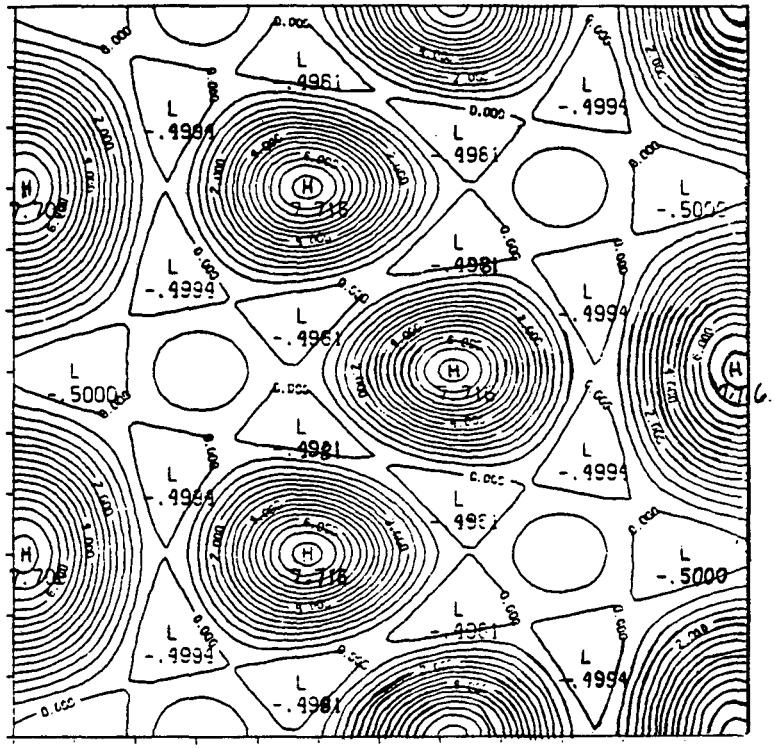


Figure 3.2.1 Level curves of k(u)

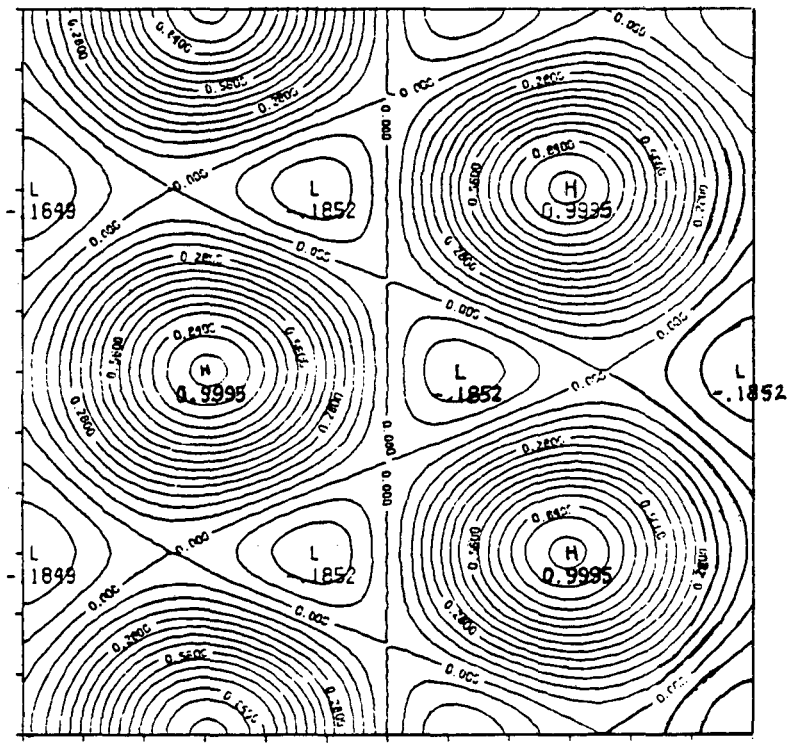


Figure 3.2.2 Level curves of h(u)

where $(\vartheta, \varphi_{max}(\vartheta))$ is on one of the boundary arcs $\overline{VE}$ or $\overline{CE}$.

In order to generate this table, we needed explicit expressions for the boundary of triangle VCE. The arc $\overline{VC}$ is simply part of the meridian $\varphi = 0$. Since $\overline{VE}$ is the projection onto $\mathbf{S}^2$ of the line segment between V and E, it lies on a great circle, i.e., the plane through $\overline{VE}$ passes through the origin. The line through the origin, normal to this plane, intersects $\mathbf{S}^2$ at two points. Let Z be one of these points. Then every point, A, on the great circle satisfies $A \cdot Z = 0$. If $A = (\sin\vartheta\cos\varphi, \sin\vartheta\sin\varphi, \cos\vartheta)$ and $Z = (\sin\vartheta_Z\cos\varphi_Z, \sin\vartheta_Z\sin\varphi_Z, \cos\vartheta_Z)$, this condition produces the equation

$$\varphi = \varphi_Z - \cos^{-1}(-\cot\vartheta_Z \cot\vartheta),$$

Since $\overline{VE}$ intersects the equator at $\varphi = \frac{\pi}{10}$, we know that $\varphi_Z = \frac{\pi}{10} \pm \frac{\pi}{2}$. We arbitrarily choose

$$\varphi_Z = \frac{\pi}{10} + \frac{\pi}{2} = \frac{3\pi}{5}$$

and go on to determine $\cot\vartheta_Z$. Let $Z = (z_1, z_2, z_3)$. Then

$$\cot\vartheta_Z = \frac{z_3}{z_1} \cdot \cos\varphi_Z .$$

$Z \cdot V = 0$ provides the relationship $2z_1 + z_3 = 0$, or $\frac{z_3}{z_1} = -\tan\vartheta_V$, and the equation for the arc $\overline{VE}$ is

$$\varphi_{max}(\vartheta) = \frac{3\pi}{5} - \cos^{-1}(\cos\frac{3\pi}{5}\cot\vartheta \tan\vartheta_V)$$

Similarly, the equation for the arc $\overline{CE}$ is

$$\varphi_{max}(\vartheta) = \frac{3\pi}{5} - \cos^{-1}(\cos\frac{3\pi}{5}\cot\vartheta \tan\vartheta'_C)$$

In Fig. 3.2.4, we plotted the $(h(\bar{u}), k(\bar{u}))$-values for $\bar{u}$ on the boundary of triangle VCE to get R, the range of (h, k). If, upon solving system (3.2.2), we find that $(\alpha_m, \beta_m) \notin R$, for some m, then there is no quadrature formula corresponding to the solution $(\alpha_1, \beta_1), \ldots, (\alpha_K, \beta_K)$.

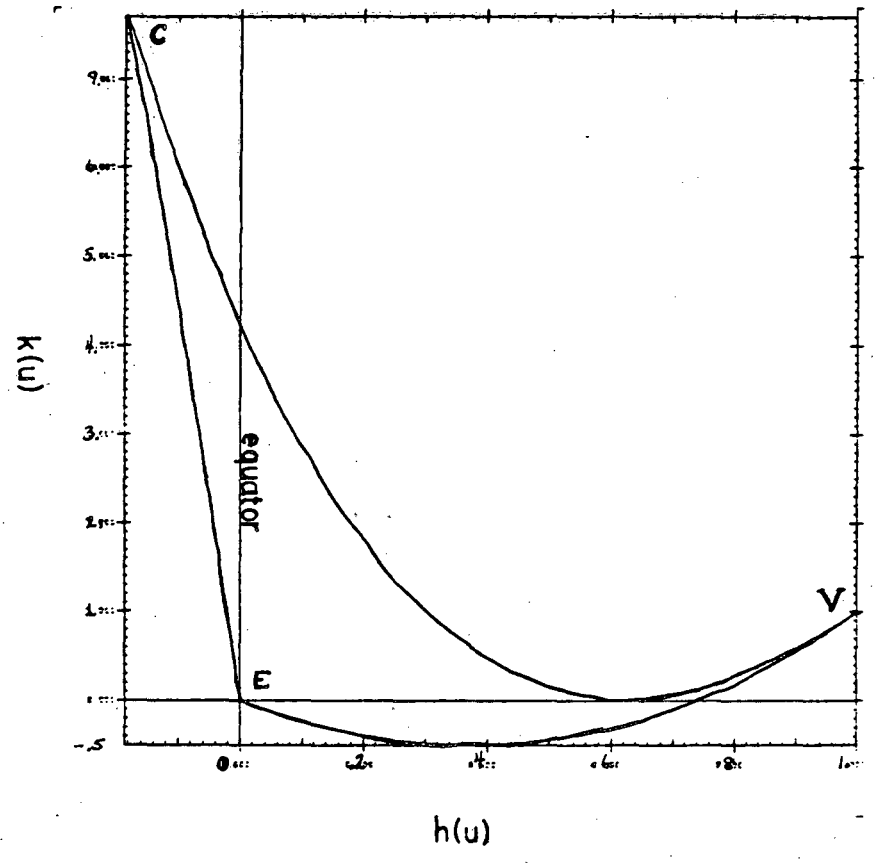


Figure 3.2.4

2.2 Solution of the System of Equations

If we denote $h(C)$ by α_c and $k(C)$ by β_c, we can rewrite (3.2.2) as

$$v + c \cdot \alpha_c^i \cdot \beta_c^j + 60 \cdot \sum_{m=1}^{K} \alpha_m^i \beta_m^j = \frac{v + c + e + 60K}{4\pi} \int_{S^2} q_{ij}(\overline{u}), \qquad (3.2.3)$$

since $h(V) = k(V) = 1$ and $h(E) = k(E) = 0$.

$\alpha_c \approx -.185185198$, $\beta_c \approx 7.7160501$, and in Table 4 (Section 3.4), we list the values of $\frac{1}{4\pi}\int_{S^2} q_{ij}(\overline{u})$ for the first 20 q_{ij}. Thus, the sums $\sum_{m=1}^{K} \alpha_m^i \beta_m^j$ have values which can be calculated:

$$\sum_{m=1}^{K} \alpha_m^i \beta_m^j = \frac{1}{60}\left[\frac{v + c + e + 60K}{4\pi} \int_{S^2} q_{ij}(\overline{u}) - v - c \cdot \alpha_c^i \cdot \beta_c^j\right] \qquad (3.2.4)$$

While working with a fixed K, we will use the notation

$$T_{ij} \equiv \text{R.H.S. of (3.2.4)},$$

with special notation for $j = 0$ or 1:

$$S_i \equiv T_{i0} \qquad T_i \equiv T_{i1}$$

We can solve system (3.2.2) explicitly for $K \leq 4$. We demonstrate the procedure for the case $K = 4$. For $K > 4$, we turn to numerical methods to solve (3.2.2). We present the solutions for the cases $K = 5$ and $K = 10$.

K = 4

The first 8 monomials q_{ij} and their degrees are

q_{ij}	h	k	h^2	hk	h^3	k^2	h^2k	h^4
deg	6	10	12	16	18	20	22	24

$\alpha_1, \ldots, \alpha_4$ are the roots of some monic 4th degree polynomial

$$f(\alpha) \equiv \alpha^4 + c_1\alpha^3 + c_2\alpha^2 + c_3\alpha + c_4.$$

The coefficients c_i and the sums $S_i = \sum_{m=1}^{4} \alpha_m^i$ are symmetric functions of $\alpha_1, \ldots, \alpha_4$. They are related by Newton's formulas [3]:

$$\begin{aligned}
S_1 + c_1 &= 0 \\
S_2 + c_1S_1 + 2c_2 &= 0 \\
S_3 + c_1S_2 + c_2S_1 + 3c_3 &= 0 \\
S_4 + c_1S_3 + c_2S_2 + c_3S_1 + 4c_4 &= 0
\end{aligned}$$

Thus, we can calculate the coefficients of $f(\alpha)$ from the values (3.2.4) for S_i. If the roots of this $f(\alpha)$ are all real, then we have the 4 α-values, $\alpha_i = h(\bar{u}_i)$.

Now, 3 of the 4 remaining equations are linear in $\beta_1, \ldots, \beta_4$. We can write them in matrix form as

$$\begin{bmatrix} 1 & 1 & 1 \\ \alpha_1 & \alpha_2 & \alpha_3 \\ \alpha_1^2 & \alpha_2^2 & \alpha_3^2 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} + \beta_4 \cdot \begin{bmatrix} 1 \\ \alpha_4 \\ \alpha_4^2 \end{bmatrix} = \begin{bmatrix} T_0 \\ T_1 \\ T_2 \end{bmatrix},$$

This gives us $\beta_1, \beta_2, \beta_3$ as linear functions of β_4, which makes the last equation -- the one which corresponds to k^2 -- a quadratic in β_4.

If β_4 is real, we have 1 or 2 sets of $\beta_1, \ldots, \beta_4$, i.e., 1 or 2 solutions $(\alpha_1, \beta_1), \ldots, (\alpha_4, \beta_4)$. If, for each pair (α_m, β_m) of a solution, there exists a point $\bar{u}_m$ such that $h(\bar{u}_m) = \alpha_m$, $k(\bar{u}_m) = \beta_m$, then we have an invariant 24th-degree quadrature formula.

Table 3 summarizes the outcome of this procedure for the different choices of special invariant sets.

At the end of this chapter, we list the (ϑ, φ) - and the (α, β)-values of the 4 general nodes of each quadrature formula. Figures 3.2.5 through 3.2.7 show their location in the triangle VCE. We tested these formulas on the 11-ellipsoid phantom (eyes, ears, nose and mouth omitted) with $N_s \approx 2d + 1$, where $d - 1$ is the order of the formula, i.e, 24. The L^2 error is calculated from the reconstructed values on a $64x64$ grid of the plane $z = .381$, with the understanding that the reconstructed value is 0 at any gridpoint outside the circle $x^2 + y^2 = 1 - (.381)^2$.

Table 3

v	c	e	# Dirs	Solutions / Formulas
0	0	0	240	No solns (2 complex α_m)
12	0	0	246	2 solns / 1 formula (1 β_m not in range of k)
0	20	0	250	No solns (2 complex α_m)
0	0	30	255	No solns (2 complex α_m)
12	20	0	256	No solns (2 complex α_m)
12	0	30	261	No solns (β_4 not real)
0	20	30	265	No solns (2 complex α_m)
12	20	30	271	2 solns / 2 formulas

K = 5

The 9th and 10th q_{ij} are

$$hk^2 \text{ (degree = 26)} \quad \text{and} \quad h^3k \text{ (degree = 28)}.$$

Since h^5 is not one of the first 10 q_{ij}, we have no value for S_5. Thus, c_5 -- and, therefore, $\alpha_1, \ldots, \alpha_5$ -- cannot be determined, and we cannot solve this system of equations in the same way that we found all the solutions of the $K = 4$ case. With some modification, however, we can combine that procedure with numerical algorithms to obtain *some* of the solutions.

If we make some initial guess for α_5, we can calculate

$$R_i \equiv \sum_{m=1}^{4} \alpha_m^i = S_i - \alpha_5^i, \qquad 1 \le i \le 4.$$

Then $R_1, \ldots, R_4$ can be used to find the coefficients $c_1, \ldots, c_4$ of the 4th-degree polynomial whose roots are $\alpha_1, \ldots, \alpha_4$. Thus, we have $\alpha_1, \ldots, \alpha_4$, which depend on α_5 in some complicated way.

As before, the equations which correspond to k, hk, h^2k, h^3k are linear in $\beta_1, \ldots, \beta_5$. Making an initial guess for β_5, we can solve the following matrix equation for $\beta_1, \ldots, \beta_4$:

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 \\ \alpha_1^2 & \alpha_2^2 & \alpha_3^2 & \alpha_4^2 \\ \alpha_1^3 & \alpha_2^3 & \alpha_3^3 & \alpha_4^3 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \end{bmatrix} = \begin{bmatrix} T_0 \\ T_1 \\ T_2 \\ T_3 \end{bmatrix} - \beta_5 \cdot \begin{bmatrix} 1 \\ \alpha_5 \\ \alpha_5^2 \\ \alpha_5^3 \end{bmatrix}$$

Then, the equations for k^2 and hk^2 form a system of 2 equations which depends on α_5 and β_5. We solve this system numerically for the unknowns α_5 and β_5.

More specifically, we used IMSL subroutines ZCPOLY (a polynomial root-finder) LEQ2C (a matrix-solver), and ZSCNT (a non-linear-system-solver, secant method). The α_m and β_m were allowed to be complex throughout the

computation, but were accepted as a solution only if they were real. Using this method, we found solutions for only 2 choices of special sets -- $(v, c, e) = (12,0,0)$ and $(v, c, e) = (12,20,0)$. The locations of the general nodes of these formulas are listed at the end of this chapter, along with the results of the simulation experiments.

Remark: An apparently more natural way to find (α_m, β_m) numerically is to try to solve the last 2 equations for S_5 and T_4, instead of α_5 and β_5. I.e., make initial guesses for S_5 and T_4, solve Newton's formulas for $c_1, \ldots, c_5$, and obtain $\alpha_1, \ldots, \alpha_5$ as the roots of this 5th-degree polynomial. Then the matrix equation for the β_m would be simply

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 & \alpha_5 \\ \alpha_1^2 & \alpha_2^2 & \alpha_3^2 & \alpha_4^2 & \alpha_5^2 \\ \alpha_1^3 & \alpha_2^3 & \alpha_3^3 & \alpha_4^3 & \alpha_5^3 \\ \alpha_1^4 & \alpha_2^4 & \alpha_3^4 & \alpha_4^4 & \alpha_5^4 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \\ \beta_5 \end{bmatrix} = \begin{bmatrix} T_0 \\ T_1 \\ T_2 \\ T_3 \\ T_4 \end{bmatrix}$$

Although this approach seems more straightforward, we could not find suitable initial guesses for S_5 and T_5 to obtain a solution.

K = 10

This case is solved by the same procedure as $K = 5$. The 11th through 20th q_{ij} are

q_{ij}	h^5	k^3	h^2k^2	h^4k	h^6	hk^3	h^3k^2	h^5k	k^4	h^7 or h^2k^3
deg	30	30	32	34	36	36	38	40	40	42

If we take h^2k^3 for the 20th q_{ij}, we need to initialize 4 values of α_m and 4 values of β_m. We then try to solve a system of 8 equations -- those which involve k^2, k^3 and k^4. Of course, initial values must be chosen more carefully, and convergence is much slower than in the $K = 5$ case. We found solutions for 2 choices of special sets -- $(v,c,e) = (12,0,30)$ and $(v,c,e) = (12,20,30)$. The locations of the general nodes of these formulas are listed at the end of this chapter, along with the results of the simulation experiments.

3. Equilibrium Distributions

Let $\bar{u}_1, \ldots, \bar{u}_N$ be points on $\mathbf{S}^2$ and suppose that there are positive point charges at each point $\bar{u}_i$ and at $-\bar{u}_i$. Then the electrostatic potential at each $\bar{u}_i$, excluding the potential due to the charge at $\bar{u}_i$ itself, is given by:

$$Q_i \equiv \frac{1}{2} + \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{1}{|\bar{u}_i - \bar{u}_j|} + \frac{1}{|\bar{u}_i + \bar{u}_j|}.$$

If $\bar{u}_1, \ldots, \bar{u}_N$ are chosen to minimize the total potential energy of this system

$$Q \equiv \sum_{i=1}^{N} Q_i = \frac{N}{2} + \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{1}{|\bar{u}_i - \bar{u}_j|} + \frac{1}{|\bar{u}_i + \bar{u}_j|},$$

then $\pm\bar{u}_1, \ldots, \pm\bar{u}_N$ is an *equilibrium distribution* for the $2N$ point charges, i.e., at each $\bar{u}_i$, the electric field due to the other point charges,

$$\vec{E}_i \equiv \frac{\bar{u}_i}{2} + \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{\bar{u}_i - \bar{u}_j}{|\bar{u}_i - \bar{u}_j|^2} + \frac{\bar{u}_i + \bar{u}_j}{|\bar{u}_i + \bar{u}_j|^2},$$

is a scalar multiple of the position vector $\bar{u}_i$.

In [4], Grünbaum proposed that, for large N, a set of directions chosen in this way would be a good set of nodes for a uniform-weight quadrature formula. Having shown that the directions $\bar{u}_1, \ldots, \bar{u}_N$ which minimize the quantity

$$\sum_{i,j=1}^{N} \sum_{m=0}^{2p} P_{2m}(\bar{u}_i \cdot \bar{u}_j) \tag{3.3.1}$$

are the nodes for a quadrature formula which is exact for spherical polynomials of degree $\leq 2p$, he observed that

$$\frac{1}{|\bar{u}_i - \bar{u}_j|} + \frac{1}{|\bar{u}_i + \bar{u}_j|} = 2 \sum_{m=0}^{\infty} P_{2m}(\bar{u}_i \cdot \bar{u}_j).$$

This suggests that, for large N, the electrostatic potential Q is a reasonable approximation to the quantity (3.3.1).

If (ϑ_i, φ_i) are the spherical coordinates of $\bar{u}_i$, then Q is a function of $2N$ variables. Numerical minimization of this function is possible when $N \approx 50$, cumbersome when $N \approx 100$, and almost impossible when $N \geq 200$.

If N is an integer multiple of 60, however, we can significantly reduce the number of variables by requiring that the $\bar{u}_i$ consist of $\frac{N}{60}$ icosahedral orbits. Then Q becomes a function of only $\frac{N}{30}$ variables. E.g., for $N = 60$, we look for a single point $\bar{u}_1$ whose orbit $\{\rho\bar{u}_1 : \rho \varepsilon G\}$ minimizes Q over all other orbits.

We can also reduce the number of operations needed to calculate Q and its derivatives:

Let $d_{ij} \equiv \frac{1}{|\bar{u}_i - \bar{u}_j|} + \frac{1}{|\bar{u}_i + \bar{u}_j|}$. Since $d_{ij} = d_{ji}$,

$$Q - \frac{N}{2} = \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} d_{ij} = 2 \sum_{i=2}^{N} \sum_{j=1}^{i-1} d_{ij} \equiv 2D,$$

and minimizing D will minimize Q.

For arbitrary $\bar{u}_1, \ldots, \bar{u}_N$, calculating D requires the computation of $\frac{1}{2}N(N-1)$ quantities d_{ij}. If the set of points $\bar{u}_1, \ldots, \bar{u}_N$ consists of K general icosahedral orbits, $N = 60K$, then only $30K^2 + 29K$ values of d_{ij} need to be calculated. To show this, we will write $Q - \frac{N}{2}$ as

$$Q - \frac{N}{2} = \sum_{\substack{\text{same} \\ \text{orbit}}} d_{ij} + \sum_{\substack{\text{diff} \\ \text{orbit}}} d_{ij}$$

where the first summation involves only points $\bar{u}_i$ and $\bar{u}_j$ which are in the same orbit, and the second summation involves only points $\bar{u}_i$ and $\bar{u}_j$ which are in different orbits.

To begin, we break up the summation over i by orbits:

$$Q - \frac{N}{2} = \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}} d_{ij}$$

$$= \sum_{i=1}^{60} \left[\sum_{\substack{j=1 \\ j \neq i}}^{60} d_{ij} + \sum_{j=61}^{N} d_{ij} \right] + \sum_{i=61}^{120} \left[\sum_{j=1}^{60} d_{ij} + \sum_{\substack{j=61 \\ j \neq i}}^{120} d_{ij} + \sum_{j=121}^{N} d_{ij} \right]$$

$$+ \cdots + \sum_{i=N-59}^{N} \left[\sum_{j=1}^{N-60} d_{ij} + \sum_{\substack{j=N-59 \\ j \neq i}}^{N} d_{ij} \right]$$

$$= \sum_{i=1}^{60} \sum_{\substack{j=1 \\ j \neq i}}^{60} d_{ij} + \sum_{i=61}^{120} \sum_{\substack{j=61 \\ j \neq i}}^{120} d_{ij} + \cdots + \sum_{i=N-59}^{N} \sum_{\substack{j=N-59 \\ j \neq i}}^{N} d_{ij}$$

$$+ 2 \left[\sum_{i=1}^{60} \sum_{j=61}^{N} d_{ij} + \sum_{i=61}^{120} \sum_{j=121}^{N} d_{ij} + \cdots + \sum_{i=N-119}^{N-60} \sum_{j=N-59}^{N} d_{ij} \right]$$

Now the symmetry of the orbits enables us to reduce each double summation to 60 times a single summation:

If $\bar{u}_i$ and $\bar{u}_j$ belong to the orbit of $\bar{u}_1$, then

$$\sum_{\substack{j=1 \\ j \neq i}}^{60} d_{ij} = \sum_{j=2}^{60} d_{1j}$$

and so, for $\bar{u}_i$ and $\bar{u}_j$ in the *same* orbit,

$$\sum_{i=1}^{60} \sum_{\substack{j=1 \\ j \neq i}}^{60} d_{ij} = 60 \sum_{j=2}^{60} d_{1j} .$$

If $\bar{u}_i$ is in the orbit of $\bar{u}_1$, then

$$\sum_{j=61}^{N} d_{ij} = \sum_{j=61}^{N} d_{1j}$$

and so, for $\bar{u}_i$ and $\bar{u}_j$ in *different* orbits,

$$\sum_{i=1}^{60} \sum_{j=61}^{N} d_{ij} = 60 \sum_{j=61}^{N} d_{1j} .$$

Both of these statements are true for the orbits of $\bar{u}_{61}, \bar{u}_{121}, \ldots, \bar{u}_{N-59}$. Thus, we have

$$Q - \frac{N}{2} = 2D = 60 \left[\sum_{j=2}^{60} d_{1j} + \sum_{j=62}^{120} d_{61,j} + \cdots + \sum_{j=N-58}^{N} d_{N-59,j} \right]$$

$$+ 120 \left[\sum_{j=61}^{N} d_{1j} + \sum_{j=121}^{N} d_{61,j} + \cdots + \sum_{j=N-59}^{N} d_{N-119,j} \right]$$

and computing D requires the calculation of $59K$ same-orbit d_{ij}'s and

$$(N - 60) + (N - 120) + \cdots + 60 = 60[(K-1) + \cdots + 2 + 1] = 30K(K-1)$$

different-orbit d_{ij}'s.

There is a similar reduction of computation in the calculation of the partial derivatives. We used IMSL routine ZXCGR, a conjugate-gradient method, and obtained solutions to the K-general-node cases, for $K = 4, 5, 10$. Starting from the K nodes of one of the exact quadrature formulas (Section 3.2), convergence occurred in 33, 39, and 78 iterations, respectively. We calculated the electric field $\vec{E}_i$ for each base-node $\bar{u}_i$. The angle between $\vec{E}_i$ and $\bar{u}_i$ is always less than 3°.

4. Tables and Figures for Chapter Three

Values of $\frac{1}{4\pi}\int_{S^2} q_{ij}$ for the first 20 q_{ij}

Table 4

q_{ij}	deg	$\frac{1}{4\pi}\int_{S^2} q_{ij}$	q_{ij}	deg	$\frac{1}{4\pi}\int_{S^2} q_{ij}$
h	6	$\frac{5}{21}$	h^5	30	.21852725
k	10	$\frac{125}{77}$	k^3	30	123.688858
h^2	12	$\frac{475}{3003}$	h^2k^2	32	.4485985
hk	16	$-\frac{3125}{51051}$	h^4k	34	.103166625
h^3	18	$\frac{106625}{969969}$	h^6	36	.184429625
k^2	20	$\frac{338125}{46189}$	hk^3	36	-14.72420693
h^2k	22	$\frac{113125}{2028117}$	h^3k^2	38	.0379491
h^4	24	$\frac{439625}{5148297}$	k^4	40	733.8222725
hk^2	26	-2.1098055	h^5k	40	.09613535
h^3k	28	.1014723	h^2k^3	42	2.280482148

We computed the first 8 integrals by using MACSYMA (Project MAC's SYmbolic MAnipulation System) to do the following:

(1) expand h^ik^j with $x = \sin\vartheta\cos\varphi$ and $y = \sin\vartheta\sin\varphi$,

(2) discard any term which contains an odd power of z (h and k are homogeneous even polynomials with only even powers of y. In each polynomial, a

term contains an odd power of x if and only if it contains an odd power of z. Hence, the same is true of the terms of $h^i k^j$.)

(3) integrate the remaining terms with respect to φ, from 0 to 2π,

(4) replace z^2 by $\cos^2\vartheta$, $\sin^2\vartheta$ by $1 - \cos^2\vartheta$, multiply by $\sin\vartheta$, and integrate with respect to ϑ, from 0 to π.

For $26 \leq \deg q_{ij} < 60$, we computed the integrals using a polynomial manipulation package written in APL by Jeffrey Shallit to perform steps (1) and (2), and an APL program written by John Hughes to compute the integral of each term by the formula:

$$\int_{S^2} x^{2k} y^{2n} z^{2p} = P \cdot T,$$

where

$$P = 2\pi \cdot \frac{(2k-1)!!}{(2k)!!} \cdot \left\{ (-1)^0 \binom{n}{0} + \frac{2k+1}{2k+2} \left[(-1)^1 \binom{n}{1} + \frac{2k+3}{2k+4} \left[(-1)^2 \binom{n}{2} \right.\right.\right.$$
$$\left.\left.\left. + \cdots + \frac{2(n+k)-1}{2(n+k)} \left[(-1)^n \binom{n}{n} + 0 \right] \right] \right] \right\}$$

$$T = 2 \left[\frac{1}{2p+1} - \binom{n+k}{1} \frac{1}{2p+3} + \binom{n+k}{2} \frac{1}{2p+5} \right.$$
$$\left. + \cdots + (-1)^{n+k} \binom{n+k}{n+k} \frac{1}{2p+2n+2k+1} \right]$$

Nodes and reconstruction results of Exact Uniform - Weight Formulas

We list the spherical coordinates and (α, β) - values of the K - general node formulas. Non-zero values of v, c and/or e indicate that these special invariant sets are used in a formula. Note that the special sets consist of antipodal pairs, so only ***half*** of each set is actually used in the simulation experiments. Thus, the total number of directions is $N = 60K + \frac{1}{2}(v + c + e)$. N_s is the number of plane integrals measured along each direction.

$K = 4$									
v	c	e	N	ϑ	φ	$h(\vartheta,\varphi)$	$k(\vartheta,\varphi)$	N_s	L^2-error
12	0	0	246	1.6232 1.5613 1.4507 1.3347	.03185 .19740 .13230 .04405	-.08916 .01097 .25113 .62706	5.4207 1.0594 .1915 -.0535	51	14.57
12	20	30	271	1.5940 1.5296 1.4154 1.3150	.10973 .09414 .14144 .03809	-.03679 .08149 .33285 .68259	3.5070 2.1110 -.2134 -.0055	55	14.44
12	20	30	271	1.5932 1.5279 1.4213 1.3114	.10016 .11180 .12397 .05683	-.03679 .08149 .33285 .68259	3.6697 1.8242 -.0557 -.0394	55	14.41

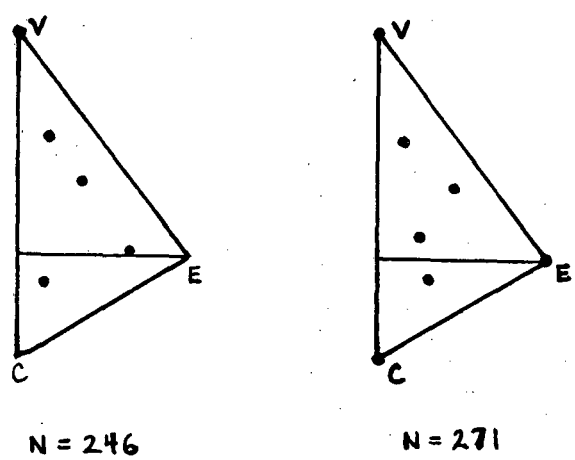


Figure 3.4.1

$K = 5$									
v	c	e	N	ϑ	φ	$h(\vartheta,\varphi)$	$k(\vartheta,\varphi)$	N_s	L^2-error
12	0	0	306	1.6666	.08716	-.12499	5.7056	61	13.61
				1.5388	.09918	.06122	2.2688		
				1.5106	.23667	.06299	-.0089		
				1.4290	.06889	.34689	.3898		
				1.2899	.10636	.69198	-.1137		
12	20	0	316	1.6265	.13787	-.06995	3.6685	63	13.28
				1.5147	.22476	.06353	.1092		
				1.5260	.02706	.09815	2.6350		
				1.4024	.12772	.37947	-.2181		
				1.3040	.04494	.70798	.0161		

$K = 10$									
v	c	e	N	ϑ	φ	$h(\vartheta,\varphi)$	$k(\vartheta,\varphi)$	N_s	L^2 error
12	0	30	621	1.7019	.07222	-.1532	6.6124	87	12.17
				1.6091	.05598	-.0660	4.7897		
				1.5762	.12958	-.0084	2.6717		
				1.5600	.21520	.0109	.7500		
				1.5037	.08725	.1423	1.5813		
				1.4857	.11915	.1735	.8550		
				1.4070	.16449	.3299	-.3773		
				1.3946	.06629	.4463	.0599		
				1.3299	.06235	.6302	-.0988		
				1.2357	.07160	.8420	.3261		
12	20	30	631	1.6343	.04165	-.1030	5.6339	87	11.33
				1.6622	.14625	-.0925	4.1808		
				1.5472	.16617	.0346	1.3528		
				1.5423	.04916	.0592	2.9464		
				1.5113	.21170	.0753	.1864		
				1.4687	.07571	.2349	.9661		
				1.3998	.17469	.3355	-.4398		
				1.3932	.05252	.4570	.1055		
				1.3201	.08245	.6414	-.1455		
				1.2434	.04452	.8463	.3528		

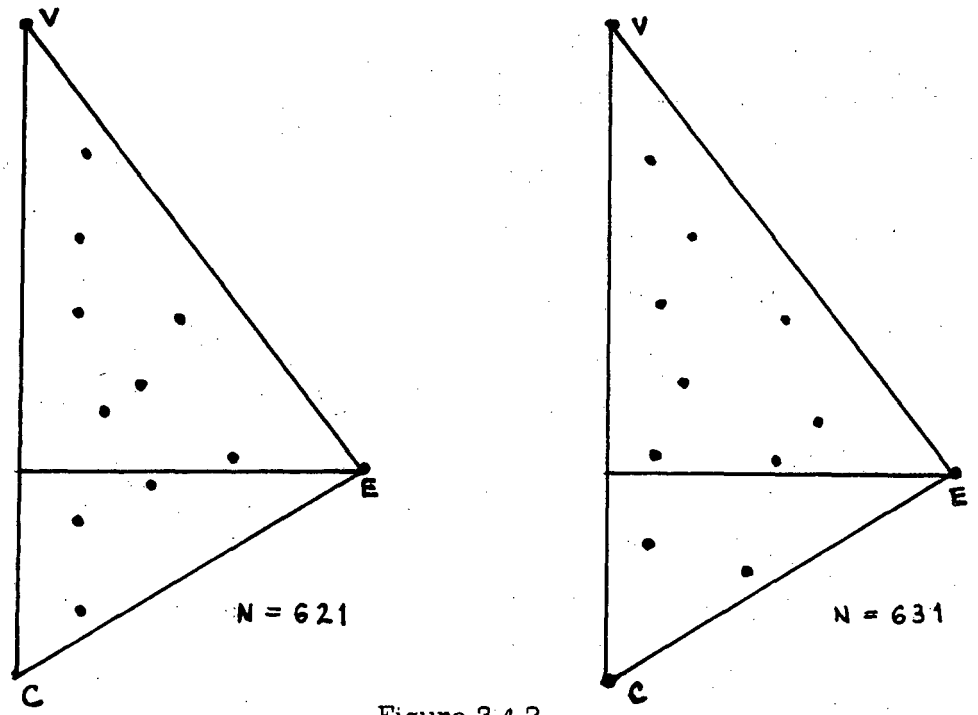


Figure 3.4.2

The actual implementation of these quadrature formulas raises an interesting question. Recall that for the purpose of reconstruction, we are only interested in numerically integrating *even* functions of $\bar{u}$. Hence, we think of the quadrature nodes as "directions" and make some effort to avoid redundancy in this set of directions. The orbit of a general node $\bar{u}_m$ contains 60 distinct *directions*, unless $\bar{u}_m$ is on a median or an edge of the icosahedron, which happens rarely. The special invariant sets, however, consist of antipodal pairs, so implementation of a quadrature formula uses only 6 vertices and/or 10 centroids and/or 15 midpoints of edges. Since the (α_m, β_m) are the solutions of a system of equations which assumes twice as many special points, it seems reasonable to count the contributions of the special points twice, as if they had been calculated at each point of an antipodal pair. But this produces a larger L^2 error in the reconstruction than simply weighting each direction equally.

Nodes of Equilibrium Distribution Formulas

In the following tables, we list the (ϑ_i, φ_i) coordinates of these solutions, their (α_i, β_i) values, and the values of $\cos^{-1}(\vec{E}_i \cdot \bar{u}_i)$ for each base-node. Figures 3.3.1 through 3.3.3 show their locations in the triangle VCE. We tested these formulas on the 11 - ellipsoid phantom (eyes, ears, nose and mouth omitted). The optimal values of N_s for these formulas are approximately the same as the optimal values of N_s for the exact uniform - weight formulas. The L^2 error is calculated from the reconstructed values on a $64x64$ grid of the plane $z = .381$, with the understanding that the reconstructed value is 0 at any gridpoint outside the circle $x^2 + y^2 = 1-(.381)^2$. The reconstruction results are given on the last line of each table.

$K = 4$				
ϑ	φ	$h(\vartheta,\varphi)$	$k(\vartheta,\varphi)$	$\cos^{-1}(E_i \cdot \bar{u}_i)$
1.6316	.07067	-.09466	5.1887	.036871
1.5397	.20726	.03639	.5869	.043576
1.4509	.08714	.27756	.5752	.026749
1.2962	.06465	.71565	-.0035	.028169
$N_s = 51$ L^2-error = 14.48				

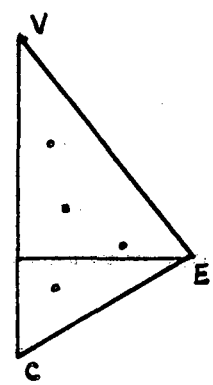


Figure 3.3.1

$K = 5$				
ϑ	φ	$h(\vartheta,\varphi)$	$k(\vartheta,\varphi)$	$\cos^{-1}(E_i \cdot \bar{u}_i)$
1.6486	.07067	-.11399	5.6090	.037480
1.5493	.21481	.02277	.6120	.043860
1.5109	.06655	.12990	1.9611	.046866
1.4038	.12968	.37388	-.2206	.040497
1.2779	.05564	.76563	.1135	.025763
$N_s = 65$ L^2-error = 13.17				

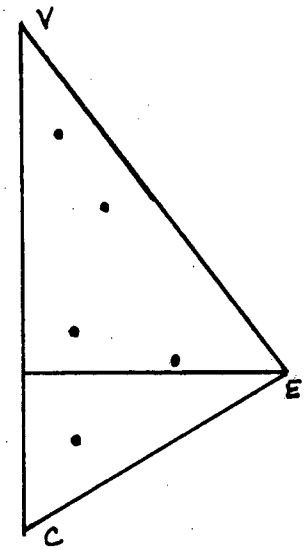


Figure 3.3.2

$K = 10$				
ϑ	φ	$h(\vartheta,\varphi)$	$k(\vartheta,\varphi)$	$\cos^{-1}(E_i \cdot \bar{u}_i)$
1.6811	.04897	-.14880	6.6206	.032826
1.6129	.15235	-.05187	3.0169	.055148
1.5844	.05391	-.02525	4.1095	.047568
1.5544	.24632	.01225	.2858	.047864
1.4999	.17246	.11572	.4592	.031852
1.4927	.06136	.17650	1.5753	.046858
1.4077	.15688	.33656	-.3409	.058872
1.3973	.04679	.44741	.1579	.052083
1.3153	.08847	.64829	-.1533	.030515
1.2270	.03998	.87933	.4709	.018955
$N_s = 89$ L^2-error = 11.01				

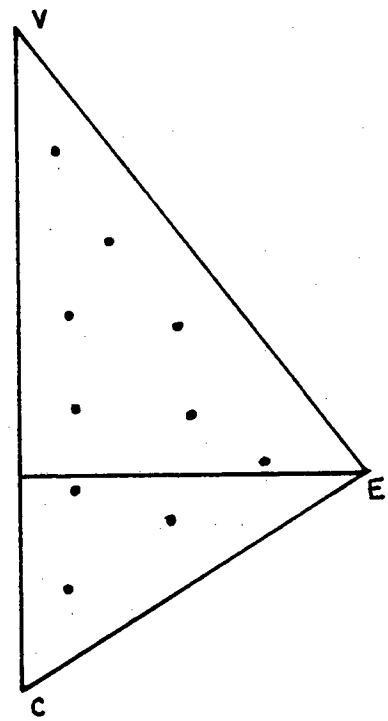


Figure 3.3.3

Chapter Four: Summary of Results

1. Simulation Experiments

We tested five methods by simulating the reconstruction of Shepp's head phantom with the high - contrast features removed. The L^2 error

$$\left\{ \sum_{i,j=1}^{64} [f(\bar{x}_{ij}) - \bar{f}(\bar{x}_{ij})]^2 \right\}^{1/2}$$

was computed from the values of $\bar{f}$ on a 64 x 64 grid of the plane $z = .381$. $\bar{f}$ was assumed to be 0 (i.e., was not calculated) outside the disk $x^2 + y^2 = 1 - (.381)^2$. Table 5 summarizes the results of these experiments. Notice that Shepp's set of directions is tested with two values of N_s.

Table 5

11 - ellipsoid phantom , 64 x 64 grid of $z = .381$

Method (Sec. ref.)	N	N_s	L^2 error
Shepp (Sec. 1.3)	625	101	14.15
Louis (Sec. 1.4)	630	71	13.36
Shepp (Sec. 1.5)	625	71	12.89
Exact (Sec. 3.2)	631	87	11.33
Louis	1225	97	11.09
Shepp	1089	93	11.04
Equilibrium (Sec. 3.3)	600	89	11.01

Figures 4.1.1 through 4.1.7 plot the values of $\bar{f}$ at 128 points of the line $y = .23$, which passes through the left and right ventricles. Figures 4.1.8 through 4.1.14 plot the values of $\bar{f}$ at 128 points of the line $y = -.605$, which passes through the three small tumors, "old f,g,e".

Shepp 625, Nsamp = 101
y = .23

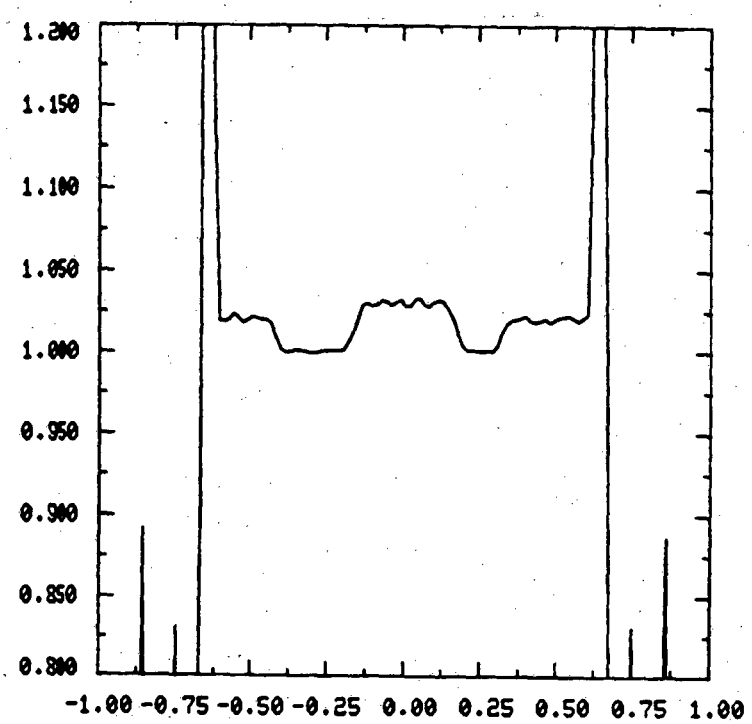
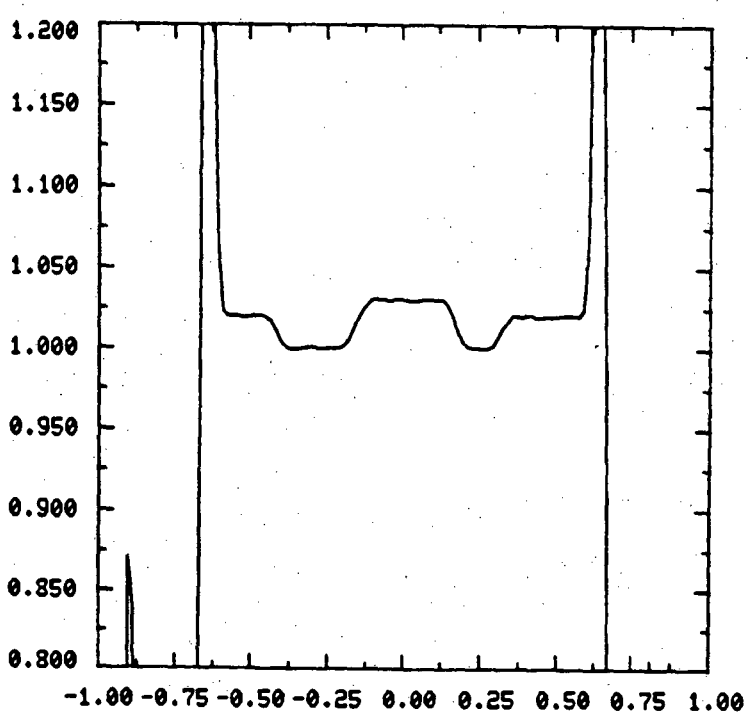


Fig. 4.1.1

Louis 630
y = .23

Fig. 4.1.2



Shepp 625, Nsamp = 71
y = .23

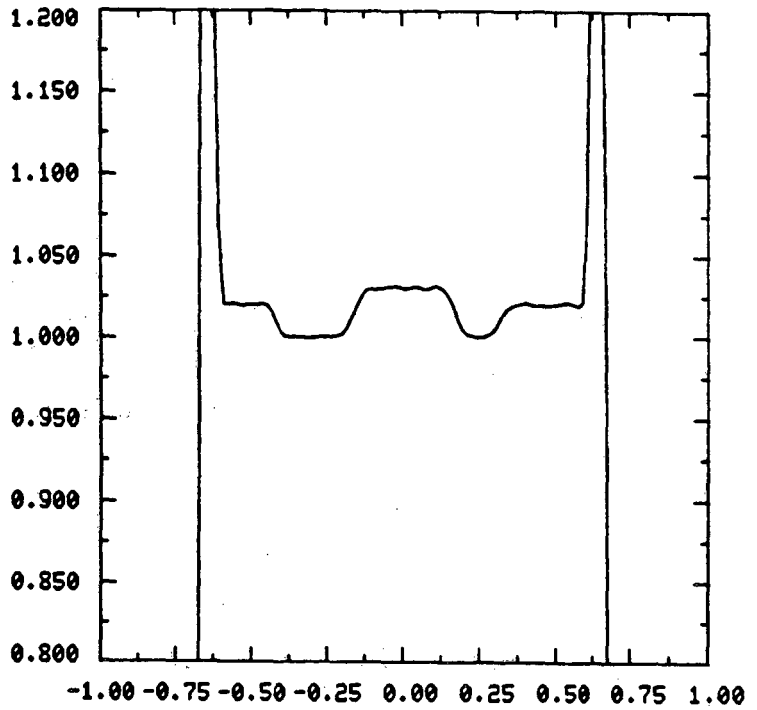
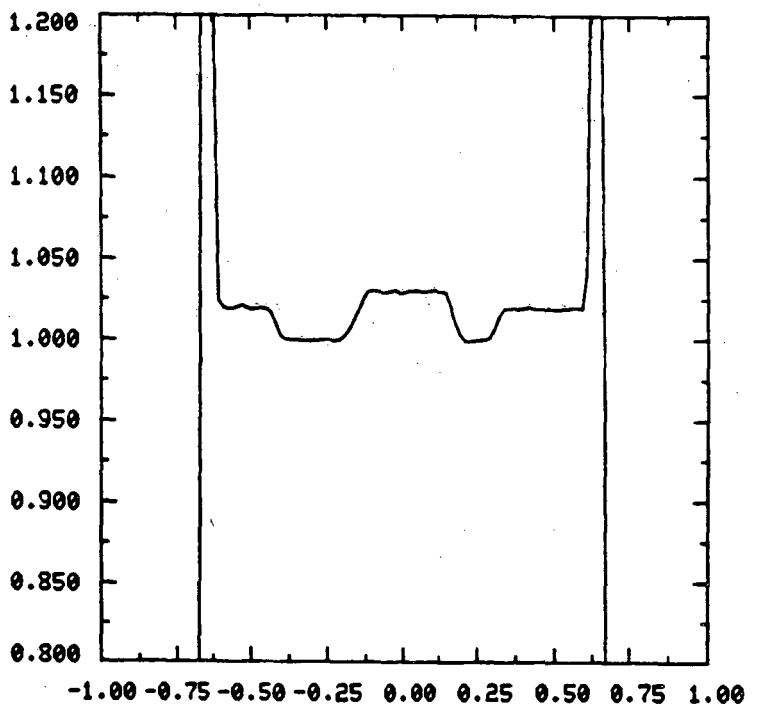


Fig. 4.1.3

Exact 631
y = .23

Fig. 4.1.4



Louis 1225
y = .23

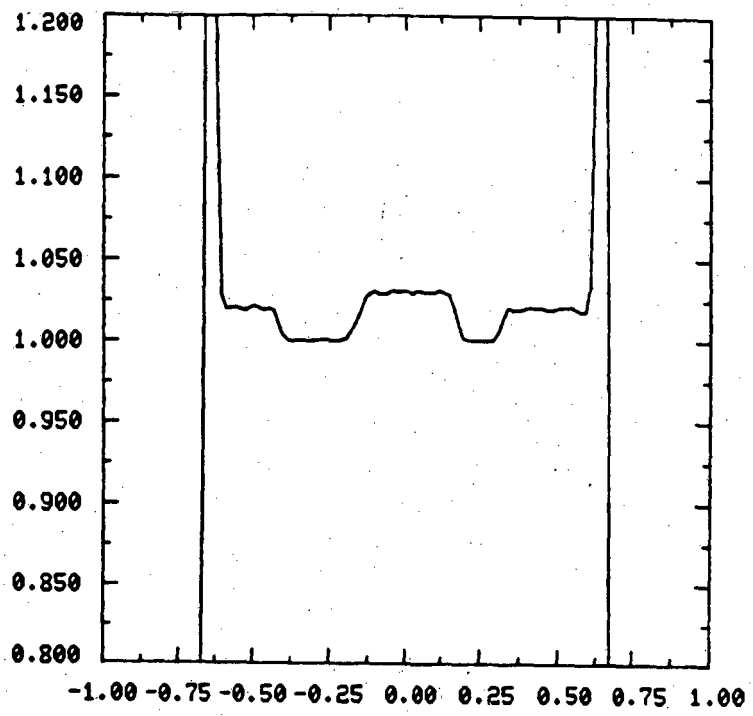
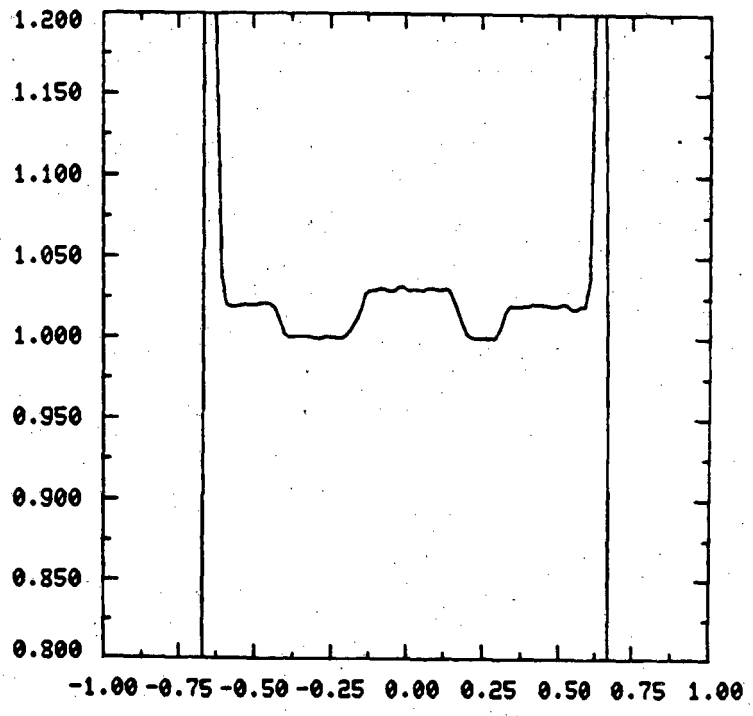


Fig. 4.1.5

Shepp 1089
y = .23

Fig. 4.1.6



Equil 600
y = .23

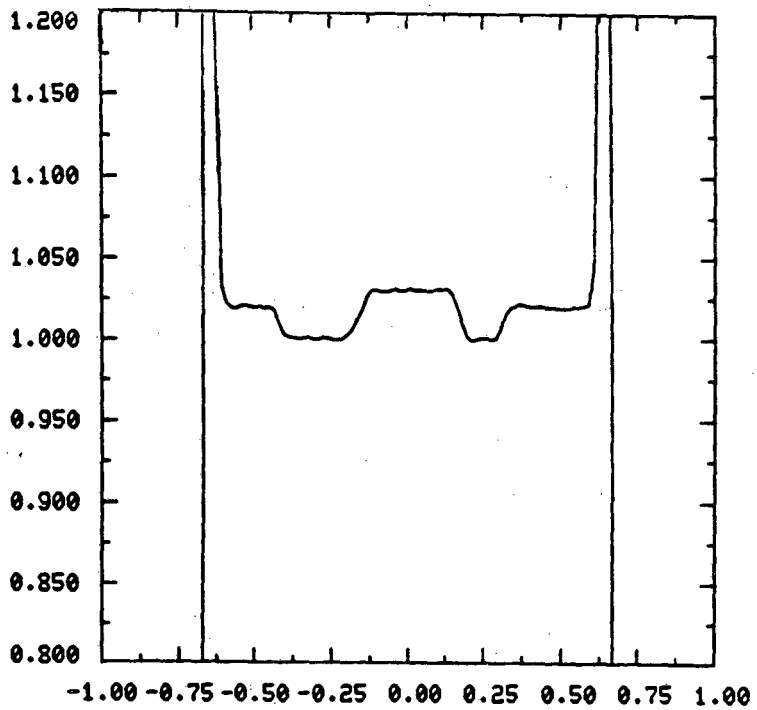
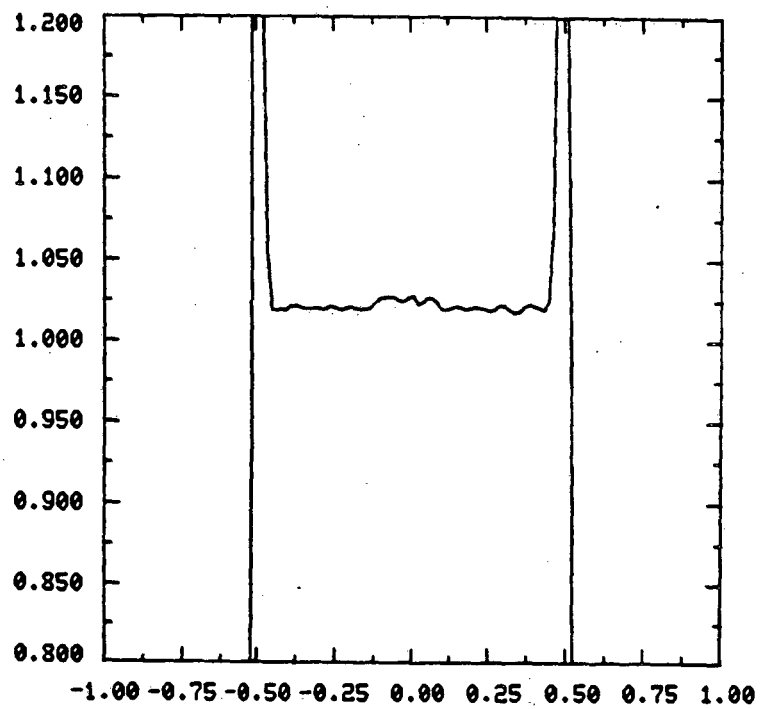


Fig. 4.1.7

Fig. 4.1.8

Equil 600
y = -.605



Shepp625, Nsamp = 101
y = -.605

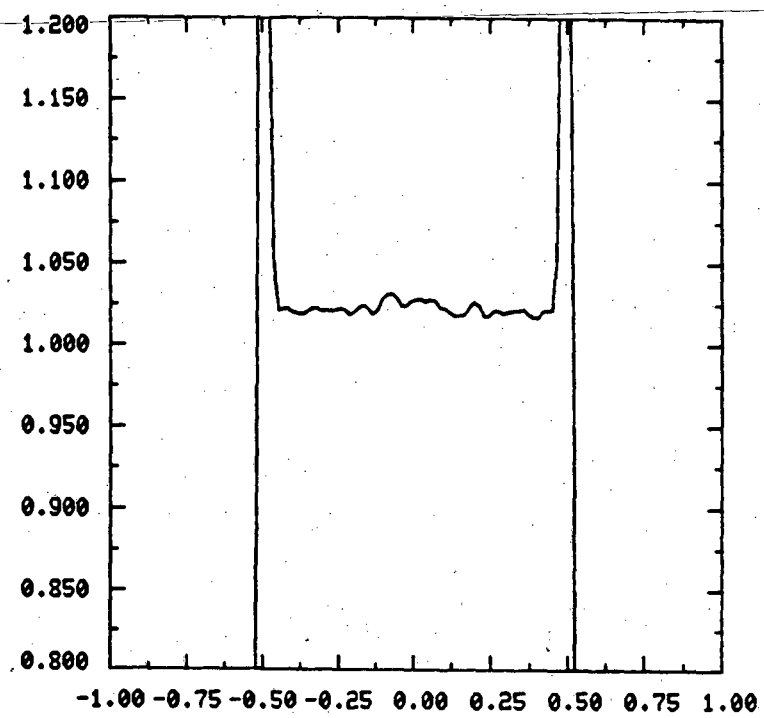
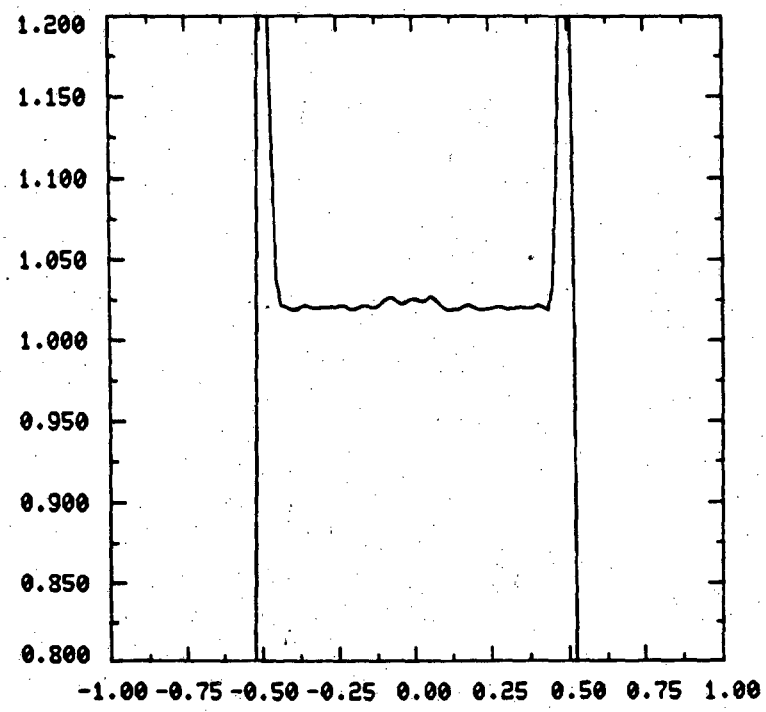


Fig. 4.1.9

Louis 630
y = -.605

Fig. 4.1.10



Shepp 625, Nsamp = 71
y = -.605

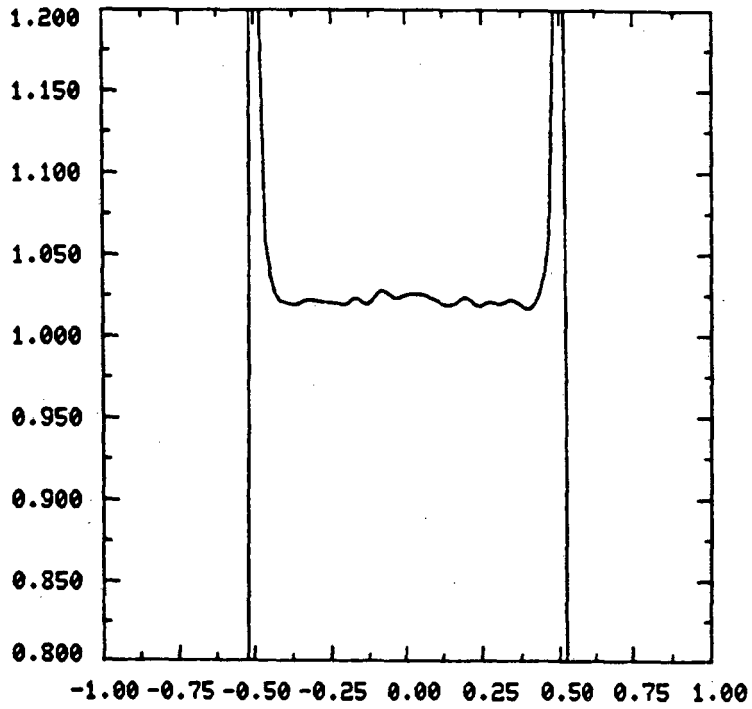
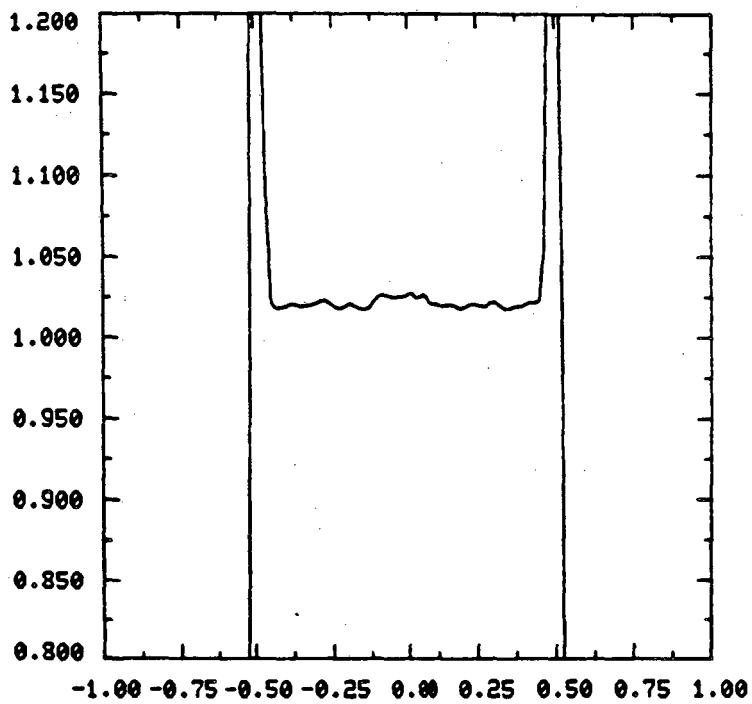


Fig. 4.1.11

Exact 631
y = -.605

Fig. 4.1.12



Louis 1225
y = -.605

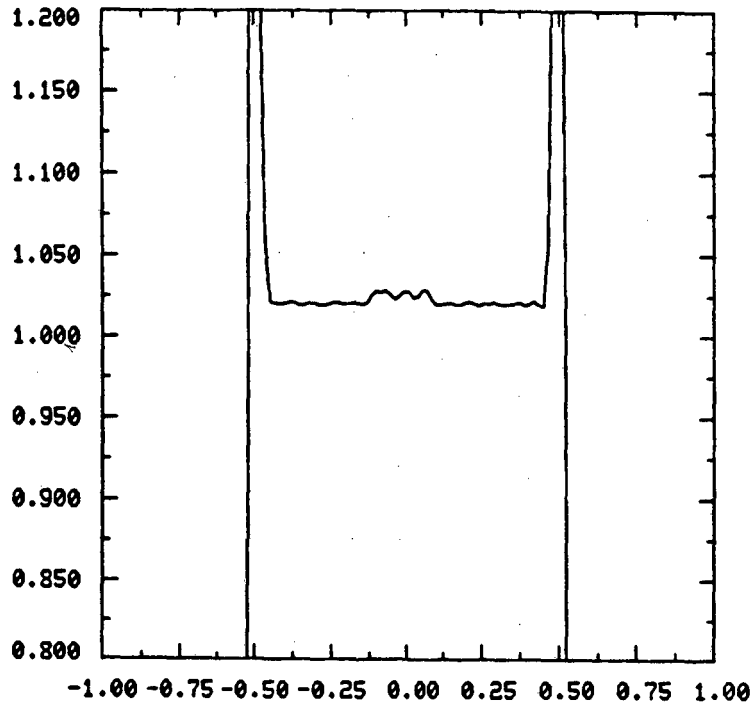
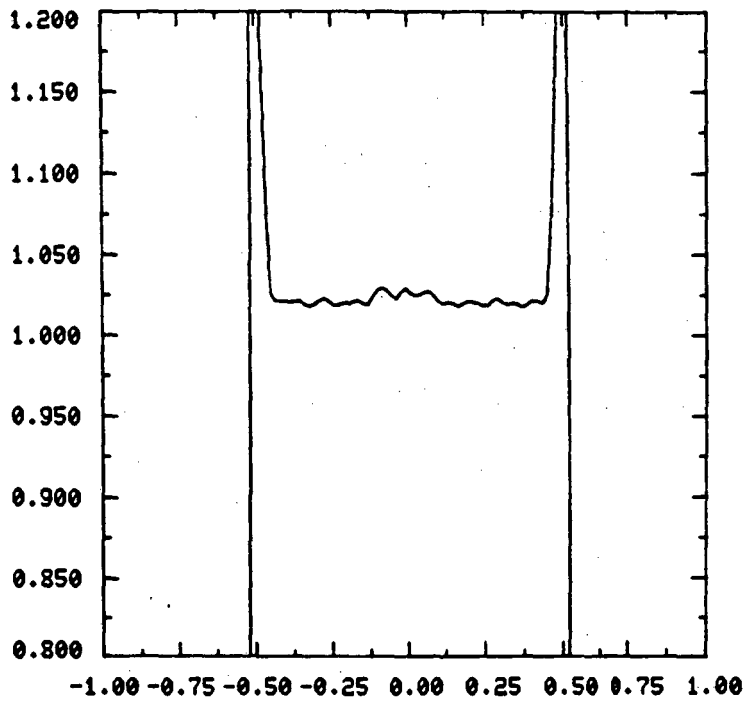


Fig. 4.1.13

Fig. 4.1.14

Shepp 1089
y = -.605



2. Comparison of Methods

In this section, we discuss the merits and weaknesses of the quadrature formulas which we have described. A highly efficient formula is clearly more desirable than a less efficient one. Reconstruction of an object as complex as a human head, however, involves the numerical integration of an approximation of a very discontinuous function. Since $P(t,\bar{u})$ as a function of t is only piecewise differentiable, the approximation to its second derivative, $Q(t_i,\bar{u})$, contains many large positive and negative peaks. Hence, it is also important that a quadrature formula be of high order. Thus, a second consideration in comparing methods is the ease with which we can derive a formula of a given (high) order, using a particular method.

Product-Space Formulas

This method is clearly the most convenient of those we have described. A Kth-order formula is obtained by taking $N_\varphi = K + 1$, and $M_\vartheta = N_\varphi$, for Shepp's method, $M_\vartheta = N_\varphi + 1$, for Louis's method, or $M_\vartheta = \frac{2}{3}N_\varphi$, for our "optimal" method. The efficiency of Louis's method is $\frac{1}{3}$; the efficiency of Shepp's method is approximately the same, and the efficiency of our method approaches $\frac{1}{2}$ as K increases.

Another drawback to these formulas concerns the spacing of the quadrature nodes and the large variation in the weights. The nodes lie on N_ϑ latitudes which are spaced at intervals of $\frac{\pi}{M_\vartheta}$. There are N_φ nodes on each circle $\vartheta = \vartheta_i$, and the arc-length of this circle is $2\pi\sin\vartheta_i$. Thus, for values of ϑ near 0 or π (the poles), the nodes are very close together, whereas for values of ϑ near $\frac{\pi}{2}$ (the

equator), the nodes are much farther apart. Since the weight of each node on the circle $\vartheta = \vartheta_i$ is $\sin\vartheta_i$, these methods, in effect, have many nodes near the pole(s) but assign them very little weight. A more efficient use of quadrature nodes would be to space and weight them more uniformly.

Gauss-type Icosahedral Formulas

The invariant quadrature formulas described in Chapter Two automatically integrate most of the spherical harmonics of each degree. Thus, the coordinates and weights of a few base nodes will satisfy the small number of remaining constraints, producing, for example, Konyaev's 151-point formula which is exact for even functions of degree $\leq$ 28. The efficiency of these formulas is close to 1, and the action of the icosahedral rotation group distributes the quadrature nodes uniformly over the sphere. In addition, the magnitudes of the weights are more equal. The weights of our 91-point 18-degree formula (Sec. 2.3), for example, are all on the order of 0.1. The weights of Konyaev's 28-degree formula all have magnitude 10^{-3}.

Unfortunately, finding the coordinates and weights of the base nodes requires intricate manipulation of the system of non-linear equations which they must satisfy. Far from the simplicity of the product-space formulas, where a new formula can be obtained by changing a single number, each of these invariant formulas is the end-product of a complete re-working of the system of non-linear constraints into a sequence of linear and simpler non-linear problems. Finally, neither McLaren's nor Konyaev's method seems capable of producing quadratures of higher order than Konyaev's 28-degree formula.

Uniform-Weight Icosahedral Formulas

The product-space formulas are very easy to derive, but not very efficient. The Gauss-type quadratures are very efficient, but difficult to derive. Our uniform-weight formulas are a compromise between these two extremes. They are more efficient than the former and easier to derive than the latter. Actually, their efficiency, as measured by E_m, hovers around $\frac{1}{2}$ and does not appear to be much higher than that of our "optimal" product-space formula. The fact that they perform better in simulation experiments than product-space formulas may be due to the absence of large values of E_m for all m. The equilibrium quadratures, in particular, integrate harmonics of high degree with relatively small errors.

The procedure for deriving an equilibrium quadrature formula is practically "automated". A good set of starting values is needed for the numerical optimization routine, but no other changes are required. The procedure for the exact quadrature, on the other hand, calls for a rearrangement of the constraints, and a different set of equations must be solved for each new value of K, the number of base nodes. Thus, although the exact formulas perform almost as well as the equilibrium formulas in the simulation experiments, the equilibrium distribution is more likely to provide a systematic way of producing efficient quadrature formulas.

Future Research

Our method for finding the nodes of icosahedral equilibrium quadrature formulas eliminates the need for intricate manipulation of the constraints. Instead, we rely on a numerical algorithm which may converge slowly or not at all, depending on the starting vector. Because of the symmetries in the function

$D = Q - \frac{N}{2}$, it might be possible to devise an optimization routine, specifically tailored for this function, with better convergence properties. We plan to explore this possibility, in conjunction with a search for a reliable starting vector. To produce the 4-, 5- and 10-base-node equilibrium quadratures, we took as starting values the base nodes of one of the exact quadrature formulas. Clearly, this is not a practical method for choosing starting points for formulas which use more base-nodes, since we do not have an exact formula of order > 10. We are optimistic that the following procedure will generate a set of $6K$ starting points from a known set of K base-nodes.

Our icosahedron **T** has five *first neighbors*, i.e., there are five distinct icosahedra which are associated with **T** in the following way:

Let **D** be the dodecahedron which is dual to **T**, i.e., its vertices are the centroids C_i of **T**. Five distinct cubes can be inscribed in **D**. Their vertices are the vertices of **D**, and their edges are diagonals of the pentagonal faces of **D**. For each of these five cubes, there is another dodecahedron which can be circumscribed around it. These dodecahedra are distinct and are dual to five different icosahedra. A rotation by $\frac{\pi}{2}$ about a midpoint of an edge of **T** rotates **T** into one of these neighboring icosahedra. The same rotation takes our K base-nodes into K base-nodes of the neighboring icosahedron. Thus, by performing the appropriate five rotations through $\frac{\pi}{2}$, we get a total of $6K$ points. In this way, we hope to obtain the starting points for a $6K$-base-node equilibrium quadrature formula.

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