Computing Hyperelliptic Integrals for Surface Measure of Ellipsoids

CHARLES F. DUNKL and DONALD E. RAMIREZ
University of Virginia

An algorithm for computing a class of hyperelliptic integrals and for determining the surface measure of ellipsoids is described. The algorithm is used to construct an omnibus optimal-design criterion.

Categories and Subject Descriptors: G.1.4 [**Numerical Analysis**]: Quadrature and Numerical Differentiation—*multiple quadrature*; G.3 [**Mathematics of Computing**]: Probability and Statistics

General Terms: Algorithms

Additional Key Words and Phrases: Elliptic integral, expected radius, Lauricella's hypergeometric function, optimal designs, surface measure

1. INTRODUCTION

We begin by defining the multivariate elliptic integral $|||\,\boldsymbol{\Sigma}\,|||$ for a positive definite matrix $\boldsymbol{\Sigma}$ with eigenvalues $\gamma_1 \geq \cdots \geq \gamma_n > 0$ as

$$|||\,\boldsymbol{\Sigma}\,||| = \mathscr{E}((\mathbf{U}'\,\boldsymbol{\Sigma}\,\mathbf{U})^{1/2}) = \mathscr{E}((\mathbf{U}'\,\boldsymbol{\Lambda}\,\mathbf{U})^{1/2}), \tag{1.1}$$

where $\mathbf{U}$ is the uniformly distributed vector random variable on the unit sphere Ω in $\mathbb{R}^n$ and where $\boldsymbol{\Lambda} = \operatorname{diag}(\gamma_1, \ldots, \gamma_n)$. Each point $\mathbf{u}$ in Ω is naturally associated with a point $\mathbf{x} \in \mathbb{R}^n$ in the ellipsoid

$$\frac{x_1^2}{\gamma_1} + \cdots + \frac{x_n^2}{\gamma_n} = 1, \tag{1.2}$$

where $x_i = (\gamma_i)^{1/2} u_i$ $(1 \leq i \leq n)$. The length of the vector $\mathbf{x}$ is $(\mathbf{x}'\mathbf{x})^{1/2} = (\mathbf{u}'\,\boldsymbol{\Lambda}\,\mathbf{u})^{1/2}$, and thus, $|||\,\boldsymbol{\Sigma}\,||| = |||\,\boldsymbol{\Lambda}\,|||$ is the expected radius of the ellipsoid (1.2).

We will show that the $(n-1)$-dimensional elliptic (hyperelliptic) integral can be transformed into a univariate integral. We show in Section 5 that the

C. F. Dunkl's research was partially supported by NSF Grant DMS-88-02400. D. E. Ramirez's research was partially supported by the Center for Advanced Studies at the University of Virginia.
Authors' address: Department of Mathematics, University of Virginia, Charlottesville, VA 22903.

surface measure of an ellipsoid can be expressed as a multivariate elliptic integral. The resulting univariate integral can be efficiently computed with the Romberg method.

The paper is organized as follows. Section 2 presents the procedure for transforming the $(n-1)$-dimensional multivariate elliptic integral into a single-variable integral with a domain of integration $[0, 1]$. Section 3 presents a transformation of the univariate integral into a form suitable for numerical evaluation by the Romberg method. Upper and lower bounds for the hyperelliptic integrals are given in Section 4. The relationship between the multivariate elliptic integral and the surface measure of an ellipsoid is derived in Section 5, solving the ancient problem of efficiently computing the surface measure of ellipsoids. Section 6 discusses the Fortran implementation of the algorithm presented here. Section 7 concludes by showing how multivariate elliptic integrals can be used to find optimal designs for a class of response surface designs involving second-order terms.

2. REDUCTION OF HYPERELLIPTIC INTEGRALS

Let Σ be a positive definite matrix with eigenvalues $\gamma_1 \geq \cdots \geq \gamma_n > 0$. The value of $|||\Sigma|||$ can be expressed in hyperspherical coordinates of the form

$$\sigma_n^{-1} \int_0^{2\pi} \int_0^{\pi} \cdots \int_0^{\pi} (\gamma_1 u_1^2 + \cdots + \gamma_n u_n^2)^{1/2} \cdot (\sin \omega_1)^{n-2} \cdots (\sin \omega_{n-2}) \, d\omega_1 \cdots d\omega_{n-2} \, d\omega_{n-1}, \tag{2.1}$$

where

$$\begin{aligned} u_1 &= \cos \omega_1, \\ u_2 &= \sin \omega_1 \cos \omega_2, \\ &\vdots \\ u_{n-1} &= \sin \omega_1 \cdots \sin \omega_{n-2} \cos \omega_{n-1}, \\ u_n &= \sin \omega_1 \cdots \sin \omega_{n-2} \sin \omega_{n-1}, \end{aligned}$$

$(0 \leq \omega_i \leq \pi \ (1 \leq i \leq n-2)$, and $0 \leq \omega_{n-1} < 2\pi)$, and with σ_n from formula (5.2). When $n = 2$, the value of $|||\Sigma|||$ can be represented in terms of the complete elliptic integral $E(k, \pi/2)$ of the second kind,

$$|||\Sigma||| = \frac{2}{\pi}(\gamma_1)^{1/2} E\left(k, \frac{\pi}{2}\right), \tag{2.2}$$

where $k^2 = 1 - (\gamma_2/\gamma_1)$. Accordingly, we call $|||\Sigma|||$ the *multivariate elliptic integral* for general n.

The first step is to change the domain of integration from the sphere to the simplex E in $\mathbb{R}^n$, defined by $t_1 + \cdots + t_n = 1$, $t_i \geq 0$ $(1 \leq i \leq n)$. This applies to integrands depending only on u_i^2 $(1 \leq i \leq n)$, so that the integral can be taken over the first octant. Let $u_i^2 = t_i$, where $du_i = (t_i)^{-1/2}/2\, dt_i$ $(1 \le i \le n)$, so

$$\begin{aligned} d\mathbf{u} &= \frac{k}{2^n}(t_1 \cdots t_n)^{-1/2}\, d\mathbf{t} \\ &= c(t_1 \cdots t_n)^{-1/2}\, d\mathbf{t}, \end{aligned} \tag{2.3}$$

with k, c constants of proportionality. The evaluation of c is based on the Dirichlet formula [Exton 1976, p. 222]:

$$\int_E t_1^{\alpha_1 - 1} \cdots t_n^{\alpha_n - 1}\, d\mathbf{t} = \frac{\Gamma(\alpha_1) \cdots \Gamma(\alpha_n)}{\Gamma(\alpha_1 + \cdots + \alpha_n)}. \tag{2.4}$$

Use (2.4) with $\alpha_1 = \cdots = \alpha_n = 1/2$, so

$$1 = \int_\Omega d\mathbf{u} = c\int_E (t_1 \cdots t_n)^{-1/2}\, d\mathbf{t} = \frac{c\left(\Gamma\left(\frac{1}{2}\right)\right)^n}{\Gamma\left(\frac{n}{2}\right)}, \tag{2.5}$$

and

$$c = \frac{\Gamma\left(\frac{n}{2}\right)}{\left(\Gamma\left(\frac{1}{2}\right)\right)^n}. \tag{2.6}$$

Let

$$y_i = \gamma_i/\gamma_1 \quad \text{with } 0 < y_i \le 1,$$

and let

$$x_i = 1 - y_i \quad \text{with } 0 \le x_i < 1$$

$(1 \le i \le n)$. Then

$$\begin{aligned} (\gamma_1 t_1 + \cdots + \gamma_n t_n)^{1/2} &= (\gamma_1)^{1/2}\left(\sum_{i=1}^n y_i t_i\right)^{1/2} \\ &= (\gamma_1)^{1/2}\left(1 - \sum_{i=1}^n x_i t_i\right)^{1/2}. \end{aligned} \tag{2.7}$$

For $0 \le x_i < 1$ $(1 \le i \le n)$, define the function

$$\begin{aligned} F(x_1, \ldots, x_n) &:= F_\nu(x_1, \ldots, x_n) \\ &= c\int_E \left(1 - \sum_{i=1}^n x_i t_i\right)^\nu (t_1 \cdots t_n)^{-1/2}\, d\mathbf{t}, \end{aligned} \tag{2.8}$$

where the domain of integration is over the simplex E with $t_1 + \cdots + t_n = 1$ and with the parameter $\nu = 1/2$ in the remainder of this paper. Expression (2.8) is Carlson's R-function with parameters $R_\nu(\frac{1}{2}, \ldots, \frac{1}{2};\, y_1, \ldots, y_n)$ [Carlson

1972; Exton 1976, p. 225]. This function is a special case of the Lauricella F_D function. The important property that F possesses is a form of homogeneity in the variables $x_1, \ldots, x_n$ [Carlson 1963; Exton 1976, p. 216]. This will permit the $(n-1)$-dimensional integral

$$|||\Sigma||| = (\gamma_1)^{1/2} F\left(0, 1 - \frac{\gamma_2}{\gamma_1}, \ldots, 1 - \frac{\gamma_n}{\gamma_1}\right) \tag{2.9}$$

to be transformed into a univariate integral. The homogeneity property is shown in Theorem 2.1 for completeness:

THEOREM 2.1. *For* $0 \le x_i < 1$ $(1 \le i \le n)$,

$$F(x_1, \ldots, x_n) = -2 \sum_{i=1}^{n} (1 - x_i) \frac{\partial F}{\partial x_i}.$$

PROOF. With $1 \le j \le n$,

$$\frac{\partial F}{\partial x_j} = -\frac{1}{2} \int_E t_j \left(1 - \sum_{i=1}^{n} x_i t_i\right)^{-1/2} c(t_1 \cdots t_n)^{-1/2}\, d\mathbf{t}, \tag{2.10}$$

and since $t_1 + \cdots + t_n = 1$,

$$\begin{aligned} \sum_{j=1}^{n} (1 - x_j) \frac{\partial F}{\partial x_j} &= -\frac{1}{2} \int_E \left(\sum_{j=1}^{n} (1 - x_j) t_j\right) \left(1 - \sum_{i=1}^{n} x_i t_i\right)^{-1/2} c(t_1 \cdots t_n)\, d\mathbf{t} \\ &= -\frac{1}{2} \int_E \left(1 - \sum_{i=1}^{n} x_i t_i\right)^{1/2} c(t_1 \cdots t_n)^{-1/2}\, d\mathbf{t} \\ &= -\frac{1}{2} F, \end{aligned} \tag{2.11}$$

which concludes the proof of Theorem 2.1. □

We now show how to convert the multivariate elliptic integral into a univariate integral. The function B is the beta function, where $B(a, b) = (\Gamma(a)\Gamma(b))/(\Gamma(a + b))$.

THEOREM 2.2. *For* $0 \le x_i < 1$ $(1 \le i \le n)$,

$$F(x_1, \ldots, x_n) = \frac{1}{nB\left(\frac{1}{2}, \frac{n+1}{2}\right)} \int_0^1 u^{-1/2} (1 - u)^{(n-1)/2} \phi(u)\, du,$$

where

$$\phi(u) = \left(\sum_{i=1}^{n} \frac{1 - x_i}{1 - u x_i}\right) \left(\prod_{i=1}^{n} (1 - u x_i)\right)^{-1/2}.$$

PROOF. Use the multinomial expansion [Srivastava and Karlsson 1985, p. 329] to write

$$\left(1 - \sum_{i=1}^{n} x_i t_i\right)^{1/2} = \sum_{m_1,\dots,m_n=0}^{\infty} \left(\frac{1}{2}\right)_{|\mathbf{m}|} \frac{(x_1 t_1)^{m_1}}{m_1!} \cdots \frac{(x_n t_n)^{m_n}}{m_n!} \tag{2.12}$$

for $|\sum_{i=1}^{n} x_i t_i| < 1$, and where $\mathbf{m} = (m_1, \dots, m_n) \in \mathbb{Z}_+^n$ and $|\mathbf{m}| = m_1 + \cdots + m_n$. Using (2.12) in (2.10),

$$\begin{aligned} \frac{\partial F}{\partial x_j} &= -\frac{1}{2} \sum_{|\mathbf{m}|=0}^{\infty} \left(\frac{1}{2}\right)_{|\mathbf{m}|} \frac{x_1^{m_1}}{m_1!} \cdots \frac{x_n^{m_n}}{m_n!} \\ &\quad \cdot \int_E t_1^{m_1-1/2} \cdots t_j^{m_j+1/2} \cdots t_n^{m_n-1/2} c\, d\mathbf{t} \\ &= -\frac{1}{2} \frac{\Gamma\left(\frac{n}{2}\right)}{\left(\Gamma\left(\frac{1}{2}\right)\right)^n} \sum_{|\mathbf{m}|=0}^{\infty} \left(\frac{1}{2}\right)_{|\mathbf{m}|} \frac{x_1^{m_1}}{m_1!} \cdots \frac{x_n^{m_n}}{m_n!} \\ &\quad \cdot \frac{\Gamma\left(m_1 + \frac{1}{2}\right) \cdots \Gamma\left(m_j + \frac{3}{2}\right) \cdots \Gamma\left(m_n + \frac{1}{2}\right)}{\Gamma\left(|\mathbf{m}| + \frac{n+2}{2}\right)}. \end{aligned} \tag{2.13}$$

With $\Gamma(z + n) = (z)_n \Gamma(z)$, we reduce further to

$$\begin{aligned} &-\frac{1}{2} \frac{\Gamma\left(\frac{n}{2}\right)}{\left(\Gamma\left(\frac{1}{2}\right)\right)^n} \frac{\left(\Gamma\left(\frac{1}{2}\right)\right)^{n-1} \Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{n+2}{2}\right)} \sum_{|\mathbf{m}|=0}^{\infty} \left(\frac{1}{2}\right)_{|\mathbf{m}|} \\ &\quad \cdot \frac{\left(\frac{1}{2}\right)_{m_1} \cdots \left(\frac{3}{2}\right)_{m_j} \cdots \left(\frac{1}{2}\right)_{m_n}}{\left(\frac{n+2}{2}\right)_{|\mathbf{m}|}} \frac{x_1^{m_1}}{m_1!} \cdots \frac{x_n^{m_n}}{m_n!} \\ &= -\frac{1}{2n} \sum_{|\mathbf{m}|=0}^{\infty} \frac{\left(\frac{1}{2}\right)_{|\mathbf{m}|} \left(\frac{1}{2}\right)_{m_1} \cdots \left(\frac{3}{2}\right)_{m_j} \cdots \left(\frac{1}{2}\right)_{m_n}}{\left(\frac{n+2}{2}\right)_{|\mathbf{m}|}} \frac{x_1^{m_1}}{m_1!} \cdots \frac{x_n^{m_n}}{m_n!}. \end{aligned} \tag{2.14}$$

The series expansion of the Lauricella F_D function is

$$F_D(a, b_1, \ldots, b_n; c; x_1, \ldots, x_n) = \sum_{|\mathbf{m}|=0}^{\infty} \frac{(a)_{|\mathbf{m}|}(b_1)_{m_1} \cdots (b_n)_{m_n}}{(c)_{|\mathbf{m}|}} \frac{x_1^{m_1}}{m_1!} \cdots \frac{x_n^{m_n}}{m_n!}. \tag{2.15}$$

(See Exton [1976, p. 41] where the typographical error is corrected by (2.15).) This series has an integral representation with $c > a > 0$ as

$$\frac{1}{B(a, c-a)} \int_0^1 u^{a-1}(1-u)^{c-a-1} \prod_{i=1}^{n} (1 - ux_i)^{-b_i} \, du. \tag{2.16}$$

(See Exton [1976, p. 49], where the typographical error is corrected by (2.16).) For $n = 2$, the series (2.15) is the classical Appell series $F_1[a, b_1, b_2; c; x_1, x_2]$, which has a single Eulerian integral representation (e.g., Srivastava and Karlsson [1985, pp. 22 and 276]).

Apply (2.16) to (2.14), yielding

$$\frac{\partial F}{\partial x_j} = -\frac{1}{2nB\left(\frac{1}{2}, \frac{n+1}{2}\right)} \int_0^1 u^{-1/2}(1-u)^{(n-2)/2} \cdot (1 - ux_j)^{-1} \prod_{i=1}^{n} (1 - ux_i)^{-1/2} \, du. \tag{2.17}$$

Finally, use (2.17) in Theorem 2.1. This completes the proof of Theorem 2.2. □

The function $F(x_1, \ldots, x_n)$ of Theorem 2.2 is the Carlson function $R_{1/2}(1/2, \ldots, 1/2; y_1, \ldots, y_n)$. This function can be written as a combination of functions of type $R_{-1/2}$ [Carlson 1977, p. 99],

$$R_{1/2}(1/2, \ldots, 1/2; y_1, \ldots, y_n) = \frac{1}{n} \sum_{i=1}^{n} y_i R_{-1/2}(1/2, \ldots, 3/2, \ldots, 1/2; y_1, \ldots, y_n), \tag{2.18}$$

where the 3/2 term appears in the ith position. Since functions of type $R_{-1/2}$ can be written in terms of a single univariate integral [Carlson 1977, p. 153], the same is true for the function $R_{1/2}$. This had been noted by Carlson [1977, p. 260], where an explicit representation for $R_{1/2}$ with $n = 3$ is given. (We are grateful to the referee for these references.)

3. REMOVING SINGULARITIES

In the previous section, we have shown that the multivariate elliptic integral (1.3) can be represented as a univariate integral with domain of integration [0, 1] and integrand $\phi(u)$ of Theorem 2.2. With Σ as a positive definite matrix, where $\gamma_1 \geq \cdots \geq \gamma_n > 0$, the values $x_i = 1 - \gamma_i/\gamma_1$ satisfy $0 \leq x_i < 1$ $(1 \leq i \leq n)$. Thus, $\phi(u)$ has singularities at $u = 1/x_i > 1$ $(1 \leq i \leq n)$. The distance between the domain of integration and the nearest singularity of $\phi(u)$ is

$$\frac{1}{x_n} - 1 = \frac{\gamma_n}{\gamma_1 - \gamma_n}. \tag{3.1}$$

An efficient implementation of the algorithm for computing the multivariate elliptic integral has been given by Dunkl and Ramirez [1994]. We have found that the Romberg algorithm of Dunkl [1962] (see, e.g., Davis and Rabinowitz [1984, p. 493] is a convenient method for numerically evaluating the multivariate elliptic integral.

Floating-point arithmetic makes it more desirable to cope with singularities near zero, and thus, we make the substitution $v = 1 - u$ to transform the integral of Theorem 2.2 to

$$F(x_1, \ldots, x_n) = \frac{1}{nB\left(\frac{1}{2}, \frac{n+1}{2}\right)} \int_0^1 (1-v)^{-1/2} \cdot \left(\prod_{j=2}^{n} \frac{v}{y_j + x_j v} \right)^{1/2} \left(1 + \sum_{j=2}^{n} \frac{y_j}{y_j + x_j v} \right) dv, \tag{3.2}$$

where $1 - x_i u = (x_i + y_i) - x_i u = y_i + x_i(1-u)$, $x_1 = 0$, and $y_1 = 1$; this substitution has removed a potential source of numerical inaccuracy due to subtraction.

To remove the singularity $(1-v)^{-1/2}$ at $v = 1$, we implement a modification of the Kahan [1980] substitution to provide for faster convergence (see also Davis and Rabinowitz [1984, p. 441]). Kahan suggested the substitution $v = g(x) = 3x^2 - 2x^3$ with $dv = 6x(1-x)\,dx$ and $(1-v)^{-1/2} = (1-x)^{-1}(1+2x)^{-1/2}$. The transformation $g(x) = v$ satisfies $g(0) = 0$, $g(1) = 1$, and $g'(1) = 0$. Note that $(1-v)^{-1/2} dv = 6x(1+2x)^{-1/2} dx$.

Our computer experiments have shown that efficiency can be further improved with the substitution $v = g(x) = 5x^4 - 4x^5$ with $dv = 20x^3(1-x)\,dx$ and $(1-v)^{-1/2} = (1-x)^{-1}(1 + 2x + 3x^2 + 4x^3)^{-1/2}$ so that $(1-v)^{-1/2} dv = 20x^3(1 + 2x + 3x^2 + 4x^3)^{-1/2} dx$. The integral of Theorem 2.2 now has the form

$$F(x_1, \ldots, x_n) = \frac{20}{nB\left(\frac{1}{2}, \frac{n+1}{2}\right)} \int_0^1 x^3 (1 + 2x + 3x^2 + 4x^3)^{-1/2} \psi(x)\, dx, \tag{3.3}$$

where

$$\psi(x) = \left(\prod_{j=2}^{n} \frac{5x^4 - 4x^5}{y_j + x_j(5x^4 - 4x^5)} \right)^{1/2} \left(1 + \sum_{j=2}^{n} \frac{y_j}{y_j + x_j(5x^4 - 4x^5)} \right). \tag{3.4}$$

Note that the value of the integrand in (3.3) at $x = 1$ is $10^{-1/2}(1 + \sum_{j=2}^{n} y_j)$.

4. HYPERELLIPTIC INEQUALITIES

In Section 3 we have presented an efficient algorithm for numerically computing the multivariate elliptic integral $|||\,\mathbf{\Sigma}\,|||$. We now compute hyperelliptic inequalities for $|||\,\mathbf{\Sigma}\,|||$.

THEOREM 4.1. *For $\mathbf{\Sigma}$, a positive definite matrix with eigenvalues $\gamma_1 \geq \cdots \geq \gamma_n > 0$,*

$$\frac{1}{n}\sum_{i=1}^{n}(\gamma_i)^{1/2} \leq |||\,\mathbf{\Sigma}\,||| \leq \left(\frac{1}{n}\mathrm{tr}(\mathbf{\Sigma})\right)^{1/2}. \tag{4.1}$$

PROOF. The upper bound follows from the convexity of the function $x \to x^2$, together with the previously quoted result that $\mathscr{E}(\mathbf{U}'\,\mathbf{\Sigma}\,\mathbf{U}) = \mathrm{tr}(\mathbf{\Sigma})/n$.

For the lower bound, apply Cauchy's inequality to a vector $\mathbf{u}$ in the unit sphere Ω,

$$\begin{aligned}\sum_{i=1}^{n}(\gamma_i^{1/2}u_i)u_i &\leq \left(\sum_{i=1}^{n}\gamma_i u_i^2\right)^{1/2}\left(\sum_{i=1}^{n}u_i^2\right)^{1/2}\\ &= \left(\sum_{i=1}^{n}\gamma_i u_i^2\right)^{1/2}.\end{aligned} \tag{4.2}$$

Integrate, with respect to normalized surface measure $d\boldsymbol{\omega}$, recalling for each $1 \leq i \leq n$ that

$$\int_{\Omega} u_i^2\, d\boldsymbol{\omega} = \frac{1}{n}\int_{\Omega}(u_1^2 + \cdots + u_n^2)\, d\boldsymbol{\omega} = \frac{1}{n}. \tag{4.3}$$

This completes the proof of Theorem 4.1. □

These bounds can be achieved, and our computer experiments have shown that the upper bound is particularly tight when γ_1/γ_n is relatively close to unity.

Since the multivariate elliptic integral $|||\,\mathbf{\Sigma}\,|||$ is the multiple of the Carlson function $R_{1/2}$, the bounds for $R_{1/2}$ [Carlson 1966] can be transformed into (4.1). (We thank the referee for this reference.)

5. SURFACE MEASURE OF ELLIPSOIDS

We next address the ancient problem of efficiently computing the surface measure of an ellipsoid. For our notation, let $0 < \delta_1 \leq \cdots \leq \delta_n$ be the semiaxes for the ellipsoid in $\mathbb{R}^n$, given by

$$\left(\frac{x_1}{\delta_1}\right)^2 + \cdots + \left(\frac{x_n}{\delta_n}\right)^2 = 1, \tag{5.1}$$

and let the surface measure of this ellipsoid be denoted by $\mathscr{S}(\delta_1, \ldots, \delta_n)$.

The surface measure σ_n of the unit sphere in $\mathbb{R}^n$ is

$$\sigma_n = \mathscr{S}(1, \dots, 1) = \frac{2\pi^{n/2}}{\Gamma\left(\frac{n}{2}\right)}. \tag{5.2}$$

Given the values $\delta_1, \dots, \delta_n$ for the semiaxes, let $\mathbf{\Gamma}$ be a positive definite matrix with eigenvalues $\gamma_i = \delta_i^{-2}$; for example, let $\mathbf{\Gamma} = \operatorname{diag}(\gamma_1, \dots, \gamma_n) = \operatorname{diag}(\delta_1^{-2}, \dots, \delta_n^{-2})$. The relationship between the surface measure and the multivariate elliptic integral is demonstrated in our next theorem:

THEOREM 5.1. *For* $0 < \delta_1 \le \cdots \le \delta_n$,

$$\mathscr{S}(\delta_1, \dots, \delta_n) = \sigma_n \left(\prod_{i=1}^{n} \delta_i \right) |||\mathbf{\Gamma}|||$$
$$= \sigma_n \frac{|||\mathbf{\Gamma}|||}{\det(\mathbf{\Gamma}^{1/2})}.$$

PROOF. The surface of the ellipsoid is defined by

$$G(\mathbf{x}) = \sum_{i=1}^{n} (x_i/\delta_i)^2 - 1 = 0.$$

The normal vector $\mathbf{n(x)}$ to the surface $G(\mathbf{x}) = 0$ is given by

$$\mathbf{n(x)} = \nabla G(\mathbf{x}) = 2\left(\frac{x_1}{\delta_1^2}, \dots, \frac{x_n}{\delta_n^2} \right)'. \tag{5.3}$$

The angle $\Theta \in [0, \pi]$ between $\mathbf{x}$ and $\nabla G(\mathbf{x})$ satisfies

$$\cos(\Theta) = \frac{\nabla G(\mathbf{x}) \cdot \mathbf{x}}{|\nabla G(\mathbf{x})|\,|\mathbf{x}|} = \left(\sum_{i=1}^{n} \frac{x_i^2}{\delta_i^4} \right)^{-1/2} \Big/ |\mathbf{x}|. \tag{5.4}$$

Partition the surface of the ellipsoid into a large number N of curvilinear simplexes with $(n-1)$-surface measure ΔS_p $(1 \le p \le N)$. Choose a representative point $\mathbf{x}^{(p)}$ in each subregion $(1 \le p \le N)$. The subregions ΔS_p define a partition of the volume of the ellipsoid into n-dimensional cones with volumes ΔV_p, each with height h_p. We relate the surface measure of the ellipsoid to its volume.

The volume of the cone ΔV_p is approximately given by

$$\Delta V_p = \frac{1}{n} h_p \Delta S_p, \tag{5.5}$$

where the height h_p is related to the directed cosine of the angle $\Theta^{(p)}$ between the normal vector $\mathbf{n}(\mathbf{x}^{(p)})$ and the representative point $\mathbf{x}^{(p)}$ by (using (5.4))

$$h_p = |\mathbf{x}^{(p)}|\cos(\Theta^{(p)})$$
$$= \left(\sum_{i=1}^{n} \frac{(x_i^{(p)})^2}{\delta_i^4} \right)^{-1/2}. \tag{5.6}$$

Define $\mathbf{u}^{(p)}$ by $u_i^{(p)} = x_i^{(p)}/\delta_i$ $(1 \le i \le n)$, so $\mathbf{u}^{(p)}$ has length $|\mathbf{u}^{(p)}| = 1$, and

$$\begin{aligned} \Delta S_p &= n\left(\sum_{i=1}^{n} \frac{(u_i^{(p)})^2}{\delta_i^2}\right)^{1/2} \Delta V_p \\ &= n\left(\prod_{i=1}^{n} \delta_i\right)\left(\sum_{i=1}^{n} \frac{(u_i^{(p)})^2}{\delta_i^2}\right)^{1/2} \Delta U_p, \end{aligned} \tag{5.7}$$

where $\Delta V_p = (\prod_{i=1}^{n} \delta_i)\Delta U_p$, thus transforming the volume of the cones ΔV_p, which have partitioned the volume of the ellipsoid into the volume of the cones ΔU_p, which form a partition of the volume of the unit sphere.

Now let ΔU_p correspond to a partition of the surface measure of the unit sphere, say, $\Delta\omega_p$. The analog to (5.5) is

$$\Delta U_p = \frac{1}{n}\Delta\omega_p. \tag{5.8}$$

Passing to the limit as the terms in (5.7) are summed using (5.8) yields

$$\mathscr{S}(\delta_1, \ldots, \delta_n) = \sigma_n\left(\prod_{i=1}^{n} \delta_i\right)\int_{\Omega}\left(\frac{u_1^2}{\delta_1^2} + \cdots + \frac{u_n^2}{\delta_n^2}\right)^{1/2} d\boldsymbol{\omega}. \tag{5.9}$$

This completes the proof of Theorem 5.1. □

The expression for $\mathscr{S}$ as an $(n-1)$-dimensional integral was shown by Lehmer [1950]. (We thank I. J. Good for this reference.) Carlson [1966] observed that the integral representation given by Lehmer was a multiple of $R_{-1/2}(1/2, \ldots, 1/2;\ \delta_1^{-2}, \ldots, \delta_n^{-2})$.

Theorem 5.1 allows a coefficient of sphericity CS to be defined for an ellipsoid with semiaxes $\delta_1, \ldots, \delta_n$ and with surface measure $\mathscr{S}(\delta_1, \ldots, \delta_n)$. The sphere with the same volume as the given ellipsoid has radius $r = (\prod_{i=1}^{n} \delta_i)^{1/n}$. The surface measure of the sphere is

$$\sigma_n r^{n-1} = \sigma_n\left(\prod_{i=1}^{n} \delta_i\right)^{(n-1)/n}.$$

As before, set $\boldsymbol{\Gamma} = \mathrm{diag}(\delta_1^{-2}, \ldots, \delta_n^{-2})$.

The ratio of $\mathscr{S}(\delta_1, \ldots, \delta_n)$ to $\sigma_n r^{n-1}$ is a dimensionless quantity that is greater than or equal to one, with a value equal to one when all semiaxes are equal. Thus, with $\boldsymbol{\Delta} = \mathrm{diag}(\delta_1, \ldots, \delta_n)$,

$$\begin{aligned} CS(\boldsymbol{\Delta}) &= \frac{\mathscr{S}(\delta_1, \ldots, \delta_n)}{\sigma_n r^{n-1}} \\ &= \left(\prod_{i=1}^{n} \delta_i\right)^{1/n} |||\boldsymbol{\Gamma}||| \ge 1. \end{aligned} \tag{5.10}$$

Note that (5.10) yields a lower bound for $|||\Gamma|||$ with

$$\left(\prod_{i=1}^{n} \gamma_i^{1/2}\right)^{1/n} = \left(\prod_{i=1}^{n} \delta_i\right)^{-1/n} \leq |||\Gamma|||, \tag{5.11}$$

which is weaker than the lower bound given by Theorem 4.1, since the geometric mean is dominated by the arithmetic mean.

6. IMPLEMENTATION OF THE ALGORITHM

Dunkl and Ramirez [1994] presented an efficient implementation of the procedures contained in this paper in Fortran. Given eigenvalues $\gamma_1 \geq \cdots \geq \gamma_n > 0$ of Σ, their subroutine ELLPTI computes the value of $|||\Sigma|||$, the bounds for $|||\Sigma|||$, the estimated error for $|||\Sigma|||$ from the Romberg method, and the surface measure of the corresponding ellipsoid, with its error estimate.

6.1 Time and Accuracy

Table I shows the number of function evaluations needed to compute the surface measure of varying ellipsoids with axes the power of 2 $(1, 2, \ldots, 2^{n-1})$, where $n = 5$ and 10, respectively, and with varying error tolerances. The estimated error is also displayed. These calculations were performed using the WATFOR-77 compiler and a DOS-based PC-compatible machine with an 80286 processor and double-precision mode.

6.2 Related Algorithms

The routine ELLPTI incorporates the Romberg integration algorithm of Dunkl [1962] (see, e.g., Davis and Rabinowitz [1984, p. 493]).

For values $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_n > 0$, a measure of the distance between the domain of integration and the nearest singularity is given by $\gamma_n/(\gamma_1 - \gamma_n)$ (see (3.1)). To lessen the effect of singularities at the end points of the domain of integration, we modified the basic cubic spline substitution suggested by Kahan [1980] (see also Davis and Rabinowitz [1984, p. 441]) to a fifth-order substitution, since Romberg extrapolation works better on smoother functions.

6.3 Test Results

6.3.1 One can use the IMSL subroutine RNSPH and the Monte Carlo method to estimate multivariate elliptic integrals. With $\gamma_1 = \gamma_2 = 4/3$ and $\gamma_3 = 2/3$, $|||\sum||| = 1.049$ with 10,000 replications. The routine ELLPTI will provide ten-digit accuracy with only 128 function evaluations.

6.3.2 The surface area of an ellipsoid in $\mathbb{R}^3$ can be computed by Legendre's formula with Jacobi functions; see, for example, Lawden [1984, p. 102]. With semiaxes 2, 2, and 1, Lawden's formula (4.2.19) shows that the surface area is 34.688. With semiaxes 2, 1, and 1, formula (4.2.20) shows that the surface area is 21.478. With semiaxes 1, 0.5186497, and 0.3420201, formula (4.2.16) has $\nu = 70$ degrees, $k = 0.8$, $D(\nu, k) = 1.05975$, $F(\nu, k) = 1.43230$, and a surface area of 4.56124.

Table I. Comparison of Number of Function Evaluations Needed to Compute the Surface Measure of Ellipsoids

n	Relative error	Evaluations	Surface measure	Estimated error
5	1 E-4	32	12,926.7356	0.11 E0
	1 E-8	128	12,926.7351	0.11 E-4
	Exact		12,926.73509934	
10	1 E-4	32	29,713.5552 E10	0.26 E10
	1 E-8	128	29,713.5540 E10	0.25 E6
	Exact		29,713.55397781 E10	

6.3.3 Cesàro [1897, p. 338] computed the surface area of the ellipsoid in $\mathbb{R}^3$, with semiaxes a, b, and c having the ratio $a^2 : b^2 : c^2 = 3:2:1$, to be $2.52620923\pi a^2$. With $\delta_1 = 6^{-1/2}$, $\delta_2 = 3^{-1/2}$, and $\delta_3 = 2^{-1/2}$ (equivalently, with $\gamma_1 = 6$, $\gamma_2 = 3$, and $\gamma_3 = 2$), the surface area is 3.96816018. Our algorithm yields ten significant digits with only 128 evaluations of the function $\psi(x)$ of (3.4).

We know of no other algorithm for computing the surface measure of ellipsoids when four or more of the semiaxes are different.

7. A GEOMETRIC APPROACH TO OPTIMAL REGRESSION DESIGNS

The problem of optimal regression design is to choose "as well as possible" the design $\boldsymbol{\xi} = \{(x_1, y_1), \ldots, (x_N, y_N)\}$, in order to make observations $w_1, \ldots, w_N$ on the variable w when

$$w_i = \beta_0 + \beta_1 x_i + \beta_2 y_i + \beta_{12} x_i y_i + \beta_{11} x_i^2 + \beta_{22} y_i^2 + e_i, \tag{7.1}$$

where e_i are the unknown independent normal errors with $\sigma^2 > 0$ $(1 \le i \le N)$; for an example, see Silvey and Titterington [1973]. (For convenience, we have restricted (7.1) to a second-order response surface.) Associated with a design $\boldsymbol{\xi}$ is the experimental design matrix $\mathbf{X}(\boldsymbol{\xi})$, whose rows are $(1, x_i, y_i, x_i y_i, x_i^2, y_i^2)$, and its moment matrix $\mathbf{M}(\boldsymbol{\xi}) = \mathbf{X}'(\boldsymbol{\xi})\mathbf{X}(\boldsymbol{\xi})$. A good design has $\mathbf{M}(\boldsymbol{\xi})$ "as large as possible"; or equivalently, it has $\mathbf{M}^{-1}(\boldsymbol{\xi})$ "as small as possible." (We are assuming that $\mathbf{M}(\boldsymbol{\xi})$ has full rank.)

An often-used criterion for the measure of $\mathbf{M}(\boldsymbol{\xi})$ is its determinant, and a design $\boldsymbol{\xi}_0$ that maximizes $\det(\mathbf{M}(\boldsymbol{\xi}))$ (or, equivalently, that minimizes $\det(\mathbf{M}^{-1}(\boldsymbol{\xi}))$) over a class of permitted designs is said to be D-optimal. The design $\boldsymbol{\xi}$ can be associated with the six-dimensional ellipsoid $\epsilon(\boldsymbol{\xi})$, given by

$$\mathbf{x}'\mathbf{M}^{-1}(\boldsymbol{\xi})\mathbf{x} = 1. \tag{7.2}$$

The volume of this ellipsoid is proportional to $(\det \mathbf{M}(\boldsymbol{\xi}))^{1/2}$, and the ellipsoid has semiaxes equal to the square roots of the eigenvalues of $\mathbf{M}(\boldsymbol{\xi})$. Thus, the D-optimal-design problem can be regarded as that of finding the ellipsoid $\epsilon(\boldsymbol{\xi})$ of maximal volume.

One unfortunate problem with the D-criterion is that the volume of $\epsilon(\xi)$ can be large when only one of its semiaxes is large, or, equivalently, when only one of the eigenvalues of $\mathbf{M}^{-1}(\xi)$ is small. To overcome this inherent problem, we propose the expected radius $|||\mathbf{M}^{-1}(\xi)|||$ as an all-purpose geometric measure of the size of the ellipsoid $\epsilon(\xi)$. For a random unit vector $\mathbf{U}$ in $\mathbb{R}^n$, the value $(\mathbf{U}'M^{-1}(\xi)\mathbf{U})^{1/2}$ is proportional to the standard error of the linear parametric function $\mathbf{U}'\boldsymbol{\beta}$. Thus, $|||\mathbf{M}^{-1}(\xi)|||$ is a statistical measure of the mean standard error of a random linear estimator, and the optimal design ξ_0 will maximize $|||\mathbf{M}^{-1}(\xi)|||$ over the class of permitted designs.

Wardrop and Myers [1990] used D-optimality and D_s-optimality to find optimal designs for a class of response surface designs involving second-order terms. (The D_s-optimality criterion is based on applying the D-optimality criterion to the second-order terms in the partitioned matrix $(\mathbf{X}'\mathbf{X})^{-1}$.) One of their classes of designs is the equiradial design consisting of n_1 equally spaced points on the unit circle and n_0 values at the origin. Wardrop and Myers [1990] showed that the optimal D-design has the ratio 5 : 1 of perimeter points to center points, while the optimal D_s-design has the ratio 3 : 1. We apply the expected radius criterion to find the design that is optimal with respect to $|||\mathbf{M}^{-1}(\xi)|||$, our omnibus geometric criterion.

Let $\lambda = n_1/N$ be the proportion of perimeter points. The moment matrix $\mathbf{M}(\lambda)$ satisfies

$$\frac{1}{N}\mathbf{M}(\lambda) = \frac{1}{8}\begin{bmatrix} 8 & 0 & 0 & 4\lambda & 4\lambda & 0 \\ 0 & 4\lambda & 0 & 0 & 0 & 0 \\ 0 & 0 & 4\lambda & 0 & 0 & 0 \\ 4\lambda & 0 & 0 & 3\lambda & \lambda & 0 \\ 4\lambda & 0 & 0 & \lambda & 3\lambda & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda \end{bmatrix} \tag{7.3}$$

(see, e.g., Waldrop and Myers [1990]).

The eigenvalues of (7.3) can be shown to be $\lambda/2$, $\lambda/2$, $\lambda/4$, $\lambda/8$, and $((\lambda/2 + 1) \pm (1 - \lambda + 9/4\lambda^2)^{1/2})/2$. The eigenvalues of $N\mathbf{M}^{-1}(\lambda)$ are proportional to the inverse of these values. Using ELLPTI, a numerical search for the minimum of $|||\mathbf{M}^{-1}(\lambda)|||$ shows that the optimal value of λ is $\lambda = 0.71959$, with a minimum value of $|||\mathbf{M}^{-1}(\lambda)||| = 2.3952/N$. Thus, the optimal equiradial design has 72 percent of the values on the perimeter.

REFERENCES

CARLSON, B. C. 1977. *Special Functions of Applied Mathematics*. Academic Press, New York.

CARLSON, B. C. 1972. Intégrandes à deux formes quadratiques. *C. R. Acad. Soc. Paris 274*, 15, 1458–1461.

CARLSON, B. C. 1966. Some inequalities for hypergeometric functions. *Proc. Amer. Math. Soc. 17*, 1, 32–39.

CARLSON, B. C. 1963. Lauricella's hypergeometric function F_D. *J. Math. Anal. Appl. 7*, 3, 452–470.

CESÀRO, E. 1897. *Elementi di Calcolo Infinitesimale*. Lorenzo Alvano, Naples, Italy.

DAVIS, P. J. AND RABINOWITZ, P. 1984. *Methods of Numerical Integration*. 2nd ed. Academic Press, Orlando, Fla.

DUNKL, C. F. 1962. Romberg quadrature to prescribed accuracy. SHARE File No. 7090-1481, TYQUAD.

DUNKL, C. F. AND RAMIREZ, D. E. 1994. Algorithm 736 Hyperelliptic integrals and the surface measures of ellipsoids. *ACM Trans. Math. Softw. 20*, 4. This issue.

EXTON, H. B. 1976. *Multiple Hypergeometric Functions and Applications*. Halsted Press, New York.

KAHAN, W. M. 1980. Handheld calculator evaluates integrals. *Hewlett-Packard J. 31,* 8, 23–32.

LAWDEN, D. F. 1984. *Elliptic Functions and Applications*. Springer-Verlag, New York.

LEHMER, D. H. 1950. Approximations to the area of n-dimensional ellipsoid. *Can. J. Math. 2,* 3, 267–282

SILVEY, S. D. AND TITTERINGTON, D. H. 1973. A geometric approach to optimal design theory. *Biometrika 60*, 1, 21–32.

SRIVASTAVA, H. M. AND KARLSSON, P. W. 1985. *Multiple Gaussian Hypergeometric Series*. Halsted Press, New York.

WARDROP, D. AND MYERS, R. 1990. Some response surface designs for finding optimal conditions. *J. Stat. Plann. Inference 25,* 1, 7–28.

Received October 1991; revised October 1992; accepted November 1992