Optimal designs for 3D shape analysis with spherical harmonic descriptors

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Abstract

We determine optimal designs for some regression models which are frequently used for describing 3D shapes. These models are based on a Fourier expansion of a function defined on the unit sphere in terms of spherical harmonic basis functions. In particular it is demonstrated that the uniform distribution on the sphere is optimal with respect to all Φ_p-criteria proposed by Kiefer (1974) and also optimal with respect to a criterion which maximizes a p-mean of the r smallest eigenvalues of the variance-covariance matrix. This criterion is related to principal component analysis, which is the common tool for analyzing this type of image data. Moreover, discrete designs on the sphere are derived, which yield the same information matrix in the spherical harmonic regression model as the uniform distribution and are therefore directly implementable in practice. It is demonstrated that the new designs are substantially more efficient than the commonly used designs in 3D-shape analysis.

Keywords and Phrases: Shape analysis, spherical harmonic descriptors, optimal designs, quadrature formulas, principal component analysis, 3D-image data

AMS Subject Classification: 62K05, 65D32

1 Introduction

Over the last decade, tools for acquiring and visualizing 3D models have become integral components of data processing in many fields including medicine, chemistry, architecture, agriculture and biology. Volumetric shape analysis permits an evalutation of the actual structures that are implicitly represented in 3D image data. For the analysis, description and comparison of shapes of various structures shape descriptors, which are able to handle very different shapes and to represent their global and local features are of increasing interest [see e.g. Brechbühler, Gerig and Kübler (1995), Novotni and Klein (2003), Székely, Kelemen, Brechbühler and Gerig (1996), Ding Nesumi, Takano and Ukai (2000), Funkhouser, Min, Kahzdan, Chen, Halderman and Dobkin (2003), Kazhdan, Funkhouser and Rusinkiewicz (2003) among many others]. Spherical harmonic shape descriptors usually describe the surface in terms of a relatively small number of coefficients of a spherical harmonic expansion of the radius as a function on the unit sphere [see e.g. Ding et al. (2000) or Brechbühler et al. (1995)], i.e.

$$r(\theta,\phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} c_\ell^m Y_\ell^m(\theta,\phi) \tag{1.1}$$

where $\theta \in [0,\pi], \phi \in (-\pi,\pi]$, the quantities

$$c_\ell^m = \frac{1}{4\pi} \int_0^\pi \int_{-\pi}^{\pi} r(\theta,\phi) Y_\ell^m(\theta,\phi) d\phi \sin\theta d\theta \tag{1.2}$$

are the usual "Fourier" coefficients and

$$\{Y_\ell^m(\theta,\phi) \mid m \in \{-\ell,-\ell+1,\ldots,\ell\}; \ell \in \mathbb{N}_0\}$$

is a complete orthonormal basis on the unit sphere. Let $r_i = r(\theta_i,\phi_i)$ denote the observed radius of the 3D shape at polar angle θ_i and azimuthal angle ϕ_i [in other words the corresponding point of the shape has spherical coordinates $(r_i \sin\theta_i \cos\phi_i, r_i \sin\theta_i \sin\phi_i, r_i \cos\theta_i)^T$] and assume that data

$$\{(r_i,\theta_i,\phi_i) \mid i = 1,\ldots,n\}$$

is available for one object. Usually, a truncated expansion of order d is applied as an approximation of (1.1), where the coefficients c_ℓ^m are determined by the least squares critierion

$$\min_{c_\ell^m} \Big\{ \sum_{i=1}^{n} \Big(r_i - \sum_{\ell=0}^{d} \sum_{m=-\ell}^{\ell} c_\ell^m Y_\ell^m(\theta_i,\phi_i) \Big)^2 \Big\} \tag{1.3}$$

and the estimated coefficients in this expansion (appropriately normalized) are then used for describing and analyzing the 3D shapes. For this purpose typical tools from multivariate statistics (cluster, discriminant or principal component analysis) are applied [see Ding et al. (2000), Kazhdan et al. (2003), Kelemen et al. (1999) among many others].

A common design of experiment for this situation is a uniform distribution on the rectangle $[0,\pi] \times (-\pi,\pi]$ realized by a grid or a uniform design taking observations on several circles with equal distance on the z-axis [see e.g. Ding et al. (2000)]. In the literature on shape analysis these designs are mainly motivated by its easy implementation. If the grid is fine enough or a sufficiently large number of circles on the unit sphere is used the matrix B^TB of the least squares estimate $\hat{c} = (B^TB)^{-1}B^Tr$ approximates a diagonal matrix, which simplifies the numerical calculation in the statistical analysis. Here $r = (r_1, \dots, r_n)$ is the vector of measured radii and $B = (Y_\ell^m(\theta_i, \phi_i))_i^{\ell,m}$ is the design matrix corresponding to the least squares problem (1.3) [see Brechbühler et al. (1995)].

In the present paper we consider the problem of finding optimal designs for 3D shape analysis based on spherical harmonic descriptors. In Section 2 we present some more details on spherical harmonic descriptors and basic results on the theory of optimal experimental design. In the same section we also demonstrate that the uniform distribution on the unit sphere is optimal with respect to any of Kiefer's (1974) Φ_p-criteria if the interest of the experimenter is in the estimation of the complete vector

$$c = (c_0^0, c_1^{-1}, c_1^0, c_1^1, \dots, c_d^{-d})^T \in \mathbb{R}^{(d+1)^2}$$

or a certain subset of the parameters. It is also shown that for any $t \leq (d+1)^2$ this design maximizes the *pth* mean of the r largest eigenvalues of the variance-covariance matrix $(B^TB)^{-1}$. Therefore the uniform distribution on the sphere is particulary efficient for principal component analysis, which is the main tool for summarizing the information contained in the spherical harmonic coefficients obtained by (1.3) [see e.g. Ding et al. (2000) or Kazhdan et al. (2003)]. Because this design is continuous with density $\frac{1}{4\pi} \sin\theta d\theta d\phi$, it is not directly implementable in practice. Therefore for a finite sample size we determine in Section 3 discrete designs, which give the same information matrix as the uniform distribution on the sphere. For this reason these designs are also optimal with respect to Kiefer's (1974) Φ_p-criteria and optimal with respect to a criterion, which maximizes a p-mean of the r smallest eigenvalues of the information matrix and is related to principal component analysis. In Section 4 we present several examples, which illustrate the advantages of our approach, and determine optimal uniform designs, which take in each direction only one observation and are for this reason particular attractive to practitioners. We also reanalyze a design used by Ding et al. (2000) for principal component analysis and demonstrate that the designs derived in the present paper are substantially more efficient. Finally, some more technical details are given in the Appendix.

2 Spherical harmonic descriptors and optimal design

An orthogonal system $\{Y_\ell^m(\theta, \phi) \mid \ell \in \mathbb{N}_0; m \in \{-\ell, -\ell+1, \dots, \ell\}\}$ of functions on the unit sphere satisfies

$$\frac{1}{4\pi} \int_0^\pi \int_{-\pi}^\pi Y_\ell^m(\theta, \phi) Y_{\ell'}^{m'}(\theta, \phi) d\phi \sin\theta d\theta = 0 \qquad (2.1)$$

whenever $(m, \ell) \neq (m', \ell')$. The common system used in shape analysis [see Brechbühler et al. (1995) or Ding et al. (2000)] is obtained by the normalization

$$\frac{1}{4\pi} \int_0^\pi \int_{-\pi}^\pi (Y_\ell^m(\theta, \phi))^2 d\phi \sin\theta d\theta = 1$$

and given by the spherical harmonic functions

$$
\begin{aligned}
Y_n^0(\theta,\phi) &= \sqrt{2n+1}P_n^0(\cos\theta) \quad n\in\mathbb{N}_0, \\
Y_n^m(\theta,\phi) &= \sqrt{2(2n+1)\frac{(n-m)!}{(n+m)!}}P_n^m(\cos\theta)\cos(m\phi) \quad m=0,\dots,n; \quad n\in\mathbb{N}, \\
Y_n^{-m}(\theta,\phi) &= \sqrt{2(2n+1)\frac{(n+m)!}{(n-m)!}}P_n^{-m}(\cos\theta)\sin(m\phi) \quad m=-n,\dots,-1; n\in\mathbb{N},
\end{aligned} \tag{2.2}
$$

where $P_n^m(x)$ is the mth associated Legendre function of degree n satisfying the differential equation

$$
(1-x^2)P''(x)-2xP'(x)+\Big\{n(n+1)-\frac{m^2}{1-x^2}\Big\}P(x)=0. \tag{2.3}
$$

It is well known [see Andrews, Askey and Roy (1999), Chapter 9], that these functions can be represented as

$$
P_n^m(x)=(-1)^m\frac{(2m)!}{2^n m!}(1-x^2)^{\frac{m}{2}}C_{n-m}^{(m+1/2)}(x), \tag{2.4}
$$

where $C_k^{(\alpha)}(x)$ is the kth ultraspherical polynomial orthogonal with respect to the measure $(1-x^2)^{\alpha-1/2}dx$ [see Szegö (1975)]. Note also that $P_n^0(x)$ is the nth Legendre polynomial $P_n(x)$ orthogonal with respect to the Lebesgue-measure on the interval $[-1,1]$. Because orthogonal polynomials can be calculated recursively this representation allows a fast computation of the functions Y_ℓ^m and the first four spherical harmonic functions corresponding to the case $d=1$ are given by

$$
\begin{aligned}
Y_0^0(\theta,\phi) &= 1; \quad Y_1^0(\theta,\phi)=\sqrt{3}\cos\theta. \\
Y_1^{-1}(\theta,\phi) &= \sqrt{3}\sin\theta\sin\phi; \quad Y_1^1(\theta,\phi)=\sqrt{3}\sin\theta\cos\phi.
\end{aligned} \tag{2.5}
$$

Figure 1 and 2 show the spherical harmonic descriptors

$$
(Y_\ell^m(\theta,\phi)\sin\theta\cos\phi, Y_\ell^m(\theta,\phi)\sin\theta\sin\phi, Y_\ell^m(\theta,\phi)\cos\theta)^T \quad , \ m=-\ell,\dots,\ell
$$

for $\ell=0,1,2,3$, when (θ,ϕ) varies in the rectangle $[0,\pi]\times(-\pi,\pi]$.
Consider the regression model corresponding to the least squares problem (1.3)

$$
E[Y\mid\theta,\phi]=c^Tf_d(\theta,\phi); \quad \mathrm{Var}[Y\mid\theta,\phi]=\sigma^2>0, \tag{2.6}
$$

where

$$
f_d(\theta,\phi)=\Big(Y_0^0(\theta,\phi),Y_1^{-1}(\theta,\phi),Y_1^0(\theta,\phi),Y_1^1(\theta,\phi),\dots,Y_d^{-d}(\theta,\phi),\dots,Y_d^d(\theta,\phi)\Big)^T\in\mathbb{R}^{(d+1)^2} \tag{2.7}
$$

is the vector of spherical harmonic functions of order d and

$$
c=(c_0^0,c_1^{-1},c_1^0,c_1^1,\dots,c_d^{-d},\dots,c_d^d)^T\in\mathbb{R}^{(d+1)^2}
$$

the corresponding vector of parameters. Note that there appear $(d+1)^2$ spherical harmonic functions in the model (2.6). An approximate design is a probability measure on the set $[0,\pi]\times(-\pi,\pi]$.

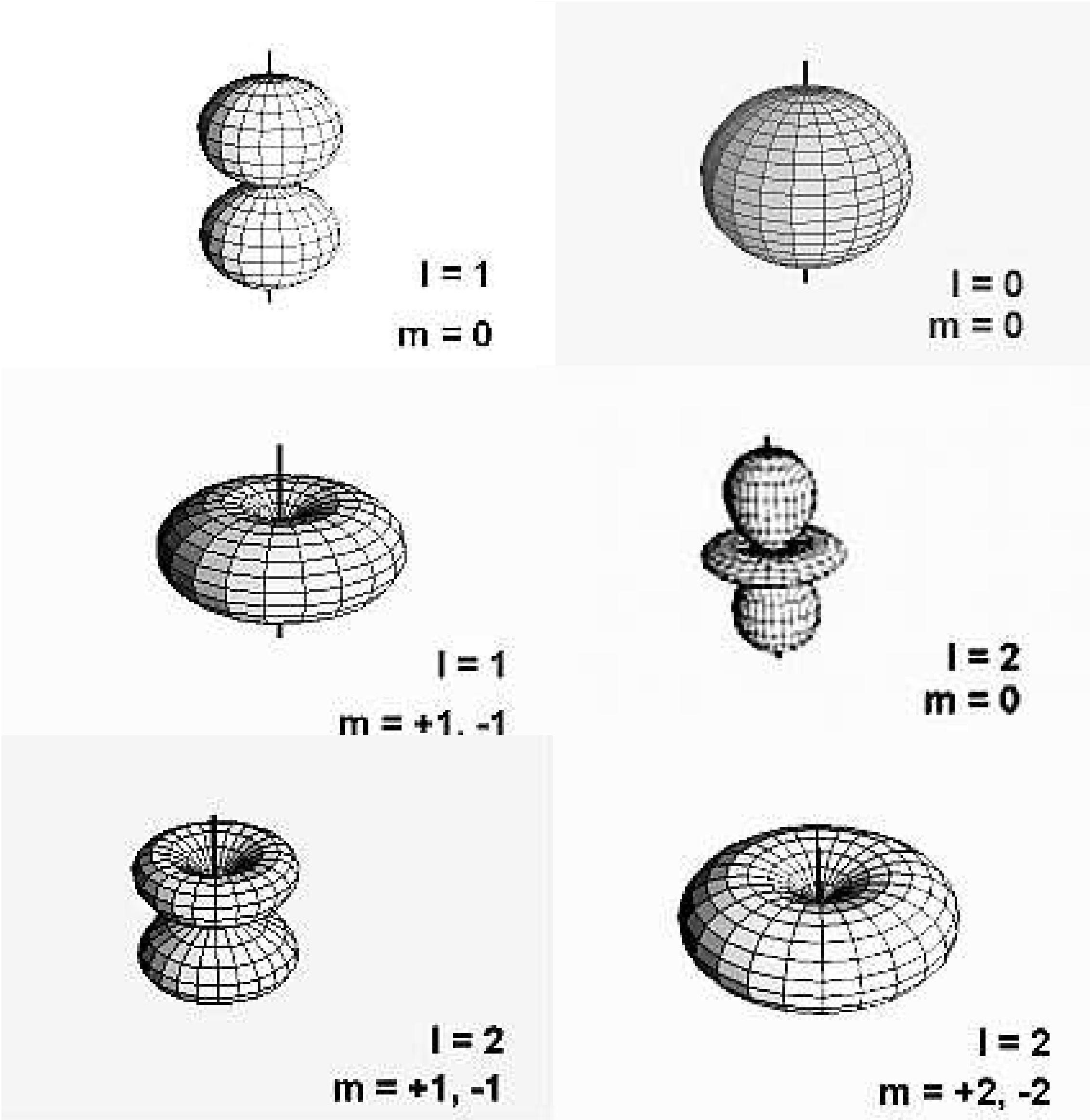

Figure 1: *Spherical harmonic descriptors* $(Y_\ell^m(\theta,\phi)\sin\theta\cos\phi, Y_\ell^m(\theta,\phi)\sin\theta\sin\phi, Y_\ell^m(\theta,\phi)\cos\theta)^T$ *for* $m=-\ell,\ldots,\ell$, $\ell=0,1,2$.

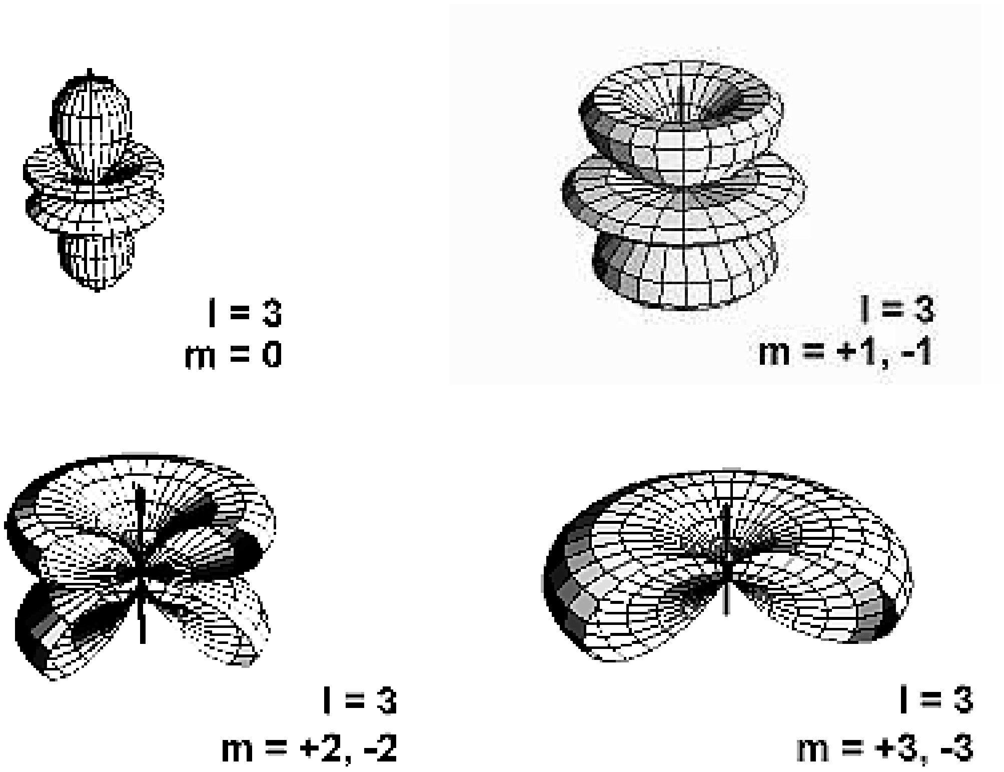

Figure 2: *Spherical harmonic descriptors* $(Y_\ell^m(\theta,\phi)\sin\theta\cos\phi, Y_\ell^m(\theta,\phi)\sin\theta\sin\phi, Y_\ell^m(\theta,\phi)\cos\theta)^T$ *for* $m=-\ell,\dots,\ell$, $\ell=3$.

For a probability measure with finite support the support points, say $z_i=(\theta_i,\phi_i)$, determine the points on the sphere, where the radius of the 3D shape is observed and the corresponding weights, say w_i, give the relative proportion of total observations, say w_i, taken in a particular direction. For a given design ξ with finite support the covariance matrix of the least squares estimate for the vector c is approximately proportional to the information matrix

$$M(\xi)=\int_{-\pi}^{\pi}\int_0^{\pi} f(\theta,\phi)f^T(\theta,\phi)d\xi(\theta,\phi) \tag{2.8}$$

(this is essentially the matrix B^TB mentioned in the introduction) and an optimal approximate design maximizes an appropriate function of this matrix. There are numerous criteria proposed in the literature, which can be used to discriminate between competing designs [see Silvey (1980) or Pukelsheim (1993)] and we will restrict ourselves to the famous family of Φ_p-criteria introduced by Kiefer (1974) and a new optimality criterion, which has not been considered so far in the literature and is related to principal component analysis.

To be precise, let $K\in\mathbb{R}^{(d+1)^2\times s}$ denote a given matrix of rank $s\le(d+1)^2$ and assume that the main interest of the experimenter is in the estimation of s linear combinations K^Tc. If n observations are taken according to an approximate design [possibly by applying an appropriate rounding procedure to a design with finite support or by using a discretization of a continuous design; see Pukelsheim and Rieder (1992)], then the covariance matrix of the least squares estimate for K^Tc is approximately given by

$$\frac{\sigma^2}{n}(K^T M^-(\xi)K),$$

where A^- denotes a generalized inverse of the matrix A and we assume that the linear combinations K^Tc are estimable by the design ξ, that is

$$\text{range}\,(K) \subset \ \text{range}\,(M(\xi));$$

see Pukelsheim (1993). Let $-\infty \le p < 1$; following Kiefer (1974) we call the design ξ^* Φ_p-optimal for estimating the linear combinations K^Tc if ξ^* maximizes the expression

$$\Phi_p(\xi) = (\text{tr}(K^T M^-(\xi)K)^{-p})^{\frac{1}{p}} \tag{2.9}$$

among all designs for which K^Tc is estimable. If $K = I_{(d+1)^2}$ is the identity matrix of order $(d+1)^2 \times (d+1)^2$, then ξ^* is briefly called Φ_p-optimal. Note that the cases $p = 0$ and $p = -\infty$ correspond to the frequently used D- and E-optimality criterion, i.e.

$$\Phi_0(\xi) = \det(K^T M^-(\xi)K)^{-1} \ ; \ \ \Phi_{-\infty}(\xi) = \lambda_{\min}((K^T M^-(\xi)K)^{-1}), \tag{2.10}$$

while the A-criterion is obtained for the choice $p = -1$, i.e.

$$\Phi_{-1}(\xi) = (\text{tr}\,(K^T M^-(\xi)K)^{-1}. \tag{2.11}$$

In the following we are interested in a design, which is particulary efficient for the estimation of the coefficients corresponding to the $(2k+1)$ spherical harmonic functions

$$Y_k^{-k}, Y_k^{-k+1}, \ldots, Y_k^k$$

of the vector of regression functions defined in (2.7), where $k \in \{0, \ldots, d\}$ denotes a given "level of resolution". For this define $0_{k,s}$ as the $(2k+1) \times (2s+1)$ matrix with all entries equal to 0, let $q \in \mathbb{N}_0$, consider the indices $0 \le k_0 < k_1 < k_2 < \ldots < k_q \le d$ and define the matrix

$$K^T = K^T_{k_0,\ldots,k_q} = \Big(K_{i,j}\Big)_{i=0,\ldots,q}^{j=0,\ldots,d} \tag{2.12}$$

by

$$K_{i,j} = \begin{cases} 0_{k_i,j} & \text{if } j \ne k_i \\ I_{2k_i+1} & \text{if } j = k; \end{cases} \tag{2.13}$$

$(i = 0, \ldots, q; j = 0, \ldots, d)$. Note that $K \in \mathbb{R}^{(d+1)^2 \times s}$, where $s = \sum_{i=0}^q (2k_i + 1)$ and that K^Tc gives the vector with coefficients

$$\Big\{c_{k_\ell}^m \Big| m \in \{-k_\ell, -k_\ell + 1, \ldots, k_\ell\}; \quad \ell = 0, \ldots, q\Big\}. \tag{2.14}$$

Two cases are of particular interest here and are therefore mentioned separately. If $q = d$, then

$$K^T_{0,\ldots,d} = I_{(d+1)^2} \tag{2.15}$$

and precise estimation of the full vector of parameters is the main goal for the construction of the optimal design. On the other hand if $q = 0$, only the coefficients corresponding to the $(2k_0 + 1)$ spherical harmonic functions $Y_{k_0}^{-k_0}, \dots, Y_{k_0}^{k_0}$ are of interest and the corresponding matrix is given by

$$K_{k_0}^T = \Big[\ 0_{k_0,0} \ \vdots\ \dots\ \vdots\ 0_{k_0,k_0-1} \ \vdots\ I_{2k_0+1} \ \vdots\ \dots\ \vdots\ 0_{k_0,d}\ \Big] \ \in\ \mathbb{R}^{(2k_0+1)\times(d+1)^2}. \tag{2.16}$$

Note that the general matrix defined by (2.12) consists of $(q+1)$ (block-) rows of the form (2.16). The following result shows that for matrices of this form the Φ_p-criteria defined in (2.9) are maximized by the uniform distribution on the sphere independently of $p \in [-\infty, 1)$.

Theorem 2.1. *Let $p \in [-\infty, 1)$, $0 \le k_0 < \dots < k_q \le d$ be given indices and denote $K = K_{k_0,\dots,k_q}$ as the matrix defined by (2.12) and (2.13). A Φ_p-optimal design ξ^* for estimating the linear combinations $K^T c$ in the spherical harmonic regression model (2.6) is given by the uniform distribution on the sphere, i.e.*

$$\xi^*(d\theta, d\phi) = \frac{1}{4\pi}\sin\theta d\theta d\phi. \tag{2.17}$$

Moreover, the corresponding information matrix in the spherical harmonic regression model is given by $M(\xi^*) = I_{(2d+1)^2}$.

Proof. Let ξ^* denote the design corresponding to the density (2.17), then, due to the orthonormality of the spherical harmonic functions Y_ℓ^m, it follows that

$$M(\xi^*) = \Big(\int_0^\pi \int_{-\pi}^\pi Y_\ell^m(\theta,\phi) Y_{\ell'}^{m'}(\theta,\phi) d\phi \sin\theta \frac{d\theta}{4\pi}\Big)_{\ell,\ell',m',m} = I_{(2d+1)^2}.$$

Assume for the moment that $p > -\infty$. According to Theorem 7.20 in Pukelsheim (1993) we obtain that the measure ξ^* is Φ_p-optimal if and only if the inequality

$$f_d^T(\theta,\phi) K (K^T K)^{-p-1} K^T f(\theta,\phi) \le \ \mathrm{trace}(K^T K)^{-p} \tag{2.18}$$

holds for all $\theta \in [0, \pi]$ and $\phi \in (-\pi, \pi]$. Now the special structure of the matrix K defined in (2.12) and (2.13) yields

$$K^T K = I_s$$

where $s = \sum_{\ell=0}^q (2k_\ell + 1)$. Observing the definition of the vector $f_d(\theta,\phi)$ in (2.7) and again the definition of the matrix K the inequality (2.18) reduces to

$$\begin{aligned} s \ &\ge \sum_{\ell=0}^q \sum_{m=-k_\ell}^{k_\ell} \Big(Y_{k_\ell}^m(\theta,\phi)\Big)^2 \\ &= \sum_{\ell=0}^q (2k_\ell+1)\Big\{\Big(P_\ell^0(\cos\theta)\Big)^2 + 2\sum_{m=1}^{k_\ell} \frac{(k_\ell - m)!}{(k_\ell+m)!}\Big(P_{k_\ell}^m(\cos\theta)\Big)^2\Big\} \end{aligned} \tag{2.19}$$

for all $\theta \in [0, \pi]$ and $\phi \in (-\pi, \pi]$; where we have used the representation (2.2) and the trigonometric identity $\cos^2(m\phi) + \sin^2(m\phi) = 1$ for the last equality. From the identity

$$\begin{aligned} &P_k^0(\cos\alpha\cos\beta + \sin\alpha\sin\beta\cos\phi) \\ &\quad = P_k^0(\cos\alpha)P_k^0(\cos\beta) + 2\sum_{m=1}^k \frac{(k-m)!}{(k+m)!} P_k^m(\cos\alpha) P_k^m(\cos\beta)\cos(m\phi) \end{aligned}$$

for the Legendre functions [see Andrews, Askey and Roy (1999), p. 457] and the fact that P_k^0 is the kth Legendre polynomial it follows (with the choice $\alpha = \beta, \phi = 0$)

$$(P_k^0(\cos\alpha))^2 + 2\sum_{m=1}^{k} \frac{(k-m)!}{(k+m)!}(P_k^m(\cos\alpha))^2 = P_k^0(1) = 1.$$

Now the right hand side of the inquality (2.19) simplifies to

$$\sum_{\ell=0}^{q}(2k_\ell + 1) = s,$$

and consequently the inequality (2.19) or equivalently (2.18) holds for all $\theta \in [0, \pi]$ and $\phi \in (-\pi, \pi]$. This proves that the design ξ^* corresponding to the uniform distribution on the sphere is Φ_p-optimal for any $p \in (-\infty, 1)$ and any matrix K of the form (2.12) and (2.13). The remaining case $p = -\infty$ finally follows from Lemma 8.15 in Pukelsheim (1993).

□

It should be noted at this point that the E-criterion is of particular importance for the design of experiment in 3D-shape analysis, because many authors propose to use principal component analysis for the comparison of different shapes [see e.g. Ding et al. (2000) or Kazhdan et al. (2003) among others]. More precisely, it is proposed to summarize the information contained in the spherical harmonic coefficients by a principal component analysis based on the variance-covariance matrix of the least squares estimator obtained from (1.3), which explains the 3D-shape variation of different objects by the first, say r, principal components corresponding to the r largest eigenvalues of the matrix $M^{-1}(\xi)$. Consequently, an efficient design for principal component analysis should minimize a function of the largest r eigenvalues of the matrix $M^{-1}(\xi)$. To be precise let $r \leq (d+1)^2$, and $-p \leq \infty < 1$, then we call a design ξ^* $\Psi_{p,r}$-optimal if ξ^* maximizes

$$\Psi_{p,r}(\xi) = \Big(\sum_{j=1}^{r}\Big\{\lambda_{(j)}(M(\xi))\Big\}^p\Big)^{1/p} \tag{2.20}$$

where $\lambda_{(j)}(M(\xi))$ denotes the jth smallest eigenvalue of the matrix $M(\xi^*)$. Again the case $p = -\infty$ and $p = 0$ are obtained from the corresponding limits, that is $\Psi_{-\infty,r}(\xi) = \lambda_{(1)}(M(\xi))$ and $\Psi_{0,r}(\xi) = \prod_{j=1}^{r}\lambda_{(j)}(M(\xi))$, respectively. To the knowledge of the authors optimality criteria of this type have not been considered in the literature so far. Note also that the E- and A-optimality criterion (with $K = I_{(d+1)^2}$) are obtained for the choice $r = 1$ and $r = (d+1)^2$ with $p = -1$, respectively. The most important case for the choice of the parameter $p \in [-\infty, 1)$ is certainly obtained for $p = -1$. In the following we show that the uniform distribution on the sphere is also $\Psi_{r,p}$-optimal.

Corollary 2.2. *Let $p \in [-\infty, 1)$ and $1 \leq r \leq (d+1)^2$, then the uniform distribution on the sphere defined by (2.17) is $\Psi_{p,r}$-optimal in the spherical harmonic regression model (2.6).*

Proof. The case $p = -\infty$ is obtained from Theorem 2.1 with $K = I_{(d+1)^2}$. For $-\infty < p < 1$ note that $\Psi_{p,r}(\xi^*) = r^{1/p}$ if $p \neq 0$ and $\Psi_{0,r}(\xi^*) = 1$. If $p \neq 0$ and ξ^* would not be $\Psi_{p,r}$-optimal, then there would exist a design, say ξ, with

$$\Big(\Psi_{p,r}(\xi)\Big)^p = \sum_{j=1}^{r} \lambda_{(j)}^p(M(\xi)) < r = \Big(\Psi_{p,r}(\xi^*)\Big)^p.$$

Consequently, we obtain $\lambda_{(1)}(M(\xi)) < 1 = \lambda_{\min}(M(\xi^*))$, which implies that the uniform distribution on the sphere ξ^* is not E-optimal and contradicts Theorem 2.1. The case $p = 0$ is obtained by a similar argument and the assertion of the corollary has been established.

□

3 Discrete optimal designs

Note that the uniform distribution defined by (2.17) is not directly implementable as a design in real experiments. Therefore, for practical applications it is important to obtain discrete designs ξ which are equivalent to the uniform distribution $\xi^*(d\theta, d\phi) = \frac{1}{4\pi}\sin\theta d\theta d\phi$ in the sense that

$$M(\xi) = M(\xi^*) = I_{(d+1)^2}, \tag{3.1}$$

where $M(\xi)$ is the information matrix (2.8) of the design ξ in the spherical harmonic regression model (2.6). Note that due to Caratheodory's theorem [see Silvey (1980)] there always exist discrete designs satisfying (3.1) and in the following we will construct a broad class of discrete designs, which can easily be implemented in practice. For this purpose we need an auxiliary result about quadrature formulas, which will be proved in the appendix.

Lemma 3.1. *Assume that $r \in \mathbb{N}$ and let $-1 \le x_1 < x_2 < \ldots < x_r \le 1$ denote r points with corresponding weights $w_1, \ldots, w_r > 0$ $\Big(\sum_{i=1}^r w_i = 1\Big)$. The points x_i and weights w_i generate a quadrature formula of degree $p \ge r$, that is*

$$\sum_{i=1}^{r} w_i x_i^\ell = \frac{1}{2}\int_{-1}^{1} x^\ell dx \quad \ell = 0, \ldots, p, \tag{3.2}$$

if and only if the following two conditions are satisfied:

(A) *The polynomial $V_r(x) = \prod_{i=0}^r (x - x_i)$ is orthogonal to all polynomials of degree $p - r$ with respect to the Lebesgue-measure, that is*

$$\int_{-1}^{1} V_r(x) x^\ell dx = 0, \quad \ell = 0, \ldots, p - r. \tag{3.3}$$

(B) *The weights w_j are given by*

$$w_j = \frac{1}{2}\int_{-1}^{1} \ell_j(x) dx, \tag{3.4}$$

where

$$\ell_i(x) = \prod_{\substack{j=1 \\ j\ne i}}^{r} \frac{x - x_j}{x_i - x_j}$$

denotes the ith Lagrange interpolation polynomial with nodes $x_1, \ldots, x_r$.

It follows from condition (3.3) that $p \le 2r-1$ (otherwise there does not exist a solution of this system). Moreover, there exists at least one set of points, which satisfies condition (3.3), namely

$$\{x \mid P_r(x) = 0\}, \tag{3.5}$$

where P_r denotes the *rth* Legrendre polynomial orthogonal with respect to the Lebesgue-measure on the interval $[-1,1]$, because it is well known that this polynomial has r distinct roots located in the interval $(-1,1)$ [see Szegö (1975)]. Moreover, the corresponding weights defined by (3.4) are positive and define a Gaussian quadrature formula, i.e. a quadrature formula of degree $2r-1$ with r nodes [see e.g. Engels (1980) or Ghizetti and Ossicini (1970)]. In the following we will use this Lemma with $p = 2d$, then it follows that for any $r \in \{d+1, \ldots, 2d\}$ there exists at least one quadrature formula $\{x_i, w_i\}_{i=1}^r$ determined by the equations (3.3) and (3.4), which integrates polynomials of degree $2d$ exactly (in other words: the system of equations in (3.2) is satisfied with $p = 2d$) and the corresponding weights w_i are positive. We consider a quadrature formula of this type, define

$$\theta_i = \arccos x_i \quad i = 1, \ldots, r \tag{3.6}$$

and consider the design

$$\mu = \begin{pmatrix} \theta_1 & \ldots & \theta_r \\ w_1 & \ldots & w_r \end{pmatrix} \tag{3.7}$$

on the interval $[0, \pi]$. Similary, we define for any $t \in \mathbb{N}$ and any $\alpha \in (-\frac{t+1}{t}\pi, -\pi]$ a design $\nu = \nu(\alpha, t)$ on the interval $(-\pi, \pi]$ by

$$\nu = \nu(\alpha, t) = \begin{pmatrix} \phi_1 & \ldots & \phi_t \\ \frac{1}{t} & \ldots & \frac{1}{t} \end{pmatrix}, \tag{3.8}$$

where the points ϕ_j are given by

$$\phi_j = \alpha + \frac{2\pi j}{t} \quad j = 1, \ldots, t. \tag{3.9}$$

The following result shows that designs of the form $\mu \otimes \nu$ are discrete Φ_p- and $\Psi_{p,r}$- optimal designs for the spherical harmonic regression model (2.6).

Theorem 3.2. *Let $p \in [-\infty, 1)$, $0 \le k_0 < \ldots < k_q \le d$ and denote by $K = K_{k_0,\ldots,k_q}$ the matrix defined by (2.12). For any $t \ge 2d+1$ and any $r \in \{d+1, \ldots, 2d\}$ the design $\mu \otimes \nu$ with factors given by (3.7) (corresponding to a quadrature formula of degree $2d$) and (3.8) is Φ_p-optimal for estimating the coefficients $K^T c$ and $\Psi_{p,r}$-optimal in the spherical harmonic regression model (2.6).*

Proof. Observing the proof of Theorem 2.1 and Corollary 2.2 the assertion can be established by showing the identity

$$M(\mu \otimes \nu) = I_{(d+1)^2}. \tag{3.10}$$

For this let

$$\begin{aligned}\psi(\phi) &= (\psi_{-d}(\phi), \psi_{-d+1}(\phi), \dots, \psi_d(\phi))^T \\ &= (\sqrt{2}\sin(d\phi), \dots, \sqrt{2}\sin\phi, 1, \sqrt{2}\cos\phi, \dots, \sqrt{2}\cos(d\phi))^T,\end{aligned}$$

then the regression functions in the spherical harmonic regression model of degree d are given by

$$\gamma_{ij} P_i^{|j|}(\cos\theta) \cdot \psi_j(\phi); \quad j = -i, \dots, i,\ i = 0, \dots, d, \tag{3.11}$$

where P_i^j is the Legendre function defined by the equation (2.4) and the constants γ_{ij} are given by

$$\gamma_{ij} = \sqrt{(2i+1)\frac{(i-|j|]!}{(i+|j|)!}}$$

(note that the different scaling of the case $j = 0$ and $j \neq 0$ in (2.2) has been reflected by introducing the factor $\sqrt{2}$ in the definition of the functions ψ_j). Therefore the identity (3.10) is equivalent to the system of equations

$$\gamma_{ij}\gamma_{k\ell} \int_{-\pi}^{\pi} \int_0^{\pi} P_i^{|j|}(\cos\theta)\psi_j(\phi) P_k^{|\ell|}(\cos\theta)\psi_\ell(\phi) d\mu(\theta) d\nu(\phi) \ = \ \delta_{ik}\delta_{j\ell} \tag{3.12}$$

($j = -i, \dots, i; i = 0, \dots, d; \ell = -k, \dots, k; k = 0, \dots, d$), where δ_{ik} denotes Kronecker's symbol. Observing Fubini's theorem this system is satisfied if the equations

$$\gamma_{ij}\gamma_{k\ell} \int_0^{\pi} P_i^j(\cos\theta) P_k^\ell(\cos\theta) d\mu(\theta) = \delta_{ik}\delta_{j\ell} \tag{3.13}$$

($j = 0, \dots, i; i = 0, \dots, d; \ell = 0, \dots, k; k = 0, \dots, d$) and

$$\int_{-\pi}^{\pi} \psi_j(\phi)\psi_\ell(\phi) d\nu(\phi) = \delta_{j\ell}; \quad j, \ell = -d, \dots, d \tag{3.14}$$

can be established. It is well known [see Pukelsheim (1993)] that the last identity is satisfied for measures of the form (3.8). In order to prove the remaining identity (3.13) recall that the measure μ corresponds to a quadrature formula, which integrates polynomials of degree $2d$ exactly. Moreover, it follows from the representation (2.4) that for an even $m \in \{0, \dots, n\}$ the Legendre function $P_n^m(x)$ is a polynomial of degree n, while for any odd $m \in \{0, \dots, n\}$ the function $P_n^m(x)/\sqrt{1-x^2}$ is a polynomial of degree $n-1$. Observing the equation (3.14) we can restrict ourselves to the case $j = \ell$ for which the integrand $P_i^j(x)P_k^j(x)$ in (3.13) is always a polynomial of degree $i + k \leq 2d$, which contains the factor $(1 - x^2)$ if j is odd. Consequently, we obtain from (3.2) (with $p = 2d$)

$$\int_0^{\pi} P_i^j(\cos\theta) P_k^j(\cos\theta) d\mu(\theta) = \sum_{\ell=1}^{r} w_\ell P_i^j(x_\ell) P_k^j(x_\ell) = \frac{1}{2}\int_{-1}^{1} P_i^j(x) P_k^j(x) dx = \frac{\delta_{ik}}{\gamma_{ij}\gamma_{kj}},$$

where the last property follows from the orthogonality of the Legendre functions [see Andrews, Askey and Roy (1999)]. This implies (3.12) [or equivalently (3.10)] and proves the theorem.

□

Remark 3.3. It should be noted that the mapping $(\theta, \phi) \to (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ from the rectangle $[0, \pi] \times (-\pi, \pi]$ onto the unit sphere S_2 maps all points of the form $(0, \phi)$ and (π, ϕ) with $\phi \in (-\pi, \pi]$ on the points $(0, 0, 1)$ and $(0, 0, -1)$ on S_2, respectively. Moreover, it is easy to see that the vector $f_d(\theta, \phi)$ defined in (2.7) satisfies for all $\phi \in (-\pi, \pi]$

$$\begin{aligned} f_d(0, \phi) &= (1, 0, \ldots, 0)^T \in \mathbb{R}^{(d+1)^2}, \\ f_d(\pi, \phi) &= (-1, 0, \ldots, 0)^T \in \mathbb{R}^{(d+1)^2}. \end{aligned}$$

As a consequence various points of the designs $\mu \otimes \nu$ constructed by Theorem 3.2 could be identified on the unit sphere, if the support of the factor μ contains the point 0 or π. To be precise let $\bar{\mu}$ denote the measure obtained from μ by omitting the points 0 and π, define μ_0 as the measure, which puts masses $\mu(\{0\})$ and $\mu(\{\pi\})$ at the points $(0, 0)^T$ and $(\pi, 0)^T$, respectively, then the measure

$$\mu_0 + \bar{\mu} \otimes \nu$$

has the same information matrix as the measure $\mu \otimes \nu$. Note that in the case $\mu(\{0\}) + \mu(\{\pi\}) = 0$ it follows that $\bar{\mu} = \mu$, because the points 0 and π are no support points of the design μ.

Example 3.4. Consider the spherical harmonic regression model of degree $d = 1$ and the case $r = d+1 = 2$. From Lemma 3.1 with $p = 2d = 2$ it follows that the polynomial $V_2(x) = (x-1)(x+1/3)$ satisfies

$$\int_{-1}^{1} V_2(x)dx = 0.$$

The points $x_1 = -1/3$ and $x_2 = 1$ generate a quadrature formular of degree 2 on the interval $[-1, 1]$ with corresponding weights

$$w_1 = \int_{-1}^{1} \frac{x-1}{(-4/3)} \frac{dx}{2} = \frac{3}{4}; \quad w_2 = \int_{-1}^{1} \frac{x+1/3}{4/3} \frac{dx}{2} = \frac{1}{4}.$$

According to Theorem 3.2 any design of the form

$$\mu \otimes \nu(\alpha, t) = \begin{pmatrix} 0 & \arccos(-\frac{1}{3}) \\ \frac{1}{4} & \frac{3}{4} \end{pmatrix} \otimes \nu(\alpha, t)$$

with $t \geq 3, \alpha \in (-\frac{t+1}{t}\pi, -\pi]$ is Φ_p-optimal for estimating the parameters $K^T_{k_0,k_q} c$ $(q \leq 1)$ and $\Psi_{p,r}$-optimal in the first order spherical harmonic regression model (2.6). A typical example is given by the 6 point design

$$\mu \otimes \nu = \begin{pmatrix} 0 & \arccos(-\frac{1}{3}) \\ \frac{1}{4} & \frac{3}{4} \end{pmatrix} \otimes \begin{pmatrix} -\frac{\pi}{3} & \frac{\pi}{3} & \pi \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix},$$

and by Remark 3.3 the design with equal masses at the points $(0, 0)$, $(\arccos(-\frac{1}{3}), -\frac{\pi}{3})$, $(\arccos(-\frac{1}{3}), \frac{\pi}{3})$ and $(\arccos(-\frac{1}{3}), \pi))$ has the same information matrix as the design $\mu \otimes \nu$, namely the identity matrix I_4.

Remark 3.5. Note that there are numerous possibilities to construct a discrete design with an information matrix equal to $I_{(d+1)^2}$ in the spherical harmonic regression model (2.6). According to Theorem 3.2 a quadrature formula with $r \in \{d+1, \ldots, 2d\}$ nodes $x_1, \ldots, x_r$ with positive weights is required, which integrates polynomials up to degree $2d$ exactly. By (3.7) this formula gives the factor μ of the optimal design $\mu \otimes \nu$, where the second factor is any design of the form (3.8) with $t \geq 2d+1$. By Lemma 3.1 the quadrature formula is determined by the equations

$$\int_{-1}^{1} V_r(x) x^\ell dx = 0 \quad \ell = 0, \ldots, 2d-r. \tag{3.15}$$

If $P_j(x)$ denotes the jth Legendre polynomial orthogonal with respect to the Lebesgue-measure on the interval $[-1, 1]$, then the polynomial $V_r(x)$ can be represented as a linear combination of the Legendre polynomials $P_0(x), \ldots, P_r(x)$ and the orthogonality in (3.15) implies for some constants $a_{2d-r+1}, \ldots, a_r$

$$V_r(x) = \sum_{j=2d-r+1}^{r} a_j P_j(x). \tag{3.16}$$

Note that the constants $a_{2d-r+1}, \ldots, a_r$ have to be chosen such that $V_r(x)$ has r real roots in the interval $[-1, 1]$ and such that the corresponding weights defined by (3.4) are positive. This is in general a non-trivial problem. However, one can easily describe a class of quadrature formulas, for which this property is satisfied. For this let $P_j^{(\alpha,\beta)}(x)$ denote the jth Jacobi polynomial orthogonal with respect to the measure $(1-x)^\alpha (1+x)^\beta dx$ on the interval $[-1, 1]$ [see Szegö (1975)]. For any $r \geq d+1$ it follows from these orthogonality properties that the identity (3.15) is satisfied for the polynomials

$$P_r^{(0,0)}(x), \quad (1-x) P_{r-1}^{(1,0)}(x), \quad (1+x) P_{r-1}^{(0,1)}(x), \quad (1-x^2) P_{r-1}^{(1,1)}(x). \tag{3.17}$$

Note that $P_r^{(0,0)}(x)$ is proportional to the Legendre polynomial $P_r(x)$ and consequently the representation of the form (3.16) is obvious in this case choosing $a_{r-1} = \ldots = a_{2d-r+1} = 0$. Moreover, if p is the degree of one of these polynomials it follows from classical results on orthogonal polynomials that each of the polynomials in (3.17) has precisely p roots in the interval $[-1, 1]$. It is shown in Bouzitat (1949) that the weights corresponding by formula (3.4) to these roots are positive [see also Ghizetti, Ossicini (1970)], and as a consequence we obtain a quadrature formula of degree $2d$ on the interval $[-1, 1]$, say $\{x_j, w_j\}_{j=1,\ldots,p}$. The corresponding design μ obtained from (3.6) and (3.7) gives in combination with any design ν of the form (3.8) a Φ_p-optimal design $\mu \otimes \nu$ for estimating the parameters $K_{k_1,\ldots,k_q}^T c$ in the spherical harmonic regression model (2.6). This design is also $\Psi_{p,r}$-optimal, by Corollary 2.2. We finally note that the roots of the polynomials in (3.17) are the support points of D-optimal designs in heteroscedastic polynomial regression models [see Studden (1980, 1982)].

Although there are numerous designs on the rectangle $[0, \pi] \times (-\pi, \pi]$ with information matrix in the spherical harmonic regression model (2.6) given by $I_{(d+1)^2}$, the support points of the factor corresponding to the polar angle θ have to cover a sufficiently large range of the interval $[0, \pi]$ in order to obtain a Φ_p-optimal design in the sense of Theorem 3.2. This is the statement of the final theorem of this section, which will be proven in the appendix.

Theorem 3.6. *Let x_1^* denote smallest root of the Legendre polynomial $P_{d+1}(x)$ and define $z^* = \arccos|x_1^*|$. If $z > z^*$, then there exists no design on the rectangle $[z, \pi - z] \times (-\pi, \pi]$ with information matrix $I_{(d+1)^2}$ in the spherical harmonic regression model (2.6).*

4 Further discussion

4.1 The second order spherical harmonic model

Consider the case $d = 2$ corresponding to the second order spherical harmonic model with 9 regression functions. We calculate the designs corresponding to the four cases in (3.17) for the choice $r = d + 1 = 3$. From $P_3(x) = x(5x^2 - 3)/2$ we obtain the support points of the probability measure μ corresponding to the polar angle θ as

$$\theta_1 = \arccos\sqrt{\frac{3}{5}}\ ;\ \theta_2 = \arccos 0 = \frac{\pi}{2}\ ;\ \theta_3 = \arccos(-\sqrt{\frac{3}{5}}) \tag{4.1}$$

and the corresponding weights are given by

$$w_2 = \frac{1}{2}\int_{-1}^{1}\frac{x^2 - 3/5}{(-3/5)}dx = \frac{4}{9}\ ,\quad w_1 = w_3 = (1 - w_2)/2 = \frac{5}{18}\ . \tag{4.2}$$

Similary, if the polynomial $(x^2 - 1)P_2^{(1,1)}(x) = \frac{3}{4}(x^2 - 1)(5x^2 - 1)$ is used for the construction of a quadrature formula, we obtain

$$\theta_1 = \arccos 1 = 0\ ;\ \theta_2 = \arccos\sqrt{\frac{1}{5}}\ ;\ \theta_3 = \arccos(-\sqrt{\frac{1}{5}})\ ;\ \theta_3 = \arccos(-1) = \pi; \tag{4.3}$$

and the weights are obtained from the representation (3.4) and given by

$$w_1 = w_4 = \frac{1}{12}\ ,\quad w_2 = w_3 = \frac{5}{12}. \tag{4.4}$$

The measure ν corresponding to the azimuthal angle ϕ is given by (3.8), where $t \geq 5$. The projections of the support points of the two measures onto the unit sphere are depicted on the left and right panel of Figure 3, where for the second component a design with $t = 5$ support points and $\alpha = -\pi$ is used. It should be noted that it follows from Remark 3.3 that the design $\mu \otimes \nu$ obtained from (4.3) and (4.4) for the factor μ and $\nu = \nu(\alpha, 5)$ corresponds to uniform design on the sphere with 12 support points. A general construction of uniform designs will be discussed in the following paragraph. We finally illustrate the two other non-symmetric cases in (3.17). For the supporting polynomial we obtain

$$(1 - x)P_2^{(1,0)}(x) = \frac{1 - x}{2}(5x^2 + 2x - 1),$$

which gives for the support points of the factor μ of the product design $\mu \otimes \nu(\alpha, t)$

$$\theta_1 = \arccos 1 = 0;\quad \theta_2 = \arccos\Big(\frac{-1 + \sqrt{6}}{5}\Big);\quad \theta_2 = \arccos\Big(\frac{-1 - \sqrt{6}}{5}\Big) \tag{4.5}$$

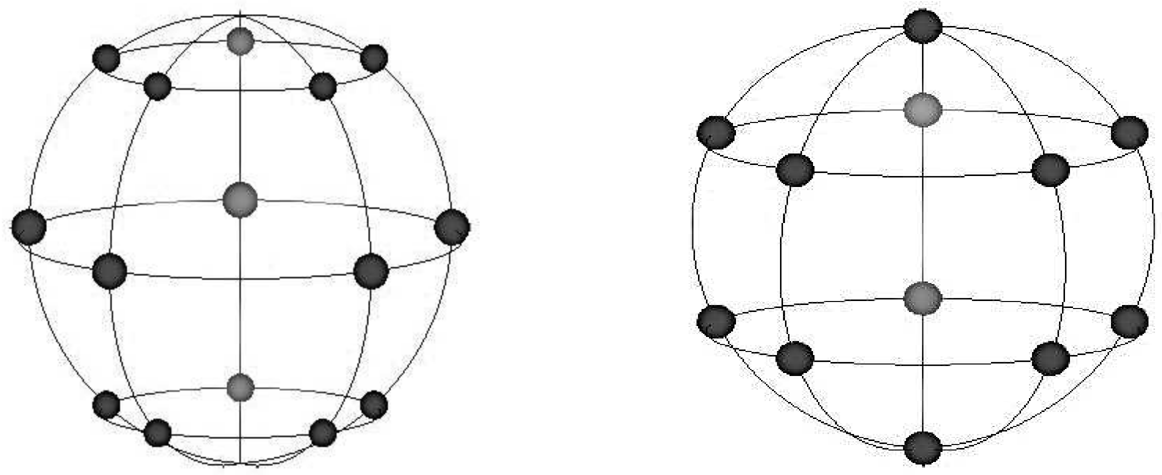

Figure 3: *Projections of the suppport points of the optimal design in the second order spherical harmonic regression model (2.6). The left panel correspond to the optimal design defined by (4.1), while the right panel represents the design (4.3).*

with corresponding weights

$$w_1 = \frac{1}{9}; \quad w_2 = \frac{1}{36}(16 + \sqrt{6}); \quad w_3 = \frac{1}{36}(16 - \sqrt{6}).$$

The fourth case of a factor μ of a design $\mu \otimes \nu(\alpha, t)$ yielding I_9 as information matrix in the second order spherical harmonic model (2.6) is obtained by symmetry, that is

$$\begin{aligned} \theta_1 &= \arccos\Big(\frac{1+\sqrt{6}}{5}\Big); \quad \theta_2 = \arccos\Big(\frac{1-\sqrt{6}}{5}\Big); \quad \theta_3 = \arccos(1) = \pi; \\ w_1 &= \frac{1}{36}(16 - \sqrt{6}); \quad w_2 = \frac{1}{36}(16 + \sqrt{6}); \quad w_3 = \frac{1}{9}. \end{aligned} \tag{4.6}$$

The projections of the support points onto the unit sphere of the corresponding product designs $\mu \times \nu(\alpha, t)$ with $\alpha = -\pi$ and $t = 5$ are depicted in the left and right panel of Figure 4. Note that the two cases are related by a reflection of the support points at the equator.

4.2 Optimal designs with equal weights

Note that the designs provided by Theorem 3.2 are in general not uniform designs, which would have equal weights at their support points. Because designs with this structure are particulary attractive from a practical point of view we will briefly discuss the possibility of their construction in this section. Note that for the determination of an optimal design in the spherical harmonic regression model (2.6) with equal weights at its supports by the procedure introduced in Section 3 it is necessary to find a quadrature formula, which has equal weights at its support points and integrates polynomials of degree $2d$ exactly. This problem has a long history in mathematics [see Engels (1980)].

It follows from Lemma 3.1 that such a formula must have at least $d+1$ nodes. Moreover, quadrature formulas with the minimal number of n nodes and equal weights, which integrate polynomials of

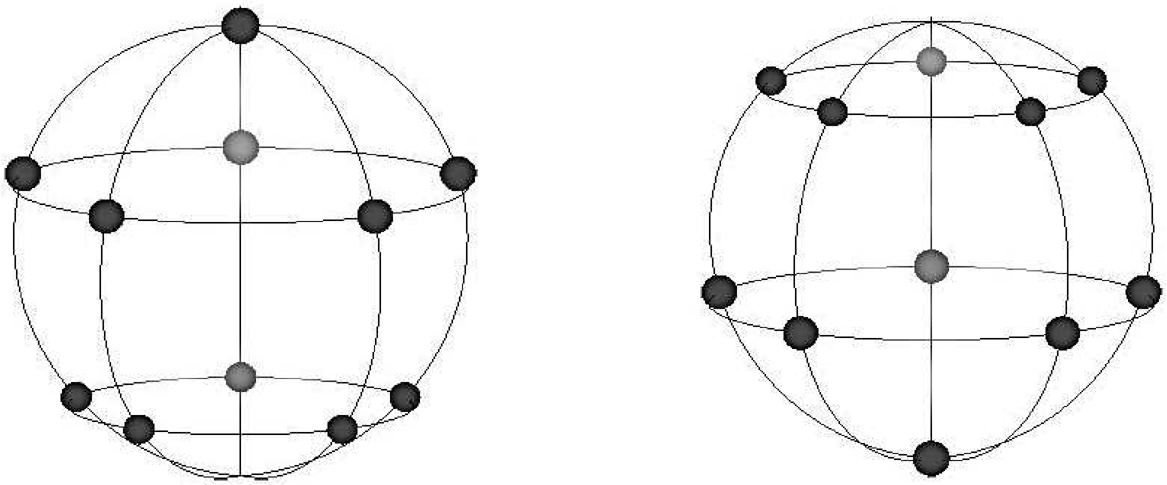

Figure 4: *Projections of the suppport points of the optimal design in the second order spherical harmonic regression model (2.6). The left panel correspond to the optimal design defined by (4.5), while the right panel represents the design (4.6).*

degree n exactly only exist in the cases $n = 0, 1, \ldots, 7, 9$ [see Engels (1980), p. 58]. In the present context these formulas correspond to uniform designs for the polar angle θ in the case $d = 1, 2, 3, 4$ which give in combination with a design of the form (3.8) a Φ_p- or $\Psi_{p,r}$-optimal design in the spherical harmonic regression model (2.6) with equal weights at its support points. The corresponding nodes of the quadrature formula required for the factor μ are depicted in the first four rows of Table 4.1. If $d \geq 5$ quadrature formulas with equal weights on $2d$ points integrating polynomials of degree $2d$ exactly do not exist and more nodes are required for the construction of such formulas. We determined formulas of this type numerically for $d = 5, 6, 7$ and depicted them in the second part of Table 4.1. Note that these formulas use the origin and that the number of nodes increases rapidly. For example, if $d = 7$, we only found a quadrature formula with 23 support points and equal weights, which integrates polynomials of degree 14 exactly.

d	x_0	$\pm x_1$	$\pm x_2$	$\pm x_3$	$\pm x_4$	$\pm x_5$	$\pm x_6$	$\pm x_7$	$\pm x_8$	$\pm x_9$	$\pm x_{10}$	$\pm x_{11}$
1	-	.577	-	-	-	-	-	-	-	-	-	-
2	-	.188	.795	-	-	-	-	-	-	-	-	-
3	-	.267	.423	.866	-	-	-	-	-	-	-	-
4	0	.168	.529	.601	.912	-	-	-	-	-	-	-
5	0	.223	.247	.443	.671	.724	.939	-	-	-	-	-
6	0	.008	.282	.358	.458	.566	.760	.778	.954	-	-	-
7	0	.174	.177	.186	.328	.502	.533	.542	.712	.797	.852	.965

Table 4.1. *Quadrature formulas with equal weights at their nodes. These formulas correspond to a uniform design μ_u of the form (3.7) for the polar angle θ. The resulting design $\mu_u \otimes \nu(\alpha, t)$ with $\nu(\alpha, t)$ defined by (3.8) and $t \geq 2d + 1$ is a Φ_p- or $\Psi_{p,r}$-optimal design in the spherical harmonic regression model (2.6) of degree d with equal weights at its support points.*

4.3 Some efficiency considerations

It might be of interest to compare some of the commonly used designs from the literature on the analysis of 3D shapes with the $\Psi_{p,r}$- and Φ_p-optimal designs obtained in the present paper. Examplarily, we consider two uniform designs of the form $\mu \otimes \nu$, where the components are given by

$$(4.7) \qquad \mu = \begin{pmatrix} \frac{i}{n_1+1} \\ \frac{1}{n_1} \end{pmatrix}_{i=1,\dots,n_1}, \quad \nu = \begin{pmatrix} \frac{2i\pi}{n_2} - \pi \\ \frac{1}{n_2} \end{pmatrix}_{i=1,\dots,n_2}$$

and the design

$$(4.8) \qquad \mu = \begin{pmatrix} \arccos(1 - \frac{2i}{n_1+1}) \\ \frac{1}{n_1} \end{pmatrix}_{i=1,\dots,n_1}, \quad \nu = \begin{pmatrix} \frac{2i\pi}{n_2} - \pi \\ \frac{1}{n_2} \end{pmatrix}_{i=1,\dots,n_2}$$

respectively. Note that the design $\mu \otimes \nu$ defined by (4.7) corresponds to a uniform distribution on the grid in the rectangle $[0, \pi] \times [-\pi, \pi]$, while a design $\mu \otimes \nu$ of the form (4.8) yields a design on the sphere which takes observations on several circles with equal distance on the z-axis. This design was used by Ding et al. (2000) for a principal component analysis of the variance-covariance matrix of the least squares estimator (1.3) in the spherical harmonic regression model of degree 7. In Table 4.2 and 4.3 we consider the problem of designing an experiment for the estimation of the full parameter vector c or for the principal component analysis in the spherical harmonic regression model (2.6). We show the D-, E- and A- efficiencies of these designs for various values of n_1 and n_2 in the spherical harmonic models of degree 1, 2, 3, 4. The tables also contain the $\Psi_{-1,r}$-efficiencies, which are defined by

$$(4.9) \qquad \mathrm{eff}_{\Psi,p,r}(\xi) = \frac{\Psi_{p,r}(\xi)}{\sup_\eta \Psi_{p,r}(\eta)}.$$

For the sake of brevity we choose the design for the azimuthal angle ϕ as the design defined by (3.8) - other uniform designs for this component will yield substantially lower efficiencies and are therefore not depicted. As a consequence the efficiencies of the design $\mu \otimes \nu$ do not depend on n_2 (provided that $n_2 \geq 2d + 1$, which will be assumed throughout this section).

For the first order spherical harmonic regression model we observe very good D- and A- efficiencies of the designs (4.7) and (4.8). However, the E-efficiencies and the $\Psi_{p,r}$-efficiencies of these designs are substantially smaller, in particular those efficiencies obtained for the design (4.8) with moderate values of n_1. For spherical harmonic models of larger degree both designs will still yield high D-efficiencies, the designs defined by (4.7) yield reasonable A-efficiencies, but its E- and $\Psi_{-1,r}$-efficiencies are substantially smaller. Moreover, the A- and E- efficiencies of the design (4.8) are very low. The $\Psi_{-1,r}$-efficiencies of this design are slightly larger but still not satisfactory. It is also interesting to note that the efficiencies of the design (4.7) are decreasing with the number n_1 while they are increasing for the design (4.8).

From these calculations and additional results, which are not depicted for the sake of brevity, we observe that designs with a uniform distribution on a grid in the rectangle $[0, \pi] \times (-\pi, \pi]$ should only be used if the maximization of the D-criterion is the preliminary goal of the design of the experiment. Whenever prinicpal component analysis is the main goal of the experiment or the precise estimates of the parameters itself are required some more care is necessary in the design of experiment for analysing 3D-shapes. In this case the loss of efficiency when using uniform designs on a grid in the rectangle $[0,\pi]\times[-\pi,\pi]$ or a uniform design taking observations on several circles with equal distance on the z-axis can be substantial. In most cases there exist substantially more efficent designs for the analysis in a spherical harmonic regression model. The advantages of the optimal designs derived in the present paper will also be illustrated in the following example.

		design (4.7)					design (4.8)				
d	n_1	eff_D	eff_E	eff_A	$\mathrm{eff}_{\Psi_{-1,2}}$	$\mathrm{eff}_{\Psi_{-1,3}}$	eff_D	eff_E	eff_A	$\mathrm{eff}_{\Psi_{-1,2}}$	$\mathrm{eff}_{\Psi_{-1,3}}$
1	3	1.000	1.000	1.000	1.000	1.000	0.940	0.500	0.870	0.667	0.789
	4	0.997	0.938	0.994	0.938	0.957	0.964	0.600	0.923	0.750	0.857
	5	0.993	0.900	0.986	0.900	0.931	0.976	0.667	0.949	0.800	0.894
	6	0.989	0.875	0.979	0.875	0.913	0.983	0.714	0.964	0.833	0.916
	7	0.986	0.857	0.973	0.857	0.900	0.987	0.750	0.973	0.857	0.931
2	4	0.991	0.801	0.982	0.838	0.851	0.902	0.229	0.745	0.331	0.427
	5	0.987	0.805	0.974	0.824	0.831	0.935	0.323	0.838	0.435	0.539
	6	0.981	0.794	0.964	0.807	0.811	0.954	0.399	0.888	0.512	0.617
	7	0.976	0.782	0.955	0.793	0.796	0.965	0.461	0.918	0.571	0.674
	8	0.972	0.772	0.947	0.782	0.785	0.973	0.511	0.937	0.617	0.716

Table 4.2. *D-, E- and A- and $\Psi_{-1,r}$-efficiencies ($r=2,3$) of the uniform designs (4.7) and (4.8) in a first and second order spherical harmonic model.*

		design (4.7)					design (4.8)				
d	n_1	eff_D	eff_E	eff_A	$\mathrm{eff}_{\Psi_{-1,2}}$	$\mathrm{eff}_{\Psi_{-1,3}}$	eff_D	eff_E	eff_A	$\mathrm{eff}_{\Psi_{-1,2}}$	$\mathrm{eff}_{\Psi_{-1,3}}$
3	5	0.980	0.799	0.961	0.802	0.803	0.874	0.094	0.600	0.146	0.199
	6	0.975	0.784	0.953	0.784	0.787	0.911	0.155	0.733	0.223	0.296
	7	0.970	0.768	0.944	0.768	0.772	0.934	0.214	0.811	0.292	0.377
	8	0.965	0.756	0.936	0.756	0.760	0.948	0.269	0.859	0.352	0.444
	9	0.961	0.747	0.929	0.747	0.751	0.959	0.318	0.891	0.404	0.500
4	6	0.969	0.739	0.942	0.755	0.761	0.851	0.035	0.434	0.057	0.081
	7	0.965	0.747	0.936	0.751	0.753	0.890	0.067	0.600	0.102	0.142
	8	0.961	0.739	0.929	0.742	0.743	0.916	0.103	0.709	0.149	0.203
	9	0.956	0.731	0.922	0.733	0.734	0.933	0.142	0.781	0.196	0.261
	10	0.952	0.724	0.915	0.726	0.727	0.945	0.180	0.830	0.240	0.314

Table 4.3. *D-, E- and A- and $\Psi_{-1,r}$-efficiencies ($r=2,3$) of the designs (4.7) and (4.8) in the spherical harmonic model of degree 3 and 4.*

4.4 A concluding example

In order to demonstrate the benefits of our designs we finally reanalyze the design used by Ding et al. (2000) for shape analysis of Citrus species. These authors used observations at 360 points measured in 10 circles using the equal height sampling method for the z-axis. By chosing $d = 7$ the data for the surface shape were expanded into the first 64-terms of spherical harmonic functions. The information contained in the spherical harmonic coefficients was summarized by a principal component analysis using the first seven principal components. Note that the design of Ding et al. (2000) corresponds to a design of the form (4.8) with $n_1 = 10$ and $n_2 = 36$. In the first row of Table 4.4 we show the efficiencies of this design with respect to the optimal designs obtained in this paper. The first factor of an optimal (uniform) design can be obtained from the quadrature formula corresponding to the spherical harmonic regression model of degree 7 in Table 4.1. We observe only for the D-criterion a reasonable efficiency. For all other criteria the design used by Ding et al. (2000) is very inefficient. The optimal designs proposed in this paper (or appropriate approximations) will yield substantial smaller variances of the least squares estimates for linear combinations of the parameters.

We finally note that the optimal designs obtained in this paper are approximate and do not have masses, which are multiples of $1/360$. However, a very efficient design for the inference in the spherical harmonic regression model of degree 7 using 360 different points can easily be obtained as follows. The quadrature formula obtained from Table 4.1 has equal masses as 23 nodes and yields a design of the form (3.7), say $\{\theta_i, 1/23\}_{i=1}^{23}$, where $\theta_i = \arccos x_i$ and $x_1, \dots, x_{23}$ are the points listed in Table 4.1 for the case $d = 7$. We propose to combine this design with two designs of the form (3.8) to obtain an efficient exact design. More precisely we propose to use the uniform distribution ξ_U^* at the points

$$\begin{aligned} \mathcal{U} \;=\; & \Big\{(\theta_i, \frac{\pi(2j-15)}{15}) \;\Big|\; i = 1, \dots, 8;\; j = 1, \dots, 15\Big\} \\ & \cup \Big\{(\theta_i, \frac{\pi(2j-16)}{16}) \;\Big|\; i = 9, \dots, 23;\; j = 1, \dots, 16\Big\} \end{aligned} \tag{4.10}$$

as design for the spherical harmonic regression model of degree 7. The efficiencies of the exact design ξ_U^* are depicted in the second row of Table 4.4 and we observe that this design, which advises the experimenter to take one observation at each point of $\mathcal{U}$, is highly efficient with respect to all optimality criteria under consideration.

$\mathrm{eff}_{\Psi,-1,r}$											
1	2	3	4	5	6	7	8	9	10	eff_A	eff_D
0.003	0.006	0.008	0.011	0.013	0.016	0.019	0.021	0.024	0.026	0.149	0.840
0.958	0.958	0.958	0.958	0.958	0.958	0.958	0.958	0.958	0.958	0.987	0.992

Table 4.4. *D-, A-, E- and efficiencies $\mathrm{eff}_{\Psi,-1,r}$ ($r = 2, \dots, 10$) in the spherical harmonic regression model of degree 7 of the design used by Ding et al. (2000) which is given by (4.8) with $n_1 = 10$ and $n_2 = 36$ (first row). The second row gives the efficiencies of the design defined by (4.10), which takes one observation at each point of the set $\mathcal{U}$.*

5 Appendix: technical details

5.1 Proof of Lemma 3.1.

Assume that condition (A) and (B) of Lemma 3.1 are satisfied and let $Q(x)$ denote an arbitrary polynomial of degree p. By Bezout's theorem the polynomial Q can be represented in the form

$$Q(x) = P(x)V_r(x) + R(x), \tag{5.1}$$

where $V_r(x) = \prod_{j=1}^r (x - x_j)$, the polynomial $P(x)$ is of degree $p - r$ and the degree of $R(x)$ is less than r. Because the degree of R is at most $r - 1$ it can be represented as

$$R(x) = \sum_{j=1}^r \ell_j(x) R(x_j), \tag{5.2}$$

and we obtain from the conditions (A) and (B) of the Lemma

$$\begin{aligned} \frac{1}{2}\int_{-1}^{1} Q(x)dx &= \frac{1}{2}\int_{-1}^{1} R(x)dx = \frac{1}{2}\sum_{j=1}^r R(x_j)\int_{-1}^{1} \ell_j(x)dx \\ &= \sum_{j=1}^r R(x_j)w_j = \sum_{j=1}^r Q(x_j)w_j. \end{aligned}$$

Using the functions $Q(x) = x^\ell$ ($\ell = 0, \dots, p - r$) yields the identities in (3.2).
For a proof of the converse we assume that (3.2) is valid and obtain for $\ell = 0, \dots, p - r$

$$\int_{-1}^{1} V_r(x)x^\ell dx = \sum_{j=1}^r V_r(x_j)x_j^\ell w_j = 0,$$

which gives condition (A). On the other hand condition (B) follows from the identity

$$\frac{1}{2}\int_{-1}^{1} \ell_j(x)dx = \sum_{i=1}^r w_j \ell_j(x_i) = w_j$$

observing the property $\ell_j(x_i) = \delta_{ij}$ for the Lagrange interpolation polynomials.

□

5.2 Proof of Theorem 3.6.

Let ξ denote an arbitrary discrete design on the rectangle $[0, \pi] \times (-\pi, \pi]$ and denote by $\theta_1, \dots, \theta_N$ the distinct first coordinates of the corresponding support points of ξ. Obviously ξ can be represented as

$$\xi = \sum_{i=1}^N \xi_i, \tag{5.3}$$

where the designs ξ_i are defined by

$$\xi_i = \begin{pmatrix} (\theta_i, \phi_{i1}) & \dots & (\theta_i, \phi_{iN_i}) \\ w_{i1} & \dots & w_{iN_i} \end{pmatrix}$$

(with $N_i \in \mathbb{N}$) and represent the part of ξ corresponding to the support points with first coordinate equal to θ_i $(i = 1, \dots, N)$. Define $x_i = \cos\phi_i$, $w_i = \sum_{j=1}^{N_i} w_{ij}$ $(i = 1, \dots, N)$ and consider the design

$$\eta = \eta_\xi = \begin{pmatrix} x_1 & \dots & x_N \\ w_1 & \dots & w_N \end{pmatrix}. \tag{5.4}$$

If the design ξ satisfies the condition $M(\xi) = I_{(d+1)^2}$ it follows for the submatrix corresponding to the $(d+1)$ regression functions $Y_\ell^0(\theta, \phi) = \sqrt{2\ell+1} P_\ell^0(\cos\theta)$ $(\ell = 0, \dots, d)$

$$\begin{aligned} I_{d+1} &= \Big(\int_0^\pi \int_{-\pi}^\pi Y_\ell^0(\theta,\phi) Y_k^0(\theta,\phi) d\xi(\theta,\phi) \Big)_{\ell,k=0}^d \\ &= \Big(\sum_{i=1}^N \sum_{j=1}^{N_i} w_{ij} \sqrt{2\ell+1}\sqrt{2k+1} P_\ell^0(x_i) P_k^0(x_i) \Big)_{\ell,k=0}^d \\ &= \Big(\sqrt{2\ell+1}\sqrt{2k+1} \sum_{i=1}^N w_i P_\ell(x_i) P_k(x_i) \Big)_{\ell,k=0}^d \end{aligned} \tag{5.5}$$

(note that $P_\ell^0(x) = P_\ell(x)$ is the ℓth Legendre polynomial). On the other hand the orthogonality relation for the Legendre polynomials [see Szegö (1975)] yields

$$\frac{1}{2} \int_{-1}^1 P_\ell(x) P_k(x) dx = \frac{\delta_{\ell k}}{2\ell+1};\ \ell, k = 0, \dots, d; \tag{5.6}$$

and it follows from (5.5) that the quadrature formula defined by the design η in (5.4) integrates polynomials of degree $2d$ exactly. The assertion of Theorem 3.6 now follows from the following auxiliary lemma.

□

Lemma 5.1. *For any $n \in \mathbb{N}$ let Ξ denote the set of all probability measures on the interval $[-1, 1]$ of the form (5.4), which integrate polynomials of degree n exactly, i.e.*

$$\frac{1}{2} \int_{-1}^1 x^\ell dx = \sum_{j=1}^n w_j x_j^\ell; \quad \ell = 0, \dots, n, \tag{5.7}$$

then

$$\min_{\eta \in \Xi} \min \Big\{ v \in \mathbb{R}^+ \mid supp\, \eta \subset [-v, v] \Big\} = |x_1^*|$$

where x_1^* is the smallest root of the rth Legendre polynomial $P_r(x)$ and $r = \lfloor n/2 \rfloor + 1$. Moreover, the minimum is attained by the measure

$$\eta^* = \begin{pmatrix} x_1^* & \dots & x_r^* \\ w_1^* & \dots & w_r^* \end{pmatrix}, \tag{5.8}$$

where the points $x_1^*, \dots, x_r^*$ are the roots of the Legendre polynomial $P_r(x)$, $w_i = \frac{1}{2}\int_{-1}^{1} \ell_i(x)dx$ $(i = 1, \dots, r)$ and $\ell_i(x)$ is the Lagrange interpolation polynomial with nodes $x_1^*, \dots, x_r^*$.

Proof of Lemma 5.1. For a design η on the interval $[-1, 1]$ let

$$u(\eta) := \min\{v \in \mathbb{R}^+ \mid supp\, \eta \subset [-v, v]\} \tag{5.9}$$

denote the half of the minimal length of intervals which contain the support of η and define for each $N \in \mathbb{N}$ the set $\Xi_N \subset \Xi$ as the set of all probability measures with N support points satisfying (5.7) (note that $\Xi = \cup_{N\in\mathbb{N}}\Xi_N$). Because for a design η of the form (5.4) the equations in (5.7) can be written as

$$\frac{1}{2}\int_{-1}^{1} \begin{pmatrix} 1 \\ \vdots \\ x^n \end{pmatrix} dx = \sum_{j=1}^{N} w_j \begin{pmatrix} 1 \\ \vdots \\ x_j^n \end{pmatrix}, \tag{5.10}$$

it follows from Caratheodory's theorem [see Silvey (1980)] that there exists a measure, say $\tilde{\eta}$, with at most $n + 1$ support points $x_{j_1}, \dots, x_{j_{n+1}}$ $(1 \le j_1 < j_2 < \dots < j_{n+1} \le N)$ such that (5.7) is satisfied. Consequently, we obtain

$$\inf_{\eta\in\Xi} u(\eta) = \inf_{\eta\in\Xi_{n+1}} u(\eta). \tag{5.11}$$

If

$$\eta = \begin{pmatrix} x_1 & \dots & x_{n+1} \\ w_1 & \dots & w_{n+1} \end{pmatrix} \in \Xi_{n+1}$$

with $-1 \le x_1 < \dots < x_{n+1} \le 1$ is any probability measure on the interval $[-1, 1]$, which satisfies (5.7), then by Lemma 3.1 the weights can be represented as

$$w_i = \frac{1}{2}\int_{-1}^{1} \ell_i(x)dx,$$

where $\ell_i(x)$ is the *ith* Lagrange interpolation polynomial with nodes $x_1, \dots, x_{n+1}$. Assume that $|x_1| = u(\eta)$ and define for $\varepsilon > 0$ $\tilde{\eta}$ as the measure with weights

$$\tilde{w}_i = \frac{1}{2}\int_{-1}^{1} \prod_{\substack{j=1 \\ j\neq i}}^{n+1} \frac{x - \tilde{x}_j}{\tilde{x}_i - \tilde{x}_j} dx \quad i = 1, \dots, n+1 \tag{5.12}$$

at the points $\tilde{x}_1 = x_1 + \varepsilon, \tilde{x}_2 = x_2, \dots, \tilde{x}_{n+1} = x_{n+1}$. If ε is sufficiently small it follows that all weights $\tilde{w}_j$ are positive which implies $\tilde{\eta} \in \Xi_{n+1}$ and $\tilde{x}_1 > x_1$. In the case $|x_{n+1}| = u(\eta)$ we apply exactly the same argument to the point x_{n+1} and obtain a measure $\tilde{\eta}$ with $u(\tilde{\eta}) < u(\eta)$. Consequently, the infimum in (5.11) cannot be attained in Ξ_{n+1}, i.e.

$$\inf_{\eta \in \Xi} u(\eta) = \inf_{\eta \in \Xi_n} u(\eta). \tag{5.13}$$

We now prove that the infimum on the right hand side cannot be attained in Ξ_t, whenever $t > \lfloor n/2 \rfloor + 1 = r$. For this consider a mesure

$$\eta = \begin{pmatrix} x_1 & \dots & x_t \\ w_1 & \dots & w_t \end{pmatrix} \in \Xi_t.$$

Recall from Lemma 3.1 that the weights have to satisfy (3.4) (with $t = r$) and that by (3.3) the support points satisfy

$$\int_{-1}^{1} \prod_{j=1}^{t} (x - x_j) x^\ell dx = 0; \quad \ell = 0, \dots, n-t. \tag{5.14}$$

Without loss of generality we assume that $|x_1| = u(\eta)$ and we will again construct a design with a smaller value of $u(\eta)$. For this we define $\tilde{x}_1 = x_1 + \varepsilon$, $\tilde{x}_j = x_j$; $j = 3 + n - t, \dots, t$;

$$\psi(x) = (x - \tilde{x}_1) \prod_{j=3+n-t}^{t} (x - \tilde{x}_j) \tag{5.15}$$

and construct the remaining points, say $\tilde{x}_2, \dots, \tilde{x}_{n-t+2}$, such that the resulting measure with weights of the form (3.4) at the points $\tilde{x}_1, \dots, \tilde{x}_t$ defines a quadrature formula of degree n. A necessary condition for this property is given by

$$\int_{-1}^{1} \psi(x) \prod_{j=2}^{n-t+2} (x - \tilde{x}_j) x^\ell dx \ = \ 0; \quad \ell = 0, \dots, n-t \tag{5.16}$$

and a straightforward calculation shows that these equations are equivalent to the system

$$\frac{\partial}{\partial \tilde{x}_i} \int_{-1}^{1} \psi(x) \prod_{j=2}^{n-t+2} (x - \tilde{x}_j)^2 dx \ = \ 0; \quad i = 2, \dots, n-t+2, \tag{5.17}$$

which determines the points $\tilde{x}_j = \tilde{x}_j(\varepsilon)$ $(j = 2, \dots, n-t+2)$ implicitly as a function of the parameter ε, where $\tilde{x}_j(0) = x_j$ $(j = 2, \dots, n-t+2)$. We now consider the Jacobi matrix of the system (5.17)

$$J(\tilde{x}, \varepsilon) = \Big(\frac{\partial^2}{\partial \tilde{x}_j \partial \tilde{x}_j} \int_{-1}^{1} \psi(x) \prod_{k=2}^{n-t+2} (x - \tilde{x}_k)^2 dx \Big)_{i,j=2}^{n-t+2} , \tag{5.18}$$

where we use the notation $\tilde{x} = (\tilde{x}_2, \dots, \tilde{x}_{n-t+2})$. This matrix can be calculated using the quadrature formula corresponding to the measure η. For this note that $\tilde{x}(0) = (x_2, \dots, x_{n-t+2})$ and define the polynomial

$$g_i(x) = 2\psi(x) \prod_{j=2, j \neq i}^{n-t+2} (x - x_j)^2 dx \ . \tag{5.19}$$

Note that the degree of g_i is less or equal than n. If $e_i \in \mathbb{R}^i$ denotes the ith unit vector we obtain

$$
\begin{aligned}
e_i^T J(\tilde{x}(0),0)e_i &= \int_{-1}^{1} g_i(x)dx = \sum_{j=1}^{t} g_i(x_j)w_j \\
&= g_i(x_i)w_i = 2w_i(x_i - x_1) \prod_{j=n-t+3}^{t} (x_i - x_j) \prod_{j=2,j\neq i}^{n-t+2} (x_j - x_i)^2 \neq 0;
\end{aligned}
$$

and by a similar calculation $e_i^T J(\tilde{x}(0),0)e_j = 0$ whenever $i \neq j$ $(i,j = 2,\ldots,n-t+2)$. Consequently $J(\tilde{x}(0),0)$ is diagonal with $\det J(\tilde{x}(0),0) \neq 0$. It now follows from the implicit function theorem [see Gunning and Rossi (1965)] that for sufficiently small ε there exist analytic functions $\tilde{x}_2(\varepsilon),\ldots,\tilde{x}_{n-t+2}(\varepsilon)$ such that (5.16) is satsified for the points $\tilde{x}_1,\ldots,\tilde{x}_t$. This implies that for sufficiently small ε the weights defined by (5.12) are positive and the design

$$
\tilde{\eta} = \begin{pmatrix} \tilde{x}_1 & \ldots & \tilde{x}_t \\ \tilde{w}_1 & \ldots & \tilde{w}_t \end{pmatrix} \tag{5.20}
$$

defines a quadrature formula of degree n with positive weights, i.e. $\tilde{\eta} \in \Xi_t$. If necessary (in the case $|x_t| = u(\eta)$) we use a similar argument for the largest support point of the probability measure η and obtain finally a probability measure $\tilde{\eta} \in \Xi_t$ such that $u(\tilde{\eta}) < u(\eta)$. In other words: the infimum on the right hand side of (5.13) cannot be obtained in Ξ_t, if $t > \lfloor n/2 \rfloor + 1$. From (5.15) it is easy to see that this construction is not possible if $t < r = \lfloor n/2 \rfloor + 1$. Moreover, it is well known [see for example Ghizzetti and Ossicini (1970)] that a quadrature formula, which integrates polynomials of degree n exactly must have at least r support points. Moreover, if it has r support points it is uniquely determined and given by the probability measure η^* defined in (5.8), which completes the proof of Lemma 5.1.

□

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