QUADRATURE ON A SPHERICAL SURFACE

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Abstract. Approximately calculating integrals over spherical surfaces in $\mathbb{R}^3$ can be done by simple extensions of one dimensional quadrature rules. This, however, does not make use of the symmetry or structure of the integration domain and potentially better schemes can be devised by directly using the integration surface in $\mathbb{R}^3$. We investigate several quadrature schemes for integration over a spherical surface in $\mathbb{R}^3$, such as Lebedev quadratures and spherical designs, and numerically test their performance on a set of test functions.

1. Introduction

In various applications the need arises for the calculation of integrals over spherical surfaces in $\mathbb{R}^3$. Examples being calculations using density functional theory (DFT) in computational chemistry [16], a theory used to calculate molecular properties, or solving systems involving radiative transfer equations, e.g. [15].

Integrals over a spherical surface can be brought into a standard form, namely an integral over the unit sphere $\mathbb{S}^2 = \{\mathbf{x} \in \mathbb{R}^3 : \|\mathbf{x}\|_2 = 1\}$

$$I[f] \equiv \int_{\mathbb{S}^2} f(\mathbf{x}) \,\mathrm{d}\Omega = \int_0^{2\pi} \int_0^{\pi} f(\varphi, \theta) \sin\varphi \,\mathrm{d}\varphi \,\mathrm{d}\theta, \tag{1}$$

where $f : \mathbb{S}^2 \to \mathbb{R}$ and the second integral is in the spherical coordinates representation. The case of vectorial functions is a trivial extension from this scalar problem.

Often the precise form of f is either too complicated to integrate analytically or is not known explicitly and can only be sampled at individual points on $\mathbb{S}^2$. It is therefore crucial to be able to compute approximations to integrals of the form (1). One of the most common ways to arrive at such approximations is by use of a numerical scheme, or quadrature, where we approximate the integral by a weighted sum over a finite collection of points $\{\mathbf{x}_i\} \subset \mathbb{S}^2$

$$\int_{\mathbb{S}^2} f(\mathbf{x}) \,\mathrm{d}\Omega \approx \sum_{i=0}^{N-1} w_i f(\mathbf{x}_i) \equiv Q[f], \tag{2}$$

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where w_i denote the weights and $Q[f]$ the quadrature of the exact integral. The theory of quadratures for one-dimensional integrals has a long history and many results can be found in literature, see e.g. [8, 28]. Some of this theory can be extended to the case of integrals of the form (1), a noteworthy difference however is that the distribution of points $\{\mathbf{x}_i\}$ over the surface of the unit sphere is a non-trivial problem on its own.

The discretisation of the unit sphere using a product of one-dimensional quadrature points is likely to be the most trivial extension of standard quadrature theory, but better results could potentially be achieved by using methods more bespoke to the unit sphere. We will therefore look into the problem of the discretisation of the unit sphere using amongst others rotationally invariant sets of points inspired by an early contribution by Sobolev [26].

This paper furthermore explores some of the existing quadrature schemes available to approximate the standard form of spherical integrals (1), using both equally weighted and non-uniformly weighted point sets. We will compare different schemes in terms of convergence and a measure of their efficiency.

2. Quadrature schemes on a sphere

In the construction of a quadrature scheme we have freedom in not only the position of the node set $\{\mathbf{x}_i\}$, but in the choice of the weights w_i as well. A wide variety of quadratures can, however, be derived under the assumption of fixed weights, i.e. the weights do not have to be constructed in conjunction with the nodes. In this case all weights will have to be equal and such quadrature schemes are known as Chebyshev quadratures. In the case where we need to determine both weights and nodes we will speak of Gauss quadratures. Before we start of with quadrature schemes we state some useful theory about the representation of the class of square-integrable functions on the unit sphere, i.e. $L^2(\mathbb{S}^2) = \{\int_{\mathbb{S}^2} |f|^2 \,\mathrm{d}\Omega < \infty\}$.

2.1. Spherical harmonics and efficiency of quadratures.

Square-integrable functions on the unit sphere can be expanded in terms of the spherical harmonics orthonormal basis on the unit sphere [2]. The spherical harmonical functions are given by

$$Y_n^m(\theta,\varphi) = \frac{1}{\sqrt{2\pi}} P_n^m(\cos\varphi) e^{im\theta}, \qquad -n \leq m \leq n, \quad n, m \in \mathbb{N}, \tag{3}$$

where P_n^m are the normalised associated Legendre functions, m is the order of the spherical harmonic and n the degree. We define the finite subset of spherical harmonics up to degree N as $\Pi^N = \mathrm{span}\{Y_n^m(\theta,\varphi) : 0 \leq n \leq N, -n \leq m \leq n\}$. Using these spherical harmonics we can write any $f \in L^2(\mathbb{S}^2)$ as

$$f(\theta,\varphi) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} c_{mn} Y_n^m(\theta,\varphi), \tag{4}$$

where the coefficients c_{mn} can be found via inner products with the basis functions

$$c_{mn} = \int_{\mathbb{S}^2} f(\theta,\varphi) \bar{Y}_n^m(\theta,\varphi) \,\mathrm{d}\Omega. \tag{5}$$

The decay rate of the coefficients depends on the smoothness of the function f and in effect this determines the convergence rate of the spherical harmonics expansion.

From this expansion we can deduce that it would be advantageous for a quadrature scheme to integrate all spherical harmonics up to a certain degree p, i.e. Π^p. This idea was used by McLaren [21] to define the efficiency of quadrature schemes as the ratio of the number of spherical harmonics L to which the scheme produces exact integration to the number of degrees of freedom of the scheme. If a quadrature rule makes use of N points, the number of degrees of freedom will be $3N$ as per integration node a coordinate (θ, φ) and a weight w_i must be specified. By imposing the requirement of exact integration of all spherical harmonics up until degree p one can see that $L = (p+1)^2$ yielding the formula for efficiency as stated by McLaren

$$E = \frac{(p+1)^2}{3N}. \tag{6}$$

2.2. **Gauss quadratures.**

2.2.1. *Products of one-dimensional quadratures.* Using the formulation of (1) in spherical coordinates we can view the integral over the unit sphere as a product of two one-dimensional integrals over θ and φ. As a result we can use quadrature rules for one-dimensional integrals repeatedly to arrive at a quadrature scheme for (1)

$$Q[f] = \sum_{i=0}^{N-1} w_i \sum_{j=0}^{M-1} v_j f(\theta_i, \varphi_j) = \sum_{i=0}^{N-1} \sum_{j=0}^{M-1} \tilde{w}_{ij} f(\theta_i, \varphi_j). \tag{7}$$

The weights $\tilde{w}_{ij}$ are still to be determined by the choice of two one-dimensional quadrature rules. Note that because of the requirement to integrate exactly the spherical harmonics up to a given degree p it is common practice to use an equally spaced scheme, such as the trapezoidal methoad, in θ and Gauss-Legendre scheme for φ. An equally spaced grid of M points ensures exact integration of

$$\int_0^{2\pi} e^{im\theta} \,\mathrm{d}\theta, \tag{8}$$

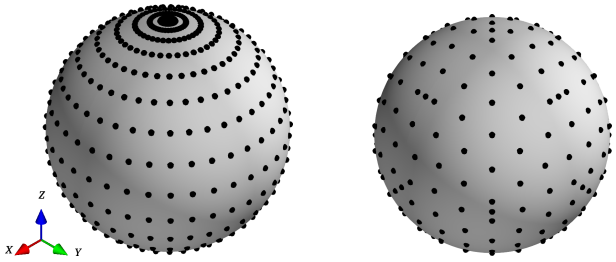
for $|m| \leq M$ whereas a Gauss-Legendre scheme of order n guarantees exact integration of all polynomials $p_l(x)$ up until degree $l = 2n - 1$ over the interval [-1,1]. We can use this and rewrite this such that we get exact results for integrals of the form

$$\int_0^{\pi} p_l(\cos\varphi) \sin\varphi \,\mathrm{d}\varphi. \tag{9}$$

Note though that the associated Legendre polynomials P_n^m are not in fact polynomials if m is odd, but the exact integration still holds [2]. In order to integrate all spherical harmonics up until degree p we would need $(p+1)/2$ points for the φ integral and $(p+1)$ points for the θ integral, yielding a total of $(p+1)^2/2$ points. This results in an efficiency of $E = 2/3$ as was already pointed out by McLaren [21].

The generation of the nodes and weights, up to very high order, can be done in a fast manner using modern techniques, see for example [28], which makes it an easily adaptable scheme. However, a common critique of this Cartesian product scheme, which we will call Gaussian product from now on, is that the distribution of the nodes is clustered around the poles, as can be seen in Figure 1a. One consequence of this is that the grid distance between points close to the poles shrinks significantly.

This could become an issue if the grid is used in solving time-dependent problems where the grid-size often forms a limiting factor for the stable time steps that are allowed.



(A) Gaussian product grid with $N = 800$.

(B) Lebedev grid with $N = 266$.

FIGURE 1. Distribution of nodes for Gauss quadratures.

2.2.2. *Lebedev quadratures.* More in the spirit of the one-dimensional Gauss quadratures we can set out to determine both the nodes and weights at the same time over the whole sphere. In order to do so we impose the constraint that we want to integrate all spherical harmonics up to degree p exactly. This yields a (possibly large[1]) system of non-linear equations which in theory could then be solved to find the nodes and weights, a difficult if not impossible task in general.

It is therefore that we focus here on ideas which stem from a seminal paper by Sobolev [26]. Suppose we have a rotationally invariant integrand f. As the integration domain $\mathbb{S}^2$ is rotationally invariant itself, it would only be natural to try to determine rotationally invariant quadrature schemes. This can be made more precise by letting $G \subset O(3)$ be a finite rotation group on the sphere possibly including inversion. A quadrature scheme is called invariant under G if for all $g \in G$ we have

$$Q[f] = Q[f \circ g]. \tag{10}$$

If we let $\Pi^p_G = \{f \in \Pi^p : f = f \circ g \quad \forall g \in G\}$ be the subset of spherical harmonics up to degree p invariant under G we can state the following theorem.

Theorem 1 (Sobolev [26])**.** *Let Q be a quadrature scheme invariant under the group G. Then, Q is exact for all functions $f \in \Pi^p$ if and only if Q is exact for all functions $f \in \Pi^p_G$.*

This greatly reduces the number of non-linear equations that need to be solved to derive a rotationally invariant scheme as it suffices to only impose exact integration on the invariant spherical harmonics in Π^p_G. Sobolev also states bounds for the size of Π^p_G, which effectively determines the size of the system of non-linear equations which needs to be solved.

We will discuss here one of the most common quadratures based on this idea, Lebedev quadrature. Lebedev constructed a class of quadratures invariant under the octahedron rotation group with inversion $G = O_h$ by working out the invariant spherical harmonics and solving the non-linear equations for degrees up to $p =$

[1]Note that the size of Π^p grows as $(p+1)^2$ with the degree p.

131 [19, 17, 18]. An example of a resulting Lebedev grid can be seen in Figure 1b. Pre-computed numerical values for the nodes and weights have been collected from [7]. Note that the construction of Lebedev quadratures can be tedious as it requires the simultaneous solution to a large number of non-linear equations, which makes this quadrature less adaptive compared to the Gaussian product quadrature. Furthermore, Murray, Handy and Laming [22] argue that it is considerably harder to make use of symmetry in integrands f as the structure of the grid does not allow a trivial decomposition as is the case for the Gaussian product scheme.

The efficiency of the scheme however clearly wins compared to the Gaussian product scheme as it asymptotes towards the conjectured optimal value of $E = 1$ as can be seen in Figure 2. This shows that by using Lebedev quadrature we can achieve the same kind of accuracy as with the Gaussian product scheme using less quadrature points by and order of roughly $\frac{2}{3}$. As a result the Lebedev quadratures need less function evaluations and if the nodes and weights are precomputed this will result in a faster integration scheme.

Sobolev's theorem obviously allows for extensions using different symmetry groups and indeed some initial work by McLaren derived a single quadrature rule using the icosahedron symmetry group [21]. A more substantial extension appeared recently by Ahrens and Beylkin, who constructed a generalised algorithmic approach, albeit of high algorithmic complexity $\mathcal{O}(N^3)$, which can construct quadratures based on both octahedron and icosahedron groups with inversion up to any given order [1].

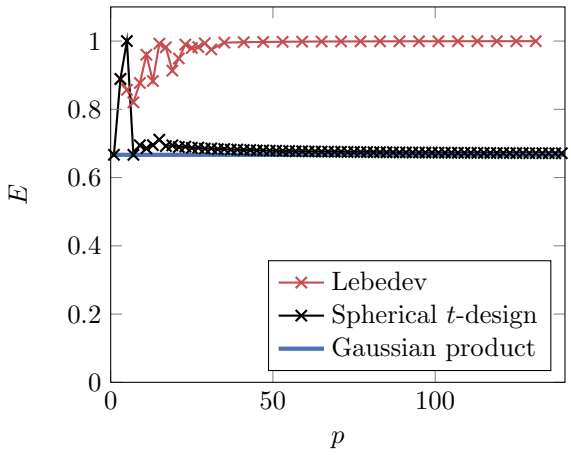


FIGURE 2. Efficiency E as defined in (6) as a function of the maximal degree p of exact integration for various quadratures on the sphere.

2.3. **Chebyshev quadratures.** Another approach to deriving quadratures on the sphere starts from the assumption that the weights of all the N integration nodes are equal. As pointed out by Lebedev [17] quadratures of this type will minimise a probability error if the function values are subject to normally distributed errors, something which could be the case if the integrand can only be empirically sampled. As one wants to correctly integrate the constant function $f \equiv 1$ this implies that

the weights must satisfy

$$w_i = \frac{4\pi}{N}, \qquad i = 0, \dots, N-1. \tag{11}$$

The remaining question now is how the nodes should be scattered along the sphere to achieve optimal quadrature schemes. As the weights are equal for all nodes, this suggests the seemingly trivial answer that the nodes should be uniformly spread out over the sphere. Although this is true in essence, a crucial caveat soon emerges, what does "uniformly spread out" mean in the context of a sphere and how do we calculate these points. This problem has generated a large amount of research in various parts of mathematics and we will only shortly discuss a few possible ways to distribute points on a sphere, see [6] for a more complete recent survey.

2.3.1. *Uniform distribution of points on a sphere - Spherical designs.* If we impose the standard requirement that a quadrature is exact for all spherical harmonics up until order p in the case of equal weights we arrive at the spherical designs. Initially defined by Delsarte, Goethals and Seidel [10] as a problem in algebraic combinatorics its connection with quadratures was soon made. A set of N points $\{\mathbf{x}_i\}$ is called a spherical t-design if

$$\int_{\mathbb{S}^2} f(\mathbf{x}) \, \mathrm{d}\Omega = \frac{4\pi}{N} \sum_{i=0}^{N-1} f(\mathbf{x}_i), \qquad \forall f \in \Pi^t. \tag{12}$$

Obviously one wants to find spherical designs with a minimal amount of nodes and this a subject of active research [13, 3, 6]. The platonic solids can be seen as spherical designs and other early examples were found by Lebedev who, using his formalism of invariant quadratures, derived a 96 and 168 point spherical design of order 11 and 15 respectively [17]. However, the question of the existence of efficient spherical designs for arbitrary degree was only proved in 1984 and gave no indication as to how many points were needed for these designs [24]. A recent breakthrough showed the existence of t-designs for $\mathbb{S}^2$ with $\mathcal{O}(t^2)$ points [5], which is promising as this guarantees that the efficiency will be $E = \mathcal{O}(1)$.

For the actual computation of spherical designs we state one of the initial papers with accompanying website containing the datasets [13, 14] which derived spherical designs up to order $p = 21$. More recent developments and algorithms for the solution of systems of non-linear equations made it possible to find spherical designs up to much higher order [12]. For this paper we used datasets containing spherical designs up to high orders from [29], which lists both symmetrical and unsymmetrical spherical designs, a difference which we will shortly see expressed in the next section in the context of numerical performance. For an example of a spherical 21-design see Figure 3c. We can clearly see that the points appear to be more uniformly spread out compared to the other quadratures that we saw before in Figure 1.

The efficiency of the spherical designs can be seen in Figure 2 and we note that asymptotically it seems that $E \approx \frac{2}{3}$, which would put these quadratures on par with the Gaussian product scheme. Note however that we have used the original McLaren formula (6) to determine E and this assumes 3 degrees of freedom per node. If we instead would interpret the fixed equal weights as a loss of degrees of freedom so that per point there are only 2 degrees of freedom we would get $E \approx 1$.

2.3.2. *Random distribution of points on a sphere - Monte Carlo.* Another approach to Chebyshev quadratures is to use a Monte Carlo scheme where instead of a regular grid we use a randomly generated grid yielding a non-deterministic quadrature scheme. This quadrature can be applied to a more general class of integrals over a multidimensional volume V

$$J[f] = \int_V f(\mathbf{x})\,\mathrm{d}\Omega. \tag{13}$$

It is argued that Monte Carlo integration becomes increasingly competitive for higher-dimensional integrals as it does not suffer from the curse of dimensionality [23].

Let us assume we have acquired a set of N randomly generated nodes $\{\mathbf{x}_i\}$. The question how to sample these will be discussed later. If we use the following notation for the averaging of a function g

$$\langle g \rangle = \frac{1}{N} \sum_{i=0}^{N-1} g(\mathbf{x}_i), \tag{14}$$

we can state the fundamental principle for the Monte Carlo integration which follows from the law of large numbers

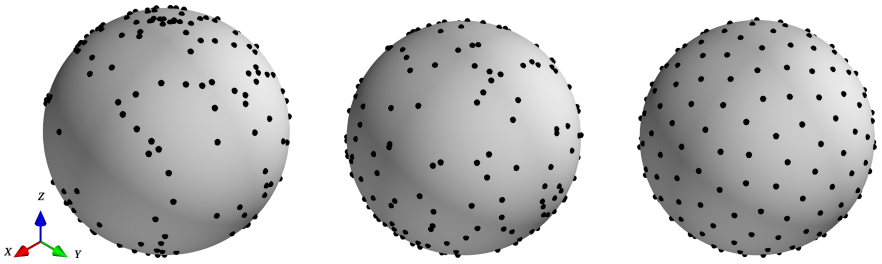
$$J[f] \approx V\langle f \rangle \pm \frac{1}{\sqrt{N}} \sqrt{V^2 \mathrm{Var}(f)}. \tag{15}$$

Here $\mathrm{Var}(f)$ denotes the sample variance of f over our nodes and is given by

$$\mathrm{Var}(f) = \langle f^2 \rangle - \langle f \rangle^2. \tag{16}$$

The error term containing the variance of the integrand is only a rough indication as it is not a strict error bound, which is often the case for deterministic quadratures, and can seriously underestimate the true error if for example the integrand has a very much localised behaviour which could be completely missed by the random grid. Under the assumption of a roughly constant sample variance we see that a Monte Carlo quadrature should take the form $Q[f] = V\langle f \rangle$, which has exactly the same form as spherical designs (12) if the integration is taken over $\mathbb{S}^2$. An estimate of the error using the variance is then given to be $\mathcal{O}(N^{-1/2})$, which is indeed independent of the dimension of the integral.

The actual implementation of a Monte Carlo method for the sphere can be achieved in at least two different ways. The first one starts from the integral formulation (1) in spherical coordinates and therefore uniformly samples random points $(\theta, \varphi) \in [0, 2\pi] \times [0, \pi]$. The function to average over is in this case not equal to the original integrand $f(\theta, \varphi)$, but $f(\theta, \varphi)\sin(\theta)$. The result of a grid simulation using the procedure is a grid with points more concentrated near the poles of the sphere as can be seen in Figure 3a. To resolve this clustering issue we can generate random points uniformly on the sphere instead such that any small unit of area has a similar number of points on average. This can be achieved by letting θ uniform on $[0, 2\pi]$ and u uniform on $[0, 1]$ to construct $\varphi = \arccos(2u - 1)$. A resulting uniformly distributed random grid is depicted in Figure 3b and shows indeed no general clustering over nodes. If this type of grid is used the quadrature function is the original integrand f just as for the spherical designs.



(A) Cartesian product random grid with $N = 240$.

(B) Uniform random grid with $N = 240$.

(C) Spherical t-design for $t = 21$ with $N = 240$.

FIGURE 3. Distribution of nodes for Chebyshev quadratures.

2.4. **Minimal energy quadratures.** Another field of active research into point distribution on spheres and related quadratures is that of energy minimalising point distributions. Without going into much detail we will sketch some of the ideas to derive quadratures using this formalism. For a more detailed exposure we refer to [9, 6, 4] and references therein.

The idea of finding near-uniform node sets on the sphere can be approached in a different manner by considering the nodes as particles confined to the sphere. If we define an interaction potential energy functional between these particles of the form

$$E_K(\mathbf{x}_1, \dots, \mathbf{x}_N) = \sum_{\substack{i,j \\ i \neq j}} K(\mathbf{x}_i, \mathbf{x}_j), \tag{17}$$

the configuration that minimises this energy can be used as a point distribution. Common energy functionals are the Riesz kernel $K(\mathbf{x}_i, \mathbf{x}_j) = \|\mathbf{x}_i - \mathbf{x}_j\|^{-s}$ or the logarithmic kernel $K(\mathbf{x}_i, \mathbf{x}_j) = -\log(\|\mathbf{x}_i - \mathbf{x}_j\|)$ and their minimisation leads to what is known as Fekete problems. The Riesz kernel can be seen as a generalisation of the Thompson problem, in which one tries to find the position of electrical point charges distributed on a conducting sphere [6]. The logarithmic kernel leads to a configuration in which the product of the mutual distances between the points is maximised [4] and the search for an algorithmic approach in determining these so called Fekete points is the subject of Smale's 7th problem [25].

Having found such minimal energy configurations one can either choose to use a Chebyshev quadrature and thus use the configuration as if it were a spherical design [9] or one can choose a Gauss quadrature style approach and determine separately an optimal set of weights. In the latter case the most straightforward way to acquire the weights would be to again enforce exact integration up of Π^p up until a specified order p, see for example [11] for the construction of such quadratures and related issues.

3. Numerical results

We will compare four different quadrature rules that were discussed in the previous section, namely the Gaussian product quadrature, Lebedev quadrature, spherical designs and Monte Carlo quadrature. As noted in the previous section we use

pre-computed nodes and weights for the Lebedev quadrature [7] and for the spherical designs [29]. For the spherical designs we use the symmetric node set. In the Gaussian product quadrature we use M points to discretise θ and $2M$ points to discretise φ and then generate the complete grid by taking their Cartesian product resulting in $N = 2M^2$ points. For the Monte Carlo quadrature we will also compare the two types of nodal distributions as discussed in the previous section.

In order to compare the numerical performance of the different schemes we apply them to a set of test functions with different levels of smoothness and look at the resulting relative error defined by

$$e[f] = \left| \frac{I[f] - Q[f]}{I[f]} \right|, \tag{18}$$

as a function of the number of integration nodes N.

3.1. **Test functions.** We choose a set of test functions based on a set used in literature before to compare quadratures on the sphere [11, 27]

$$f_1(x, y, z) = 1 + x + y^2 + x^2 y + x^4 + y^5 + x^2 y^2 z^2, \tag{19}$$

$$\begin{aligned} f_2(x, y, z) = {} & \frac{3}{4} \exp\left(-(9x-2)^2/4 - (9y-2)^2/4 - (9z-2)^2/4\right) \\ & + \frac{3}{4} \exp\left(-(9x+1)^2/49 - (9y+1)/10 - (9z+1)/10\right) \\ & + \frac{1}{2} \exp\left(-(9x-7)^2/4 - (9y-3)^2/4 - (9z-5)^2/4\right) \\ & - \frac{1}{5} \exp\left(-(9x-4)^2 - (9y-7)^2 - (9z-5)^2\right) \end{aligned}, \tag{20}$$

$$f_3(x, y, z, \alpha) = (1 + \tanh(-\alpha(x + y - z))/\alpha, \tag{21}$$

$$f_4(x, y, z, \alpha) = (1 - \operatorname{sign}(x + y - z))/\alpha, \tag{22}$$

$$f_5(x, y, z, \alpha) = (1 - \operatorname{sign}(\pi x + y))/\alpha. \tag{23}$$

The functions are designed to have spherical harmonics expansions (4) with increasing convergence rates. Only the first test function has a finite expansion, with spherical harmonics of order up to 6, and the other functions have infinite expansions. Note that f_4 can be seen as a discontinuous function analogue to f_3 with only two levels along the sphere, which divide the sphere in half. Its expansion will converge very slowly and we can therefore expect slow convergence for any quadrature.

The exact values of the integral to which we compare the quadrature results are taken from [11]

$$I[f_1] = \frac{216\pi}{35}, \tag{24}$$

$$I[f_2] = 6.6961822200736179523\ldots, \tag{25}$$

$$I[f_3] = \frac{4\pi}{\alpha}, \tag{26}$$

$$I[f_4] = \frac{4\pi}{\alpha}, \tag{27}$$

$$I[f_5] = \frac{4\pi}{\alpha}. \tag{28}$$

3.2. **Results.** As can be seen in Figure 4 the rapid converging spherical harmonics expansion results in a fast convergence of the quadrature schemes. Both the spherical design and the Lebedev quadrature need fewer points to arrive at an approximation up to machine precision compared to the Gaussian product. This could be expected from the schemes respective efficiencies. We can also see an error convergence for the Monte Carlo methods as expected, $\mathcal{O}(N^{-1/2})$. Monte Carlo 1 uses points picked from a uniform distribution over the sphere and Monte Carlo 2 uses the uniformly points on the Cartesian product $[0,\pi]\times[0,2\pi]$ and both methods seem to yield comparable results.

The increase in the relative error for Lebedev quadrature is possibly due to the fact that the nodes are only approximately known and small errors in the nodes or weights could yield a small loss of accuracy. It has to be noted that the calculation of the spherical designs has been a recent endeavour (2015) whereas the Lebedev node values seem to stem from an older C code (1999) by Lebedev and Laikov [20] which could be a reason for a difference in relative precision of the quadratures.

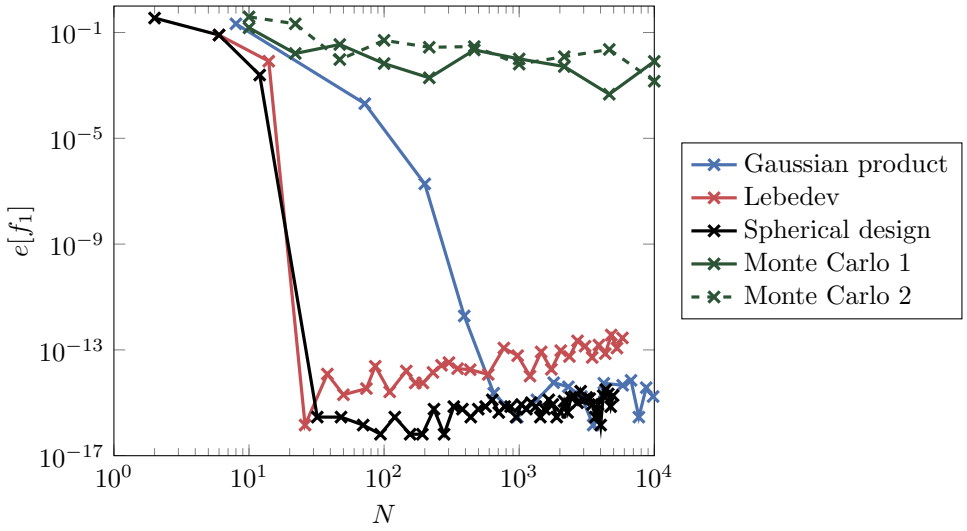


FIGURE 4. Relative errors $e[f_1]$ for different quadratures as a function of the number of integration nodes N.

If we now consider f_2 we see in Figure 5 that we need more points to achieve machine precision as could be expected from the fact that the spherical harmonics expansion now is an infinite series. The quadratures will achieve machine precision integration if they exactly integrate all spherical harmonics up to the degree for which the coefficients in the expansion become smaller than machine precision. Again we see the trend that the spherical design and Lebedev quadrature need less points compared to the Gaussian product quadrature, but their convergence behaviour is very similar.

If we continue to a supposedly even more slowly converging spherical harmonic expansion, that for f_3, we see something remarkably happening in Figure 6. First of all we see that Lebedev quadrature and spherical designs result in exact integration for all N. Furthermore we see a clear distinction between the two different types

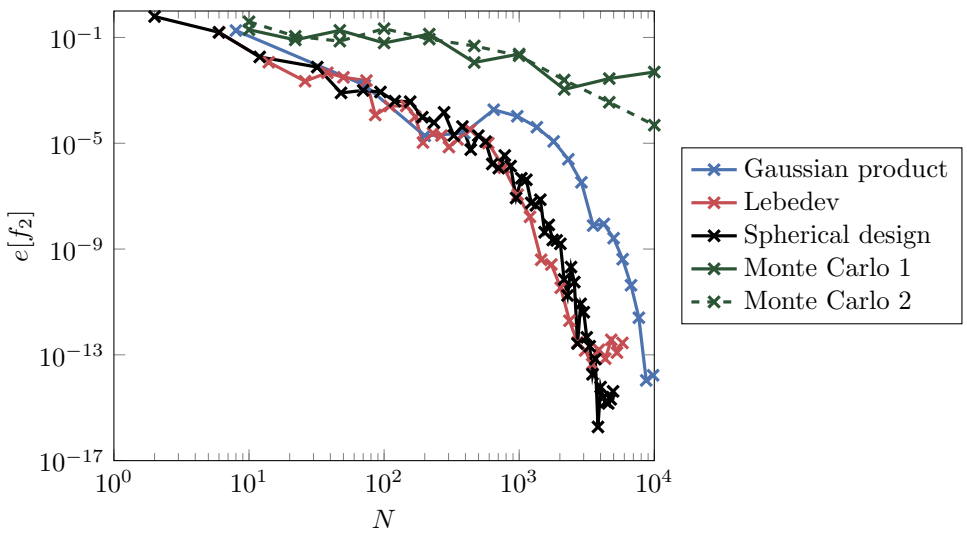


FIGURE 5. Relative errors $e[f_2]$ for different quadratures as a function of the number of integration nodes N.

of Gaussian product quadratures. This can all be traced back to the fact that the function f_3 satisfies a certain symmetry. The plane $x+y-z=0$ divides the sphere in two equal halves over which the tanh part of f_3 is anti symmetric. As a result the spherical expansion of f_3 will be of the form

$$f_3(\theta,\varphi) = c_{00}Y_0^0(\theta,\varphi) + \sum_{\substack{n=1\\ n \text{ odd}}}^{\infty} \sum_{m=-n}^{n} c_{mn}Y_n^m(\theta,\varphi). \tag{29}$$

We call a quadrature grid symmetric if for any $\mathbf{x}$ in the grid its antipode $-\mathbf{x}$ is also part of the grid. It is easy to convince oneself that any quadrature with a symmetric grid will integrate all spherical harmonics of odd degree exactly. And as a result we find that such quadratures will yield exact integration of f_3 using an arbitrary number of nodes. This symmetric property holds indeed for the Lebedev quadrature and spherical designs, which explains their extraordinary good convergence when applied to f_3.

As for the Gaussian product quadrature we can apply similar arguments. If we take for the θ discretisation $2M$ points the resulting grid will be non symmetric and we see the standard Gaussian product convergence behaviour, but now for a less smooth function. If on the other hand we take $2M+1$ points for the θ discretisation we arrive at a symmetric grid and thus will exactly integrate f_3 as we can see in Figure 6. Why the latter version does not integrate exactly for $N < 10^2$ remains unclear.

If we consider the discontinuous functions f_4, f_5 we see again a clear effect of symmetry. We see that for f_4 the spherical designs result in exact integration and this holds for the $(2M+1)$ adapted Gaussian product for large enough N too. Again this will be due to a symmetric grid and the fact that the function itself is antisymmetric in a way that divides the sphere in two halves. However, what is interesting to note is that the Lebedev quadrature behaves very irregularly,

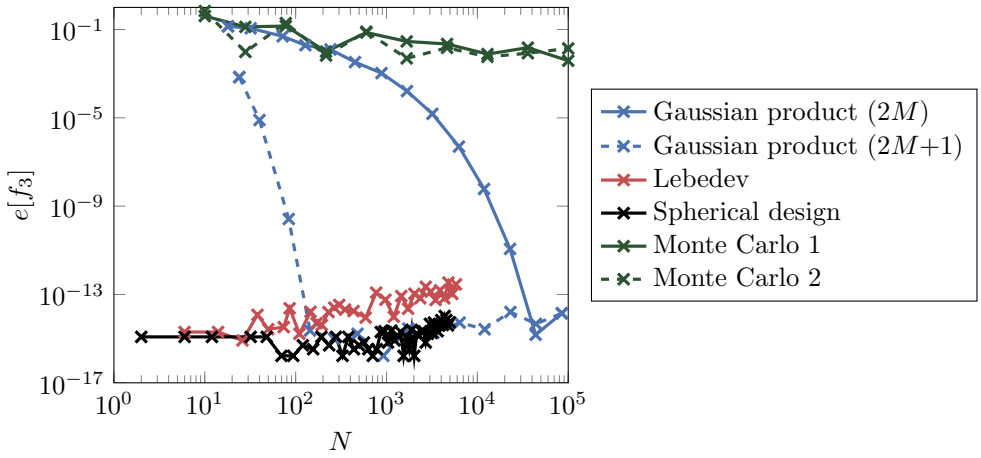


FIGURE 6. Relative errors $e[f_3]$ for different quadratures as a function of the number of integration nodes N for $\alpha = 12$. For the Gaussian product we take two different grids, one with an even number of points $2M$ for the θ grid and one with an odd number of points $2M + 1$.

switching between exact integration and behaviour as bad as Monte Carlo. This is due to the fact that for this choice of function f_4 there will be points of the Lebedev grid which will lie on the discontinuity line of the function. As a result errors will be introduced in the quadrature. If none of the integration nodes lies along the discontinuity, as is the case for spherical designs, the quadrature will be exact.

We can change the function slightly so that we shift the line of discontinuity so that for spherical designs there will be grid points too located at the discontinuity line of the function. As a result the exact integration will break down as can be seen in Figure 8. The $(2M + 1)$ adapted Gaussian product however still manages to do exact integrations if N is large enough.

Noteworthy furthermore is the fact that in the case of the original Gaussian product quadrature we observe a convergence rate of the quadrature of $\mathcal{O}(N^{-1/2})$, which means that it is on par with Monte Carlo methods. The Lebedev quadrature and spherical designs seem to do better and show an error which seems to be $\mathcal{O}(N^{-1})$.

4. Conclusion

In this paper we reviewed the problem of finding quadrature schemes on a spherical surface in $\mathbb{R}^3$. A large variety of quadratures exist and in this paper we have focussed on four of these, a Cartesian product of one-dimensional quadratures, Lebedev quadrature, spherical designs and Monte Carlo quadrature. Theory and background on the different quadratures was given in Section 2. In Section 3 the quadratures were compared by using a set of test functions which differ in how challenging they are to integrate. We found that overall the spherical designs and Lebedev quadratures seem to perform best under most general assumptions. The Cartesian product quadrature shows a similar convergence rate, albeit slightly slower because it uses more points. The advantage of this approach, however, is

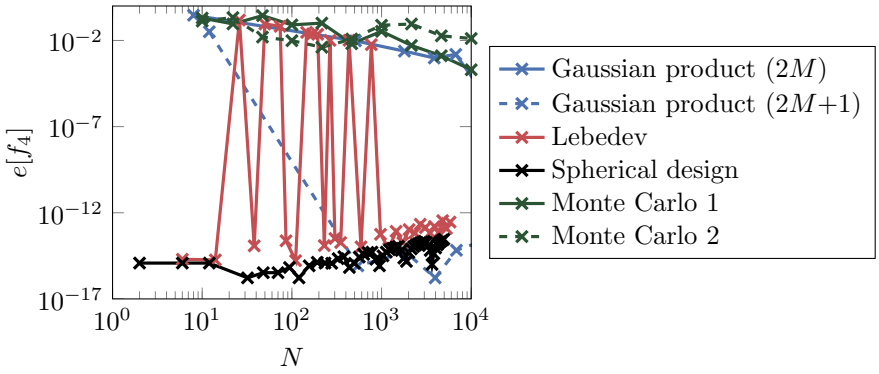


FIGURE 7. Relative errors $e[f_4]$ for different quadratures as a function of the number of integration nodes N for $\alpha = 12$.

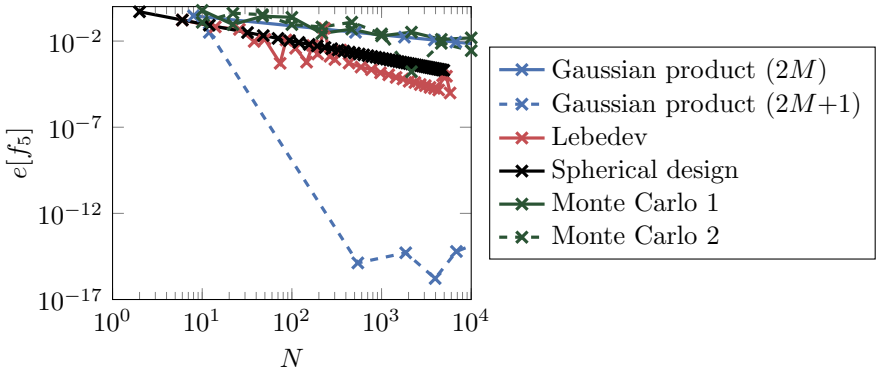


FIGURE 8. Relative errors $e[f_5]$ for different quadratures as a function of the number of integration nodes N for $\alpha = 12$.

that the quadrature is easy to generate for large orders, something which is not yet the case for Lebedev quadrature or spherical designs.

Several extensions of the work in this paper exist and are mentioned throughout the text. Of particular interest we think is Smale's 7th problem which asks for an algorithmic way to (cheaply) find minimising energy distributions over a sphere which could then be used for quadratures. Along the same line a cheap algorithm which can generate Lebedev-type quadratures up to arbitrary order remains to be found.

We would like to add to the list of possible extensions the problem of finding good quadrature schemes for integration on spherical surfaces $\mathbb{S}^d \in \mathbb{R}^d$ where d is not necessarily equal to 3, see for example [6, 9, 3].

Lastly another approach to quadratures on the sphere could be to take a different set of basis functions used to expand the integrand, such as radial basis functions. This is a type of basis which is often used in interpolation along scattered nodes on the sphere and it can be used to generate quadrature rules as well [27].

Appendix A. Code

Python code for the quadratures discussed and to generate the figures in this paper is freely available for personal use from

https://bitbucket.org/CasperBeentjes/quadratures-on-unit-sphere.

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