NOTE 8

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Version two: title change, - half section on pdf's,
+ 'toss away' example, + repositioning technique
via direction cosines, all posted on 10.03.2012

UNIFORMLY DISTRIBUTED RANDOM DIRECTIONS IN BOUNDED SPHERICAL AREAS

PART I: **Conventional Approaches for Attitude purposes**

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Abstract The well known link between spacecraft attitude and unit vectors in dimension three and four is at the origin of requirements to simulate random directions or equivalently generate points on the S^2 and S^3 spheres. In this first part the attention will be focused onto uniform distributions contained in single limited areas bounded by small and great circles which are typically generated by the usual formulation of definite integrals over polar co-ordinates. An example of a 'toss away method' is worked out in the case of a spherical triangle to show how these conventional areas can further be exploited to obtain uniform direction distributions in arbitrary spherical figures. It will further be shown that, in dimension four, areas useful for attitude purposes are in fact spherical subspaces obtained by constraints which specifically apply to rotations represented by the Rodrigues four-vector. Part II is devoted to uniform random distributions contained inside general trigonometrical circumferences and implemented without toss away intervention on S^2, employing a novel analytical area ratio method. Moreover, a direct algorithm based on pseudo co-ordinates and adapted to spherical rectangles is presented as well.

INTRODUCTION

Let us start by noticing that the direction of a sensing target or the orientation of the spin axis of a spin stabilized satellite corresponds to a unit vector or equivalently a point on the three dimensional unit sphere mathematically denoted by S^2. These directions may be constrained by system requirements, or by the presence of optical baffles, or by some other limitations. Such constraint boundaries normally translate into closed geometrical figures on the unit sphere. In the same way, the instantaneous three axis attitude corresponds to a three dimensional rotation which is fully defined by the four scalar Euler-Rodrigues parameters or by what we call the Rodrigues four-vector[1]. This vector happens to be a unit vector and thereby a three axis attitude corresponds to a point on the four dimensional sphere S^3. If a roll-pitch-yaw motion is constrained within given limits – for instance a random start point of a three-axis attitude simulation which corresponds to a random rotation constrained in size and starting from a initial given attitude – the constraint usually correspond to a closed subspace on the four dimensional sphere. Providing the basic background to cover these random direction generation needs for a limited class of

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special spherical figures is the aim of this note. The corresponding algorithms are presented here and in our Notes 10.

We have not found dedicated contributions dealing with geometrically isolated distributions on spheres. Moreover, the intuitive approximations which are employed for random direction generation in limited areas of the three or four dimensional spheres in the fields of measurement, estimation and control do normally not get the attention which is required to guarantee the quality of the result. The spherical surface parts we will handle here should be considered to be examples giving the background allowing the construction of random direction **p**robability **d**istribution **f**unction(s) or pdf's as far as feasible. In this part we will more in particular first look at the possibilities to manipulate the integration limits of the definite integrals involving the standard pdf's and the corresponding expectations which allow a close verification of the random direction generation efficiency. This will first be performed for S^2, a case which does not involve any interpretation difficulties. To this we will add a toss away example involving an arbitrary spherical triangle. For S^3 we will explicitly identify the properties of the particular unit vectors we are looking for, before presenting methods comparing to those derived for S^2.

HISTORICAL BACKGROUND

The numerical generation of uniform direction distributions on the complete spherical surface of any finite dimension has been studied since the middle of the twentieth century. If one is only interested in this global type of uniform random direction simulation one may find some information in Watson[2] as well as in Fischer[3], but for dimension four the list provided by Shuster[4] is the better choice. We may nevertheless complement these references by highlighting the origin of a few methods. It all started with the upcoming availability of electronic computing. The first contributor we identified, was the famous mathematician John Von Neumann[5]. He proposed in 1951 to simulate uniform directions in two dimensions by first generating two uniformly distributed coordinates inside a square and toss away those coordinates not laying inside or on the inscribed circle. He further proposed to transform these two co-ordinates in a unit vector without using a square root. A trick which also has its equivalent for dimension four[6]. When one considers a sphere in a cube the proportion of co-ordinates to be tossed away for higher dimensions grows rapidly and is already 47% in dimension three. Therefore this algorithm is usually avoided in practice. Soon afterwards Mueller[7] reported that by obtaining n random numbers belonging to the same normal distribution and just normalizing this n-tuple one obtains a unit vector which is uniformly random in dimension n. In the same year (1959) Hicks and wheeling[8] derived a method to extend a uniform random direction in dimension $n-1$ to an equally uniformly distributed n-dimensional unit vector in dimension n. Next to come were the, in our opinion, two numerically most efficient algorithms namely the algorithm of Sibuya[9] in 1964 and the one of Tashiro[10] in 1977. The former is tailored to and optimal for uniform random distributions of even dimension, the latter applies to odd dimensions. They should thus be applied especially in higher dimensions if a huge number of random directions needs to be generated in the shortest possible processing time. But even if a few hundred random directions have to be simulated at once, the method relying on the normal distribution is by far the most comfortable being hardly prone to implementation errors. In this paper we will only describe such global uniform random direction simulations which allow a modification which is, in one way or another, useful for constructing algorithms applicable to limited areas.

THE POLE OR REFERENCE DIRECTION

All the algorithms we will derive, are based on very particular choices of the position of the spherical figure in which we generate uniformly distributed random points. This original position is independent of the ultimate practical position where the direction vectors have to be located. This means that in the majority of the applications a simple repositioning algorithm will have to be systematically applied to each generated random point of a given sample. At the same occasion each point will be tranformed in a unit vector which is the actual random direction we are aiming for. The figures we consider will all first be located so that either their center or one of their corners coincide with the pole of a polar co-ordinate system. The figure itself in which random point have to be simulated is called the area of applicability which we represent by S. It is assumed that the pdf is non-zero only inside S.

In line with general practice, in dimension k we will choose the last Cartesian co-ordinate x_k to be the pole or reference direction so that polar co-ordinates on the unit sphere S^2 correspond to

$$x_1 = \cos\alpha \, \sin\epsilon, \qquad x_2 = \sin\alpha \, \sin\epsilon, \qquad x_1 = \cos\epsilon \tag{1}$$

In astronomy α is a 'right ascension', while ϵ is generally called a 'colatitude' from dimension three onwards. We will also employ these denominations here. For we will also look at the unit sphere S^3 in dimension $k = 4$ the polar co-ordinates used in that case are

$$x_1 = \cos\alpha_1 \sin\alpha_2 \sin\epsilon, \quad x_2 = \sin\alpha_1 \sin\alpha_2 \sin\epsilon, \quad x_3 = \cos\alpha_2 \sin\epsilon, \quad x_4 = \cos\epsilon \tag{2}$$

When we work with unit vectors, we represent the positive polar direction by $\mathbf{v}_0$ and any other arbitrary direction by $\mathbf{v}_e$. The angle between these vectors is thus a colatitude, or simply ϵ, what we formally represent by the inner product:

$$< \mathbf{v}_0 \cdot \mathbf{v}_e > = \cos\epsilon \tag{3}$$

The name 'mode' which one finds in the literature about random directions is given to the statistical mean direction(s) of a sample of 'observed' directions contained in an area S. Normally the 'mode' needs to be found or an empirical pdf has to be determined around an observed mode, in contrast to our problem where a well defined statistical situation has to be simulated. Therefore, the 'mode' is not an adequate notion in the present context. The distributions considered here will be called **L**imited **A**rea **U**niform **D**istribution (LAUD).

PDF'S FOR SPHERICAL AREAS

The two types of orthogonal co-ordinate systems, indicated when dealing with geometry on spheres, are the Cartesian co-ordinates on the one hand and the spherical co-ordinates on the other hand. For the latter we have just before selected the polar variant which involves a colatitude ϵ. This section recalls the conventions employed for a pdf which relies on polar co-ordinates

If we restrict ourselves to continuous distributions a pdf $p(x_1, \ldots, x_k)$ is a positive, finite and single valued increasing function integrating to one over its validity area S as follows:

$$1 = \int_S p(x_1, \ldots x_k)\, dx_1, \ldots dx_k \tag{4}$$

Thus, by convention, the pdf includes any metric factors which are dictated by the properties of the underlying manifold and the corresponding co-ordinates employed. This convention allows to give the well known general definition for the mathematical expectation of an arbitrary function $f(x_1, \ldots x_k)$ integrable over S, namely:

$$\mathrm{E}\,(f) = \int_S f(x_1, \ldots x_k)\, p(x_1, \ldots x_k)\, dx_1, \ldots dx_k$$

without having to care about the potential underlying geometry.

For our particular case a little introduction is given in Note 4, explaining the well known method to derive the infinitesimal surface elements for a k-dimensional sphere. If more background is desired, we refer to the very readable chapters VII and VIII of the classical book by A.P. Wills [11]. For S^2 and S^3 these elements are:

$$dS_2 = \sin\epsilon\, d\alpha\, d\epsilon, \qquad dS_3 = \sin\alpha_1\, \sin^2\epsilon\, d\alpha_1\, d\alpha_2\, d\epsilon \tag{5}$$

respectively. In our problem we have to simulate an arbitrary number of random directions which, in the end, must have the same density per area unit everywhere in S, or in other words: distributed uniformly in S. Because the probability to find a direction in an area unit must the same everywhere, this corresponds to a probability model function

$$h(\alpha,\, \epsilon) = \frac{1}{\int_S\, dS_2}$$

as if S^2 were a plane. To arrive at the required shape prescribed by (4) including the effect of the polar manifold we write

$$1 = \int_S h(\alpha,\, \epsilon)\, dS_2 = \int_S \frac{\sin\epsilon}{\int_S\, dS_2}\, d\alpha\, d\epsilon = \int_S p(\alpha,\, \epsilon)\, d\alpha\, d\epsilon \tag{6}$$

Consequently the pdf's expressed in polar co-ordinates for an area S on S^2 and S^3 are:

$$p_2(\alpha,\, \epsilon) = \frac{\sin\epsilon}{\int_S\, dS_2}, \qquad p_3(\alpha_1, \alpha_2,\, \epsilon) = \frac{\sin\alpha_1\, \sin^2\epsilon}{\int_S\, dS_3} \tag{6}$$

respectively. This indicates that from dimension three onwards, the probability density of any type of uniform random distribution has to be zero at the pole ($\epsilon = 0$). This is a well known statistical insight also occurring with other types of distributions. It is caused by the fact that the surface element dS itself becomes zero at $\epsilon = 0$. Pdf's expressed in other parameters not relying on a spherical colatitude co-ordinate, do not show this peculiarity, as is the case in the paper by Weinberger [12].

The pdf's we will work out have the main purpose to allow the correct simulation of random directions having the properties inherent to the pdf they are derived from. To this end we will, in a number of cases, have to perform probability transformations from a uniformly distributed real number in a given line interval to a random spherical co-ordinate which is also uniformly distributed on the sphere. This is achieved by the well known relation between the cumulative distribution function $F_x(\eta)$ corresponding to the pdf $p(x)$ – integrated up to the new transformed random variable η – with the random variable ξ distributed uniformly between zero and one, or

$$\xi \;=\; F_x(\eta) \;=\; \int_{-\infty}^{\eta} p(x)\, dx \tag{7}$$

The integration involved normally leads to a non-linear function of the unknown η, while ξ is the input to (7). If an explicit analytical expression for η cannot be obtained on the basis of (7), we will systematically apply the method of the chord to solve the non-linear function for η as a function of ξ. This is feasible because the right hand side of (7) is an increasing function of η. The transformation (7) works for one variable only. The straight forward application of (7) is thus only possible if the pdf for a random direction can be factorized as follows:

$$p(\alpha_1, \ldots, \alpha_{k-2}, \epsilon) = p_\epsilon \prod_{i=1}^{k-2} p_i(\alpha_i)$$

which is the case in this Note. This factorization is no longer possible in area ratio methods presented in Note 10. In that case the difficulty will be overcome by a step by step factitious integration allowing each time the application of (7). In fact the integration result will be obtained indirectly by means of analytical area expressions.

UNIFORM DISTRIBUTIONS ON S^2

Global Uniform Distributions

All known algorithms to simulate uniformly distributed random directions on the complete S^2 sphere, which only rely on the generation of *uniformly* distributed *scalars*, permit a particularization to spherical caps, rings and parts of them, except the ball in the box case. We therefore look to the former as an introduction to LAUDs on the sphere in three dimensions. To easily include the intervention of uniformly distributed random numbers we introduce the convention that, for the *generation process* of a uniformly distributed random number ξ inside a prescribed interval (a, b) on a line, we will write

$$\xi_i \;=\; \rho_u^{(i)} \qquad a \le \xi \le b \tag{8}$$

where ρ_u is the process itself and i stands for the i-th random number involved if more than one different statistically independent random number is required for the simulation of a single random direction.

We know that the surface of a three dimensional unit sphere is equal to 4π. Hence, we can divide the corresponding surface integral by 4π or:

$$1 \;=\; \frac{1}{4\pi} \int_{\epsilon=0}^{\pi} \int_{0}^{2\pi} \sin\epsilon \; d\epsilon \; d\alpha \tag{9}$$

which directly compares to (6). From this integral we derive that the pdf of the global uniform distribution expressed in polar co-ordinates, is simply:

$$p(\alpha,\,\epsilon) \;=\; p_\alpha p_\epsilon \;=\; \Big(\frac{1}{2\pi}\Big)\,\Big(\frac{\sin\epsilon}{2}\Big) \tag{10}$$

Consequently, obtaining a random angle α is equivalent to generating a uniformly distributed random number in an interval of length 2π. The variables ϵ is distributed like a sine function requiring the intervention of (7) yielding:

$$\eta \;=\; \arccos\,(1\;-\;2\,\xi) \tag{11}$$

The (a) pdf based algorithm for generating pseudo random directions on S^2 as a whole proceeds as follows:
a1. $\xi_1 \;=\; \rho_u^{(1)}$ with $0 \le \xi \le 1$
a2. get $\epsilon \;=\; \eta$ by applying (11)
a3. $\alpha \;=\; \xi_2 \;=\; \rho_u^{(2)}$ with $-\pi \le \xi < \pi$
a4. $x_1 \;=\; \cos\alpha\sin\epsilon,\quad x_2 \;=\; \sin\alpha\sin\epsilon,\quad x_3 \;=\; \cos\epsilon$
The character (a) just used is employed to denote the particular algorithm which is redundantly referred to by a name, here 'pdf'.

The pdf based algorithm just described and the algorithm of Hicks and Wheeling[8] limited to dimension three are almost equivalent. To describe the central idea of their procedure in our notations, we start from p_ϵ in (10) and write $n_{0k} = \int_0^{\pi/2} \sin^{k-2}\epsilon\, d\epsilon$ for the normalization constant limited to ϵ in an hemisphere of dimension k. Substituting $\sin\epsilon$ by s and employing the fact that $d\epsilon = \cos^{-1}\epsilon\; d(\sin\epsilon)$ leads to

$$2\,\xi \;=\; \frac{1}{n_0}\int_0^\eta \frac{s^{k-2}\,ds}{+\sqrt{1\;-\;s^2}} \tag{12}$$

With $n_0 = 1/2$ for $k = 3$ this is a partial alternative for (11), because we still have to add a random sign to the random value of s. By comparing this with Tashiro's algorithm[10], in the special case of dimension three, we see that also that is the same, because the integral in (12) can be transformed as follows:

$$\xi \;=\; \int_0^\eta \frac{s\,ds}{\sqrt{1\;-\;s^2}} = \sqrt{1-\eta^2} \;=\; \sqrt{1-\sin^2\epsilon} \;=\; \cos\epsilon$$

Thus, ξ between zero and one simply maps onto $\cos\epsilon$ with ϵ between zero and $\pi/2$. To cover the two hemispheres the known minute adaptation in the following (b) Tashiro procedure is proposed:
b1 $\cos\epsilon \;=\; \xi_1 \;=\; \rho_u^{(1)}$ with $-1 \le \xi \le +1$
b2 $\alpha \;=\; \xi_2 \;=\; \rho_u^{(2)}$ with $-\pi \le \xi \le +\pi$
b3 $x_1 \;=\; \sqrt{1-\cos^2\epsilon}\,\cos\alpha,\; x_2 \;=\; \sqrt{1-\cos^2\epsilon}\,\sin\alpha,\; x_3 \;=\; \cos\epsilon$
which, indeed, is numerically the shortest approach.

Spherical Caps and Derived LAUDs

The integration limits of (9) can be selected so as to define an area of S^2 comprised between the colatitude angles ϵ_a and ϵ_b and the right ascensions α_a and α_b as follows:

$$1 \;=\; \frac{1}{n_r}\int_{\epsilon_a}^{\epsilon_b}\int_{\alpha_a}^{\alpha_b} \sin\epsilon \; d\epsilon \; d\alpha \tag{13}$$

with

$$n_r = (\alpha_b - \alpha_a)(\cos\epsilon_a \,-\, \cos\epsilon_b) \tag{14}$$

subject to the constraints $0 \leq \epsilon_a < \epsilon_b \leq \pi$ and $-\pi \leq \alpha_a < \alpha_b \leq \pi$. The break down of the relevant pdf is now:

$$p_r(\alpha,\epsilon) \;=\; \Big(\frac{1}{\alpha_b \,-\, \alpha_a}\Big)\Big(\frac{\sin\epsilon}{\cos\epsilon_a \,-\, \cos\epsilon_b}\Big) \tag{15}$$

We thereby obtain the numerically optimal and statistically rigorous (c) Extended Tashiro procedure which simulates independent random directions in restricted areas by only setting particular integration limits for the polar co-ordinates in (12), namely:

c1 $\cos\epsilon \,=\, \xi_1 \,=\, \rho_u^{(1)}$ with $\cos\epsilon_b \leq \xi \leq \cos\epsilon_a$
c2 $\alpha \,=\, \xi_2 \,=\, \rho_u^{(2)}$ with $\alpha_a \leq \xi \leq \alpha_b$
c3 $x_1 \,=\, \sqrt{1-\cos^2\epsilon}\,\cos\alpha,\; x_2 \,=\, \sqrt{1-\cos^2\epsilon}\,\sin\alpha,\; x_3 \,=\, \cos\epsilon$

With the help of this procedure we can simulate uniform direction distributions inside:
- spherical caps with $\epsilon_a = 0$ but $\epsilon_b < \pi$ while $\alpha_2 - \alpha_1 = 2\pi$,
- spherical rings with $0 < \epsilon_a, \;\; \epsilon_b < \pi$ and $\alpha_2 - \alpha_1 = 2\pi$,
- (complete) lunes with $\epsilon_a = 0$ and $\epsilon_b = \pi$ while $\alpha_2 - \alpha_1 < 2\pi$,
- lune triangles where either $\epsilon_a \neq 0$ and $\epsilon_b = \pi$, or $\epsilon_a = 0$ and $\epsilon_b \neq \pi$ while $\alpha_2 - \alpha_1 < 2\pi$ (this is a triangle which is not subject to the rules applicable to the spherical triangles dealt with in spherical trigonometry due to the presence of one side which is a small circle arc),
- spherical co-ordinate quadrangles which are a mixture of the preceeding boundary definitions. Their main geometric properties require that there are two parallel small circle arcs intersecting two meridians going through the polar axis perpendicular onto the plane of the small circles.

The reference system in which we have generated the random points on the sphere, is usually not the same as the reference system in which the simulated points are ultimately employed. A simple method to perform the required transformation, is described later on at the end of the spherical triangle example. The method is based on the selection of three non-coplanar fixed points preferably located on the circumference of the application area and available as known vectors in the target reference system.

Checking Randomness on Spherical Caps and Derived LAUDs

As announced before the performance verification of a large random direction sample generation for any of the LAUDs introduced before can be achieved by comparing the theoretical expectations of the mean values and mean squares of the α-co-ordinate or right ascension as well as for the ϵ-co-ordinate or colatitude. This even applies to quadrangles or rings located far from the pole.

The break down of the pdf implied by (15) yields the following mathematical expectations for the right ascension:

$$\mathrm{E}\,(\alpha) \;=\; 0.5\,(\alpha_a \,+\, \alpha_b), \qquad \mathrm{E}\,(\alpha^2) \;=\; (\alpha_a^2 \,+\, \alpha_a\,\alpha_b \,+\, \alpha_b^2)/\sqrt{3} \tag{16}$$

if the figure considered has no rotational symmetry around the pole. This does not play a role for the colatitude for which we find:

$$\mathrm{E}\,(\epsilon) \;=\; MN_3(\epsilon_b) \,-\, MN(\epsilon_a), \quad \mathrm{E}\,(\epsilon^2) \;=\; MSQ_3(\epsilon_b) \,-\, MSQ(\epsilon_a) \tag{17}$$

with the functions

$$MN_3(\epsilon) \;=\; \int_0^{\epsilon} \epsilon\, p_\epsilon(\epsilon)\, d\epsilon \;=\; (\sin\epsilon \,-\, \epsilon\cos\epsilon)/(\cos\epsilon_a - \cos\epsilon_b)$$

and

$$MSQ_3(\epsilon) \;=\; \int_0^{\epsilon} \epsilon^2\, p_\epsilon(\epsilon)\, d\epsilon \;=\; (2\epsilon\sin\epsilon \,-\, (\epsilon^2 \,-\, 2)\cos\epsilon \,-\, 2)/(\cos\epsilon_a \,-\, \cos\epsilon_b)$$

where the subscript three refers to the dimension we are working in. We suggest to build the empirical mean and root mean square (RMSQ) values in parallel with the RMSQ value of ϵ derived from the empirical covariance matrix **C** involving only the x_1 and x_2 co-ordinates, namely:

$$C \;=\; \frac{1}{N}\begin{vmatrix} \Sigma\, x_1^2 & \Sigma\, x_1\, x_2 \\ \Sigma\, x_1\, x_2 & \Sigma\, x_2^2 \end{vmatrix} \tag{18}$$

where N is the number of directions in the sample. In cases of rotational symmetry (RS) the diagonal elements c_{ii} of C must theoretically be mutually equal. Even without RS the RMSQ of the colatitude is equal to

$$\epsilon_{cov} \;=\; \arcsin[(c_{11} \,+\, c_{22})^{1/2}]\ \mathrm{rad} \tag{19}$$

as derived in Note 4.

Empirically testing all these parameters makes another counting process superfluous, because if something is mistaken in the coding of the algorithm it will appear by verifying mean and RMSQ on both co-ordinates.

TOSS AWAY

By 'toss away' we mean algorithmic steps which have to be undertaken to get the right uniform distribution of random directions by first generating such directions in a larger area subject to a rejection criterion which allows to fill a precisely defined smaller area. Although there may be cases where the intervention of toss away can hardly be avoided, there are also a number of instances where employing toss away is not mandatory but could replace an intricate or equally less effective algorithm. To help us making a choice, we introduce a numerical efficiency measure consisting of two factors, namely the *geometrical* efficiency e_g and the *numerical* efficiency e_n. Quantifying this efficiency is then based on the the number of 'random number' generations required in the mean for obtaining one valid random direction satisfying all potential constraints. The efficiency shall be equal to one if we need the minimum quantity of uniformly distributed random numbers per independent random direction generation, that is equal to 2 on S^2 meaning on the sphere in dimension $k = 3$ and to 3 if $k = 4$. If more is required the efficiency shall decrease proportionally.

The geometrical efficiency is simply the ratio of the actual useful area S_U where directions are retained over the full area S_F in which the bulk of the algorithm is performed before the rejection criterion is applied, or $e_g = S_U/S_F$. If m uniformly distributed random numbers are required in excess of $k-1$ for the generation of one random direction, the corresponding numerical efficiency is obviously equal to $e_n = (k-1)/(m+k-1)$ and the total proposed efficiency measure becomes

$$e_{tot} = \frac{S_U\,(k - 1)}{S_F\,(m + k - 1)}$$

Uniform Distribution in a Spherical Triangle

This is an example where polar co-ordinates can be employed in combination with a toss away scheme. In contrast to the previous cases, where the derivation of the pdf was the major concern, here the geometrical aspects will play an overriding role. Let us start with three arbitrary defined unit vectors $\mathbf{t}_1, \mathbf{t}_2$ and $\mathbf{t}_3$ pointing to the corners of a spherical triangle. We assume that none of the arcs separating any two of the three directions is larger that π. It will be our strategy to move away from the three dimensional vector description towards the two dimensional manifold S^2 where spherical trigonometry evolves independently of the actual Cartesian orientation of the triangle. The unit vectors are only needed to compute the essential angles and arc lengths belonging to the triangle shown in Fig.1. The three arcs between the points a_i and a_j are represented by ϵ_{ij} and the dihedral angles β_i at the corners of the triangle are found from:

$$\cos\epsilon_{jk} = (\mathbf{t}_j \cdot \mathbf{t}_k) \quad \text{and} \quad \cos\epsilon_{jk} = \cos\epsilon_{ij}\,\cos\epsilon_{ik} + \sin\epsilon_{ij}\,\sin\epsilon_{ik}\cos\beta_i \qquad (20)$$

where i, j, k are a permutation of 1,2,3.

We further forget about $\mathbf{t}_1, \mathbf{t}_2$ and $\mathbf{t}_3$ for a while and locate the triangle in a favorable orientation in the polar co-ordinate system, namely with one corner coincident with the pole. Consequently, two of the sides of the triangle are then located on meridians and the spherical triangle is thus completely embedded in a lune triangle. Thereafter, we generate uniformly distributed direction in this lune triangle by assuming that the meridian comprising the point a_2 corresponds to a right ascension $\alpha = 0$ and the integration over the right ascension goes up to $\alpha = \beta_1$, whereas the colatitude needs to integrated between zero and $\zeta = \sup(\epsilon_{12}, \epsilon_{13})$. After having obtained the random point D with right ascension α_d and colatitude τ_1, one has to check whether this point is inside the triangle and if not, toss it away. In this case one repeats the procedure until a valid D is obtained. The actual geometrical check consists in verifying that the dihedral angle ω satisfies the inequality

$0 \leq \omega \leq \beta_2$ provided $\epsilon_{13} \leq \epsilon_{12}$ as depicted in Fig. 1. The dihedral angle ω is obtained by means of two applications of the cosine rule using the angles given in Fig.1, namely:

$$\cos\tau_2 \;=\; \cos\epsilon_{12}\,\cos\tau_1 \,+\, \sin\epsilon_{12}\,\sin\tau_1\,\cos\alpha_d \tag{21}$$

yielding τ_2, which was still unknown and employing it now in

$$\cos\tau_1 \;=\; \cos\epsilon_{12}\,\cos\tau_2 \,+\, \sin\epsilon_{12}\,\sin\tau_2\,\cos\omega$$

provides ω. Should $\epsilon_{12} \leq \epsilon_{13}$ apply instead, we have to derive an ω between ϵ_{13} and τ_3 and compare it with β_3. To be effective we will have to take care to locate the original triangle at the pole in way to obtain the smallest ratio of the useless area – there where toss away occurs – with respect to the area of the spherical triangle inside the lune.

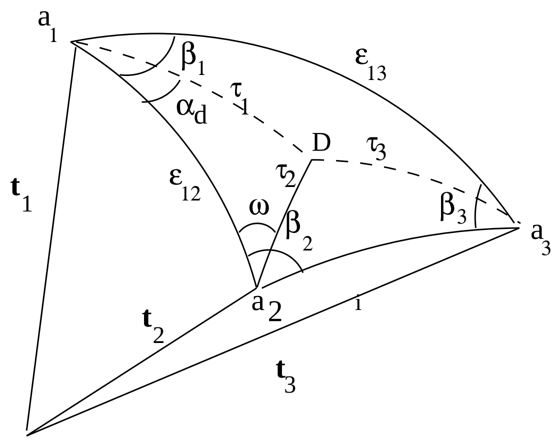

Fig. 1 Geometrical specification of the spherical triangle
and the location of a random point D

Once a valid point D has been obtained, it still needs to be converted into a unit vector $\mathbf{t_d}$ consistent with the Cartesian orientation of the triad $\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3$. On top of $\cos\tau_1$ and $\cos\tau_2$ we need the value of $\cos\tau_3$ which is easily obtained by means of the cosine rule. Thereby we have the three direction cosines of $\mathbf{t_d}$ in the skew reference system whose reference axes are along the unit vectors $\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3$. Consequently, we can write

$$\mathbf{t_d} \;=\; m_1\,\mathbf{t_1} \,+\, m_2\,\mathbf{t_2} \,+\, m_3\,\mathbf{t_3}$$

with the reference co-ordinates m_1, m_2, m_3 which one determines by solving the following basic linear equation system:

$$\left|\begin{matrix} (\mathbf{t_1}\cdot\mathbf{t_d}) \\ (\mathbf{t_2}\cdot\mathbf{t_d}) \\ (\mathbf{t_3}\cdot\mathbf{t_d}) \end{matrix}\right| = \left|\begin{matrix} \cos\tau_1 \\ \cos\tau_2 \\ \cos\tau_3 \end{matrix}\right| = \left|\begin{matrix} 1 & \cos\epsilon_{12} & \cos\epsilon_{13} \\ \cos\epsilon_{12} & 1 & \cos\epsilon_{23} \\ \cos\epsilon_{13} & \cos\epsilon_{23} & 1 \end{matrix}\right| \left|\begin{matrix} m_1 \\ m_2 \\ m_3 \end{matrix}\right| \tag{22}$$

The matrix involved is known to be positive definite, because the corresponding Gramm determinant is non-zero if the triad is not coplanar. Further, this matrix is always the same for all random directions inside the same spherical triangle enclosed by the triad $\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3$. Hence, the burden involved to perform the transformation from spherical trigonometry back to a three dimensional vector space is almost negligible. This is one of those examples which show the power behind the synergy of spherical trigonometry and vector calculus.

In Note 10 a numerical example is given for the random direction generation inside a given spherical triangle. In that context the present toss away scheme is compared with a novel analytical area ratio method proposed there for the triangle as well. At that occasion the actual efficiencies of both algorithms are assessed

UNIFORM DISTRIBUTION ON S^3

The Global Uniform Distribution

The global distribution which involves the complete surface of S^3 is in fact a special case of a LAUD consisting of a spherical cap around the pole. Hence, it may be advantageous to start with the surface integral for a cap of arc radius ϵ_0 yielding the surface which contains the normalization constant $n_{\epsilon 0}$, namely:

$$\int_0^{\epsilon_0} \int_{\alpha_1=0}^{\pi} \int_{\alpha_2=0}^{2\pi} \sin\alpha_1 \sin^2\epsilon \; d\epsilon \; d\alpha_1 \; d\alpha_2 \;=\; 4\pi\,(0.5\epsilon_0 - \; 0.25\sin(2\epsilon_0)) \;=\; 4\pi\, n_{\epsilon_0} \qquad (23)$$

For the full sphere $\epsilon_0 = \pi$ and its surface becomes $2\pi^2$. Consequently, the pdf of the cap on S^3 can be factorized as follows:

$$p_{u3,\epsilon_0}(\epsilon, \alpha_1, \alpha_2) \;=\; p_{\epsilon_0}(\epsilon)\, p_{\alpha_1}(\alpha_1)\, p_{\alpha_2}$$

with

$$p_{\epsilon_0}(\epsilon) \;=\; \frac{\sin^2\epsilon}{(0.5\epsilon_0 - \; 0.25\sin(2\epsilon_0))}, \quad p_{\alpha_1}(\alpha_1) \;=\; \frac{\sin\alpha_1}{2}, \quad p_{\alpha_2} \;=\; \frac{1}{2\pi} \qquad (24)$$

Obviously the generation of random values of α_1 and α_2 follows the lines of the (e)-pdf algorithm in the section about Lauds on S^2. This time the random number transformation for ϵ is subject to the equation:

$$\xi \;=\; \frac{1}{n_{\epsilon_0}} \int_0^{\eta} \sin^2\eta \; d\eta \;=\; \frac{(0.5\eta - \; 0.25\sin(2\eta))}{(0.5\epsilon_0 - \; 0.25\sin(2\epsilon_0))} \qquad (25)$$

where, as usual, ξ is a random number between zero and one and η is the tranformed random ϵ angle satisfying the correct pdf in the range between zero and ϵ_0. This leads to the following pdf-based direction generation algorithm:

d1. $\xi_1 \;=\; \rho_u^{(1)}$ with $0 \le \xi \le 1$
d2. get $\alpha_1 \;=\; \eta$ by applying (11)
d3. $\alpha_2 \;=\; \xi_2 \;=\; \rho_u^{(2)}$ with $0 \le \xi < 2\pi$
d4. $\xi_3 \;=\; \rho_u^{(3)}$ with $0 \le \xi \le 1$
d5. compute $\epsilon \;=\; \eta$ by solving (25) employing ξ_3
d6. $x_1 = \cos\alpha_1 \cos\alpha_2 \sin(2\epsilon),\; x_2 = \cos\alpha_1 \sin\alpha_2 \sin(2\epsilon),\; x_3 = \sin\alpha_1 \sin(2\epsilon),\; x_4 = \cos(2\epsilon)$

We further have the Shibuya[18]-algorithm with the following implementation scheme:

e1. as for d1
e2. $\cos\eta = \sqrt{\xi_1}$, $\sin\eta = +\sqrt{1-\xi_1}$
e3. $\beta_1 = \xi_2 = \rho_u^{(2)}$ with $0 \le \xi \le 2\pi$
e4. $x_1 = \cos\eta\cos\beta_1$, $x_2 = \cos\eta\sin\beta_1$
e5. $\beta_2 = \xi_3 = \rho_u^{(3)}$ with $0 \le \xi \le 2\pi$
e6. $x_3 = \sin\eta\cos\beta_2$, $x_4 = \sin\eta\sin\beta_2$

This straight forward method relies on non-polar spherical co-ordinates. This alternative only works for even dimensions. In our opinion, the (normal) algorithm using the normal distribution on each Cartesian co-ordinate, as explained in the introduction is also the simplest to implement among the algorithms presented here and by Shuster[4]. We extensively tested the methods d, e and the normal distribution approach and verified the mean direction densities on spherical caps with 15^0 arc radius located on the co-ordinate axes (8 caps), on directions equidistant from all co-ordinate axes (16 caps), on directions equidistant from any two axes and orthogonal to the other two (24 caps) and finally on the rest of the sphere separately. All three methods work equally well. Even by reducing the arc radius of the spherical caps no clustering around the natural symmetry axes related to co-ordinates could be identified. Nevertheless, only the pdf based method 'd' is adequate when considering LAUDs on S^3.

The Target Directions on S^3

The four dimensional directions we are interested in here, are the Rodrigues four (unit) vectors, whose components were first derived by Euler[13] as an effective analytical and rational parameterization of a three dimensional orthogonal transformation of norm plus one. Such a transformation is now known as a rotation matrix which is an element of the SO(3) group. The parameterization of the 3×3 rotation matrix Q by the real numbers (q_1, q_2, q_3, q_4) is in fact

$$Q = \begin{vmatrix} q_1^2 - q_2^2 - q_3^2 + q_4^2 & 2(q_1q_2 + q_3q_4) & 2(q_1q_3 - q_2q_4) \\ 2(q_1q_2 - q_3q_4) & -q_1^2 + q_2^2 - q_3^2 + q_4^2 & 2(q_2q_3 + q_1q_4) \\ 2(q_1q_3 + q_2q_4) & 2(q_2q_3 - q_1q_4) & -q_1^2 - q_2^2 + q_3^2 + q_4^2 \end{vmatrix}$$

It was Rodrigues[14] who discovered, independently from Euler, the particular geometrical properties of these numbers and the ability to combine arbitrary rotations with their help. Let us represent the real eigenvector or rotation axis belonging to Q by the three dimensional unit vector $\mathbf{p}$ and the rotation angle around this vector by γ, then the four 'Euler-Rodrigues parameters' contain $\mathbf{p}$ and γ in the following way:

$$q_1 = p_x \sin\gamma/2, \quad q_2 = p_y \sin\gamma/2, \quad q_3 = p_z \sin\gamma/2, \quad q_4 = \cos\gamma/2 \qquad (26)$$

If $\mathbf{p}$ is expressed in right ascension α and colatitude θ and we write $\epsilon = \gamma/2$, it appears that (26) represents a point on S^3 in polar co-ordinates, the way we have defined it before. The vector representation $\mathbf{r}$ of (26) is then the Rodrigues four-vector. From (24) we know that the pdf's of α, θ and ϵ are separable. Consequently, we can express constraints on any of these parameters separately or combine them with the knowledge that ϵ stands alone as rotation angle, while α and θ can be constrained so as to force the simulated rotation axes to stay within given three dimensional boundaries. These combinations are the LAUDs we address in the rest of this note.

To highlight the basic properties of $\mathbf{r}$ with respect to three dimensional rotations, we introduce the four-vector $\mathbf{p_0}$, namely $\mathbf{p_0} = |\mathbf{p} : 0|'$, where the accent denotes transposition, and $\mathbf{v_0} = |0, 0, 0, 1|'$. The Rodrigues four-vector can then be written as

$$\mathbf{r}(\mathbf{p},\epsilon) \;=\; \sin\epsilon\,\mathbf{p_0} \,+\, \cos\epsilon\,\mathbf{v_0} \tag{27}$$

We notice that

$$Q(+\mathbf{r}) \;=\; Q(-\mathbf{r}) \tag{28}$$

due to the quadratic dependence of Q with respect to the Euler-Rodrigues parameters in the matrix displayed in (26). By inspecting (27) we further observe that

$$\mathbf{r}(\mathbf{p},\epsilon) \;=\; \mathbf{r}(-\,\mathbf{p},-\,\epsilon) \tag{29}$$

independently of (28). These ambiguities are not disturbing in the majority of the applications involving Rodrigues four-vectors. And also here it does not really matter, if one takes care to enforce the natural constraint $0 \le \epsilon \le \pi$ valid for any colatitude.

Before proceeding to the general simulation cases in dimension four, it may be useful to cast a glance on such constraints which decrease the stochastic dimensionality, thus requiring simpler random direction generation algorithms.

In a *first case* we might like to simulate random rotations which have a constrained or not constrained random rotation angle 2ϵ combined with a constant rotation axis $\mathbf{p}$. From (27) it is immediately obvious that this is a one dimensional case equivalent to the random number generation of a point on a circle or an arc of it, that is on S^1. And because the surface element is one in this case, it will be sufficient to directly generate uniformly random numbers for the values of ϵ in the desired interval.

In a *second case* we may suppress a dimension by keeping ϵ constant but vary the rotation axis $\mathbf{p}$ over the complete sphere S^2 or part of it, thus a simulation in dimension three where $\mathbf{r}$ is complemented in a non-stochastic way as prescribed by (27). Equivalently, one may constrain the area, in which the rotation axis may evolve, to a plane. Let us, for example, do the random direction generation so that the fixed plane in which $\mathbf{p_e}$ must be perpendicular to the r_2-axis, then $\mathbf{p_e} = |\cos\alpha,\, 0,\, \sin\alpha|'$. Further, both α and ϵ are simultaneously and independently random so as to yield a direction on S^3 where the $y-$co-ordinate has always to be zero. This is equivalent to a direction on S^2 with the components $|\cos\alpha\sin\epsilon,\, \sin\alpha\sin\epsilon,\, \cos\epsilon|'$ to be distributed globally over S^2; a problem discussed earlier. Assume now that we do not really aim at the $x, y-$plane, but at a plane moved away by a fixed rotation Q_t, then the actual Rodrigues-four vector is reached by applying systematically Q_t to $\mathbf{p_e}$, or:

$$\mathbf{r} \;=\; \mathbf{r}(\mathbf{p},\epsilon) \;=\; \sin\epsilon \begin{vmatrix} Q_t\,\mathbf{p_e} \\ \cdots \\ 0 \end{vmatrix} + \cos\epsilon\,\mathbf{v_0}$$

It is important to be aware that the generation of the rotation axis, hidden in $\mathbf{r}$, can be performed in the context of a geometrically simple configuration before moving it systematically to the target orientation by applying the repositioning as explained before. In agreement with (27), we therefore need a reference triad consisting of three vectors $\mathbf{p_1}, \mathbf{p_2}, \mathbf{p_3}$ in the circumference limiting the location of the random vector $\mathbf{p}$ obtained..

LAUDs on S^3

Starting from (20) we can obtain all possible LAUD defined in polar co-ordinates, by assuming integration boundaries subjected to the constraints $0 \leq \epsilon_1 \leq \epsilon \leq \epsilon_2, \leq \pi,\ 0 \leq \theta_1 \leq \theta \leq \theta_2 \leq \pi$ and $\alpha_1 \leq \alpha \leq \alpha_2$ which yield the normalization value:

$$n_{(laud)} = \int_{\epsilon_1}^{\epsilon_2} \int_{\theta_1}^{\theta_2} \int_{\alpha_1}^{\alpha_2} \sin\theta \sin^2\epsilon \; d\epsilon \; d\theta \; d\alpha \tag{30}$$

with the decomposition

$$n_{(laud)} = [n_\epsilon(\epsilon_2) - n_\epsilon(\epsilon_1)]\,[n_\theta(\theta_2) - n_\theta(\theta_1)]\,[n_\alpha(\alpha_2) - n_\alpha(\alpha_1)]$$

where only the factor concerning ϵ adds something new to what we had derived in (16) and (17) for S^2 where – for the application to this case – ϵ in(17) has to be replaced by θ. From (20) we get

$$n_\epsilon(\epsilon_0) = 0.5\,\epsilon_0 - \; 0.25\,\sin(2\epsilon_0) \tag{31}$$

The corresponding pdf's remain very simple. They are

$$p_\epsilon = \frac{\sin^2\epsilon}{n_\epsilon(\epsilon_2) - n_\epsilon(\epsilon_1)}, \quad p_\theta = \frac{\sin\theta}{\cos\theta_1 - \cos\theta_2}, \quad p_\alpha = \frac{1}{\alpha_2 - \alpha_1} \tag{32}$$

Introducing the shorthands MNE_4 and MSQE_4 for the following functions, namely

$$\begin{aligned} \mathrm{MNE}_4(\epsilon_0) &= \frac{1}{n_\epsilon(\epsilon_2) - n_\epsilon(\epsilon_1)} \int_0^{\epsilon_0} \epsilon\, p_\epsilon(\epsilon)\, d\epsilon \\ &= \frac{0.25\epsilon_0^2 - 0.25\epsilon_0 \sin 2\epsilon_0 - 0.125(\cos 2\epsilon_0 - 1)}{n_\epsilon(\epsilon_2) - n_\epsilon(\epsilon_1)} \end{aligned} \tag{33}$$

and

$$\begin{aligned} \mathrm{MSQE}_4(\epsilon_0) &= \frac{1}{n_\epsilon(\epsilon_2) - n_\epsilon(\epsilon_1)} \int_0^{\epsilon_0} \epsilon^2\, p_\epsilon(\epsilon)\, d\epsilon \\ &= \frac{\epsilon_0^3/6 - 0.25(\epsilon_0^2 - 0.5)\sin 2\epsilon_0 - 0.25\epsilon_0 \cos 2\epsilon_0}{n_\epsilon(\epsilon_2) - n_\epsilon(\epsilon_1)} \end{aligned} \tag{34}$$

yields the expectations:

$$\mathrm{E}\,(\epsilon) = \mathrm{MNE}_4(\theta_2) - \mathrm{MNE}_4(\epsilon_1) \quad \text{and} \quad \mathrm{E}\,(\epsilon^2) = \mathrm{MSQE}_4(\epsilon_2) - \mathrm{MSQE}_4(\epsilon_1)$$

for a uniform distribution in the interval (ϵ_1, ϵ_2)

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