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© *N. P. Kopytov, E. A. Mityushov***UNIFORM DISTRIBUTION OF POINTS ON HYPERSURFACES: SIMULATION OF RANDOM EQUIPROBABLE ROTATIONS**

The paper describes a universal method for simulation of uniform distributions of points on smooth regular surfaces in Euclidean spaces of various dimensions. The authors give an interpretation of a set of possible values of Rodrigues–Hamilton parameters used to describe a rigid rotation as a set of points of a three-dimensional hypersphere in four-dimensional Euclidean space. The relationship between random equiprobable rotations of a rigid body and a uniform distribution of points on the surface of a three-dimensional hypersphere in four-dimensional Euclidean space is established.

Keywords: uniform distribution of points on hypersurfaces, random points on a hypersphere, quaternions, random rotations.

Introduction

In spite of the simplicity of the statement, the problem of the uniform distribution of points on the surfaces is complicated. The consideration of particular types of surfaces together with different approaches can lead to the appearance of a particular solution for each individual case. For example, there are several well-known techniques for the uniform distribution of points on a plane and on the surface of a sphere [1–3]. But methods for the uniform distribution of points on the surface of an ellipsoid [5] and surfaces defined by explicit form equations [6, 7] are less known.

In addition to papers which describe methods for the uniform distribution of points on surfaces in three-dimensional space, a number of works is devoted to methods for the uniform distribution of points on the surface of a hypersphere [2, 4, 5]. Also, there are methods for the uniform distribution of points on the surface of a hyperellipsoid [5]. Among researchers whose works are most often cited in the context of the problem of the uniform distribution of points on the surface of a hypersphere, one should mention G. Marsaglia [1], and M. E. Muller [2]. It should be noted that a separate page on the Internet site Wolfram MathWorld [4] is also devoted to this problem.

The methods mentioned above are suitable either for particular surfaces or generalized to a narrow class of surfaces. However, taking into account that the problem of the uniform distribution of points on different surfaces is important for a large amount of applied and fundamental research and, in particular, for methods of statistical and simulation mathematical modeling, there is a need to find a more universal method for the uniform distribution of points on surfaces and hypersurfaces.

In this paper the method developed by the authors to simulate the uniform distribution of points on smooth regular surfaces in Euclidean spaces of different dimensionality is briefly described.

One of possible applications of the proposed method is its use in the problems associated with the rotation of three-dimensional Euclidean space. Such rotations can be described by the group of orthogonal matrices $SO(3)$, which can be displayed on a three-dimensional hypersphere in four-dimensional Euclidean space [8]. Taking into account that in [9] general relationship of transformations groups and surfaces in multidimensional Euclidean spaces is considered, the proposed approach can be useful in a wide spectrum of scientific problems.

In this paper the possibility of using the uniform distribution of points on a three-dimensional hypersphere in four-dimensional Euclidean space to define equiprobable rotations of a rigid body is established.

§ 1. Simulation of the uniform distribution of points on smooth regular surfaces in Euclidean spaces of different dimensionality

In [10–14], the method for the uniform distribution of points on smooth regular surfaces in three-dimensional and multi-dimensional Euclidean spaces was presented by the authors. The method consists of the following stages.

1. Finding the density function of the joint distribution of surface parameters corresponding to the uniform distribution of points on the surface.
2. Generating values of parameters using the density function (obtained at stage 1) of the joint distribution and subsequent calculation of the coordinates of points.

The consideration of the problem of the uniform distribution of points on smooth regular surfaces requires a number of strict mathematical definitions.

Definition 1. Distribution of points on a smooth regular surface is called *uniform* if, under conditions of random tossing a point on this surface, the probability of its occurrence in any region of this surface is proportional to the area of this region.

Definition 2. The *geometrical probability* of hitting a point in an element of the smooth regular surface, under conditions of random tossing a point on this surface, is defined by the equality

$$P(X \in dS) = \frac{dS}{S}.$$

Here X is the point of the surface whose position is determined by a random vector, dS is the area of the surface element, and S is the whole surface area.

Definition 3. The *probability density* $f(u_1, u_2, \dots, u_m)$ of the joint distribution of parameters defining the position of a point randomly thrown on a smooth regular surface is defined by the equality

$$P(X \in dS) = f(u_1, u_2, \dots, u_m) du_1 du_2 \dots du_m.$$

The following statement can be formulated on the basis of these definitions.

Theorem. Let the functions

$$x_1(u_1, u_2, \dots, u_m), x_2(u_1, u_2, \dots, u_m), \dots, x_n(u_1, u_2, \dots, u_m),$$

where $(u_1, u_2, \dots, u_m) \in D$, define a smooth regular m -dimensional surface in n -dimensional Euclidean space. Then the density of the distribution of parameters $u_1, u_2, \dots, u_m$ determining the uniform distribution of points on this surface is defined by the function

$$f(u_1, u_2, \dots, u_m) = \begin{cases} \frac{\sqrt{g}}{\int \int \dots \int_D \sqrt{g} du_1 du_2 \dots du_m}, & (u_1, u_2, \dots, u_m) \in D; \\ 0, & (u_1, u_2, \dots, u_m) \notin D. \end{cases} \quad (1.1)$$

Here $g = \det(g_{ij})$ is the determinant of the matrix of the metric tensor on the surface. The matrix of the metric tensor on the surface has the form

$$(g_{ij}) = \begin{pmatrix} g_{11} & g_{12} & \dots & g_{1m} \\ g_{21} & g_{22} & \dots & g_{2m} \\ \dots & \dots & \dots & \dots \\ g_{m1} & g_{m2} & \dots & g_{mm} \end{pmatrix},$$

where $i, j = 1, 2, \dots, m$, $g_{ij} = \sum_{k=1}^n \frac{\partial x_k}{\partial u_i} \frac{\partial x_k}{\partial u_j}$.

Fig. 1. The uniform distribution of points on the surface of torus

P r o o f. By Definition 2, the geometric probability of hitting any point X in a surface element dS equals

$$P(X \in dS) = \frac{dS}{S}.$$

For smooth regular surfaces in multidimensional Euclidean space, the following expressions are valid:

$$dS = \sqrt{g} du_1 du_2 \dots du_m,$$

$$S = \int \int \dots \int_D \sqrt{g} du_1 du_2 \dots du_m.$$

Consequently,

$$P(X \in dS) = \frac{\sqrt{g} du_1 du_2 \dots du_m}{\int \int \dots \int_D \sqrt{g} du_1 du_2 \dots du_m}.$$

Taking into account Definition 3, the probability density is defined by the expression

$$f(u_1, u_2, \dots, u_m) = \frac{\sqrt{g}}{\int \int \dots \int_D \sqrt{g} du_1 du_2 \dots du_m}.$$

The theorem is proved.

The generation of values of parameters $u_1, u_2, \dots, u_m$ using the density function $f(u_1, u_2, \dots, u_m)$ of the joint distribution via generalized Neumann method (the acceptance-rejection method) provides the uniform distribution of points on the given surface.

Figures 1 and 2 show the uniform distribution of points on the surface of the torus and on the surface of the Klein bottle in three-dimensional Euclidean space, which was obtained using the described above method.

Fig 2. The uniform distribution of points on the surface of Klein bottle

§ 2. Rodrigues–Hamilton parameters and the simulation of equiprobable rotations of a rigid body using the uniform distribution of points on the surface of a three-dimensional hypersphere in four-dimensional Euclidean space

The most common way to describe the rotation of a rigid body is the use of Euler angles ψ, ϑ, φ . The density function of the joint distribution of Euler angles used to describe and simulate the set of equiprobable rigid body rotations is well known [15, 16]:

$$f(\psi, \vartheta, \varphi) = \frac{\sin \vartheta}{8\pi^2}. \quad (2.1)$$

As it is known [17, 18], another way to describe rotations of a rigid body is related with using the parameters of Rodrigues–Hamilton $\lambda_0, \lambda_1, \lambda_2, \lambda_3$, which are also components of a quaternion of rotation $\lambda = \lambda_0 + i\lambda_1 + j\lambda_2 + k\lambda_3$. Rodrigues–Hamilton parameters satisfy the normalization condition

$$\lambda_0^2 + \lambda_1^2 + \lambda_2^2 + \lambda_3^2 = 1 \quad (2.2)$$

and are associated with Euler angles by the relations

$$\lambda_0 = \cos \frac{\vartheta}{2} \cos \frac{\psi + \varphi}{2}, \quad \lambda_1 = \sin \frac{\vartheta}{2} \cos \frac{\psi - \varphi}{2}, \quad \lambda_2 = \sin \frac{\vartheta}{2} \sin \frac{\psi - \varphi}{2}, \quad \lambda_3 = \cos \frac{\vartheta}{2} \sin \frac{\psi + \varphi}{2}, \quad (2.3)$$

where $0 \leq \psi \leq 2\pi$, $0 \leq \vartheta \leq \pi$, $0 \leq \varphi \leq 2\pi$.

Using the geometrical interpretation of a quaternion as a four-dimensional vector of the complex space, to each quaternion $\lambda = \lambda_0 + i\lambda_1 + j\lambda_2 + k\lambda_3$ we assign the point with coordinates $x_1 = \lambda_0$, $x_2 = \lambda_1$, $x_3 = \lambda_2$, $x_4 = \lambda_3$ in four-dimensional Euclidean space. By relation (2.2), coordinates of every point will satisfy the condition

$$x_1^2 + x_2^2 + x_3^2 + x_4^2 = 1. \quad (2.4)$$

Eq. (2.4) is identical to the equation of the three-dimensional unit hypersphere in four-dimensional Euclidean space. Thus, a set of possible values of Rodrigues–Hamilton parameters can be considered as a set of points on the three-dimensional unit hypersphere in four-dimensional Euclidean space. In this case, equations (2.3) connecting Rodrigues–Hamilton parameters and Euler angles can be used as parametric equations to define this unit hypersphere:

$$x_1 = \cos \frac{\vartheta}{2} \cos \frac{\psi + \varphi}{2}, \quad x_2 = \sin \frac{\vartheta}{2} \cos \frac{\psi - \varphi}{2}, \quad x_3 = \sin \frac{\vartheta}{2} \sin \frac{\psi - \varphi}{2}, \quad x_4 = \cos \frac{\vartheta}{2} \sin \frac{\psi + \varphi}{2}, \quad (2.5)$$

where $0 \leq \psi \leq 2\pi$, $0 \leq \vartheta \leq \pi$, $0 \leq \varphi \leq 2\pi$.

Now, for the hypersphere defined by equations (2.5), using formula (1.1), we can find the density function of the joint distribution of the parameters (in this case, the Euler angles) corresponding to the uniform distribution of points on its surface. The results of mathematical symbolic transformations give the function (2.1). From this fact, we can conclude: a set of uniformly distributed points on the surface of the three-dimensional unit hypersphere in four-dimensional Euclidean space gives a set of Rodrigues–Hamilton parameters which correspond to a set of equiprobable rigid body rotations. This is a reflection of the fact of double covering $SO(3)$ group by a three-dimensional hypersphere [17]. The univalent covering $SO(3)$ group can be carried out by a half hypersphere lying on one side of any hyperplane passing through the origin.

It should be noted that the idea of representation of random rotations by points on a three-dimensional unit hypersphere in a four-dimensional space has already been considered in the scientific literature, for example, by P. H. Roberts and D. E. Winch [19]. This idea is also mentioned in the work of M. V. Borovkov and T. I. Savelova [20]. But the parameterization of a three-dimensional hypersphere, which was used in [19], differs from the parameterization, which is considered in this paper, and the question of the uniform distribution of points on a hypersphere was not considered in [19].

Conclusions

The density function of the distribution of parameters defining the uniform distribution of points on smooth regular surfaces in Euclidean spaces of different dimensionality is obtained in the general form.

The relationship between random equiprobable rotations of a rigid body and the uniform distribution of points on the surface of a three-dimensional hypersphere in four-dimensional Euclidean space is established.

In addition to uniform distributions of points on various surfaces and hypersurfaces, the investigation of non-uniform distributions of points on various surfaces and hypersurfaces has also scientific interest. The investigation of non-uniform distributions of points on surfaces can be carried out in the framework of the proposed formalism.

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Н. П. Копытов, Е. А. Митюшов

Равномерное распределение точек на гиперповерхностях: моделирование случайных равновероятных вращений

Ключевые слова: равномерное распределение точек на гиперповерхностях, случайные точки на гиперсфере, кватернионы, случайные вращения.

УДК 519.21

Описан универсальный метод для моделирования равномерных распределений точек на гладких регулярных поверхностях в евклидовых пространствах различной размерности. Представлена интерпретация множества возможных значений параметров Родрига–Гамильтона, используемых при описании вращения твердого тела как множества точек трехмерной гиперсферы в четырехмерном евклидовом пространстве. Установлена связь между случайными равновероятными вращениями твердого тела и равномерным распределением точек на поверхности трехмерной гиперсферы в четырехмерном евклидовом пространстве.

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