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Sampling random directions within an elliptical cone

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ABSTRACT

This work extends the spherical surface sampling algorithm in order to uniformly generate random directions within an elliptical cone. This has applications in Monte Carlo particle transport simulations, for example modeling asymmetric beam divergence or scattering interactions. Two methods are presented. The first obeys the strict boundary of the elliptical cone. The second relaxes this requirement, increasing the range of generated directions by up to 10% for elliptical cones of extreme eccentricity. However, the second method is able to generate directions beyond the equator.

1. Introduction

Isotropically sampling 3D directions (i.e. uniformly sampling points upon the surface of the unit sphere) is a common problem in Monte Carlo programs, with a surprising variety of solutions [1–5]. The optimal sampling algorithm [4–6] generates two independent uniform variates, η_x and η_y, over the domain $(-1, 1)$ until they satisfy $\eta_x^2 + \eta_y^2 < 1$. The acceptance probability is $\pi/4 \approx 0.79$. They are then transformed to Cartesian coordinates according to

$$\begin{aligned} x &= 2\eta_x\sqrt{1-\eta_x^2-\eta_y^2} \\ y &= 2\eta_y\sqrt{1-\eta_x^2-\eta_y^2} \\ z &= 1-2(\eta_x^2+\eta_y^2). \end{aligned} \tag{1}$$

This method maps points from the unit disk onto the surface of the unit sphere: $(\eta_x, \eta_y) \to (x, y, z)$. The transformation preserves the 2D polar angle as the 3D azimuthal angle, whilst the 2D radial distance $\eta_r = (\eta_x^2+\eta_y^2)^{1/2}$ directly determines the 3D z-coordinate.

This work extends the above algorithm in order to generate random directions within an elliptical cone. This means choosing an appropriate 2D shape from which to sample points (η_x, η_y), before they are transformed with (1). This technique could find applications in Monte Carlo particle transport simulations, such as those used in high energy physics, nuclear physics, medical physics, computer graphics rendering, and modeling of semiconductors and heat transfer. The author developed this algorithm to model asymmetric angular divergence of particle beams in the TOPAS simulation software for radiotherapy [7].

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2. Methods

2.1. Geometric configuration

The goal is to uniformly generate random directions within the boundaries of an elliptical cone. This is equivalent to uniformly sampling the surface of the unit sphere enclosed by the dashed line in Fig. 1. Precisely speaking, this is the surface of the unit sphere that is enclosed by the upper nappe of a right elliptical conical surface, whose apex coincides with the center of the sphere.

The elliptical cone is defined by the opening half-angles θ_x and θ_y, and is oriented such that these are subtended by the semi-major and semi-minor axes of the directrix. Sampled points must lie upon the surface of the unit sphere and within the conical surface, and therefore satisfy the following two relations:

$$x^2+y^2+z^2 = 1 \tag{2}$$

$$\left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 < z^2 \tag{3}$$

where

$$\begin{aligned} a &= \tan\theta_x \\ b &= \tan\theta_y. \end{aligned} \tag{4}$$

Considering the spherical sampling algorithm, it is clear that only a sub-domain of the (η_x, η_y) coordinates will yield directions within the elliptical cone. This is explicitly demonstrated in Fig. 2, which shows the (η_x, η_y) coordinates that map onto the dashed line of Fig. 1. To achieve maximal acceptance probability, we sample η_x over $(-\eta_a, \eta_a)$ and η_y over $(-\eta_b, \eta_b)$, where

$$\begin{aligned} \eta_a &= \sin(\theta_x/2) \\ \eta_b &= \sin(\theta_y/2). \end{aligned} \tag{5}$$

These expressions are derived by turning (3) into an equation and solving simultaneously with (2) at the boundary conditions. These

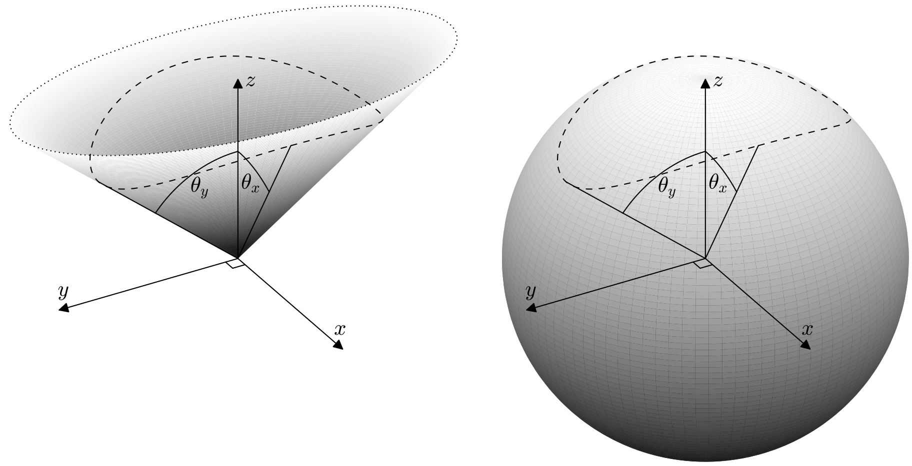

Fig. 1. The surfaces of an elliptical cone and the unit sphere, with their intersection drawn as a dashed line. The cone has $\theta_x = 30°$ and $\theta_y = 50°$.

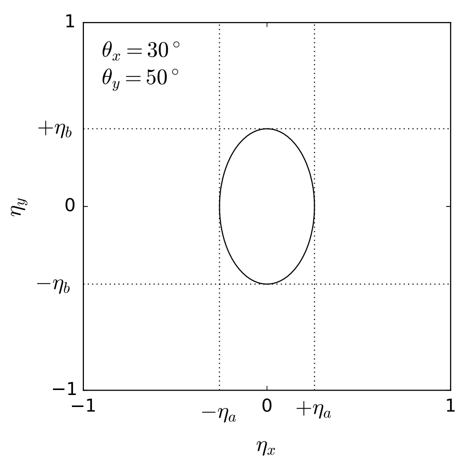

Fig. 2. The solid line indicates the (η_x, η_y) coordinates that are transformed by (1) to the coordinates of an elliptical cone with $\theta_x = 30°$ and $\theta_y = 50°$ (shown in Fig. 1).

are $y = 0$ and $\eta_y = 0$ for η_a, and $x = 0$ and $\eta_x = 0$ for η_b. Finally, a substitution is made according to (1) and a half-angle trigonometric identity is applied.

2.2. Method 1: strict cone definition

Generate two random variates, η_x uniform on $(-\eta_a, \eta_a)$ and η_y uniform on $(-\eta_b, \eta_b)$. Select the pair if both the following criteria are met:

$$\begin{aligned} \eta_x^2 + \eta_y^2 &< \frac{1}{2} \\ \left(\frac{2\eta_x}{a}\right)^2 + \left(\frac{2\eta_y}{b}\right)^2 &< \frac{\left[1 - 2(\eta_x^2 + \eta_y^2)\right]^2}{1 - (\eta_x^2 + \eta_y^2)}. \end{aligned} \tag{6}$$

Transform the selected variates to points on the sphere using (1). Selection criteria (6) enforce $z > 0$ and (3) before the coordinate transformation (1) is performed (which features a computationally expensive square-root function).

2.3. Method 2: relaxed cone definition

Generate two random variates, η_x uniform on $(-\eta_a, \eta_a)$ and η_y uniform on $(-\eta_b, \eta_b)$. Select the pair if

$$\left(\frac{\eta_x}{\eta_a}\right)^2 + \left(\frac{\eta_y}{\eta_b}\right)^2 < 1. \tag{7}$$

Transform the selected variates to points on the sphere using (1). Since the functional form of (7) is different from that of (6), it is apparent that the sampled points will not obey the strict cone definition of (3). The differences are discussed below.

3. Results and discussion

The uniformity of these two sampling methods was evaluated as recommended by Knuth [6]. First, the θ–ϕ bounding box of the generating cone was divided into 20×20 bins, and those bins enclosed by the generating cone were selected. Then, the expected number of directions within each bin was computed, accounting for the solid angle subtended by each bin and the entire generating cone. A total of 10^5 directions were generated, such that the expected number in each bin was greater than 5. Pearson's χ^2 statistic quantified the agreement between the observed and expected number of directions generated within the bins. Excessively high (low) χ^2 values indicate that the agreement is too poor (good) to be consistent with the uniform (random) generation of directions. The empirical distribution function of χ^2 was measured by repeating this process 200 times. Finally, the empirical and theoretical χ^2 distribution functions were compared using a Kolmogorov–Smirnov test. This two-level test demonstrated the uniformity of both methods (see Fig. 3).

Method 2 does not strictly obey the elliptical cone definition (3). Although the difference in the generated range of directions is usually negligible, it can become appreciable for elliptical cones with extreme eccentricity. Fig. 4a demonstrates this difference for $\theta_x = 89°$ and $\theta_y = 20°$. The acceptance probability of method 2 is constant at $\pi/4 \approx 0.79$, since it samples (η_x, η_y) points from an ellipse. However, Fig. 4b shows that the acceptance probability of method 1 can decrease by up to 10%.

A benefit of disobeying the strict cone definition is that method 2 is able to support $\theta_x > 90°$ and/or $\theta_y > 90°$ (i.e. sample directions below the equator). This is not possible in method 1, since the cone is limited to a single hemisphere. Fig. 5 displays an example of the resulting shape upon the surface of the unit sphere.

It is also possible to sample η_x and η_y from normal distributions with mean $\mu = 0$ and a standard deviation σ of η_a and η_b, respectively. The level sets of the probability density function $f(\eta_x, \eta_y)$ are ellipses, and are transformed by (1) into level sets corresponding to boundaries that can be generated by method 2. For this reason, normal sampling is a natural extension to method 2. These η_a and η_b now correspond to the angular spread from the z-axis, instead of defining the boundary to generated directions. To constrain points to the surface of the unit sphere, the variates must