

Distribution of Angle between Two Linked Triangles

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January 24, 2015

1 One Dimensional Constraint Manifold

First we consider the case in which one triangle is fixed with the coordinates $(0, 1/2, 0)$, $(0, -1/2, 0)$, $(\sqrt{3}/2, 0, 0)$. The second face will share the vertices $(0, 1/2, 0)$ and $(0, -1/2, 0)$ and its third vertex v is allowed to vary subject to the constraints of being unit distance from the other vertices. The corresponding constraint space can be described by parameterizing v by θ , the dihedral angle between faces.

$$v(\theta) = \left[\sqrt{3}/2 \cos \theta, 0, \sqrt{3}/2 \sin \theta \right]^T \quad (1)$$

Diaconis et al. outline a method for sampling uniformly from a manifold \mathcal{M} . If the manifold is of m dimensions sitting in an n dimensional ambient space, and a parameterization $f : \mathbb{R}^m \rightarrow \mathbb{R}^n$ the sampling distribution on the parameters that corresponds to a uniform sampling on \mathcal{M} is given by $h(\omega, \theta, \phi) \propto (\det [(Df)^T Df])^{1/2}$.

In this example, we have the following parameterization.

$$f(\theta) = \begin{bmatrix} 0 \\ 1/2 \\ 0 \\ 0 \\ -1/2 \\ 0 \\ \sqrt{3}/2 \\ 0 \\ 0 \\ \sqrt{3}/2 \cos \theta \\ 0 \\ \sqrt{3}/2 \sin \theta \end{bmatrix} \quad (2)$$

$$Df(\theta) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -\sqrt{3}/2 \sin \theta \\ 0 \\ \sqrt{3}/2 \cos \theta \end{bmatrix} \quad (3)$$

Thus the sampling distribution on θ is uniform.

$$h(\theta) \propto \sqrt{\det [3/4]} \quad (4)$$

$$\propto 1 \quad (5)$$

2 Three Dimensional Constraint Manifold

Now we let the common edge rotate about the x-axis while its center remains fixed at the origin. More formally, define the point $u = [0, \frac{1}{2} \cos \omega, \frac{1}{2} \sin \omega]^T$ in the y-z plane. Then, we parameterize the shared edge by $\omega \in [0, 2\pi)$ with

its endpoints being $u(\omega)$ and $-u(\omega)$. Then we use θ and ϕ to parameterize the remaining two vertices v_1 and v_2 as follows.

$$v_1 = \left[\frac{\sqrt{3}}{2} \cos \theta, \frac{\sqrt{3}}{2} \sin \theta \sin \omega, -\frac{\sqrt{3}}{2} \sin \theta \cos \omega \right]^T \quad (6)$$

$$v_2 = \left[\frac{\sqrt{3}}{2} \cos(\theta + \phi), \frac{\sqrt{3}}{2} \sin(\theta + \phi) \sin \omega, -\frac{\sqrt{3}}{2} \sin(\theta + \phi) \cos \omega \right]^T \quad (7)$$

With these parameterizations, it is trivial to verify that the constraints $|u - (-u)| = |v_1 - u| = |v_1 + u| = |v_2 - u| = |v_2 + u| = 1$ are all satisfied for any choice of (ω, θ, ϕ) . Additionally, the dihedral angle between the two triangles is given by ϕ .

We proceed in deriving the sampling distributions of the 3 parameters that corresponds to uniform sampling of the 3 dimensional constraint manifold embedded in \mathbb{R}^{12} using the method outlined in Diaconis et al. First we concatenate our parameterizations into a function $f : \mathbb{R}^3 \rightarrow \mathbb{R}^{12}$ That maps

$(\omega, \theta, \phi) \in [0, 2\pi)^3$ onto the constraint manifold.

$$f(\omega, \theta, \phi) = \begin{bmatrix} 0 \\ \frac{1}{2} \cos \omega \\ \frac{1}{2} \sin \omega \\ 0 \\ -\frac{1}{2} \cos \omega \\ -\frac{1}{2} \sin \omega \\ \frac{\sqrt{3}}{2} \cos \theta \\ \frac{\sqrt{3}}{2} \sin \theta \sin \omega \\ -\frac{\sqrt{3}}{2} \sin \theta \cos \omega \\ \frac{\sqrt{3}}{2} \cos(\theta + \phi) \\ \frac{\sqrt{3}}{2} \sin(\theta + \phi) \sin \omega \\ -\frac{\sqrt{3}}{2} \sin(\theta + \phi) \cos \omega \end{bmatrix} \quad (8)$$

$$Df(\omega, \theta, \phi) = \begin{bmatrix} 0 & 0 & 0 \\ -\frac{1}{2} \sin \omega & 0 & 0 \\ \frac{1}{2} \cos \omega & 0 & 0 \\ 0 & 0 & 0 \\ \frac{1}{2} \sin \omega & 0 & 0 \\ -\frac{1}{2} \cos \omega & 0 & 0 \\ 0 & -\frac{\sqrt{3}}{2} \sin \theta & 0 \\ \frac{\sqrt{3}}{2} \sin \theta \cos \omega & \frac{\sqrt{3}}{2} \cos \theta \sin \omega & 0 \\ \frac{\sqrt{3}}{2} \sin \theta \sin \omega & -\frac{\sqrt{3}}{2} \cos \theta \cos \omega & 0 \\ 0 & -\frac{\sqrt{3}}{2} \sin(\theta + \phi) & -\frac{\sqrt{3}}{2} \sin(\theta + \phi) \\ \frac{\sqrt{3}}{2} \sin(\theta + \phi) \cos \omega & \frac{\sqrt{3}}{2} \cos(\theta + \phi) \sin \omega & \frac{\sqrt{3}}{2} \cos(\theta + \phi) \sin \omega \\ \frac{\sqrt{3}}{2} \sin(\theta + \phi) \sin \omega & -\frac{\sqrt{3}}{2} \cos(\theta + \phi) \cos \omega & -\frac{\sqrt{3}}{2} \cos(\theta + \phi) \cos \omega \end{bmatrix} \quad (9)$$

$$(Df)^T Df = \begin{bmatrix} \frac{1}{2} + \frac{3}{4} \sin^2 \theta + \frac{3}{4} \sin^2(\theta + \phi) & 0 & 0 \\ 0 & \frac{3}{2} & \frac{3}{4} \\ 0 & \frac{3}{4} & \frac{3}{4} \end{bmatrix} \quad (10)$$

Thus the sampling distribution is computed.

$$h(\omega, \theta, \phi) \propto \sqrt{1 + \frac{3}{2} \sin^2 \theta + \frac{3}{2} \sin^2(\theta + \phi)} \quad (11)$$

3 Four Dimensional Constraint Manifold

Suppose we relax the constraints of the previous calculation. Fix the mid-point of the shared edge at the origin, but allow it the freedom to rotate in any direction. Then, the endpoints of the shared edge lie at opposite ends of the sphere with radius $1/2$. We use spherical coordinates to parameterize the axis $[-u(\phi, \omega), u(\phi, \omega)]$.

$$u(\phi, \omega) = \left(\frac{1}{2} \cos(\phi), \frac{1}{2} \sin(\phi) \cos(\omega), \frac{1}{2} \sin(\phi) \sin(\omega) \right) \quad (12)$$

Now we parameterize the remaining two vertices as $v_1 = R(2u, \theta)v_0$ and $v_2 = R(2u, \theta + \xi)v_0$ where v_0 is any fixed point satisfying $|v_0 - u| = |v_0 + u| = 1$ and $R(\hat{u}, \hat{\theta})$ is the rotation matrix with unit axis of rotation \hat{u} and angle of rotation $\hat{\theta}$.

$$v_1 = R(2u, \theta)v_0 \quad (13)$$

$$= (\cos \theta I + 4(1 - \cos \theta)uu^T + 2 \sin \theta [u]_{\times}) v_0 \quad (14)$$

$$= \cos \theta v_0 + 4(1 - \cos \theta)u(u \cdot v_0) + 2 \sin \theta (u \times v_0) \quad (15)$$

$$= \cos \theta v_0 + 2 \sin \theta (u \times v_0) \quad (16)$$

$$v_2 = R(2u, \theta + \xi)v_0 \quad (17)$$

$$= \cos(\theta + \xi)v_0 + 2 \sin(\theta + \xi)(u \times v_0) \quad (18)$$

Thus, we compute as follows.

$$f(\phi, \omega, \theta, \xi) = \begin{bmatrix} u \\ -u \\ v_1 \\ v_2 \end{bmatrix} \quad (19)$$

$$Df(\phi, \omega, \theta, \xi) = \begin{bmatrix} Du \\ -Du \\ Dv_1 \\ Dv_2 \end{bmatrix} \quad (20)$$

$$(Df)^T Df = 2(Du)^T Du + (Dv_1)^T Dv_1 + (Dv_2)^T Dv_2 \quad (21)$$

$$Du(\phi, \omega, \theta, \xi) = \begin{bmatrix} -\frac{1}{2} \sin \phi & 0 & 0 & 0 \\ \frac{1}{2} \cos \phi \cos \omega & -\frac{1}{2} \sin \phi \sin \omega & 0 & 0 \\ \frac{1}{2} \cos \phi \sin \omega & \frac{1}{2} \sin \phi \cos \omega & 0 & 0 \end{bmatrix} \quad (22)$$

$$(Du)^T Du = \begin{bmatrix} \frac{1}{4} \sin^2 \phi + \frac{1}{4} \cos^2 \phi \cos^2 \omega + \frac{1}{4} \cos^2 \phi \sin^2 \omega & \frac{1}{4} \cos \phi \cos \omega \sin \phi \sin \omega - \frac{1}{4} \cos \phi \cos \omega \sin \phi \sin \omega & 0 & 0 \\ \frac{1}{4} \cos \phi \cos \omega \sin \phi \sin \omega - \frac{1}{4} \cos \phi \cos \omega \sin \phi \sin \omega & \frac{1}{4} \sin^2 \phi \sin^2 \omega + \frac{1}{4} \sin^2 \phi \cos^2 \omega & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (23)$$

$$= \begin{bmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{4} \sin^2 \phi & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (24)$$

$$v_1 = R(2u, \theta)v_0 \quad (25)$$

$$= (\cos \theta I + 4(1 - \cos \theta)uu^T + 2 \sin \theta[u]_{\times}) v_0 \quad (26)$$

$$= \cos \theta v_0 + 4(1 - \cos \theta)u(u \cdot v_0) + 2 \sin \theta(u \times v_0) \quad (27)$$

$$= \cos \theta v_0 + 2 \sin \theta(u \times v_0) \quad (28)$$

$$v_2 = R(2u, \theta + \xi)v_0 \quad (29)$$

$$= \cos(\theta + \xi)v_0 + 2 \sin(\theta + \xi)(u \times v_0) \quad (30)$$

$$\nabla_{\phi} v_1 = 2 \sin \theta (\nabla_{\phi} u \times v_0) \quad (31)$$

$$\nabla_{\omega} v_1 = 2 \sin \theta (\nabla_{\omega} u \times v_0) \quad (32)$$

$$\nabla_{\theta} v_1 = -\sin \theta v_0 + 2 \cos \theta (u \times v_0) \quad (33)$$

$$\nabla_{\xi} v_1 = 0 \quad (34)$$

$$\nabla_{\phi} v_2 = 2 \sin(\theta + \xi) (\nabla_{\phi} u \times v_0) \quad (35)$$

$$\nabla_{\omega} v_2 = 2 \sin(\theta + \xi) (\nabla_{\omega} u \times v_0) \quad (36)$$

$$\nabla_{\theta} v_2 = -\sin(\theta + \xi)v_0 + 2 \cos(\theta + \xi)(u \times v_0) \quad (37)$$

$$\nabla_{\xi} v_2 = -\sin(\theta + \xi)v_0 + 2 \cos(\theta + \xi)(u \times v_0) \quad (38)$$

$$(39)$$

$$Dv_1 = [\nabla_\phi v_1 \quad \nabla_\omega v_1 \quad \nabla_\theta v_1 \quad \nabla_\xi v_1] \quad (40)$$

$$(Dv_1)^T Dv_1 = \begin{bmatrix} \frac{3}{4} \sin^2 \theta & 0 & 0 & 0 \\ 0 & \frac{3}{4} \sin^2 \theta \sin^2 \omega & 0 & 0 \\ 0 & 0 & \frac{3}{4} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (41)$$

$$(Dv_2)^T Dv_2 = \begin{bmatrix} \frac{3}{4} \sin^2(\theta + \xi) & 0 & 0 & 0 \\ 0 & \frac{3}{4} \sin^2(\theta + \xi) \sin^2 \omega & 0 & 0 \\ 0 & 0 & \frac{3}{4} & \frac{3}{4} \\ 0 & 0 & \frac{3}{4} & \frac{3}{4} \end{bmatrix} \quad (42)$$

$$(Df)^T Df = \begin{bmatrix} \frac{3}{4} \sin^2 \theta + \frac{3}{4} \sin^2(\theta + \xi) + \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{3}{4} \sin^2 \theta \sin^2 \omega + \frac{3}{4} \sin^2(\theta + \xi) \sin^2 \omega + \frac{1}{2} \sin^2 \phi & 0 & 0 \\ 0 & 0 & \frac{3}{4} & \frac{3}{4} \\ 0 & 0 & \frac{3}{4} & \frac{3}{4} \end{bmatrix} \quad (43)$$

$$h(\phi, \omega, \theta, \xi) \propto \sqrt{\det \left((Df)^T Df \right)} \quad (44)$$

$$\propto \sqrt{\left(\frac{3}{4} \sin^2 \theta + \frac{3}{4} \sin^2(\theta + \xi) + \frac{1}{2} \right) \left(\frac{3}{4} \sin^2 \theta \sin^2 \omega + \frac{3}{4} \sin^2(\theta + \xi) \sin^2 \omega + \frac{1}{2} \sin^2 \phi \right)} \quad (45)$$

$$\propto \sqrt{(3 \sin^2 \theta + 3 \sin^2(\theta + \xi) + 2) (3 \sin^2 \theta \sin^2 \omega + 3 \sin^2(\theta + \xi) \sin^2 \omega + 2 \sin^2 \phi)} \quad (46)$$