rotations: A Package for $SO(3)$ Data

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Abstract In this article we introduce the **rotations** package which provides users with the ability to simulate, analyze and visualize 3-dimensional rotation data. The **rotations** package includes four distributions from which to simulate data, four estimators of the central orientation and a novel approach to visualizing these data. All of the above features are available to three different parameterizations of rotations: 3-by-3 matrix form, quaternions and Euler angles.

Introduction

Data in form of three-dimensional rotations find application in several scientific areas, such as biomedical engineering, computer visioning, and geological and materials sciences. A common goal shared by these fields is to estimate the main or central orientation for a sample of rotations. That is, letting the rotation group $SO(3)$ denote the collection of all 3×3 rotation matrices, observations $\boldsymbol{R}_1, \ldots, \boldsymbol{R}_n \in SO(3)$ can be conceptualized as a random sample from a *location model*

$$\mathbf{R}_i = \boldsymbol{S}\boldsymbol{E}_i, \quad i = 1, \ldots, n, \tag{1}$$

where $\boldsymbol{S} \in SO(3)$ is the *fixed* parameter of interest indicating an orientation of central tendency, and $\boldsymbol{E}_1, \ldots, \boldsymbol{E}_n \in SO(3)$ denote i.i.d. *random* rotations which symmetrically perturb $\boldsymbol{S}$.

The **rotations** package provides users with the tools necessary to simulate data from four common choices of symmetric distributions, estimate $\boldsymbol{S}$ in (1) and visualize a sample of rotations. The remainder of this paper is organized as follows. We will begin with a discussion on how rotation data can be parameterized. Then we discuss how data generation is possible in this package. Next we discuss the different estimators used to estimate the central direction. Finally, visualizations of rotation data is presented.

Rotation Representations

The variety of applications for rotations is echoed by the number of equivalent ways to parameterize them. We consider three of the most popular: matrices in $SO(3)$, unit quaternions and Euler angles.

Matrix Form

Three-dimensional rotations can be represented by 3×3 orthogonal matrices with determinant one. All matrices with these characteristics form a group called the *special orthogonal group*, or *rotation group*, denoted $SO(3)$. Every element in $SO(3)$ can be described by an angle, $r \in [0, \pi)$ and an axis, $\boldsymbol{u} \in \mathbb{R}^3$ with $||\boldsymbol{u}|| = 1$. Thus $\boldsymbol{R} \in SO(3)$ can be thought of as rotating the coordinate axis, $\boldsymbol{I}_{3\times3}$, about the axis $\boldsymbol{u}$ by the angle r. We adopt the material scientist's terminology in calling r the misorientation angle and $\boldsymbol{u}$ the misorientation axis.

More specifically, given an angle, r, and axis, $\boldsymbol{u}$, a 3×3 rotation matrix can be formed by

$$\boldsymbol{R} = \boldsymbol{R}(r, \boldsymbol{u}) = \boldsymbol{u}\boldsymbol{u}^\top + (\boldsymbol{I}_{3\times3} - \boldsymbol{u}\boldsymbol{u}^\top)\cos(r) + \Phi(\boldsymbol{u})\sin(r) \tag{2}$$

where

$$\Phi(\boldsymbol{u}) = \Phi(u_1, u_2, u_3) = \begin{pmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{pmatrix}.$$

Quaternion Form

A second parameterization of rotations is with a *quaternion* of unit length. Quaternions are a form of imaginary numbers with one real entry and a vector of three imaginary parts that can be expressed as

$$q = x_1 + x_2 i + x_3 j + x_4 k$$

where i, j, and k are square roots of -1, i.e. $i^2 = j^2 = k^2 = -1$. We can write $q = (s, v)$ as tuple of the scalar s for coefficient $\mathbf{1}$ and vector $\boldsymbol{v}$ for the imaginary coefficients, i.e. $s = x_1$ and $v = (x_2, x_3, x_4)$.

A rotation around axis $\boldsymbol{u}$ by angle r translates to $q = (s, v)$ with

$$s = \cos(r/2), \;\; \boldsymbol{v} = \boldsymbol{u}\sin(r/2)$$

This makes q a unit quaternion.

Euler Angle Form

The final parameterization we consider is *Euler angles*. Euler angles are three dimensional vectors describing a sequence of rotations of some fixed coordinate axis. There are several versions of Euler angles and we consider the $z - x - z$ formulation. That is, if (α, β, γ) is an Euler angle for $\alpha, \gamma \in [0, 2\pi]$, and $\beta \in [0, \pi]$, rotate the z-axis counterclockwise through α radians, then rotate the x-axis through β radians and finally rotate the z-axis through γ radians.

To make this more concrete, we can form a rotation matrix from a vector of Euler angles as follows. Let $\boldsymbol{e}_1 = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}$ and $\boldsymbol{e}_3 = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}$ then

$$\boldsymbol{R} = \boldsymbol{R}(\gamma, \boldsymbol{e}_1)\boldsymbol{R}(\beta, \boldsymbol{e}_3)\boldsymbol{R}(\alpha, \boldsymbol{e}_1)$$

For each of these parameterizations

Data generation

Using (1) one can simulate a matrix $\boldsymbol{E}_i \in SO(3)$ by picking an axis $\boldsymbol{u}$ uniformly on the sphere then drawing an angle r from a distribution symmetric about 0 and bounded between $-\pi$ and π then applying (2). A matrix generated in this fashion is said to belong to the *uniform-axis random spin*, or UARS, class of distributions (Bingham et al., 2009). The choice of angular distribution distinguishes between members of this class.

The **rotate** package allows the user access to four members of the UARS class differentiated by the distributional models on r: the uniform distribution on the circle, the symmetric matrix Fisher (Langevin, 1905; Downs, 1972; Khatri and Mardia, 1977; Jupp and Mardia, 1979), the symmetric Cayley (Schaeben, 1997; León et al., 2006) and a circular-von Mises-based distribution (Bingham et al., 2009).

The uniform distribution on the circle is given by the following density function

$$C_{\mathrm{H}}(r) = \frac{1-\cos(r)}{2\pi} \tag{3}$$

for $r \in (-\pi, \pi]$. This function also plays the part of a measure on the sphere, called the Haar measure on the sphere. The function `rhaar` with input `n` will draw a sample of size n from 3 and `dhaar` with evaluate the density at a given point.

The following three distributions have only one parameter, κ, which is the concentration parameter. As κ increases, the distribution becomes more peaked about 0 and less variable. If one would prefer to specify the variability instead, the circular variance denoted ν can also be set by the user. For $r \sim F$ where F is a distribution on the circle, the circular variance is defined as $\nu = 1 - E\cos(r)$, and $E\cos(r)$ is called the mean resultant length (Mardia and Jupp, 2000).

The symmetric matrix Fisher distribution is the oldest and also the most difficult to sample from. It takes on the following distributional form

$$C_{\mathrm{F}}(r|\kappa) = \frac{1}{2\pi[\mathrm{I}_0(2\kappa) - \mathrm{I}_1(2\kappa)]} e^{2\kappa\cos(r)}[1-\cos(r)]$$

where $\mathrm{I}_p(\cdot)$ denotes the Bessel function of order p defined as $\mathrm{I}_p(\kappa) = \frac{1}{2\pi}\int_{-\pi}^{\pi}\cos(pr)e^{\kappa\cos r}dr$.

For a given κ, the function `rfisher` generates a sample of size n from this distribution using a rejection algorithm and `dfisher` evaluates the density at a given angle r.

León et al. (2006) proposed the symmetric Cayley distribution, which is identical to the de la Vallée Poussin distribution and a favorite among material scientists (Schaeben, 1997). This distribution is closely related to the beta distribution and has the distributional form

$$C_{\mathrm{C}}(r|\kappa) = \frac{1}{\sqrt{\pi}}\frac{\Gamma(\kappa+2)}{\Gamma(\kappa+1/2)}2^{-(\kappa+1)}(1+\cos r)^{\kappa}(1-\cos r).$$

`rcayley` simulates from this distribution by taking a simple transformation of random deviates from a beta distribution and `dcayley` evaluates the Cayley density at a given angle, r.

Finally the circular-von Mises-based distribution is included because the distribution is non-regular and has been applied to EBSD data (Bingham et al., 2009). An angle following this distribution has the distribution form

$$C_{\mathrm{M}}(r|\kappa) = \frac{1}{2\pi\mathrm{I}_0(\kappa)}e^{\kappa\cos(r)}.$$

Simulation from this distribution was developed by Best and Fisher (1979) and the function `rvmises` follows this procedure closely. Also, `dvmises` evaluates the density at a given angle, r.

Once an angular distribution has been chosen and a vector of n angles of rotation have been generated, the `genR` function with option `space="SO3"` creates an $n \times 9$ matrix representing a sample from the appropriate UARS member as demonstrated in the following code. If quaternions or Euler angles are desired the options `space` can be changed to `"Q4"` and `"R3"`, respectively.

```
rs <- rcayley(20, 1)
Rs <- genR(rs)
R1 <- matrix(Rs[1, ], 3, 3)
is.SO3(R1)

## [1] TRUE
```

Here `rcayley(20,1)` simulates $r_1, \ldots, r_{20}$ from $C_{\mathrm{C}}(r|\kappa = 1)$ then `genR` generates the matrices. Each row of `Rs` is an element in $SO(3)$, as demonstrated by `is.SOn`, in vector form with central orientation $\boldsymbol{I}_{3\times3}$. Any other central orientation in $SO(3)$ is possible by changing the `S` option. If a central orientation not in $SO(3)$ is proposed, however, an error is returned.

$SO(3)$ data analysis

Given a sample of n observations $\boldsymbol{R}_1, \ldots, \boldsymbol{R}_n$ generated according to (1) we offer four ways to estimate the matrix $\boldsymbol{S}$, i.e. the central orientation. These estimators are either Riemannian- or Euclidean-based in geometry and either mean- or median-based. First we discuss how the choice of geometry affects distance.

The choice of geometry results in two different metrics to measure the distance between rotation matrices $\boldsymbol{R}_1$ and $\boldsymbol{R}_2 \in SO(3)$. Under the embedding approach, the natural distance metric between two random matrices in the Euclidean distance, d_E, is induced by the Frobenius norm

$$d_E(\boldsymbol{R}_1, \boldsymbol{R}_2) = \|\boldsymbol{R}_1 - \boldsymbol{R}_2\|_F, \tag{4}$$

where $\|\boldsymbol{A}\|_F = \sqrt{\mathbf{tr}(\boldsymbol{A}^\top \boldsymbol{A})}$ denotes the Frobenius norm of a matrix $\boldsymbol{A}$ and $\mathbf{tr}(\cdot)$ denotes the trace of a matrix. The Euclidean distance between two rotation matrices corresponds to the shortest cord in $\mathcal{M}(3)$ that connects them. If $r \in [-\pi, \pi)$ denotes the misorientation angle in the angle-axis representation (2) of $\boldsymbol{R}_1^\top \boldsymbol{R}_2 \equiv \boldsymbol{R}_1^\top \boldsymbol{R}_2(r, \boldsymbol{u})$ (so that $\mathbf{tr}(\boldsymbol{R}_1^\top \boldsymbol{R}_2) = 1 + 2\cos r$), then $d_E(\boldsymbol{R}_1, \boldsymbol{R}_2) = 2\sqrt{(1 - \cos r)}$ holds.

By staying in the Riemannian space $SO(3)$ under the intrinsic approach, the natural distance metric becomes the Riemannian (or geodesic) distance, d_R, by which the distance between two rotations $\boldsymbol{R}_1, \boldsymbol{R}_2 \in SO(3)$ is defined as

$$d_R(\boldsymbol{R}_1, \boldsymbol{R}_2) = \frac{1}{\sqrt{2}} ||\mathrm{Log}(\boldsymbol{R}_1^\top \boldsymbol{R}_2)||_F = |r|, \qquad (5)$$

where $\mathrm{Log}(\boldsymbol{R})$ denotes the principle logarithm of $\boldsymbol{R}$ (i.e., $\mathrm{Log}(\boldsymbol{R}) = \mathrm{Log}(\boldsymbol{R}(\boldsymbol{u}, r)) = \boldsymbol{\Phi}(r\boldsymbol{u})$ in (2)) and $r \in [-\pi, \pi)$ is the misorientation angle of $\boldsymbol{R}_1^\top \boldsymbol{R}_2$. The Riemannian distance corresponds to the length of the shortest path that connects $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ *within* the space $SO(3)$. For this reason, the Riemannian distance is often considered the more natural metric on $SO(3)$; see Moakher (2002) for this discussion along with more details on exponential/logarithmic operators related to $SO(3)$.

We first consider estimators based on the embedding approach, which we call the projected estimators. The median-based estimator in this class is

$$\widetilde{S}_E = \mathrm{argmin}_{S \in SO(3)} \sum_{i=1}^{n} d_E(\boldsymbol{R}_i, \boldsymbol{S}). \qquad (6)$$

The function `median` with option `type="projected"` approximates $\widetilde{S}_E$ and uses an adaptation of the Weiszfeld algorithm (Weiszfeld, 1937). The mean-based estimator is

$$\widehat{S}_E = \mathrm{argmin}_{S \in SO(3)} \sum_{i=1}^{n} d_E^2(\boldsymbol{R}_i, \boldsymbol{S})$$
$$= \mathrm{argmax}_{S \in SO(3)} \mathrm{tr}(\boldsymbol{S}^\top \bar{\boldsymbol{R}}) \qquad (7)$$

and is computed by the function `mean` with option `type="projected"`. For an in-depth discussion of the algorithm used to compute this value consult Moakher (2002).

The intrinsic estimators minimize the first and second order Riemannian distances. The *geometric median* is

$$\widetilde{S}_R = \mathrm{argmin}_{S \in SO(3)} \sum_{i=1}^{n} d_R(\boldsymbol{R}_i, \boldsymbol{S}). \qquad (8)$$

An algorithm proposed by Hartley et al. (2011) is employed by the function `median` with option `type="intrinsic"`. The *geometric mean* is the L_2 analog of $\widetilde{S}_R$ given by

$$\widehat{S}_R = \mathrm{argmin}_{S \in SO(3)} \sum_{i=1}^{n} d_R^2(\boldsymbol{R}_i, \boldsymbol{S}). \qquad (9)$$

The function `mean` with option `type="intrinsic"` implements an algorithm first proposed by Manton (2004) in estimating $\widehat{S}_R$.

Confidence Area Construction

With limited theory available for estimators of the central orientation, a bootstrap method is proposed to estimate the uncertainty associated with them. The procedure implemented by the function `CIradius` is as follows where $\widehat{S}$ is any of the estimators discussed so far:

1. Estimate $\widehat{S}$ from $(\boldsymbol{R}_1, \ldots, \boldsymbol{R}_n)$
2. Sample $\boldsymbol{R}_1$,...,$\boldsymbol{R}_m$ from $(\boldsymbol{R}_1, \ldots, \boldsymbol{R}_n)$ with replacement
3. Estimate $\widehat{S}^*$ from bootstrap sample
4. Compute $\hat{T} = d_G(\widehat{S}, \widehat{S}^*)$
5. Repeat steps 1-3 B times
6. Report q% percentile of $\hat{T}$ to be the radius of the confidence 'cone'

A similar procedure was used by Bingham et al. (2010), but in place of d_R the maximum absolute angle between all three axis, which they called α, was used. It's easy to show that α is less than or equal to the geodesic distance between any two rotations making our method slightly more conservative.

Visualizations

In this section we introduce a method to visualize $SO(3)$ data via the the **ggplot2** package (Wickham, 2009). The function `plot` takes as input a $n \times 9$ matrix of $SO(3)$ observations and returns a visualization of one of the three columns. The user can specify which column to use with the `column` option, the default is one.

The four estimates of the central orientation given in the previous section can be plotted by setting `estimates show=TRUE`. The estimators are indicated by shape. One can also center the data about any observation in $SO(3)$ by setting `center=S`. Typically take `center=mean(Rs)`.

```
rs <- rvmises(50, 0.01)
Rs <- genR(rs)
plot(Rs, center = mean(Rs), show_estimates = T)
```

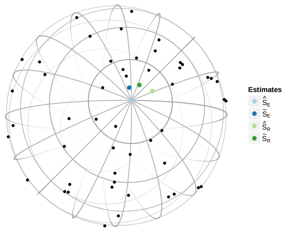

Figure 1: A plot of the a random sample from the von Mises-UARS distribution with $\kappa = 0.01$.

In figure 1 a random sample of 50 matrices following the von Mises UARS distribution with $\kappa = 0.01$ is plotted along with four estimates of the central orientation. The code to produce this plot is also given.

Summary

The **rotations** package is introduced and allows the user to create, simulate, analyze and visualize rotation data. There are three parameterizations possible in this package and four built-in distributions from which data can be simulated. The four estimators discussed in Stanfill et al. (2012) are each implemented and each can be visualized via `ggplot2`.

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