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A Permutation Test for Comparing Multiple Measures of Center in Three-Dimensional Rotation Data

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Data in the form of three-dimensional rotations arise in various fields, yet statistical techniques for modeling such data receive far less focus in the area of directional statistics than circular and spherical data. In this paper, the focus is on comparison of mean or central matrices for multiple groups of three-dimensional rotations. A permutation test is developed by using the fundamental ideas behind a traditional Analysis of Variance and a simulation study is used to investigate the power of the permutation test under various conditions. The test is then used on a biomechanics data set to compare movement around the calcaneocuboid joint for a human, chimpanzee, and baboon.

keywords: Directional data, Three-Dimensional Rotations, Permutation Test, ANOVA, Misorientation Angle, Biomechanics.

1 Introduction

Data in the form of three-dimensional rotations arise in many areas of science. One of the most classic data sets analyzed in the statistical literature for three-dimensional rotations is the vectorcardiography data considered by Downs (1972) and Khatri and Mardia (1977). Many works have considered three-dimensional rotation data sets in the study of biomechanics (Rancourt et al., 2000; Rivest et al., 2008; Haddou et al., 2010; Oualkacha and Rivest, 2009). In the area of materials science, crystal orientations have been considered by Bingham et al. (2009); Du et al. (2015); Arnold et al. (2018),

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while Sei et al. (2013) consider an application in the area of astronomy. Although three-dimensional rotation data arise in various fields, statistical techniques for modeling such data receive far less focus in the area of directional statistics than circular and spherical data (see, for example, Mardia and Jupp, 2000).

The matrix Fisher distribution is the most commonly cited distribution for three-dimensional rotation data (i.e. on the rotation group SO(3)) in the literature (Khatri and Mardia, 1977; Jupp and Mardia, 1979; Prentice, 1986; Mardia and Jupp, 2000; Rancourt et al., 2000; Sei et al., 2013) and many statistical developments for such data rely on this distributional form. Drawbacks of the continual reliance on the matrix Fisher distribution, such as complicated expressions that are difficult to evaluate and poor fit to some data sets, motivated works such as León et al. (2006), Bingham et al. (2009), and Oualkacha and Rivest (2009) to develop new distributions on SO(3). Although these works added flexibility in modeling three-dimensional rotations, there still seems to be a disconnect between methods in the statistical literature for three-dimensional rotations and the techniques that are actually employed by scientists in the application areas noted above. This could be due to the fact that development of methodology on SO(3) is highly mathematical in nature. As Pierrynowski and Ball (2009) point out, practitioners in the area of biomechanics often incorrectly calculate something as routine as an average rotation.

The need for statistical techniques that can be easily and correctly applied by scientists who collect three-dimensional rotation data, coupled with the need for flexibility in modeling that does not rely on the matrix Fisher distribution, has led to more recent works in the area of nonparametric statistics. Permutation tests for directional data were introduced by Wellner (1979), but with a mathematical focus on Riemannian manifolds. More recent works use simulations to conduct nonparametric inference for three-dimensional rotations, making them more easily accessible to scientists. Bootstrapping for estimating a central/mean rotation in SO(3) for a single data set and permutation tests for comparison of the central/mean rotations of two data sets have been explored (Stanfill et al., 2015; Bero and Bingham, 2015). These works do not, however, allow for comparison of central/mean rotations across *multiple* three-dimensional rotation data sets. Figueiredo (2017) and Ley et al. (2017) explore Analysis of Variance (ANOVA) for directional data, but these works are applicable to points on the surface of the unit sphere in $\mathbb{R}^q$ and not to the rotation group SO(3). Therefore, this paper aims to expand upon these works by using nonparametric statistics to develop an ANOVA-type procedure for comparing population central rotations across more than two groups.

In Section 2 a permutation test for comparing measures of center in multiple three-dimensional rotation data sets will be developed. This test will employ the fundamental ideas behind the ANOVA by comparing variability within the data sets to variability between the data sets. In Section 3 a simulation study will be used to investigate the power of the permutation test under various conditions. Finally, in Section 4, the permutation test will be used in a brief example to compare movement around the calcaneocuboid joint for a human, chimpanzee, and baboon. This data set was considered by Bero and Bingham (2015), but comparison could only be made on two species at a time.

2 Permutation Test for Comparing Multiple Population Mean Rotations

To employ a permutation test for comparing mean rotations across multiple three-dimensional rotation data sets, a sensible test statistic must be developed. This will be accomplished by using the underlying concepts of a traditional ANOVA test. A ratio of a measure of the variability between the data sets and a measure of the variability within the data sets will be used.

Consider k samples of data drawn from k different populations in SO(3). Denote the size of sample i as n_i, and let $\mathbf{O}_{ij} \in \mathrm{SO}(3)$ denote the j^{th} observation in the i^{th} sample. For each of the k data sets, the sample mean rotation matrix can be found (Bingham et al., 2009). Denote these k sample mean matrices as $\bar{\mathbf{O}}_1, \bar{\mathbf{O}}_2, \ldots, \bar{\mathbf{O}}_k$. To measure variability *between* these sample mean matrices, the distances from each of the sample means to the overall or grand mean matrix can be computed. The grand mean matrix, $\bar{\mathbf{O}}_G$, is the mean matrix computed from all $n_1 + n_2 + \cdots + n_k$ observations.

The distance from each individual sample mean matrix to the grand mean matrix can then be found as the misorientation angle (Bingham et al., 2009; Randle, 2003) between the two matrices

$$\mathrm{mis}(\bar{\mathbf{O}}_i, \bar{\mathbf{O}}_G) = \arccos\left(\frac{tr(\bar{\mathbf{O}}_i'\bar{\mathbf{O}}_G) - 1}{2}\right) \tag{1}$$

where tr is the trace of a matrix and $\bar{\mathbf{O}}_i'$ is the transpose of $\bar{\mathbf{O}}_i$. The total variability between the sample mean matrices can then be measured by

$$V_B = \sum_{i=1}^{k} \left(n_i \cdot \mathrm{mis}(\bar{\mathbf{O}}_i, \bar{\mathbf{O}}_G)\right) \tag{2}$$

Next, the variability *within* the groups is measured. The spread in each of the individual three-dimensional rotation data sets can be measured by using the average misorientation angle (Bingham, 2015). For data set i with individual mean $\bar{\mathbf{O}}_i$, the average misorientation angle is $\mathrm{AMA}_i = \frac{1}{n_i}\sum_{j=1}^{n_i} mis(\bar{\mathbf{O}}_{ij}, \bar{\mathbf{O}}_i)$. An overall measure of spread within all the data sets can then be found as

$$V_W = \sum_{i=1}^{k} \left(n_i \cdot \mathrm{AMA}_i\right) \tag{3}$$

Following the concept of the ANOVA for comparing means in traditional data types, the variability between the groups and the variability within the groups can be compared by taking a ratio of measures of the two sources of variability. For testing the hypotheses

H_0 : equal population mean rotation matrices for all k populations
H_a : at least two of the population mean rotation matrices differ

we can use a test statistic of

$$T = \frac{V_B}{V_W} \tag{4}$$

where V_B and V_W are defined in equations (2) and (3), respectively. If the population mean rotation matrices do in fact differ, we expect a larger V_B in comparison to V_W, giving a larger value of T. By using a nonparametric permutation test, it is not important what the actual distribution of T is. The steps of the permutation test are as listed below. (See Pesarin and Salmaso (2010) for a general work on permutation tests).

1. Calculate the statistic in (4) based on the observed data and call it T_{obs}.
2. Permute the data by combining all $n_1 + n_2 + \cdots + n_k$ observations and randomly reassigning n_1 observations to group 1, n_2 observations to group 2, etc. Calculate the test statistic in (4) for this permuted data and call it T_{perm}.
3. Repeat step 2. a large number (say 10,000) of times.
4. Let the p-value be the fraction of times that the permuted test statistic is greater than the observed test statistic; p-value $= \frac{\#\text{ of times } T_{perm} > T_{obs}}{\#\text{ of permutations}}$.

If a difference in the population mean matrices exists, then it is expected that T_{obs} will be larger than the majority of the permuted test statistics, resulting in a small p-value and rejection of the null hypothesis of equal means.

To illustrate two cases of the permutation test, consider Figure 1. Here, each three-dimensional data set is plotted as points on the sphere, where each observation is represented by three points that would correspond to three orthogonal axes. In Figure 1(a), there are three simulated data sets (in white, black, red) where the distinction between centers can be more clearly seen. In Figure 1(b), the three simulated data sets were produced from the same three population mean matrices as were used in Figure 1(a) but with much more spread within the data sets. In this instance, the distinction between the centers is not obvious. After completing the permutation test, the observed test statistic and p-value for the data in Figure 1(a) were found to be $T_{obs} = 3.48$ and p-value$< .001$. For Figure 1(b), $T_{obs} = 0.173$ and p-value $= .115$ were obtained. These plots illustrate the importance of not only comparing the difference between the sample mean matrices, but also taking into account the spread exhibited in the data as is done in a traditional ANOVA approach. While this exemplifies the permutation test for just two individual cases, in the next section the adequacy of the test is examined further by looking at a more in-depth simulation study under various conditions.

3 Simulations to Investigate Power

To further investigate the adequacy of the permutation test outlined in Section 2 for determining if multiple three-dimensional rotation data sets come from populations with differing mean rotation matrices, a simulation study was done to look at the power of the test under various parameters. Quantities that should play a role in the power of

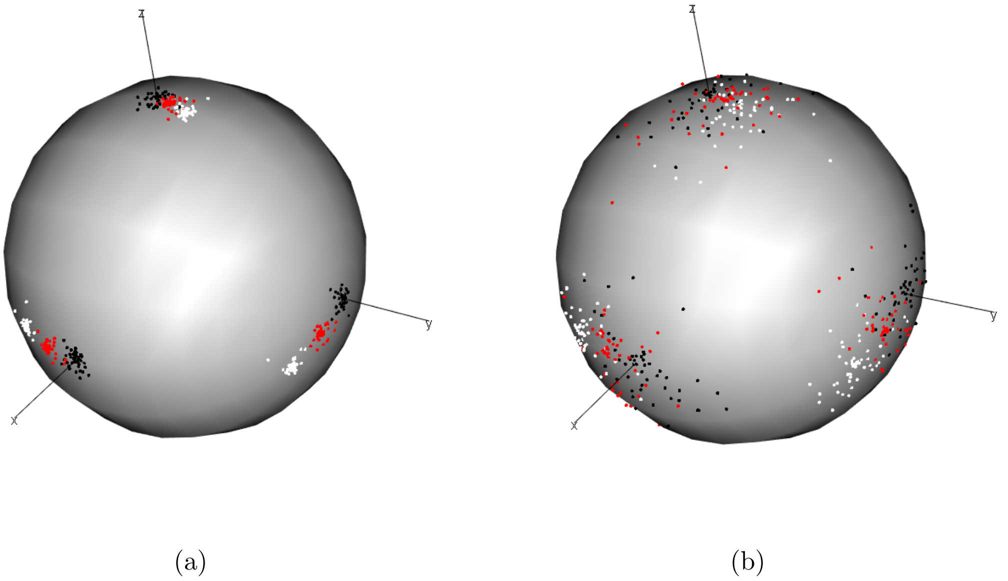
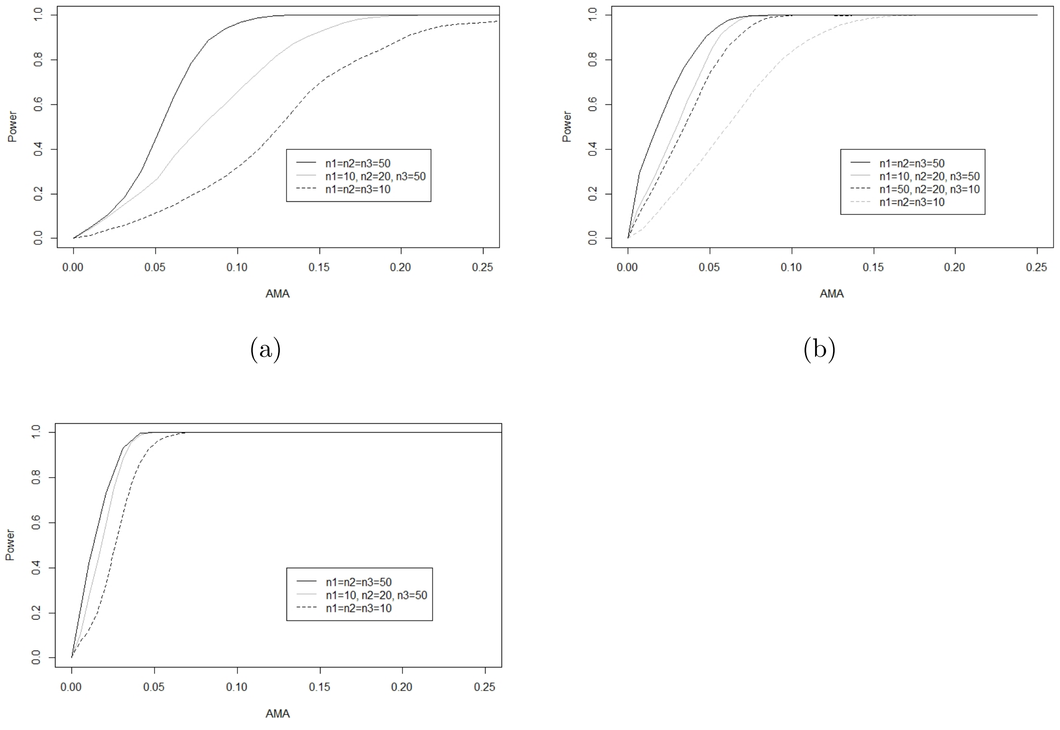


Figure 1: Plot of three simulated three-dimensional rotation data sets (each with $n = 50$) with mean rotations that (a) are significantly different and (b) are not significantly different

the test are sample sizes, variability in the individual data sets, and the difference in the true population means that the data are simulated from.

For the first part of the simulation study, three groups of data were considered. Observations were simulated from the von Mises version of the Uniform Axis-Random Spin (vM-UARS) distributions (Bingham et al., 2009), which is characterized by central rotation $\mathbf{S} \in SO(3)$ and concentration parameter $\kappa \in (0, \infty)$. The parameter κ measures spread in the distribution, with larger values of κ corresponding to rotations that are more concentrated (less spread) around the central rotation, $\mathbf{S}$. Various sample sizes ranging from 10 to 50 were used, with some cases having equal samples across the three groups and some not. Various concentration parameters ranging from $\kappa = 5$ (most spread) to $\kappa = 100$ (least spread) were used, with some cases having the same spread in all three groups and some not. Finally, the population mean rotation matrices for the three groups were allowed to differ across a spectrum of values of the average misorientation angle (AMA) between the three matrices (see Section 2 for the definition of the AMA). For each choice of AMA, sample sizes, and concentration parameters, 1000 different simulations were done. For each of the 1000 simulations, the permutation test was done (with 1000 permutations) and the p-value was recorded. The power of the test was then calculated as the proportion of times for the 1000 different simulations that the test was (correctly) found to be significant at a 0.05 level.

Plots of the power against the AMA between the true population mean matrices are provided in Figure 2 for the various combinations of sample sizes and concentration parameters. As expected, power increases as the distance between the population mean matrices (larger AMA) increases. A power of 1 is approached more quickly for larger sample sizes in each of the three plots. Additionally, as the spread of the data decreases due to a larger values of κ, the power approaches 1 more quickly. This is seen as we move from plot (a) to plot (b) to plot (c). All of these relationships between various parameters and power match what is expected, confirming that the permutation test is performing as desired in terms of power for three samples.



(a)

(b)

(c)

Figure 2: Plots of power versus the average misorientation angle between the three population central rotations for (a) $\kappa_1 = \kappa_2 = \kappa_3 = 5$, (b) $\kappa_1 = 5, \kappa_2 = 20, \kappa_3 = 100$, and (c) $\kappa_1 = \kappa_2 = \kappa_3 = 100$

For the three sample case, the observed significance level of the test was also explored. Here, the three population central matrices were set to be the same matrix. The same combinations of sample sizes and spreads as used for power were explored. For each combination of sample sizes and κ values, 1000 different simulations were done. For each of the 1000 simulations, the permutation test was done (with 1000 permutations) and the p-value was recorded. In this case, the observed significance level was calculated as the proportion of times out of 1000 that the test incorrectly rejected a null of equal population means based on a p-value below 0.05. Table 1 shows that the observed significance level bounces around 0.05 as expected for all three sample cases considered.

Table 1: Observed significance level for various choices of sample size and spread for 3 groups (missing cases are identical to the entry to the left of them in the table)

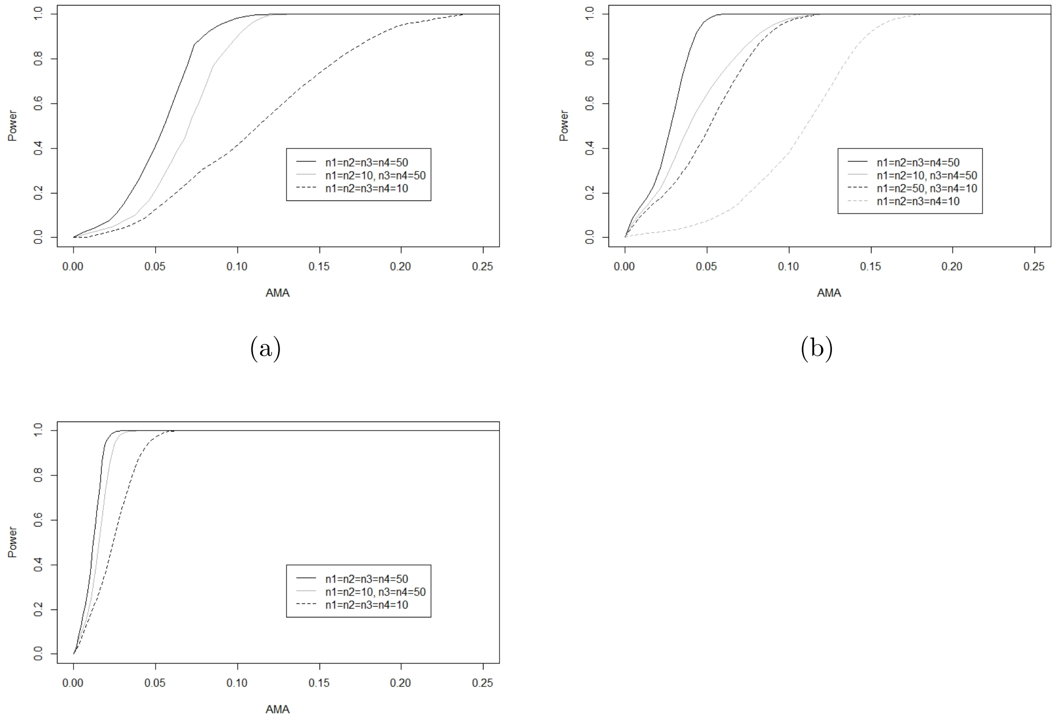
	$\kappa_1 = 5$ $\kappa_2 = 5$ $\kappa_3 = 5$	$\kappa_1 = 5$ $\kappa_2 = 20$ $\kappa_3 = 100$	$\kappa_1 = 100$ $\kappa_2 = 20$ $\kappa_3 = 5$	$\kappa_1 = 100$ $\kappa_2 = 100$ $\kappa_3 = 100$
$n_1 = n_2 = n_3 = 10$	.057	.052	-	.046
$n_1 = n_2 = n_3 = 50$	.054	.049	-	.045
$n_1 = 10, n_2 = 20, n_3 = 50$	.053	.048	.050	.045

Next, the case of 4 samples/populations was considered, both for exploring power and the observed significance level. Plots of the power against the AMA between the true population mean matrices are provided in Figure 3 for the various combinations of sample sizes and concentration parameters. The same trends are seen in these plots that were seen earlier in the three sample cases. Larger AMA, larger samples sizes, and less spread all result in larger power as expected. The observed significance levels for the four sample case are given in Table 2 and again all bounce around 0.05. Although a full-scale simulation study was not done for more than 4 groups, preliminary simulations for 5 and 6 groups show the same trends seen for 3 and 4 groups taking place.

Table 2: Observed significance level for various choices of sample size and spread for 4 groups (missing cases are identical to the entry to the left of them in the table)

	$\kappa_1 = 5$ $\kappa_2 = 5$ $\kappa_3 = 5$ $\kappa_4 = 5$	$\kappa_1 = 5$ $\kappa_2 = 20$ $\kappa_3 = 50$ $\kappa_4 = 100$	$\kappa_1 = 100$ $\kappa_2 = 50$ $\kappa_3 = 20$ $\kappa_4 = 5$	$\kappa_1 = 100$ $\kappa_2 = 100$ $\kappa_3 = 100$ $\kappa_4 = 100$
$n_1 = n_2 = n_3 = n_4 = 10$	.050	.046	-	.052
$n_1 = n_2 = n_3 = n_4 = 50$	.048	.051	-	.048
$n_1 = n_2 = 10, n_3 = n_4 = 50$	.047	.052	.049	.053

The permutation test developed here was also compared to the F-test for equality of several modal rotations presented by Rancourt et al. (2000). For all the cases explored in the simulation study, the permutation test had comparable or slightly higher power



(a) (b)

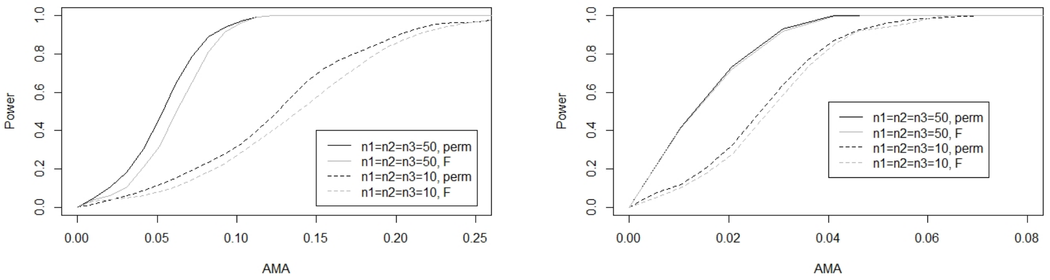
(c)

Figure 3: Plots of power versus the average misorientation angle between the four population central rotations for (a) $\kappa_1 = \kappa_2 = \kappa_3 = \kappa_4 = 5$, (b) $\kappa_1 = 5, \kappa_2 = 20, \kappa_3 = 50, \kappa_4 = 100$, and (c) $\kappa_1 = \kappa_2 = \kappa_3 = \kappa_4 = 100$

than the F-test. Selected plots of power against the AMA between the true population mean matrices are provided in Figure 4 for both the permutation test and the F-test. These plots show that the permutation test has slightly higher power than the F-test for data that is more spread (all $\kappa = 5$), with similar powers for data that is less spread (all $\kappa = 10$). This was the general trend seen across all cases explored earlier in the simulation study.

4 Application to Joint Rotation Data

We now apply the permutation test to joint rotation data as considered in Bero and Bingham (2015). The data provided by Dr. Thomas Greiner (Health Professions-Physical Therapy, University of Wisconsin-La Crosse) was collected during circumduction from a human, chimpanzee, and baboon. The foot was placed flat on the floor with the leg rotating around it in a circular motion, and movement was tracked by infra-red emit-



(a) (b)

Figure 4: Plots of power versus the average misorientation angle between the three population central rotations for both the permutation test and the F-test for (a) $\kappa_1 = \kappa_2 = \kappa_3 = 5$ and (b) $\kappa_1 = \kappa_2 = \kappa_3 = 100$

ting diodes attached to the bones on each side of a joint. Diodes may not have been placed identically on all subjects, so the rotations of all joints under consideration were measured with the Tibia-Talus joint as the reference to allow for comparison of species. Information was collected on four different joints, Cuboid-Calcaneous, Navicular-Cuboid, Navicular-Talus, and Talus-Calcaneous, using six human subjects, four chimpanzees, and seven baboons.

When considering this data, Bero and Bingham (2015) compared the species two at a time doing human/chimpanzee, human/baboon, and chimpanzee/baboon comparisons. However, we can now do comparison of all three species at once using the permutation test for comparison of multiple mean matrices. For each of the four joints in consideration, a permutation test was done with 10000 permutations. Significant differences across species were found for the Navicular-Talus joint (p-value$<$ .001) and Talus-Calcaneus joint (p-value$<$ .001). There were not significant differences found for Cuboid-Calcaneus (p-value $= 0.0942$) or Navicular-Cuboid (p-value $= 0.2148$). These results coincide with the work of Bero and Bingham (2015) where it was found that humans differed from both baboons and chimpanzees when it came to rotation of the Navicular-Talus and Talus-Calcaneus joints. While the data set considered here was small in nature, this illustrates just one instance of where the permutation test for comparing multiple mean rotations could be useful in practice.

5 Conclusion

The three-dimensional permutation test developed in this paper complements recent works that aim to provide statistical techniques that can be easily applied by scientists who collect three-dimensional rotation data. Because the permutation test is not tied to any particular distribution on SO(3) it also allows for flexibility in modeling. The test is shown to behave as expected both in terms of observed significance and power under various conditions. While the test is illustrated on a small data set in biomechanics, it's ease of implementation makes it a useful tool not only for statisticians but also for practitioners in the various fields who collect three-dimensional rotation data.

References

Arnold, R., Jupp, P., and Schaeben, H. (2018). Statistics of ambiguous rotations. *Journal of Multivariate Analysis*, 165:73–85.

Bero, D. and Bingham, M. (2015). A permutation test for three-dimensional rotation data. *Involve*, 8:735–744.

Bingham, M. A. (2015). Quantifying spread in three-dimensional rotation data: Comparison of nonparametric and parametric techniques. *Journal of Statistical Distributions and Applications*, 2:1–8.

Bingham, M. A., Nordman, D. J., and Vardeman, S. B. (2009). Modeling and inference for measured crystal orientations and a tractable class of symmetric distributions for rotations in three dimensions. *Journal of the American Statistical Association*, 104:1385–1397.

Downs, T. D. (1972). Orientation statistics. *Biometrika*, 59:665–676.

Du, C., Nordman, D., and Vardeman, S. B. (2015). Bayesian inference for a new class of distributions on equivalence classes of 3-d orientations with applications to materials science. *Technometrics*, 58:214–224.

Figueiredo, A. (2017). Bootstrap and permutation tests in anova for directional data. *Computational Statistics*, 32:1213–1240.

Haddou, M., Rivest, L.-P., and Pierrynowski, M. (2010). A nonlinear mixed effects directional model for the estimation of the rotation axes of the human ankle. *Annals of Applied Statistics*, 4:1892–1912.

Jupp, P. E. and Mardia, K. V. (1979). Maximum likelihood estimators for the matrix von mises-fisher and bingham distributions. *The Annals of Statistics*, 7:599–606.

Khatri, C. G. and Mardia, K. V. (1977). The von mises-fisher matrix distribution in orientation statistics. *Journal of the Royal Statistical Society Series B*, 39:95–106.

León, C. A., Massé, J.-C., and Rivest, L.-P. (2006). A statistical model for random rotations. *Journal of Multivariate Analysis*, 97:412–430.

Ley, C., Swan, Y., and Verdebout, T. (2017). Efficient anova for directional data. *Annals of the Institute of Statistical Mathematics*, 69:39–62.

Mardia, K. V. and Jupp, P. E. (2000). *Directional Statistics.* John Wiley and Sons.

Oualkacha, K. and Rivest, L.-P. (2009). A new statistical model for random unit vectors. *Journal of Multivariate Analysis*, 100:70–80.

Pesarin, F. and Salmaso, L. (2010). *Permutation Tests for Complex Data: Theory, Applications and Software.* John Wiley and Sons.

Pierrynowski, M. R. and Ball, K. A. (2009). Oppugning the assumptions of spatial averaging of segment and joint orientations. *Journal of Biomechanics*, 42:375–378.

Prentice, M. J. (1986). Orientation statistics without parametric assumptions. *Journal of the Royal Statistical Society Series B*, 48:214–222.

Rancourt, D., Rivest, L.-P., and Asselin, J. (2000). Using orientation statistics to investigate variations in human kinematics. *Journal of the Royal Statistical Society*, 49:81–94.

Randle, V. (2003). *Microtexture Determination and Its Applications.* London: Maney for the Institute of Materials, Minerals and Mining.

Rivest, L.-P., Baillargeon, S., and Pierrynowski, M. (2008). A directional model for the estimation of the rotation axes of the ankle joint. *Journal of the American Statistical Association*, 103:1060–1069.

Sei, T., Shibata, H., Takemura, A., Ohara, K., and Takayama, N. (2013). Properties and applications of the fisher distribution on the rotation group. *Journal of Multivariate Analysis*, 116:440–455.

Stanfill, B., Genschel, U., Hofmann, H., and Nordman, D. (2015). Nonparametric confidence regions for the central orientation of random rotations. *Journal of Multivariate Analysis*, 135:106–116.

Wellner, J. A. (1979). Permutation tests for directional data. *Annals of Statistics*, 7:929–943.