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A median estimator for three-dimensional rotation data

Melissa Bingham and Zachary Fischer

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The median is a way of measuring the center of a set of data that is robust to outlying values. However, the concept of a median for three-dimensional rotation data has been largely nonexistent. Although there are already ways to measure the center of three-dimensional rotation data using the idea of a "mean rotation", the median estimator developed here is shown to be less influenced by outlying data points. A simulation study that investigates scenarios under which the median is an improvement over the mean will be discussed. An application to a three-dimensional data set in the area of human motion will be considered.

1. Introduction

Data in the form of three-dimensional rotations are common in the areas of human motion and biomechanics, since they can be used to characterize the relative orientation of one body segment with respect to another during movement. We use data collected in a study by Rancourt, Rivest, and Asselin [Rancourt et al. 2000] to motivate the need for a median for this type of data. During the study, individuals drilled into six locations on a vertical panel, with each subject repeating the drilling five times. Infrared emitting diodes placed on the subject's hand, forearm, arm, and torso allowed for collection of orientations of the wrist, elbow, and shoulder during the drillings. Figure 1 shows five repeated wrist orientations for the drillings performed by one of the subjects studied. Since each observation is a three-dimensional rotation, it can be represented mathematically as a 3×3 orthogonal rotation matrix with determinant 1 (i.e., is a member of the rotation group $SO(3)$) and can be displayed graphically as a set of three points on the sphere, corresponding to the locations of three orthogonal axes. Notice that one of the five orientations seems to be an outlying value, as it is not clustered near the other four observations.

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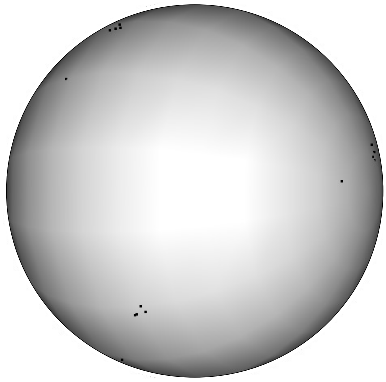

Figure 1. Five repeated wrist orientations from the drilling study (represented as a set of three points).

A common first step in data analysis is to characterize data according to some measure of center, and we attempt to do so here for the repeated drilling data. First consider using the "mean rotation" that is commonly used as a measure of center for three-dimensional rotation data [León et al. 2006; Bingham et al. 2009; Khatri and Mardia 1977]. If $\boldsymbol{O}_1, \ldots, \boldsymbol{O}_n \in \mathrm{SO}(3)$ is a random sample of three-dimensional rotations and $\overline{\boldsymbol{O}} = \sum_{i=1}^{n} \boldsymbol{O}_i$, the mean rotation is defined as $\boldsymbol{T} = \boldsymbol{V}\boldsymbol{W} \in \mathrm{SO}(3)$, where $\overline{\boldsymbol{O}} = \boldsymbol{V}\boldsymbol{\Sigma}\boldsymbol{W}$ is the singular value decomposition of $\overline{\boldsymbol{O}}$. The singular value decomposition is necessary since $\overline{\boldsymbol{O}}$ itself is not necessarily an element of SO(3) and therefore cannot serve as a mean rotation. The mean rotation of the five wrist orientations shown in Figure 1 was found and is displayed as the set of three axes in Figure 2.

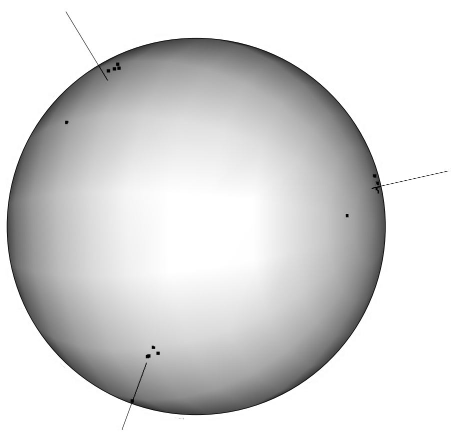

Figure 2. Five repeated wrist orientations from the drilling study (represented as a set of three points) and the mean rotation (represented as a set of three perpendicular axes).

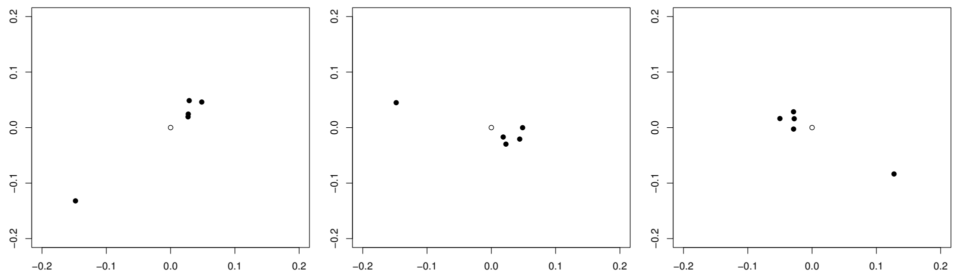

Figure 3. Stereographic projections of the five repeated wrist orientations displayed in Figure 2, with the center point representing the mean.

Figure 3 shows the same data as a stereographic projection, with the open circle at the center corresponding to the position of the mean rotation. It can be seen that the mean is not robust to outliers, as it is pulled towards the one observation that might be considered an outlier. In cases like this, a median would be preferred as a measure of center due to its robustness. While the median is typically thought of as the value that divides an ordered distribution in half, this definition is only easily applied to data that exhibit some type of natural ordering, and this property is nonexistent for three-dimensional rotation data. Therefore, we propose a possible median estimator for three-dimensional rotations in Section 2. In Section 3 we examine the effectiveness of this median through a simulation study, and in Section 4 we revisit the wrist orientations to show that the median provides a better measure of center for this data.

2. Development of a median estimator

Because three-dimensional rotation data do not have a natural ordering, we cannot simply define the median as the value that divides the ordered distribution in half. Instead we will consider the optimality property of the median when developing a possible median estimator for such data. The optimality property tells us that the mean absolute deviation attains a minimum when the deviation is measured from the median [Lee 1995], so that for a random variable X, $E|X-m|$ is minimized where $m =$ median.

To use the optimality property for three-dimensional rotations, we need a concept of "distance" (or deviation) between two orientations. For $\boldsymbol{O}_1, \boldsymbol{O}_2 \in \mathrm{SO}(3)$, there exists a vector $\boldsymbol{U} \in \mathbb{R}^3$ and an angle $r \in [0, \pi]$ such that a rotation of $\boldsymbol{O}_1$ about $\boldsymbol{U}$ by r results in $\boldsymbol{O}_2$. The angle r is sometimes referred to as a *misorientation angle* [Morawiec 2004] and we consider this angle as a measure of distance between rotations $\boldsymbol{O}_1$ and $\boldsymbol{O}_2$. Suppose $\boldsymbol{P}_1, \ldots, \boldsymbol{P}_n$ is a set of n rotations in SO(3), and let $r(\boldsymbol{P}_i, \boldsymbol{M})$ denote the misorientation angle between $\boldsymbol{P}_i$ and $\boldsymbol{M}$. We define the median rotation as the element of SO(3) that minimizes $f(\boldsymbol{M}) = \sum_{i=1}^{n} r(\boldsymbol{P}_i, \boldsymbol{M})$, so that the average deviation from all data points would be minimized by the median rotation. In the next section we compare this median rotation to the mean rotation introduced in Section 1 through a simulation study.

3. Simulation study

To examine the effectiveness of the median estimator defined in Section 2, we simulate random rotations from the uniform axis-random spin (UARS) distributions of [Bingham et al. 2009] under various conditions. The UARS distributions are a symmetric class of distributions for three-dimensional rotations, and Bingham et al. [2009] begin their development of this class by discussing a technique for data simulation. Simulation begins by starting with the 3×3 identity matrix, denoted by $\boldsymbol{I}_{3\times3}$. Then a unit vector $\boldsymbol{U}$ that is uniformly distributed on the $\mathbb{R}^3$-sphere is generated. Next, the angle $\theta \in (-\pi, \pi]$ is independently generated from a circular distribution that is symmetric about 0 and depends on a concentration parameter κ (with density $C(\theta \mid \kappa)$). Rotating $\boldsymbol{I}_{3\times3}$ around $\boldsymbol{U}$ by the angle θ results in an orientation $\boldsymbol{P}$. If this process is repeated n times, we arrive at a set of orientations $\boldsymbol{P}_1, \ldots, \boldsymbol{P}_n$ that is scattered about the center $\boldsymbol{I}_{3\times3}$. Since κ controls the angle θ that is generated from the circular distribution, it also controls the spread of the resulting orientations from their center. Now, by letting $\boldsymbol{M}_i = \boldsymbol{S}\boldsymbol{P}_i$ for $i = 1, \ldots, n$, the rotations $\boldsymbol{M}_1, \ldots, \boldsymbol{M}_n$ have center at $\boldsymbol{S}$. The rotation $\boldsymbol{M}_i$ is said to have UARS distribution with parameters $\boldsymbol{S}$ (indicating center) and κ (indicating spread), which is denoted by $\boldsymbol{M}_i \sim \mathrm{UARS}(\boldsymbol{S}, \kappa)$.

For the simulation study considered here, we will use the UARS class with θ coming from the von Mises circular distribution with mean 0. The von Mises distribution is the most commonly used circular distribution because it is symmetric and unimodal, and as $\kappa \to \infty$, the distribution approaches the normal distribution with standard deviation $1/\kappa$. The density for θ is

$$C(\theta \mid \kappa) = [2\pi I_0(k)]^{-1} \exp[\kappa \cos(\theta)], \quad \theta \in (-\pi, \pi],$$

where $I_0(\kappa)$ is the modified Bessel function of order zero. (For more on the von Mises distribution see [Mardia and Jupp 2000].) See Figure 4 for a plot of the von Mises density for $\kappa = 5$ and $\kappa = 10$, which shows how the concentration parameter κ affects the spread of the distribution. We refer to the von Mises version of the UARS class as vM-UARS.

For the simulation study considered here, we generated $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$ uniformly in SO(3). A total of n rotations, $\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_n$, were simulated from the vM-UARS

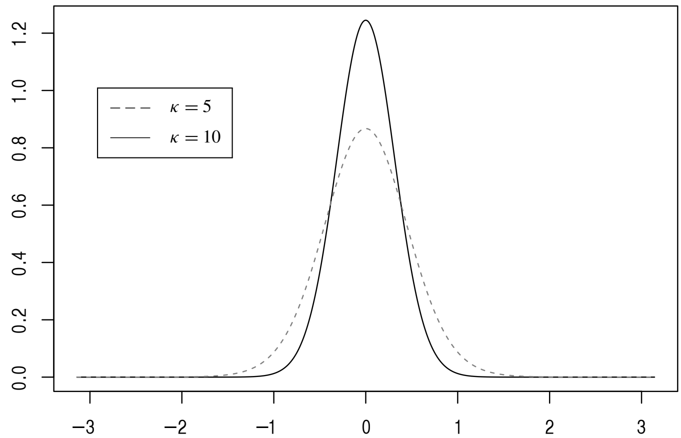

Figure 4. Von Mises circular density for concentration parameter $\kappa = 5, 10$.

distribution, with a proportion p being vM-UARS($\boldsymbol{S}_1, \kappa$) and $1 - p$ being vM-UARS($\boldsymbol{S}_2, \kappa$). We think of this data set as being composed of $100p\%$ "outliers", so that the data is centered at $\boldsymbol{S}_2$ with outliers near $\boldsymbol{S}_1$. We then found the misorientation angle between $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$, called V (i.e., $V = r(\boldsymbol{S}_1, \boldsymbol{S}_2)$). We think of V as measuring the distance between the center of the data and where the outliers are located. The values of κ considered in the simulation study were 5, 10, 50, 100, and 500. The values of n considered were 10, 50, 100, and 500. The values of p used for each choice of n are given in Table 1. Figure 5 shows a plot of $\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_{100}$ on the sphere for two different cases of κ, p, and V. In both instances, the proportion of bolder, cross-shaped points is p (representing the "outliers").

Once $\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_n$ were generated, the mean and median rotations, referred to as $\boldsymbol{N}$ and $\boldsymbol{M}$, respectively, were found. To measure the "distance" from the mean to the simulated rotations, we considered the sum of the misorientation angles $\sum_{i=1}^{n} r(\boldsymbol{Q}_i, \boldsymbol{N})$. A similar measure, $\sum_{i=1}^{n} r(\boldsymbol{Q}_i, \boldsymbol{M})$, was found for the median. We compared the mean and median by considering the difference of these distances,

	Choices for p			
$n = 10$		0.1,	0.3,	0.5
$n = 50$	0.04,	0.1,	0.3,	0.5
$n = 100$	0.01,	0.05,	0.1,	0.5
$n = 500$	0.002,	0.01,	0.1,	0.5

Table 1. Choices of p (proportion of "outliers") used in the simulation study for each value of n considered.

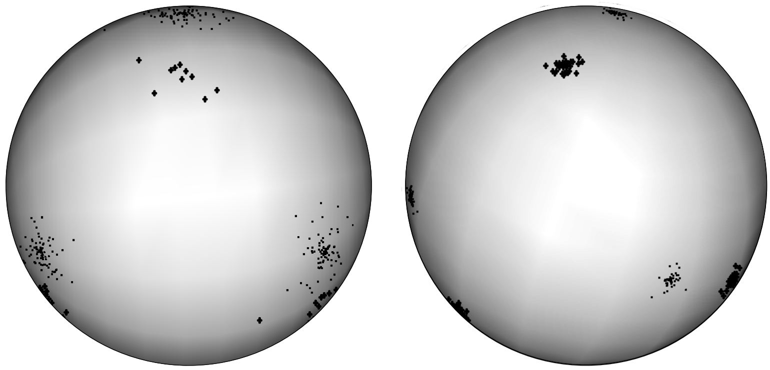

Figure 5. 100 simulated orientations with (left) $\kappa = 50$, $p = 0.10$, and $V = 0.488$ and (right) $\kappa = 500$, $p = 0.50$, and $V = 1.092$.

$R(\boldsymbol{M}, \boldsymbol{N}) = \sum_{i=1}^{n} r(\boldsymbol{Q}_i, \boldsymbol{N}) - \sum_{i=1}^{n} r(\boldsymbol{Q}_i, \boldsymbol{M})$. Note that larger values of $R(\boldsymbol{M}, \boldsymbol{N})$ indicate that the median rotation is outperforming the mean rotation.

For each combination of κ and n, 1000 rotation data sets were generated. For each data set, p was chosen randomly from the possible values listed in Table 1. A plot was then created with V, the "distance" between the uniformly selected $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$, on the horizontal axis and $R = R(\boldsymbol{M}, \boldsymbol{N})$ on the vertical axis, with different plot characters and shades of gray used to represent the various values for p. Although a total of 20 plots were made (one for each combination of κ and n), only a few, which show the general relationships seen in all plots, are provided here.

Figure 6 contains the plots for (κ, n) combinations of (5, 10), (10, 50), (50, 100), and (500, 100). As expected, when κ increases (meaning the simulated data is less spread) or n increases, the relationship between V and R becomes more defined. An interesting and unexpected feature seen in the plots is the quadratic-type relationship between V and R. We see that the maximum values of R, which coincide with the median most outperforming the mean, happen in the middle of the range of V values. One might expect that R would increase as V increases and the outliers move farther from the rest of the data. Instead, when the outliers are at a misorientation angle of π away, the mean and median are almost identical. This phenomenon is due to the fact that the three axes are orthogonal, making it impossible for them to be simultaneously pulled toward the outliers. Figure 7 contains 100 orientations plotted as a set of three points on the sphere, of which 10 would be considered outliers ($p = 0.10$). The points around the x-, y-, and z-axes have been plotted using three different colors so that it is clear which outliers belong to which cluster of points. The angle between the cluster of points of seven points and the three outliers is $V = \pi$. The mean and median are indistinguishable from one another on this plot, and both are represented by the set of three axes. If one axis were to be

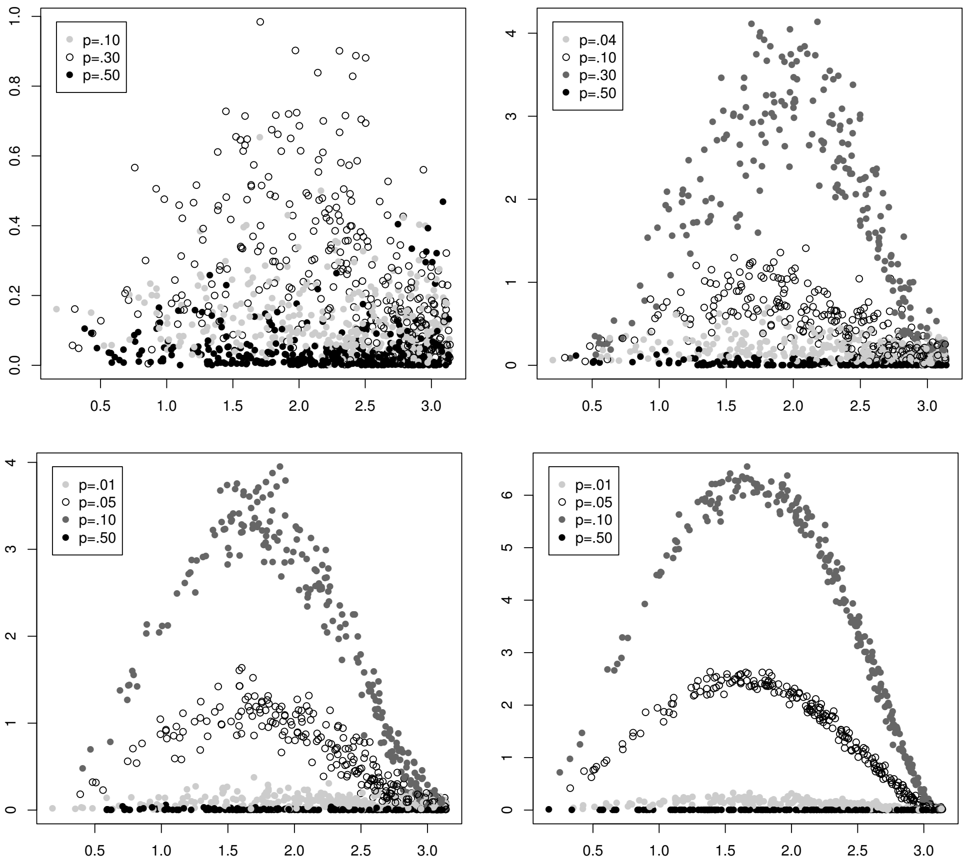

Figure 6. Plot of R (vertical axis) against V (horizontal axis) for 1000 simulated data sets using (top left) $\kappa = 5, n = 10$, (top right) $\kappa = 10, n = 50$, (bottom left) $\kappa = 50, n = 100$, and (bottom right) $\kappa = 500, n = 100$.

pulled toward the outliers, the other axes would not be able to be pulled toward the outliers and still remain orthogonal. As a result, the mean is not influenced by the outliers in this case. Therefore, the quadratic-type relationship between V and R, while unexpected, is understandable after considering the orthogonality of the axes within a three-dimensional rotation data point.

We can also discuss the plots in regards to the proportion of outliers, p. In all plots we see that with $p = 0.50$ the mean and median are generally equivalent (R near 0). This is due to the fact that with an equal number of data points coming from the two centers $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$, both the mean and median will tend to be half-way between these centers (with neither measure experiencing more pull toward one center). From the plots presented in Figure 6 it appears that, with the exception

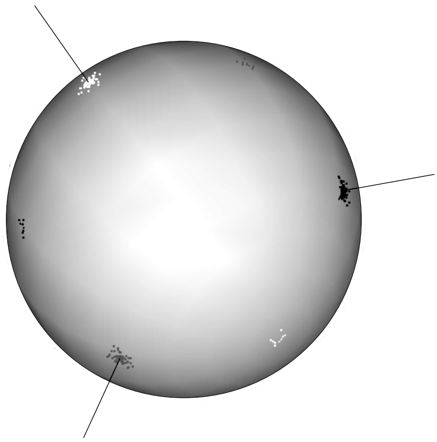

Figure 7. Plot of 100 orientations, represented as a set of three points on the sphere. Here $p = 0.10$, $V = \pi$, and the set of three axes represents the mean/median.

of $p = 0.50$, the value of R increases as the percentage of outliers increases. So the median is preferred. However, there are many other values of p that could be chosen. With $p = 0.50$ producing low values of R, it was expected that at some p we would achieve maximum values of R before again seeing a decrease. Therefore, for one of the κ and n combinations, a simulation was done with more possible values of p. Figure 8 shows the relationship between V and R for $p = 0.06$, 0.12, 0.18, 0.24, 0.30, 0.36, 0.43, and 0.50, where $\kappa = 50$ and $n = 100$. From the plot,

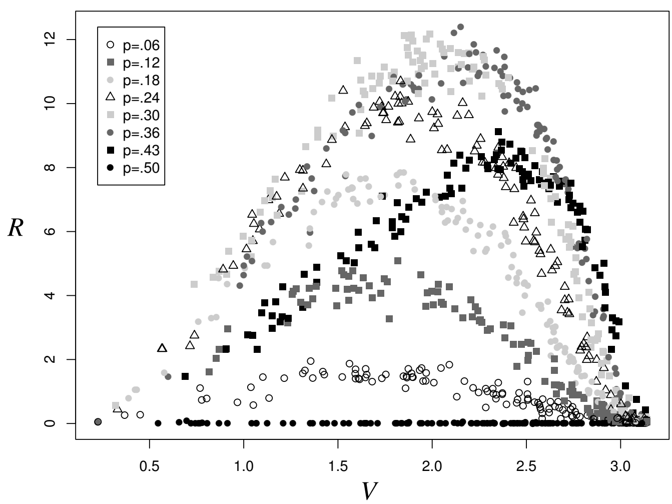

Figure 8. Plot of R against V for 1000 simulated data sets using $\kappa = 50$ and $n = 100$.

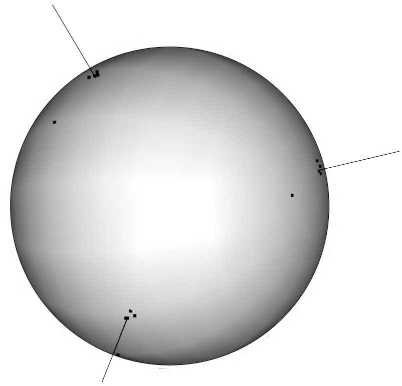

Figure 9. Five repeated wrist orientations for the drilling study (represented as a set of three points) and the median rotation (represented as a set of three perpendicular axes).

we see that the median most outperforms the mean near $p = 0.30$. As p increases from 0.30 to 0.50 the value of R begins to decrease. Even though the median is robust to outlying values, as we let p approach 0.50, it is ambiguous as to which observations would comprise the "outliers" (with $p = 0.50$ being a situation that might be best labeled as "bimodal" rather than having outliers at all).

4. Application to drilling data

Now that we have investigated the effectiveness of the median under various parameter choices, we return to the drilling data of [Rancourt et al. 2000]. In Section 1 it was seen that the mean orientation for the five repeated wrist orientations was pulled toward the outlying value. Thus, for this data set, it is desirable to use the median rotation as a measure of center. Figure 9 shows the five repeated wrist orientations on the sphere with the set of perpendicular axes now representing the median rotation. Figure 10 shows the data as a stereographic projection, with the

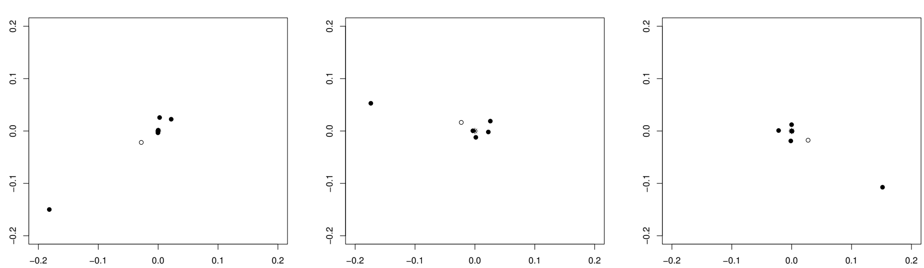

Figure 10. Stereographic projections of the five repeated wrist orientations, in black, with the center point at (0,0) representing the median and the open circle representing the mean.

point in the center at (0, 0) corresponding to the median rotation and the open circle representing the mean rotation. Both figures show the median near the center of four of the orientations, illustrating the fact that the median is not affected by the outlying value like the mean is.

This small data set with repeated drilling rotations is just one example of a situation in which a median estimator would be preferred over the mean estimator that is typically used to measure the center for three-dimensional rotation data. In subject areas where three-dimensional rotations are common, like the study of human motion, data sets with outliers are bound to show up, making the median estimator developed in Section 2 an important addition to statistics for three-dimensional rotation data.

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