# Inference for the Central Direction of Random Rotations in $SO(3)$

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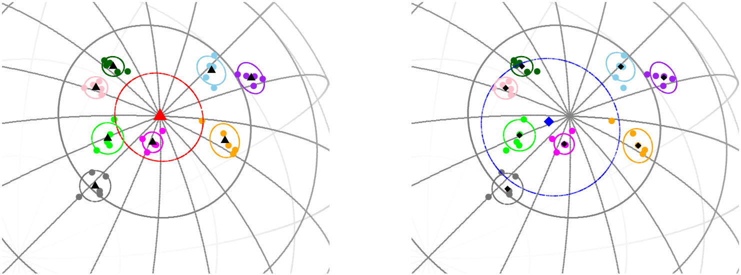
# OUTLINE

# CoDA Poster

- My CoDA poster included the following illustration of confidence regions for $SO(3)$ data
- In this talk I provide the theoretical justification for these plots



# Location Model in $SO(3)$

- $\boldsymbol{R}_1, \ldots, \boldsymbol{R}_n \in SO(3)$ random sample from

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

- Where
  - $SO(3)$ - collection of all $3 \times 3$ matrices $\boldsymbol{R}$ with $\det(\boldsymbol{R}) = 1$ and $\boldsymbol{R}^\top \boldsymbol{R} = \boldsymbol{I}$
  - $\boldsymbol{S} \in SO(3)$ - parameter measuring central tendency
  - $\boldsymbol{E}_1, \ldots, \boldsymbol{E}_n \in SO(3)$ i.i.d. random rotations (symmetrically perturb $\boldsymbol{S}$)
- Real line analog: $Y_i = \mu + e_i$ for $\mu \in \mathbb{R}$ and $e_i \in \mathbb{R}$ additive error symmetrically distributed around zero

# Rotation Matrices Construction

$\boldsymbol{R}$ associated with skew-symmetric matrix $\boldsymbol{\Phi}(\boldsymbol{W})$

$$\boldsymbol{\Phi}(\boldsymbol{W}) = \begin{bmatrix} 0 & -w_3 & w_2 \\ w_3 & 0 & -w_1 \\ -w_2 & w_1 & 0 \end{bmatrix}$$

for $\boldsymbol{W} = (w_1, w_2, w_3) \in \mathbb{R}^3$ according to

$$\boldsymbol{R} = \exp[\boldsymbol{\Phi}(\boldsymbol{W})] = \cos(r)\boldsymbol{I} + \sin(r)\boldsymbol{\Phi}(\boldsymbol{U}) + (1 - \cos r)\boldsymbol{U}\boldsymbol{U}^\top \quad (2)$$

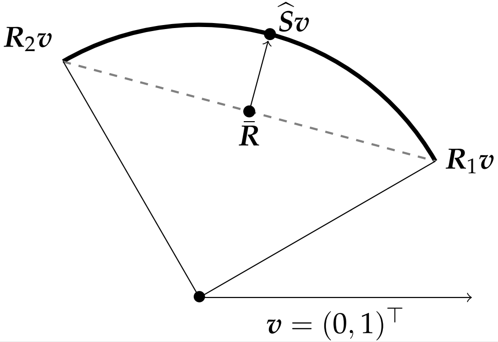
- $r = \|\boldsymbol{W}\|_F$ and $\boldsymbol{U} = \boldsymbol{W}/\|\boldsymbol{W}\|_F$
- $r$ distributed symmetrically about 0 independent of $\boldsymbol{U}$ distributed uniformly on unit sphere
- $r$ and $\boldsymbol{U}$ termed misorientation angle and axis, respectively

# Projected Mean

- The projected mean is the most developed estimator

$$\widehat{S} = \underset{S \in SO(3)}{\arg\min} \sum_{i=1}^{n} d_E^2(R_i, S) = \underset{S \in SO(3)}{\arg\max}\, \mathbf{tr}(S^\top \bar{R})$$

- $\bar{R} = \frac{1}{n}\sum_{i=1}^{n} R_i$ and $d_E(R_1, R_2) = \|R_1 - R_2\|_F$



# SETUP

- $\boldsymbol{R}_1, \ldots, \boldsymbol{R}_n \in SO(3)$ random sample from (1) with central orientation $\boldsymbol{S}$
- Use estimator $\widehat{\boldsymbol{S}} = \underset{\boldsymbol{S} \in SO(3)}{\arg\min} \sum_{i=1}^{n} d_E^2(\boldsymbol{R}_i, \boldsymbol{S})$
- $\boldsymbol{\Phi}(\hat{\boldsymbol{h}})$ skew-symmetric matrix associated with $\boldsymbol{S}^\top \widehat{\boldsymbol{S}}$

$$\exp[\boldsymbol{\Phi}(\hat{\boldsymbol{h}})] = \boldsymbol{S}^\top \widehat{\boldsymbol{S}}$$

- Define $r_{\hat{\boldsymbol{h}}} = \|\hat{\boldsymbol{h}}\|_F$ and $\boldsymbol{U}_{\hat{\boldsymbol{h}}} = \hat{\boldsymbol{h}} / \|\hat{\boldsymbol{h}}\|_F$

# Asymptotic Result

Under this setup

$$\sqrt{n}\hat{\boldsymbol{h}} \xrightarrow{d} MVN_3\left(\mathbf{0}, \frac{c}{2d^2}I\right) \tag{3}$$

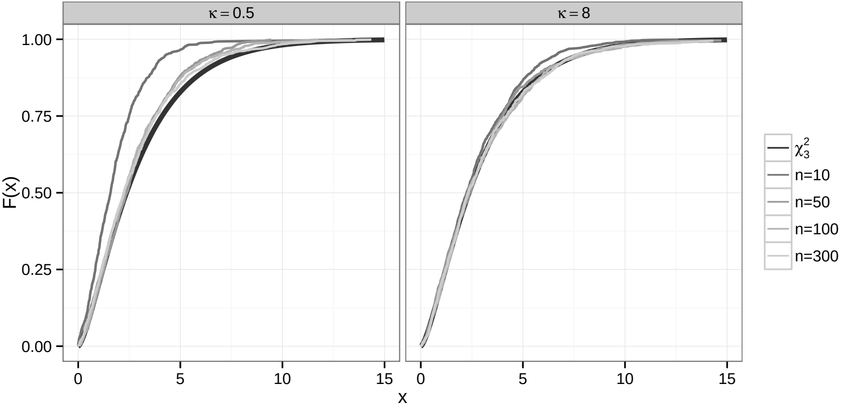
as $n \to \infty$ where

$$c = \frac{2}{3}E(1-\cos^2 r) \quad \text{and} \quad d = \frac{1}{3}E(1+2\cos r)$$

or equivalently

$$\frac{2nd^2}{c}\|\hat{\boldsymbol{h}}\|_F^2 \xrightarrow{d} \chi_3^2$$

# ECDF for Projected Mean



# Confidence Region

- By definition of the Riemannian distance $d_R$:

$$\|\hat{\boldsymbol{h}}\|_F^2 = r_{\hat{\boldsymbol{h}}}^2 = d_R(\boldsymbol{S}, \widehat{\boldsymbol{S}})^2$$

- A $100(1-\alpha)\%$ confidence region for $\boldsymbol{S}$

$$\left\{ \boldsymbol{S} \in SO(3) : \frac{2n\hat{d}^2}{\hat{c}}[d_R(\boldsymbol{S}, \widehat{\boldsymbol{S}})^2] < \chi^2_{3,1-\alpha} \right\} \tag{4}$$

where

$$\hat{c} = \frac{1}{6n}\sum_{i=1}^{n}\left\{3 - \mathbf{tr}\left[\left(\widehat{\boldsymbol{S}}^\top \boldsymbol{R}_i\right)^2\right]\right\} \quad \text{and} \quad \hat{d} = \frac{1}{3n}\sum_{i=1}^{n}\mathbf{tr}\left(\widehat{\boldsymbol{S}}^\top \boldsymbol{R}_i\right)$$

- (4) describes confidence region centered at $\widehat{S}$ with radius

$$\sqrt{\frac{\hat{c}\chi^2_{3,1-\alpha}}{2n\hat{d}^2}}$$

# PIVOTAL BOOTSTRAP[1]

1. Randomly select $n$ rotation matrices with replacement from the sample to form a bootstrap sample $\boldsymbol{R}_1^*, \ldots, \boldsymbol{R}_n^*$
2. Compute the projected mean of the bootstrap data set, $\widehat{\boldsymbol{S}}^*$ and form the test quantity $\frac{2n\hat{d}^{*2}}{\hat{c}^*}[d_R(\widehat{\boldsymbol{S}}, \widehat{\boldsymbol{S}}^*)^2]$ where $\hat{c}^*$ and $\hat{d}^*$ are computed from the bootstrap sample by replacing $\boldsymbol{R}_i$ and $\widehat{\boldsymbol{S}}$ with $\boldsymbol{R}_i^*$ and $\widehat{\boldsymbol{S}}^*$
3. Repeat steps 1 and 2, $m$ times to obtain $m$ values of the quantity $\frac{2n\hat{d}^{*2}}{\hat{c}^*}[d_R(\widehat{\boldsymbol{S}}, \widehat{\boldsymbol{S}}^*)^2]$
4. Define $\hat{q}_{1-\alpha}$ such that $P(\frac{2n\hat{d}^{*2}}{\hat{c}^*}[d_R(\widehat{\boldsymbol{S}}, \widehat{\boldsymbol{S}}^*)^2] \leq q^*_{1-\alpha}) = 1 - \alpha$
5. $\{\boldsymbol{S} \in SO(3) : \frac{2n\hat{d}^2}{\hat{c}}[d_R(\boldsymbol{S}, \widehat{\boldsymbol{S}})^2] < \hat{q}_{1-\alpha}\}$.

[1] First proposed in Dr. Zhang's M.S. Thesis completed under Dr. Dan Nordman

# Other Confidence Region Methods

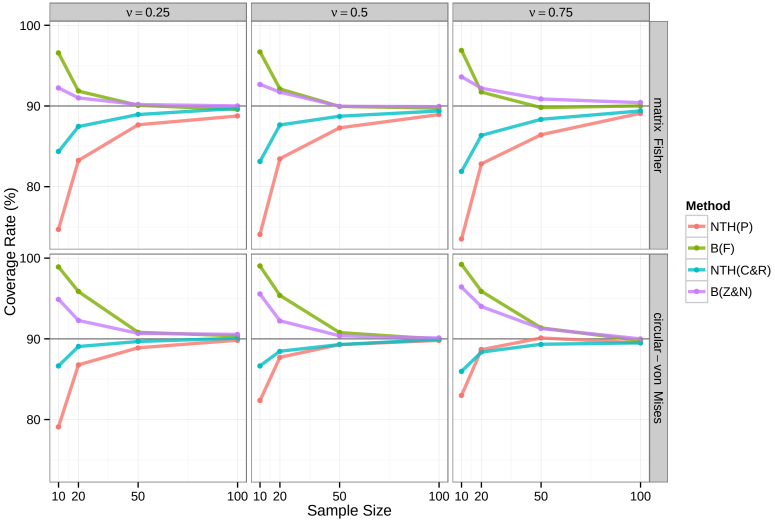
- Prentice (1986) and (1989) used asymptotics for eigenvalues and eigenvectors to construct a confidence region for $\widehat{S}$
- Fisher, Hall, Jing and Wood (1996) use the Prentice statistic and a pivotal bootstrap procedure to achieve better coverage rates
- Chang and Rivest (2001) state a result more general than (3) that is difficult to implement

# Simulation Study

Study parameters:

- Distributions: matrix Fisher, circular-von Mises
- Sample Sizes: $n = 10, 20, 50, 100$
- Circular Variances: $\nu = 0.25, 0.50$ and $0.75$
- Simulated Samples: $10,000$ per combination
- Bootstrap Sample Size: $m = 300$
- Error rate: $\alpha = 0.1$

# Coverage Rate Comparison



# Projected Median

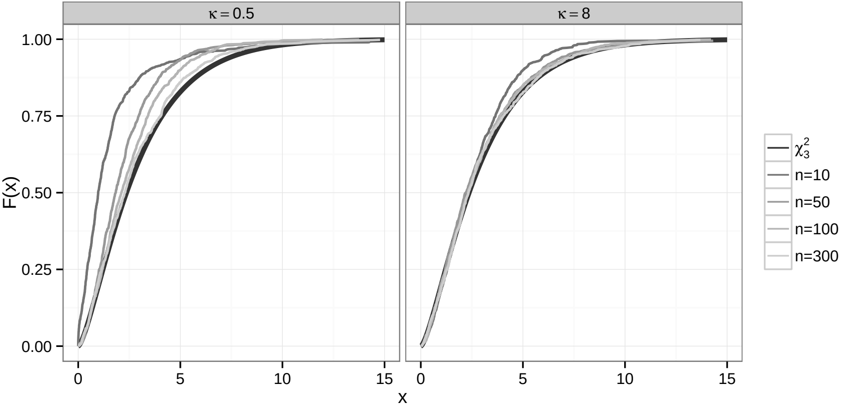
- The projected median

$$\widetilde{\boldsymbol{S}} = \operatorname*{arg\,min}_{\boldsymbol{S}\in SO(3)} \sum_{i=1}^{n} d_E(\boldsymbol{R}_i, \boldsymbol{S})$$

- (3) holds for $\widetilde{\boldsymbol{S}}$ with

$$c = \frac{1}{6}E(1+\cos r) \quad \text{and} \quad d = \frac{1}{12}E\left(\frac{1+3\cos r}{\sqrt{1-\cos r}}\right)$$

# ECDF for Projected Median



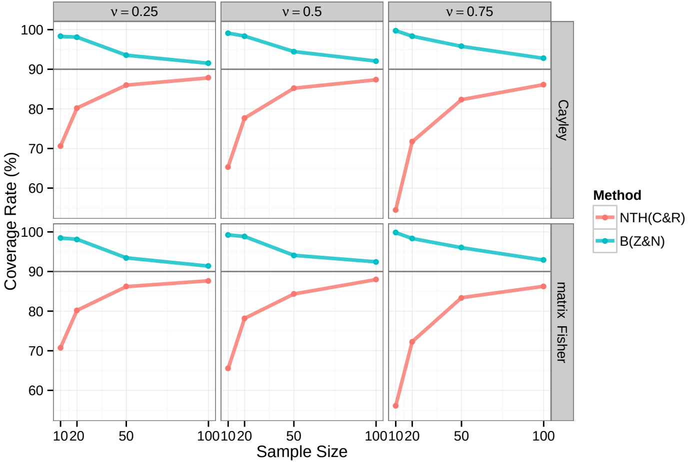
# Simulation Study for Median

- $\widetilde{S}$ cannot be written as a function of eigenvalues and eigenvectors
- The pivotal boostrap from before can still be used using by replacing $\hat{c}$ and $\hat{d}$ with

$$\tilde{c} = \frac{1}{12n}\sum_{i=1}^{n}\left[1 + \mathbf{tr}\left(\widetilde{\boldsymbol{S}}^{\top}\boldsymbol{R}_i\right)\right] \quad \text{and} \quad \tilde{d} = \frac{\sqrt{2}}{24n}\sum_{i=1}^{n}\frac{3\mathbf{tr}(\widetilde{\boldsymbol{S}}^{\top}\boldsymbol{R}_i) - 1}{\sqrt{3 - \mathbf{tr}(\widetilde{\boldsymbol{S}}^{\top}\boldsymbol{R}_i)}}$$

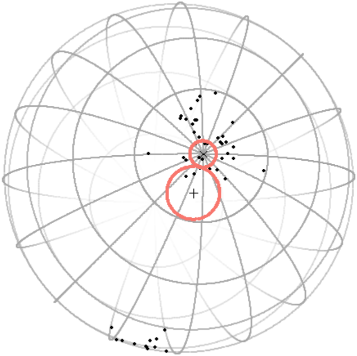
- Use same simulation parameters for the projected mean for the median

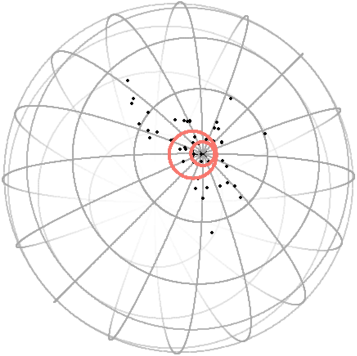
# Coverage Rate Simulation $\widetilde{S}$



# Future Work

- Look at more interesting cases, e.g. grain boundries





# Thank you

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