Statistics of Ambiguous Rotations

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1 Motivation
2 Directional Statistics and Tectonic Stress Estimation
3 Orthogonal Axial Frames
4 Ambiguous rotations in 3D
How can we do statistics with orientations of objects like these?
... some very recent NZ history
Some very recent NZ history

Kaikoura quake – 14 Nov 2016, M7.8

Some very recent NZ history
Some very recent NZ history

Cath News Asia Pacific 2017
Some very recent NZ history

www.stuff.co.nz
Some very recent NZ history

Some stranded cows
What does this have to do with directional statistics?

1. Seismology is inherently geometrical
2. Crystallography likewise
3. Needs an understanding of circular statistics – angles are special because they are **cyclic**
4. Axes are more common than directions – modifications are needed
5. Extensions to 3D spherical statistics (directions, orientations) and axes (frames)
6. Angles are generally have an inconvenient representation in 3D
What does this have to do with directional statistics?

1. Seismology is inherently geometrical.
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3. Needs an understanding of circular statistics – angles are special because they are cyclic.
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5. Extensions to 3D spherical statistics (directions, orientations) and axes (frames).
6. Angles are generally have an inconvenient representation in 3D.

New statistical methods are needed.
Directional Statistics and Tectonic Stress Estimation


Walsh, Arnold & Townend (2009), A Bayesian approach to determining and parameterising earthquake focal mechanisms, Geophys J Int, 176, 235-255;

Example: Angles in the plane (2D)

Wind directions at a site in the Italian Alps
Example: Angles in the plane (2D)

\[ \bar{\theta} = \frac{1}{n} \sum_{i=1}^{n} \theta_i \]

Familiar mean \((\bar{\theta} = 135.1^\circ)\) does not make sense
Solution is to treat the observations as **unit vectors**

\[ \mathbf{u}_i = \begin{bmatrix} \cos \theta_i \\ \sin \theta_i \end{bmatrix} \]
Averaging angles

Average the vectors

\[
\bar{u} = \frac{1}{n} \sum_{i=1}^{n} u_i
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \begin{bmatrix} \cos \theta_i \\ \sin \theta_i \end{bmatrix}
\]

\[
= \bar{R} \begin{bmatrix} \cos \bar{\theta} \\ \sin \bar{\theta} \end{bmatrix}
\]

where

\[
\bar{\theta} = \text{atan2}(\langle \sin \theta_i \rangle, \langle \cos \theta_i \rangle)
\]

\[
\bar{R}^2 = \langle \sin \theta_i \rangle^2 + \langle \cos \theta_i \rangle^2
\]
The mean of unit vectors is not a unit vector

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Length \( \bar{R} \) characterises concentration (\( \bar{R} \approx 0 \) if uniform)
Averaging angles

The mean of unit vectors is not a unit vector

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Length \( \bar{R} \) characterises concentration (\( \bar{R} \approx 0 \) if uniform)

Direction \( \bar{\theta} \) is the mean direction we want (\( \bar{\theta} = 16.7^\circ \)).
We have replaced the scalar $\theta$ with its periodic symmetry

$$\ldots \theta - 4\pi, \theta - 2\pi, \theta, \theta + 2\pi, \theta + 4\pi, \ldots$$
We have replaced the scalar $\theta$ with its periodic symmetry

\[ \ldots \theta - 4\pi, \theta - 2\pi, \theta, \theta + 2\pi, \theta + 4\pi, \ldots \]

with a 2D unit vector (with one degree of freedom)

\[ \mathbf{u} = \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix} \]

invariant under that symmetry.
Von Mises distribution (direction $\theta$, concentration $\kappa$)

$$f(\theta) = \frac{1}{2\pi I_0(\kappa)} \exp(\kappa \cos(\theta - \theta_0))$$

$$f(u) = \frac{1}{2\pi I_0(\kappa)} \exp(\kappa \mu^T u)$$

Similarity of directions is measured by the scalar product

$$\mu^T u$$

...a variety of parametric and non-parametric tests
The Rayleigh Test
The Rayleigh Test

The test statistic

\[ S = 2n\|\bar{u}\|^2 = 2n\bar{R}^2 \]

follows a \( \chi^2 \) distribution if the sample is drawn from a Uniform distribution.
A test for uniformity

The Rayleigh Test

The test statistic

\[ S = 2n||\bar{u}||^2 = 2n\bar{R}^2 \]

follows a \( \chi^2_2 \) distribution if the sample is drawn from a Uniform distribution.

- Uniform distribution
- Bimodal distribution

- No power against distributions with \( E[u] = 0 \)
- (though alternative tests exist)
A similar approach works for axes where

\[ \ldots \theta - 2\pi, \theta - \pi, \theta, \theta + \pi, \theta + 2\pi, \ldots \]

are all equivalent
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\[ \ldots \theta - 2\pi, \theta - \pi, \theta, \theta + \pi, \theta + 2\pi, \ldots \]

are all equivalent
Here we embed the axis unit vector $\pm u$

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in the space of symmetric, zero trace, rank 2 tensors

$$t(\pm u) = uu^T - \frac{1}{2} I_2$$

$$= \frac{1}{2} \begin{bmatrix} \cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta \end{bmatrix}$$
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$$\pm \mathbf{u} = \pm \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix}$$

in the space of symmetric, zero trace, rank 2 tensors

$$t(\pm \mathbf{u}) = \mathbf{u} \mathbf{u}^T - \frac{1}{2} \mathbf{I}_2$$

$$= \frac{1}{2} \begin{bmatrix} \cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta \end{bmatrix}$$

An appealing choice among possible embeddings:
Embedding axes in 2D

Here we embed the axis unit vector \( \pm u \)

\[
\pm u = \pm \begin{bmatrix}
\cos \theta \\
\sin \theta
\end{bmatrix}
\]

in the space of symmetric, zero trace, rank 2 tensors

\[
t(\pm u) = uu^T - \frac{1}{2} I_2
\]

\[
= \frac{1}{2} \begin{bmatrix}
\cos 2\theta & \sin 2\theta \\
\sin 2\theta & -\cos 2\theta
\end{bmatrix}
\]

An appealing choice among possible embeddings:

- invariant under axial symmetry \((\theta \rightarrow \theta + \pi, \pm u)\)
Here we embed the axis unit vector $\pm u$

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An appealing choice among possible embeddings:

- invariant under axial symmetry ($\theta \rightarrow \theta + \pi$, $\pm u$)
- averages to zero under a uniform distribution
Here we embed the axis unit vector $\pm \mathbf{u}$

$$\pm \mathbf{u} = \pm \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix}$$

in the space of symmetric, zero trace, rank 2 tensors

$$t(\pm \mathbf{u}) = \mathbf{u}\mathbf{u}^T - \frac{1}{2} I_2$$

$$= \frac{1}{2} \begin{bmatrix} \cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta \end{bmatrix}$$

An appealing choice among possible embeddings:

- invariant under axial symmetry ($\theta \rightarrow \theta + \pi$, $\pm \mathbf{u}$)
- averages to zero under a uniform distribution

Equivalent to familiar angle-doubling methods
Associated with a **scalar product**:

\[
\langle t(\pm u_1), t(\pm u_2) \rangle = \text{tr} \left( t(\pm u_1) t(\pm u_2) \right) = \frac{1}{2} \cos 2(\theta_1 - \theta_2)
\]
Associated with a **scalar product**:

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- Quantifies the closeness of two axes
Embedding axes in 2D

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- Quantifies the closeness of two axes
- Normalisation

\[ ||t||^2 = \langle t, t \rangle = \frac{1}{2} \]
Embedding axes in 2D

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- Quantifies the closeness of two axes
- Normalisation

\[
||t||^2 = \langle t, t \rangle = \frac{1}{2}
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- Zero for orthogonal axes \((\theta_2 = \theta_1 + (2k + 1)\pi/2, \text{ integer } k)\)
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- Zero for orthogonal axes \((\theta_2 = \theta_1 + (2k + 1)\pi/2, \text{ integer } k)\)

The scalar product forms the basis of statistical tests.
Averaging axes

Averaging observations of axes:

\[
\bar{t} = \frac{1}{n} \sum_{i=1}^{n} t_i
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} \frac{1}{2} \begin{bmatrix}
\cos 2\theta_i & \sin 2\theta_i \\
\sin 2\theta_i & -\cos 2\theta_i
\end{bmatrix}
\]

\[
= \frac{\bar{R}_2}{2} \begin{bmatrix}
\cos 2\bar{\theta} & \sin 2\bar{\theta} \\
\sin 2\bar{\theta} & -\cos 2\bar{\theta}
\end{bmatrix}
\]

\[
= \bar{R}_2 \left( \begin{bmatrix}
\cos \bar{\theta} \\
\sin \bar{\theta}
\end{bmatrix} \begin{bmatrix}
\cos \bar{\theta} & \sin \bar{\theta} \\
\sin \bar{\theta} & -\cos \bar{\theta}
\end{bmatrix} - \frac{1}{2} I \right)
\]

\[
= \bar{R}_2 \left( \bar{u} \bar{u}^T - \frac{1}{2} I \right)
\]
Averaging axes

Averaging observations of axes:

\[
\begin{align*}
\bar{t} &= \frac{1}{n} \sum_{i=1}^{n} t_i \\
&= \frac{1}{n} \sum_{i=1}^{n} \frac{1}{2} \begin{bmatrix} \cos 2\theta_i & \sin 2\theta_i \\ \sin 2\theta_i & -\cos 2\theta_i \end{bmatrix} \\
&= \frac{\bar{R}_2}{2} \begin{bmatrix} \cos 2\bar{\theta} & \sin 2\bar{\theta} \\ \sin 2\bar{\theta} & -\cos 2\bar{\theta} \end{bmatrix} \\
&= \bar{R}_2 \left( \begin{bmatrix} \cos \bar{\theta} \\ \sin \bar{\theta} \end{bmatrix} \begin{bmatrix} \cos \bar{\theta} & \sin \bar{\theta} \end{bmatrix} - \frac{1}{2} I \right) \\
&= \bar{R}_2 \left( \bar{u} \bar{u}^T - \frac{1}{2} I \right)
\end{align*}
\]

Length $\bar{R}_2$ characterises concentration ($\bar{R}_2 \approx 0$ if uniform)
Averaging axes

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= \frac{1}{n} \sum_{i=1}^{n} \frac{1}{2} \begin{bmatrix}
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\end{bmatrix} - \frac{1}{2} I \right)
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\[
= \bar{R}_2 \left( \bar{u}\bar{u}^T - \frac{1}{2} I \right)
\]

Length $\bar{R}_2$ characterises concentration ($\bar{R}_2 \simeq 0$ if uniform)
Direction $\bar{\theta}$ is the mean axis orientation we want.
Sample mean

$$\bar{t} = \frac{1}{n} \sum_{i=1}^{n} t(\pm u_i) = \frac{1}{2} \begin{bmatrix} \langle \cos 2\theta \rangle & \langle \sin 2\theta \rangle \\ \langle \sin 2\theta \rangle & -\langle \cos 2\theta \rangle \end{bmatrix}$$ (1)
Sample mean

\[ \bar{t} = \frac{1}{n} \sum_{i=1}^{n} t(\pm u_i) = \frac{1}{2} \left[ \langle \cos 2\theta \rangle \begin{pmatrix} \langle \sin 2\theta \rangle \\ -\langle \cos 2\theta \rangle \end{pmatrix} \right] \]  

(1)

then identify the axis \( \pm \bar{u} = \pm (\cos \bar{\theta}, \sin \bar{\theta})^T \) for which the scalar product

\[ \langle \bar{t}, t(\pm \bar{u}) \rangle = \frac{1}{2} (\langle \cos 2\theta \rangle \cos 2\bar{\theta} + \langle \sin 2\theta \rangle \sin 2\bar{\theta}) \]

is greatest.
Summary statistics

Sample mean

$$\bar{t} = \frac{1}{n} \sum_{i=1}^{n} t(\pm u_i) = \frac{1}{2} \begin{bmatrix} \langle \cos 2\theta \rangle & \langle \sin 2\theta \rangle \\ \langle \sin 2\theta \rangle & -\langle \cos 2\theta \rangle \end{bmatrix}$$  \hspace{1cm} (1)

then identify the axis $$\pm \bar{u} = \pm (\cos \bar{\theta}, \sin \bar{\theta})^T$$ for which the scalar product

$$\langle \bar{t}, t(\pm \bar{u}) \rangle = \frac{1}{2} (\langle \cos 2\theta \rangle \cos 2\bar{\theta} + \langle \sin 2\theta \rangle \sin 2\bar{\theta})$$

is greatest.

Sample dispersion

$$d = \frac{1}{2} - ||\bar{t}||^2$$

$$= \frac{1}{2} (1 - \langle \cos 2\theta \rangle^2 - \langle \sin 2\theta \rangle^2)$$

$$= \frac{1}{2} (1 - \bar{R}_2^2)$$
Test sample \( \{u_1, \ldots, u_n\} \) for a Uniformity
Test sample $\{u_1, \ldots, u_n\}$ for a Uniformity

The test statistic

$$S = 4n||\bar{t}||^2 = 4ntr(\bar{t}^2) = 2n\bar{R}^2$$

follows a $\chi^2_2$ distribution if the sample is drawn from a Uniform distribution (Axial version of the Rayleigh test for uniformity)
Test sample \( \{u_1, \ldots, u_n\} \) for a Uniformity

The test statistic

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follows a \( \chi^2_2 \) distribution if the sample is drawn from a Uniform distribution (Axial version of the Rayleigh test for uniformity)

\( S \) can also be used in a randomisation test for uniformity.
**Watson distribution** (mean axis $\pm \mu$, concentration $\kappa$)

$$f(u) \propto \exp \left( \kappa (\mu^T u)^2 \right)$$

Similarity measured by the scalar product

$$u^T \mu \mu^T u - \frac{1}{2}$$

... a variety of parametric and non-parametric tests
Soufrière Hills – Montserrat

Roman *et al.* 2011 used two techniques to estimate the local orientation of the axis of maximum horizontal compressive tectonic stress:
Roman et al. 2011 used two techniques to estimate the local orientation of the axis of maximum horizontal compressive tectonic stress:

- earthquake focal mechanism P axes
- shear wave splitting measurements

![Diagram showing orientations](image)
Do the inferred orientations differ from the regional stress field $\theta_0 = 32^\circ$? (one sample tests)
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FPS: No: $W = 0.136$, $p$-value=0.678
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SWS: Yes: $W = 0.067$, $p$-value=0.001
Do the inferred orientations differ from the regional stress field $\theta_0 = 32^\circ$? (one sample tests)

FPS: No: $W = 0.136$, $p$-value $= 0.678$

SWS: Yes: $W = 0.067$, $p$-value $= 0.001$
Do the two methods agree? (non-parametric two sample randomisation test for common orientation)
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(non-parametric two sample randomisation test for common orientation)

No: $D = \|\bar{t}_1 - \bar{t}_2\|^2 = 0.0198$, $p$-value=0.014.
Orthogonal Axial Frames

Now extend to 3D, and beyond ...
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An **orthogonal axial frame** (oaf) $[U]$ in 3D is a set of $r$ orthogonal unit vectors: $r \in \{1, 2, 3\}$:
Three dimensions

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(2 axes equivalent to 3: \(u_3 = u_1 \times u_2\))
Three dimensions

Represent directions by angles

- 1 axis: \((\phi, \theta)\): Unit vector

\[
\mathbf{u} = \begin{bmatrix}
\sin \theta \cos \phi \\
\sin \theta \sin \phi \\
\cos \theta
\end{bmatrix}
\]
Represent directions by angles

1 axis: \((\phi, \theta)\): Unit vector

\[
\mathbf{u} = \begin{bmatrix} 
\sin \theta \cos \phi \\
\sin \theta \sin \phi \\
\cos \theta 
\end{bmatrix}
\]

3 axes: Euler angles \((\phi, \theta, \psi)\): Orthogonal matrix

\[
\mathbf{R} = [\pm \mathbf{u}_1 \ \pm \mathbf{u}_2 \ \pm \mathbf{u}_3] = R_Z(\phi)R_Y(\theta)R_Z(\psi)
\]
Three dimensions – embedding

**Single axis in 3D – extend embedding**

\[
t([U]) = uu^T - \frac{1}{3} I_3
\]

\[
= \begin{bmatrix}
cos^2 \phi \sin^2 \theta - \frac{1}{3} & \sin \phi \cos \phi \sin^2 \theta & \cos \phi \sin \theta \cos \theta \\
\sin \phi \cos \phi \sin^2 \theta & \sin^2 \phi \sin^2 \theta - \frac{1}{3} & \sin \phi \sin \theta \cos \theta \\
\cos \phi \sin \theta \cos \theta & \sin \phi \sin \theta \cos \theta & \cos^2 \theta - \frac{1}{3}
\end{bmatrix}
\]

with scalar product

\[
\langle t([U_1]), t([U_2]) \rangle = \text{tr} (t([U_1]) t([U_2]))
\]

\[
= (u_1^T u_2)^2 - \frac{1}{3}
\]

and \( ||t||^2 = \frac{2}{3} \)
Three axes

Three orthogonal axes $[U] = (\pm \mathbf{u}_1, \pm \mathbf{u}_2, \pm \mathbf{u}_3)$:
Three axes

Three orthogonal axes \([U] = (\pm u_1, \pm u_2, \pm u_3)\):

Embedded object is a \textbf{triplet of matrices}\n
Dec 2017    Ambiguous Rotations
Three axes

Three orthogonal axes $[U] = (\pm u_1, \pm u_2, \pm u_3)$:
Embedded object is a **triplet of matrices**

$$t([U]) = (t_1([U]), t_2([U]), t_3([U]))$$

$$= (u_1u_1^T - \frac{1}{3} I_3, u_2u_2^T - \frac{1}{3} I_3, u_3u_3^T - \frac{1}{3} I_3)$$
Three axes

Three orthogonal axes $[U] = (\pm u_1, \pm u_2, \pm u_3)$:

Embedded object is a **triplet of matrices**

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$$= (u_1u_1^T - \frac{1}{3} I_3, u_2u_2^T - \frac{1}{3} I_3, u_3u_3^T - \frac{1}{3} I_3)$$

with scalar product

$$\langle t([U_1]), t([U_2]) \rangle = \sum_{j=1}^{3} \text{tr}(t_j([U_1])t_j([U_2]))$$

$$= \sum_{j=1}^{3} (u_1^T u_2)^2 - 1$$

and $\|t\|^2 = 2$. 
Three axes

Three orthogonal axes $[U] = (\pm u_1, \pm u_2, \pm u_3)$: 
Embedded object is a **triplet of matrices**

$$t([U]) = (t_1([U]), t_2([U]), t_3([U]))$$

$$= (u_1u_1^T - \frac{1}{3}I_3, u_2u_2^T - \frac{1}{3}I_3, u_3u_3^T - \frac{1}{3}I_3)$$

with scalar product

$$\langle t([U_1]), t([U_2]) \rangle = \sum_{j=1}^{3} \text{tr} (t_j([U_1])t_j([U_2]))$$

$$= \sum_{j=1}^{3} (u_{1j}^T u_{2j})^2 - 1$$

and $||t||^2 = 2$.

Averages are still just as simple

$$\bar{t} = \frac{1}{n} \sum_{i=1}^{n} t([U]_i)$$
Summary statistics

Sample mean
Summary statistics

Sample mean
Compute the average of the embedding matrices

\[ \bar{t} = \frac{1}{n} \sum_{i=1}^{n} t([U_i]) \]

\[ = \left( \frac{1}{n} \sum_{i=1}^{n} t_1([U_i]), \frac{1}{n} \sum_{i=1}^{n} t_2([U_i]), \frac{1}{n} \sum_{i=1}^{n} t_3([U_i]) \right) \]
Sample mean

Compute the average of the embedding matrices

\[
\bar{t} = \frac{1}{n} \sum_{i=1}^{n} t([U_i])
\]

\[
= \left( \frac{1}{n} \sum_{i=1}^{n} t_1([U_i]), \frac{1}{n} \sum_{i=1}^{n} t_2([U_i]), \frac{1}{n} \sum_{i=1}^{n} t_3([U_i]) \right)
\]

The sample mean \([\bar{U}]\) maximses the scalar product

\[\langle t([\bar{U}]), \bar{t} \rangle\]
Sample mean

Compute the average of the embedding matrices

\[
\bar{t} = \frac{1}{n} \sum_{i=1}^{n} t(U_i)
\]

\[
= \left( \frac{1}{n} \sum_{i=1}^{n} t_1(U_i), \frac{1}{n} \sum_{i=1}^{n} t_2(U_i), \frac{1}{n} \sum_{i=1}^{n} t_3(U_i) \right)
\]

The sample mean \([\bar{U}]\) maximises the scalar product

\[
\langle t([\bar{U}]), \bar{t} \rangle
\]

Maximisation must be performed numerically.
Summary statistics

Sample mean
Compute the average of the embedding matrices

\[
\bar{t} = \frac{1}{n} \sum_{i=1}^{n} t([U_i])
\]

\[
= \left( \frac{1}{n} \sum_{i=1}^{n} t_1([U_i]), \frac{1}{n} \sum_{i=1}^{n} t_2([U_i]), \frac{1}{n} \sum_{i=1}^{n} t_3([U_i]) \right)
\]

The sample mean \([\bar{U}]\) maximises the scalar product

\[
\langle t([\bar{U}]), \bar{t} \rangle
\]

Maximisation must be performed numerically.

Sample dispersion
Combines the separate dispersions of the three axes

\[
d = \sum_{j=1}^{3} \left[ 1 - \text{tr}((\bar{t}_j + \frac{1}{3} I_3)^2) \right]. 
\]
Test for Uniformity
Test for Uniformity

Generalises with test statistic

\[ S = 5n \| \bar{t} \|^2 = 5n \sum_{j=1}^{3} \text{tr}(\bar{t}_j^2) \sim \chi^2_{10} \]
**Test for Uniformity**

Generalises with test statistic

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Statistical tests

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**Two sample test**
Statistical tests

**Test for Uniformity**

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Randomisation test with the test statistic

\[ D = ||\bar{t}_1 - \bar{t}_2||^2 \]
Frame Bingham distributions

\[ f([U]) \propto \exp\left(\langle t([U]), (A_1, A_2, A_3) \rangle\right) \]
\[ \propto \exp\left(\sum_{j=1}^{3} u_j^T A_j u_j\right) \]

\(A_1, A_2\) and \(A_3\) are symmetric, \(3 \times 3\), trace zero matrices.
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\ldots a variety of parametric and non-parametric tests

Arnold & Jupp 2013
In an earthquake two blocks slide against each other
In an earthquake two blocks slide against each other
In an earthquake two blocks slide against each other
Earthquake Focal Mechanisms

Summarise by three unit vectors
Earthquake Focal Mechanisms

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- Fault normal $\mathbf{n}$
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Earthquake Focal Mechanisms

Summarise by three unit vectors

- Fault normal $\mathbf{n}$
- Slip vector in the fault plane $\mathbf{u}$
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$\Rightarrow$ Three axes: $\pm \mathbf{p} = \pm (\mathbf{n} - \mathbf{u})/\sqrt{2}$, $\pm \mathbf{t} = \pm (\mathbf{n} + \mathbf{u})/\sqrt{2}$, $\pm \mathbf{a} = \pm (\mathbf{p} \times \mathbf{t})$
Christchurch Earthquakes

1904–2011
22 February 2011
Example: 3D axes – oafs

PT axes in Christchurch, before and after February 2011

Before
\[ n_1 = 50 \]

After
\[ n_2 = 50 \]

- Stereonets show T, A, P axes
- Sample means are filled circles
- Did the mean orientation of the triplet of axes change after the earthquake?
  (Two sample test for consistent orientation of the three axes)
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  No: \( p \)-value 0.890

After

\( n_2 = 50 \)
Ambiguous Rotations in 3D

Extending to more complex symmetries

Fluorite

Diopside
How can we do statistics on orientations in the presence of high degrees of symmetry?
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Common orientation descriptions in 3D

- **Euler Angles**: $(\phi, \theta, \psi)$
- **Rotation Matrices**: $U \in SO(3)$

are not unique under symmetry
How can we do statistics on orientations in the presence of high degrees of symmetry?

Common orientation descriptions in 3D

- **Euler Angles**: $(\phi, \theta, \psi)$
- **Rotation Matrices**: $U \in SO(3)$

are not unique under symmetry

We have invariance under the action of a point symmetry group $K$

$$U \equiv UW_1 \equiv UW_2 \equiv \ldots \equiv UW_m \overset{\text{def}}{=} [U]$$

We need **orientation representations** invariant under $K$: **symmetric frames**
In crystallography, $K$ is one of

<table>
<thead>
<tr>
<th>$K$</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_r$ cyclic</td>
<td>$C_2$ monoclinic crystals</td>
</tr>
<tr>
<td>$D_r$ dihedral</td>
<td>$D_2$ orthorhombic crystals</td>
</tr>
<tr>
<td></td>
<td>(earthquake focal mechanisms)</td>
</tr>
<tr>
<td></td>
<td>$D_3$ trigonal crystals</td>
</tr>
<tr>
<td></td>
<td>$D_4$ tetragonal crystals</td>
</tr>
<tr>
<td></td>
<td>$D_6$ hexagonal crystals</td>
</tr>
<tr>
<td>$T$  tetrahedral</td>
<td>$O$ cubic</td>
</tr>
<tr>
<td>$Y$  icosahedral</td>
<td>cubic crystals</td>
</tr>
<tr>
<td></td>
<td>carboranes, viruses,</td>
</tr>
<tr>
<td></td>
<td>quasi-crystals, liquid crystals</td>
</tr>
<tr>
<td></td>
<td>radiolara</td>
</tr>
</tbody>
</table>
General Case in 3D

$C_2 = D_1$

$C_3$

$D_6$

$T$

$O$

$Y$
The averaging approach mixes $|K|$ rotated copies of a single distribution

$$f(U) = \frac{1}{|K|} \sum_{i=1}^{|K|} f(UW_i)$$

for $U \in SO(3)$ and $W_i \in K$
The **averaging approach** mixes $|K|$ rotated copies of a single distribution

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for $U \in SO(3)$ and $W_i \in K$

Successful, but cumbersome
Embedding approach

Extend the single direction and single axis embedding approaches
Embedding approach

Extend the single direction and single axis embedding approaches

\[ \mathbf{t} = \mathbf{u} \]

\[ \mathbf{t} = \mathbf{uu}^T - \frac{1}{2} \mathbf{l}_2 = \otimes^2 \mathbf{u} - \frac{1}{2} \mathbf{l}_2 \]
Embedding approach

Extend the single direction and single axis embedding approaches

\[ t = u \]
\[ t = uu^T - \frac{1}{2} I_2 = \otimes^2 u - \frac{1}{2} I_2 \]

with the principles:
Embedding approach

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\]

with the principles:

- Use the tensor product \( \bigotimes^r \mathbf{u} \) for \( r \)-fold axis symmetry

\[
(\bigotimes^r \mathbf{u})_{j_1 j_2 \ldots j_r} = \prod_{k=1}^{r} u_{kj_k} = u_{1j_1} u_{2j_2} \ldots u_{rj_r}
\]
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- Subtract the expectation

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for uniformly distributed \( u \)
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t = u
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\]

- Sum over axes
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\[
E[\otimes^r u]
\]

for uniformly distributed \( u \)

Gives the desired embedding.
Example: 4—fold axis $C_4$

4 directions in a plane perpendicular to $u_0$

Normal vector $u_0$ and directions $u_1, u_2, u_3, u_4$

$$t = (u_0, \sum_{i=1}^{4} \otimes^4 u_i - \frac{4}{5} \text{symm}(\otimes^2 I_3))$$
Example: Tetrahedral symmetry $T$

Directions $u_1, u_2, u_3, u_4$

$$t = \sum_{i=1}^{4} \otimes^3 u_i$$
## Embedding approach

### Embedding

<table>
<thead>
<tr>
<th>K</th>
<th>Frame</th>
<th>$t([U])$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$</td>
<td>$(u_1, u_2, u_3)$</td>
<td>$(u_1, u_2, u_3)$</td>
</tr>
<tr>
<td>$C_2$</td>
<td>$(u_0, \pm u_1)$</td>
<td>$(u_0, u_1 u_1^T - (1/3)I_3)$</td>
</tr>
<tr>
<td>$C_r$ ($r \geq 3$)</td>
<td>$(u_1, \ldots, u_r)$</td>
<td>$(u_0, \sum_{i=1}^r \otimes^r u_i - E[\cdot])$</td>
</tr>
<tr>
<td>$D_2$</td>
<td>$(\pm u_1, \pm u_2)$</td>
<td>$(u_1 u_1^T - (1/3)I_3, u_2 u_2^T - (1/3)I_3)$</td>
</tr>
<tr>
<td>$D_r$ ($r \geq 3$)</td>
<td>$(u_1, \ldots, u_r)$</td>
<td>$\sum_{i=1}^r \otimes^r u_i - E[\cdot]$</td>
</tr>
<tr>
<td>$T$</td>
<td>$(u_1, \ldots, u_4)$</td>
<td>$\sum_{i=1}^4 \otimes^3 u_i$</td>
</tr>
<tr>
<td>$O$</td>
<td>$(\pm u_1, \pm u_2, \pm u_3)$</td>
<td>$\sum_{i=1}^3 \otimes^4 u_i - E[\cdot]$</td>
</tr>
<tr>
<td>$Y$</td>
<td>$(\pm u_1, \ldots, \pm u_6)$</td>
<td>$\sum_{i=1}^r \otimes^{10} u_i - E[\cdot]$</td>
</tr>
</tbody>
</table>
## Scalar Products

<table>
<thead>
<tr>
<th>$K$</th>
<th>Frame</th>
<th>$\langle t([U]), t([V]) \rangle$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$</td>
<td>$(u_1, u_2, u_3)$</td>
<td>$u_1^T v_1 + u_2^T v_2 + u_3^T v_3$</td>
</tr>
<tr>
<td>$C_2$</td>
<td>$(u_0, \pm u_1)$</td>
<td>$u_0^T v_0 + (u_1^T v_1)^2 - 1/3$</td>
</tr>
<tr>
<td>$C_r$ ($r \geq 3$)</td>
<td>$(u_1, \ldots, u_r)$</td>
<td>$u_0^T v_0 + \sum_{i=1}^{r} \sum_{j=1}^{r} (u_i^T v_j)^r - c_r$</td>
</tr>
<tr>
<td>$D_2$</td>
<td>$(\pm u_1, \pm u_2)$</td>
<td>$(u_1^T v_1)^2 + (u_2^T v_2)^2 - 2/3$</td>
</tr>
<tr>
<td>$D_r$ ($r \geq 3$)</td>
<td>$(u_1, \ldots, u_r)$</td>
<td>$\sum_{i=1}^{r} \sum_{j=1}^{r} (u_i^T v_j)^r$</td>
</tr>
<tr>
<td>$T$</td>
<td>$(u_1, \ldots, u_4)$</td>
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<td>$O$</td>
<td>$(\pm u_1, \pm u_2, \pm u_3)$</td>
<td>$\sum_{i=1}^{3} \sum_{j=1}^{3} (u_i^T v_j)^4 - 9/5$</td>
</tr>
<tr>
<td>$Y$</td>
<td>$(\pm u_1, \ldots, \pm u_6)$</td>
<td>$\sum_{i=1}^{6} \sum_{j=1}^{6} (u_i^T v_j)^{10} - 36/11$</td>
</tr>
</tbody>
</table>
Summary statistics

Normalisation

\[ \langle t([U]), t([U]) \rangle = \| t([U]) \|^2 = \rho^2 \quad \text{for all } [U] \]
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Given a sample \([U_1], \ldots, [U_n]\): compute mean of embedded values:

\[ \bar{t} = \frac{1}{n} \sum_{k=1}^{n} t([U_k]) \]
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Sample Mean

$$[\tilde{U}] = \arg \max_{[M] \in SO(3)/K} \langle t([M]), \bar{t} \rangle$$
Normalisation

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Dispersion

\[ d = \rho^2 - \| \bar{t} \|^2 \]
The scalar product is a measure of closeness: leads to intuitive test statistics for randomisation tests:
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**Test uniformity:**

\[ T = \| \bar{\bar{t}} \|^2 \]

Reject for large values of \( T \) compared values from simulations from a uniform distribution
Statistical tests

The scalar product is a measure of closeness: leads to intuitive test
statistics for randomisation tests:

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**Test of location \([M_0]\):**

\[ T = ||\bar{t} - t([M_0])||^2 \]

Randomisation distribution reorients each sample element \([U_k]\) under the
point group symmetry of \([M_0]\)
Statistical tests

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**Two sample test:**

\[ T = ||\bar{t}_1 - \bar{t}_2||^2 \]

Randomisation distribution permutes the sample labels of the observations \([U_{11}], \ldots, [U_{1n_1}], [U_{21}], \ldots, [U_{2n_2}]\)
Embedding leads to a natural exponential family of probability distributions
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\[ f([U]|\kappa, [M]) = c(\kappa)^{-1} \exp \{ \kappa \langle t([U]), t([M]) \rangle \} \]

radially symmetric, with mode \([M]\) and concentration parameter \(\kappa\).

Generalisation of the von Mises and Fisher distributions.
Embedding leads to a natural exponential family of probability distributions

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radially symmetric, with mode \([M]\) and concentration parameter \(\kappa\).

Generalisation of the von Mises and Fisher distributions.

Similarly the **frame cardoid** distribution is a simple generalisation of the planar distribution:

\[ f([U]) = 1 + \kappa \langle t([U]), t([M]) \rangle \]
Application: Diopside (CaMgSiO): $C_2$ Symmetry

Symmetric under rotations of $180^\circ$ about a single axis

Monoclinic
Observations from an Electron Backscattering Diffraction (EBSD) experiment

Orientations at 100 locations
Diopside: $C_2$ symmetry

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Orientations at 100 locations

$p$–value < 0.001 for a test of uniformity: not Uniform
Diopside: $C_2$ symmetry

Orientations in two regions ($n_1 = 34$ and $n_2 = 37$).
Diopside: $C_2$ symmetry

Orientations in two regions ($n_1 = 34$ and $n_2 = 37$).

$p$–value 0.47 for a test of equality of orientations: No evidence for difference
Misorientation and Regression relationships

Phase transitions – solids undergoing a change of symmetry
e.g. the Martensite transformation $O \rightarrow D_4$

A whole lot of applications in seismology and crystallography
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and moon quakes ...
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Re-analyse using new methods
Thank You

Kia ora koutou