Statistics of Ambiguous Rotations

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Many thanks

With thanks to:

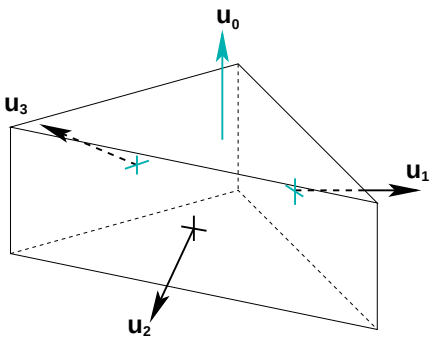
John Townend, Martha Savage, David Walsh, Carolin Boese, Jesse Dimech, Ernestynne Walsh, Steve Sherburn, Lisa Woods, Florian Bachmann

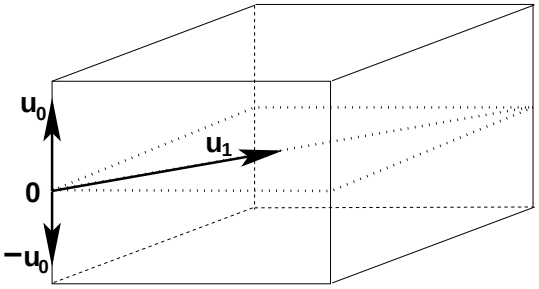
Outline

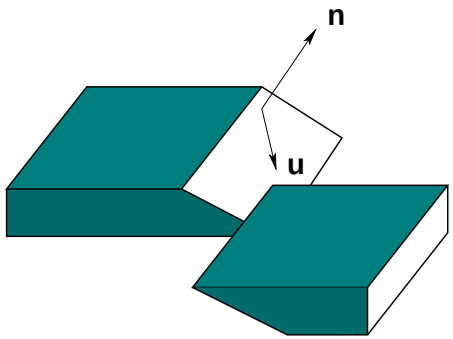
Statistics of Highly Symmetric Objects

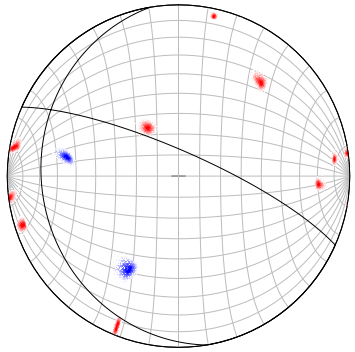


How can we do statistics with orientations of objects like these?







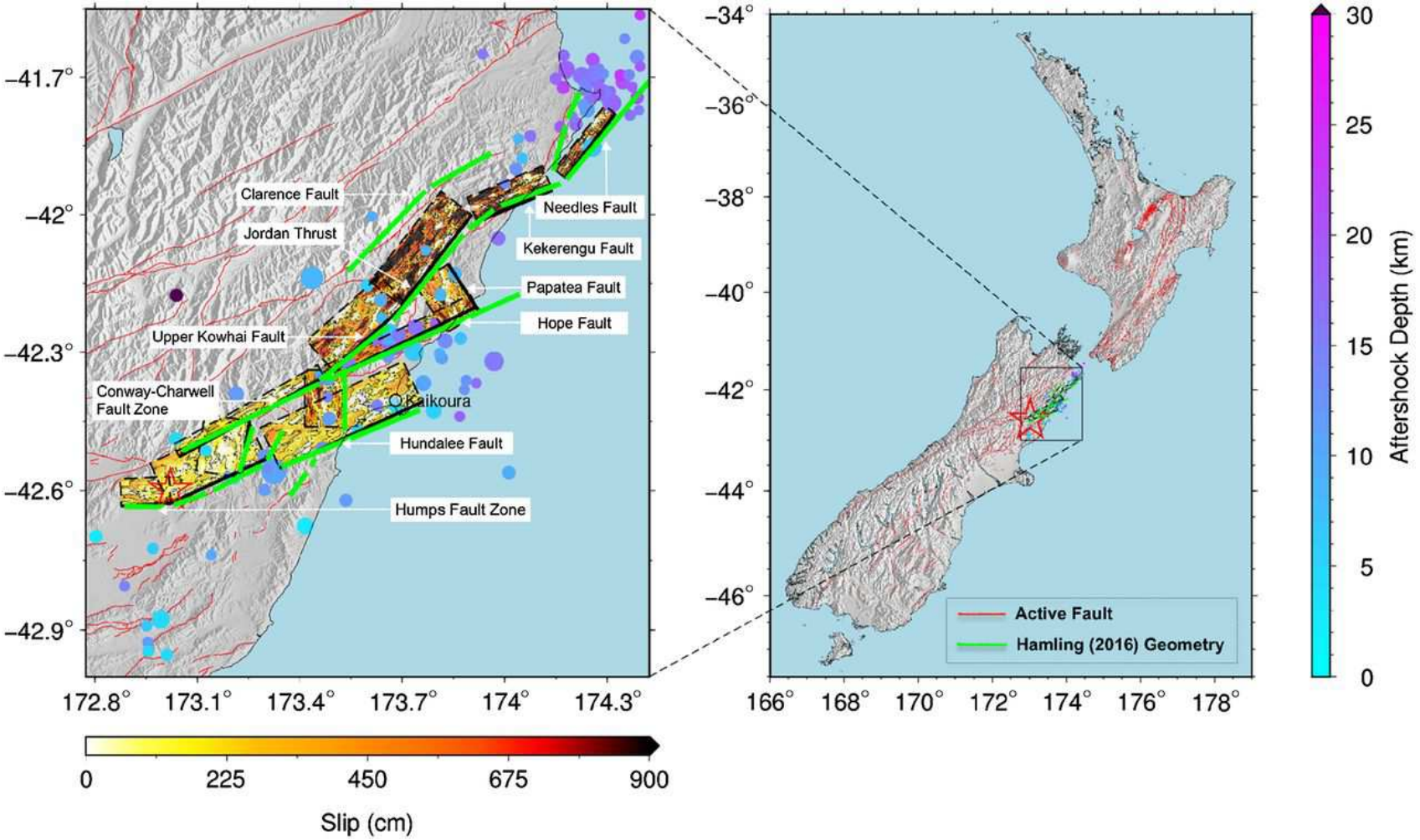


But first...

... some very recent NZ history

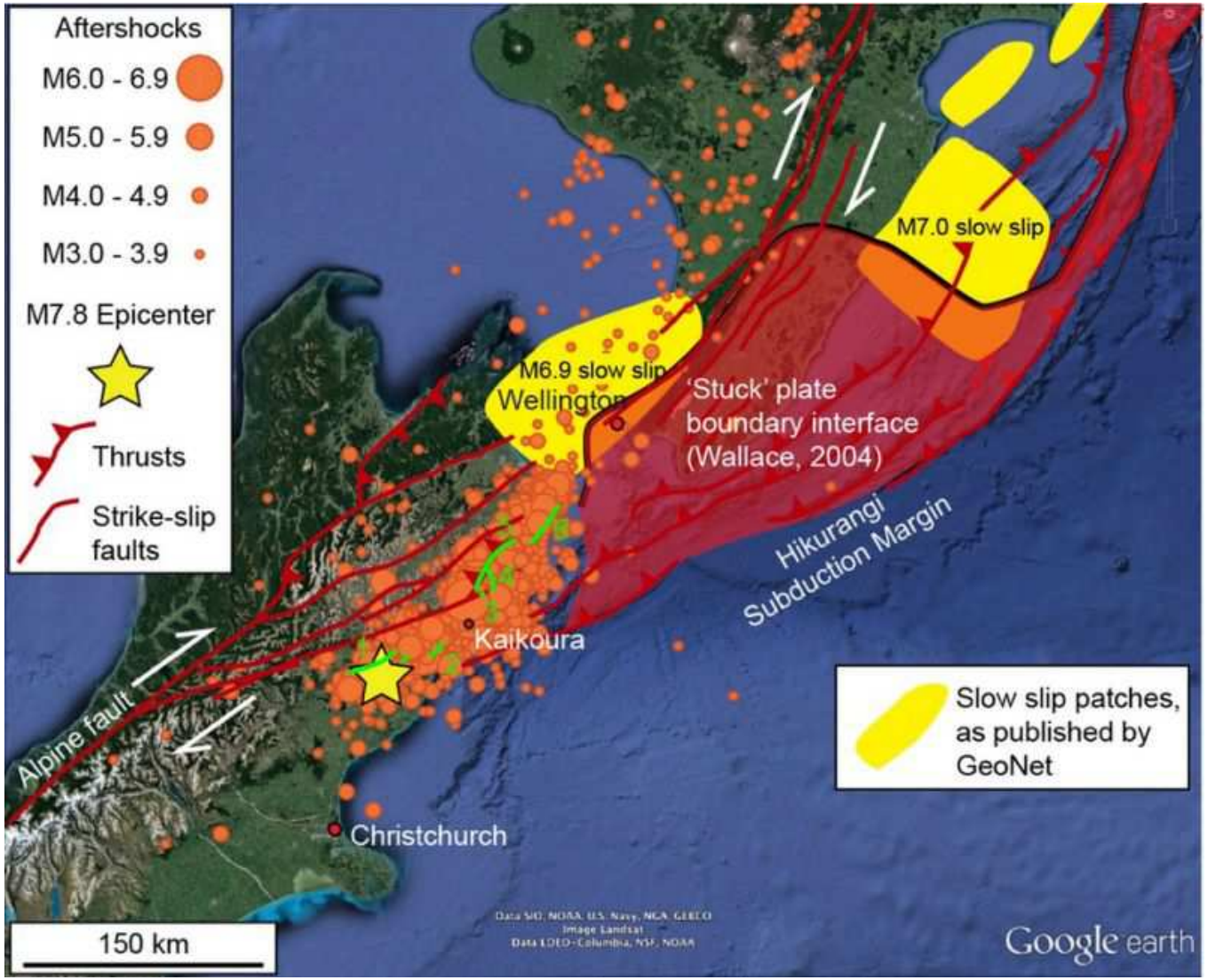
Some very recent NZ history

Kaikoura quake – 14 Nov 2016, M7.8



Bradley et al., Seismological Research Letters (2017) 88 (3): 740-756

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. Seisomology 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

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New statistical methods are needed.

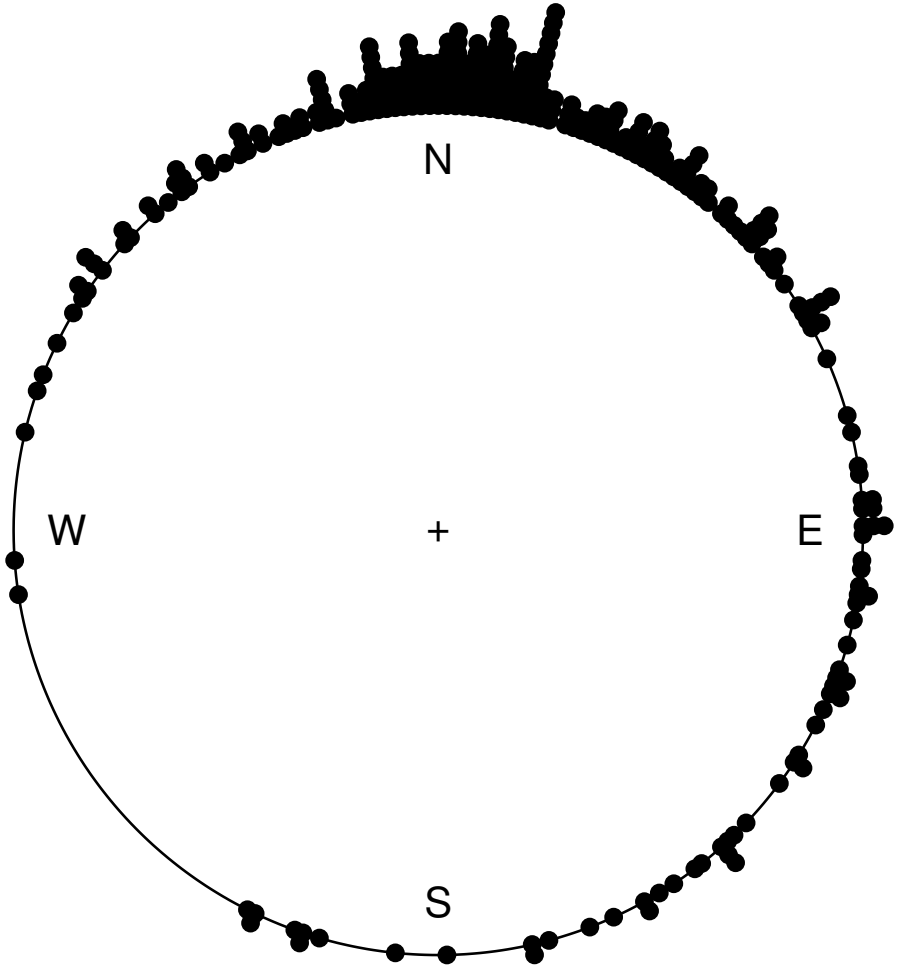
Directional Statistics and Tectonic Stress Estimation

Arnold & Townend (2007) A Bayesian approach to estimating tectonic stress from seismological data, Geophys J Int, 170, 1336-56;

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

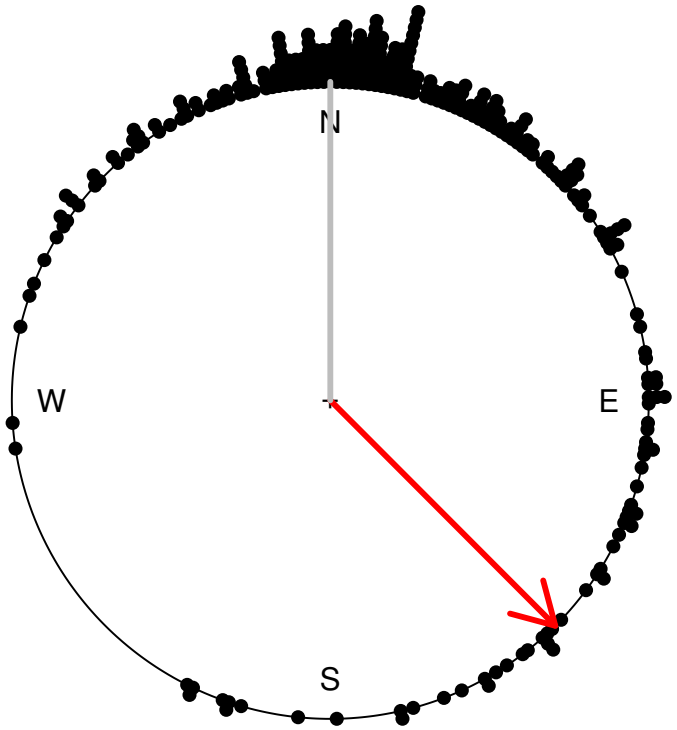
Roman et al. (2011) Analysis and forward modeling of seismic anisotropy during the ongoing eruption of the Soufrière Hills Volcano, Montserrat, 19962007, J Geophys Res, 116, B03201

Example: Angles in the plane (2D)



Wind directions at a site in the Italian Alps

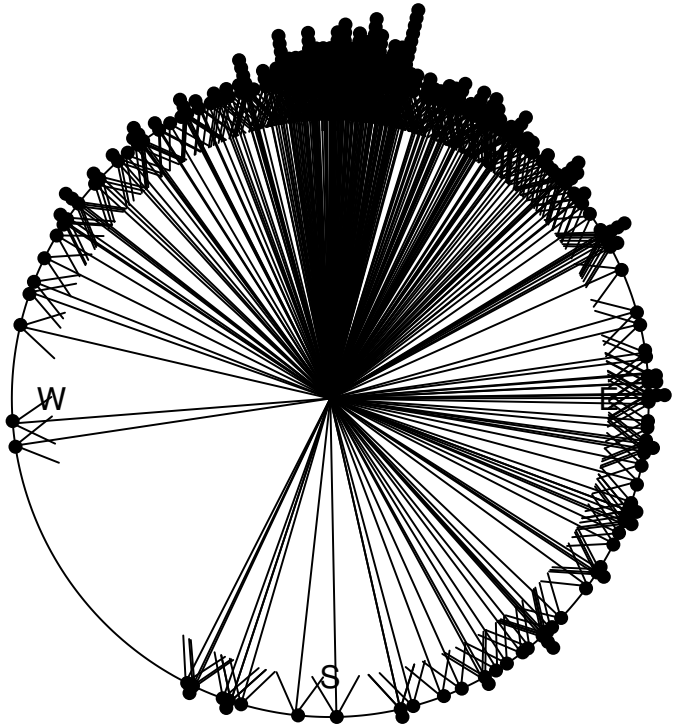
Example: Angles in the plane (2D)



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

Familiar mean ($\bar{\theta} = 135.1^\circ$) does not make sense

Averaging angles



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

$$\begin{aligned}\bar{\mathbf{u}} &= \frac{1}{n}\sum_{i=1}^{n}\mathbf{u}_i \\ &= \frac{1}{n}\sum_{i=1}^{n}\begin{bmatrix}\cos\theta_i \\ \sin\theta_i\end{bmatrix} \\ &= \bar{R}\begin{bmatrix}\cos\bar{\theta} \\ \sin\bar{\theta}\end{bmatrix}\end{aligned}$$

where

$$\bar{\theta} = \mathtt{atan2}(\langle\sin\theta_i\rangle, \langle\cos\theta_i\rangle) \qquad \bar{R}^2 = \langle\sin\theta_i\rangle^2 + \langle\cos\theta_i\rangle^2$$

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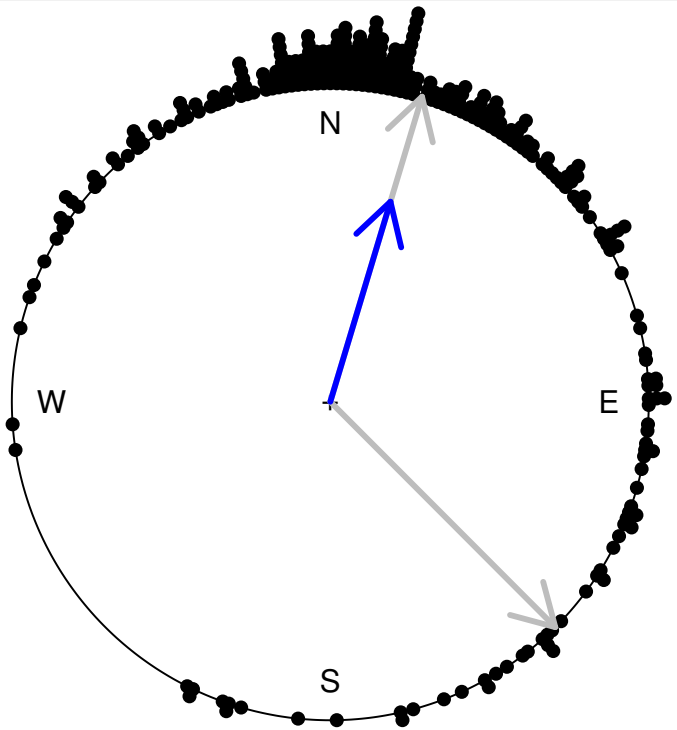

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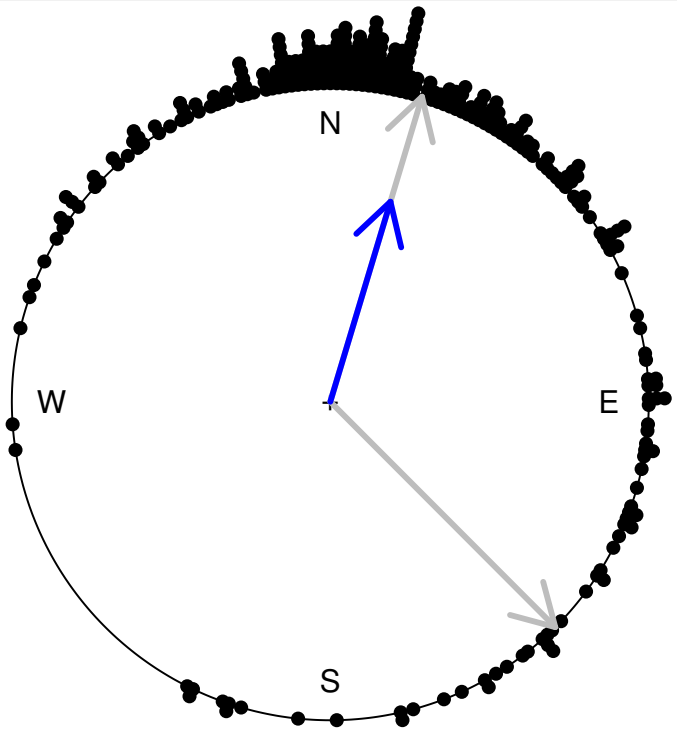

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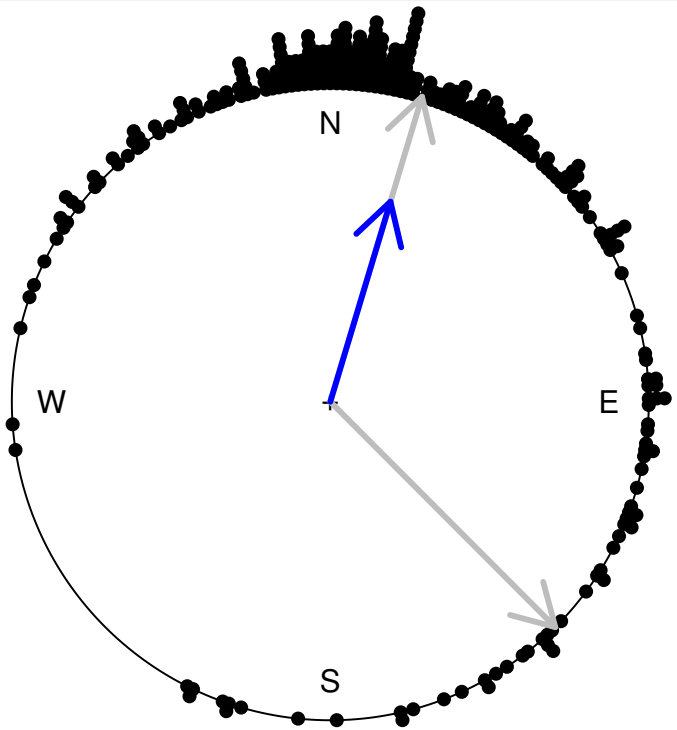

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Direction $\bar{\theta}$ is the mean direction we want ($\bar{\theta} = 16.7°$).

Averaging angles

We have replaced the scalar θ with its periodic symmetry

$$\ldots\theta - 4\pi, \theta - 2\pi, \theta, \theta + 2\pi, \theta + 4\pi, \ldots$$

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

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

invariant under that symmetry.

Inference

Von Mises distribution (direction θ, concentration κ)

$$
\begin{aligned}
f(\theta) &= \frac{1}{2\pi I_0(\kappa)} \exp\left(\kappa \cos(\theta - \theta_0)\right) \\
f(\mathbf{u}) &= \frac{1}{2\pi I_0(\kappa)} \exp\left(\kappa \boldsymbol{\mu}^T \mathbf{u}\right)
\end{aligned}
$$

Similarity of directions is measured by the scalar product

$$\boldsymbol{\mu}^T \mathbf{u}$$

. . . a variety of parametric and non-parametric tests

A test for uniformity

The Rayleigh Test

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The test statistic

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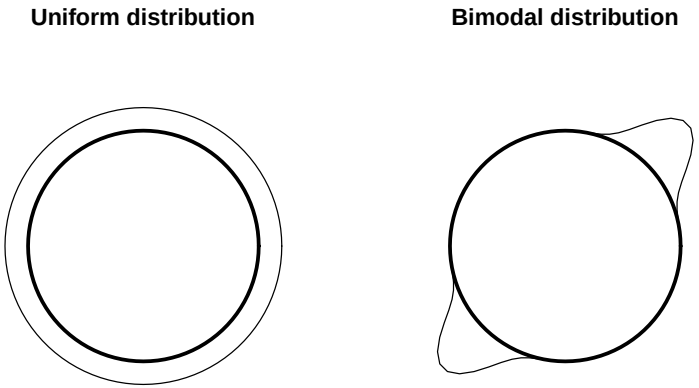
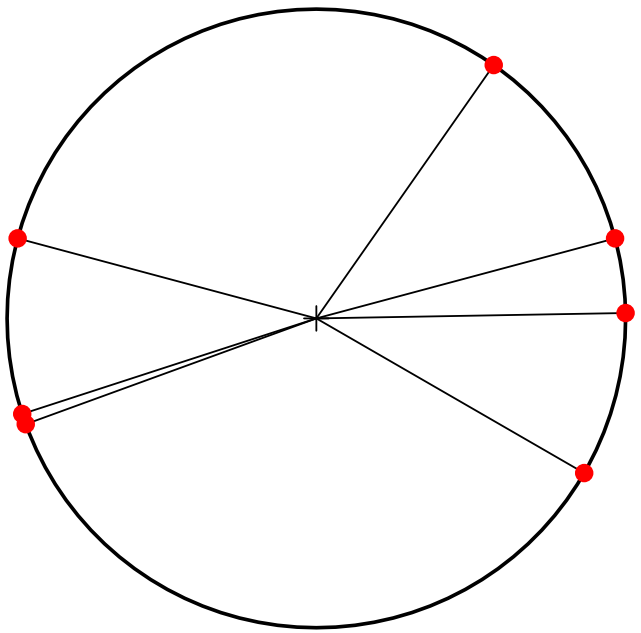


- No power against distributions with $E[\mathbf{u}] = 0$
- (though alternative tests exist)

Averaging axes



A similar approach works for **axes** where

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are all equivalent

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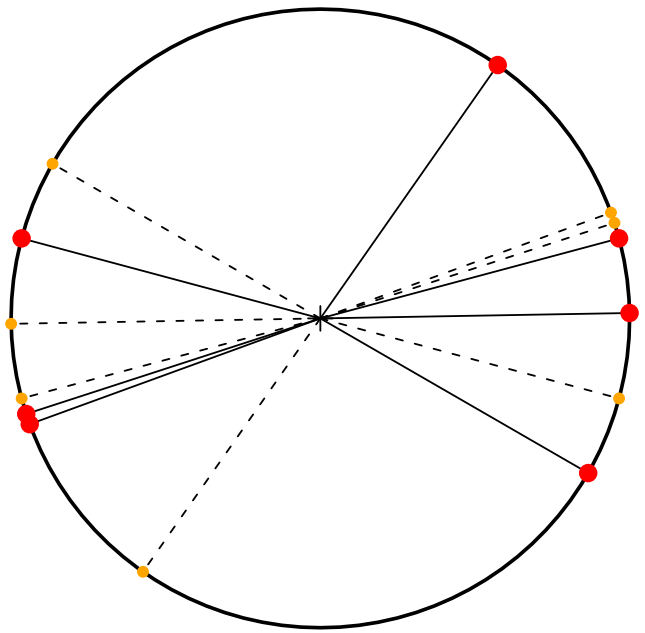

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Embedding axes in 2D

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

$$\begin{aligned} t(\pm\mathbf{u}) &= \mathbf{u}\mathbf{u}^T - \tfrac{1}{2} I_2 \\ &= \frac{1}{2} \begin{bmatrix} \cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta \end{bmatrix} \end{aligned}$$

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Equivalent to familiar angle-doubling methods

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Associated with a **scalar product**:

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The scalar product forms the basis of statistical tests.

Averaging axes

Averaging observations of axes:

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&= \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) \\
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Summary statistics

Sample mean

$$\bar{t} = \frac{1}{n}\sum_{i=1}^{n} t(\pm\mathbf{u}_i) = \frac{1}{2}\begin{bmatrix} \langle\cos 2\theta\rangle & \langle\sin 2\theta\rangle \\ \langle\sin 2\theta\rangle & -\langle\cos 2\theta\rangle \end{bmatrix} \tag{1}$$

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

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

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Sample dispersion

$$\begin{aligned} d &= \tfrac{1}{2} - ||\bar{t}||^2 \\ &= \tfrac{1}{2}(1 - \langle\cos 2\theta\rangle^2 - \langle\sin 2\theta\rangle^2) \\ &= \tfrac{1}{2}(1 - \bar{R}_2^2) \end{aligned}$$

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S can also be used in a randomisation test for uniformity.

Inference

Watson distribution (mean axis $\pm\boldsymbol{\mu}$, concentration κ)

$$f(\mathbf{u}) \quad \propto \quad \exp\left(\kappa(\boldsymbol{\mu}^T\mathbf{u})^2\right)$$

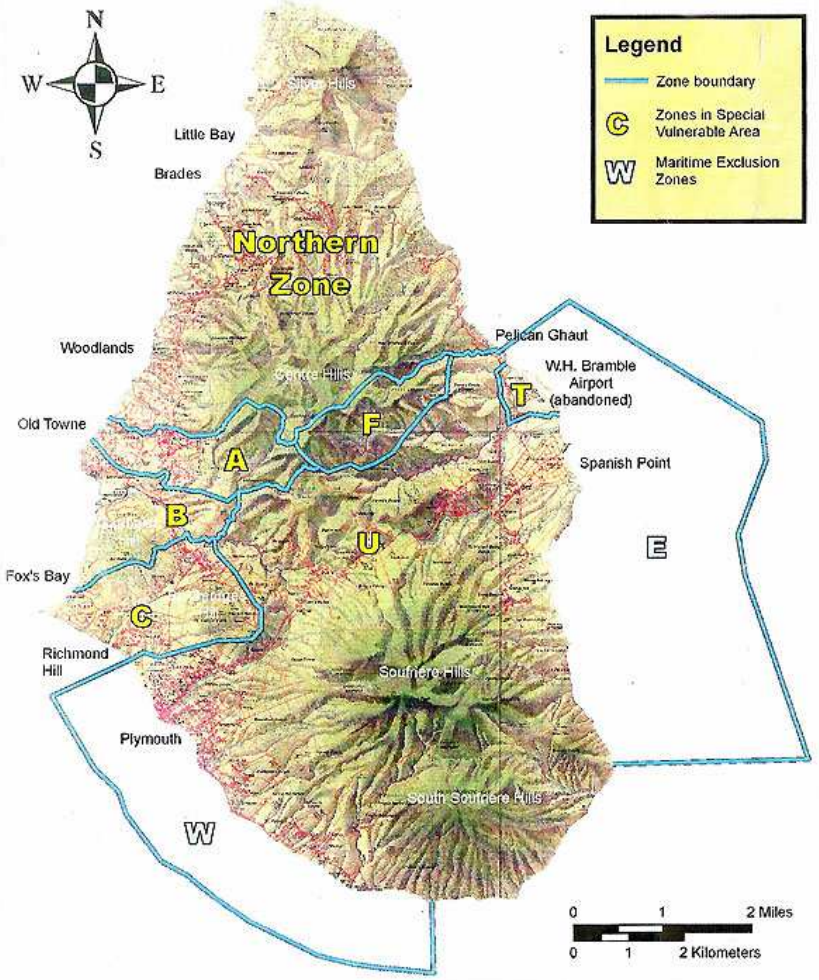
Similarity measured by the scalar product

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

. . . a variety of parametric and non-parametric tests

Example – Montserrat

Soufrière Hills – Montserrat



Hazard Level System

Soufriere Hills Volcano, Montserrat: Hazard Levels and Access Restrictions

1 August 2008

Zones in the Special Vulnerable Area

- **A** South of Nantes River, including, Salem, Hope, Frith, Flemmings, parts of Olveston and Old Towne, and upper part of Happy Hill.
- **B** Iles Bay, Belham, Waterworks, parts of Old Towne and lower part of Happy Hill.
- **C** Cork Hill, Weekes, St Georges Hill, Foxes Bay, Richmond Hill and Delvins.
- **F** Corbett Springs, Locust Valley. This zone is dedicated to farming and is defined by NDPRAC.
- **U** Formerly the Unsafe Zone.
- **T** Trant's. Limits marked by red flags, southern limit is Farm River. This zone is dedicated to sand and gravel extraction and is defined by NDPRAC. Access requires the use of special procedures for monitoring activity and rapid response.

Maritime Exclusion Zones

- **W** 2 km offshore between Sturge Park and O'Garro's.
- **E** 4 km offshore between Roches Yard and Spanish Point, decreasing to 2 km offshore from Spanish Point to Pelican Ghaut.

Sustained eruption of the Soufrière Hills, 1996-2007.

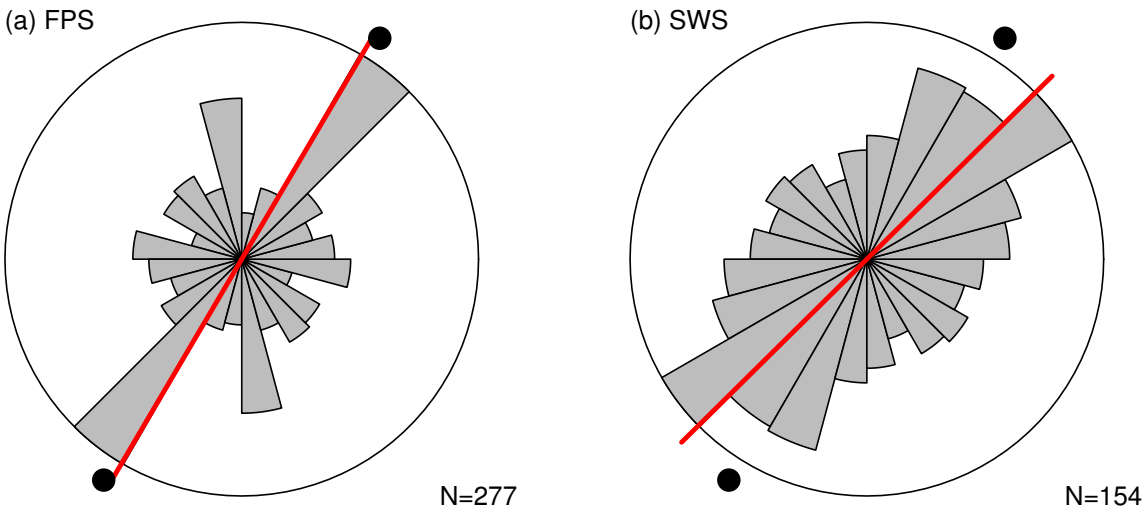
Soufrière Hills – Montserrat

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

Soufrière Hills – Montserrat

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



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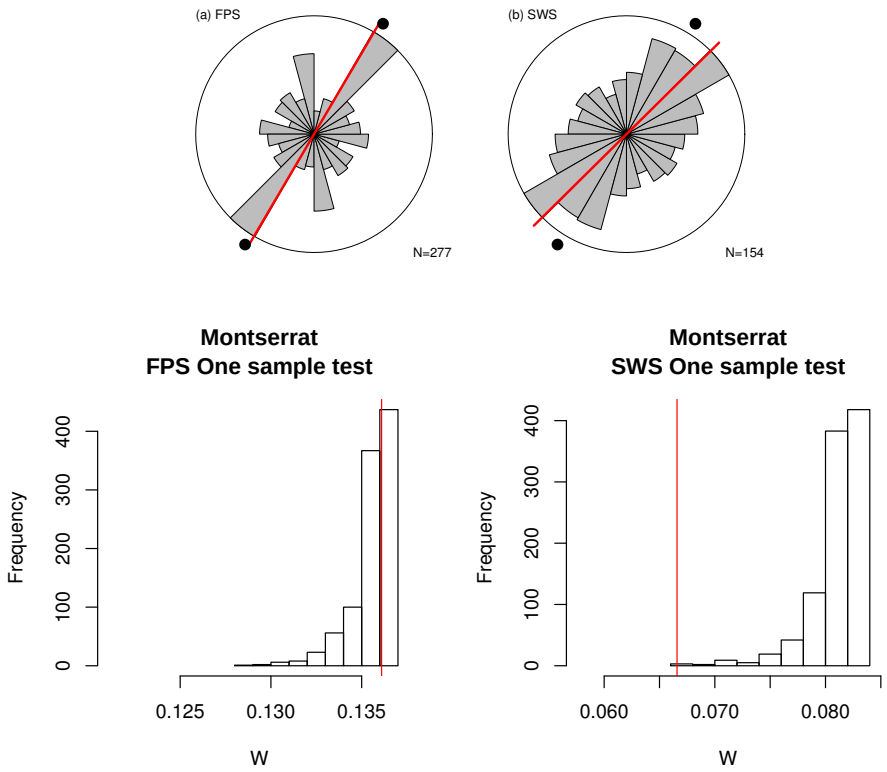
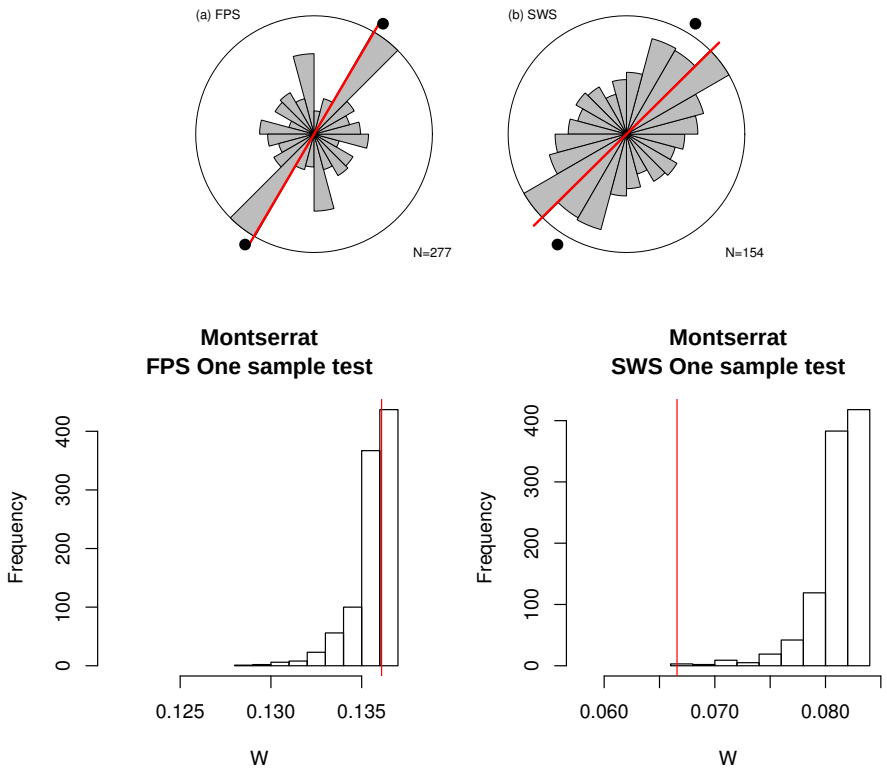


- Do the inferrred orientations differ from the regional stress field $\theta_0 = 32°$? (one sample tests)

Soufrière Hills – Montserrat



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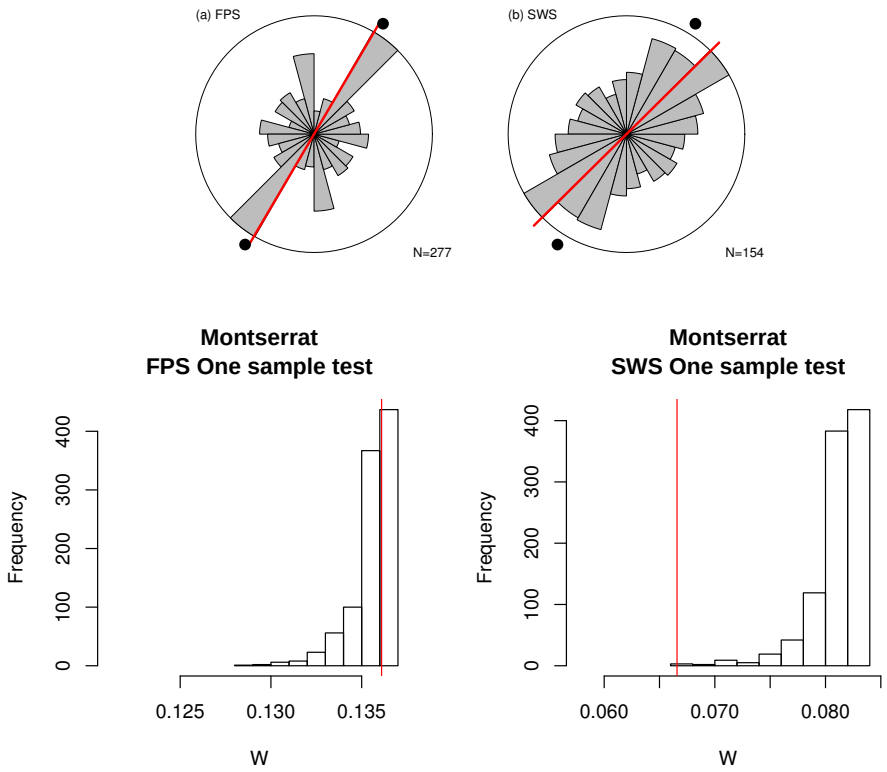

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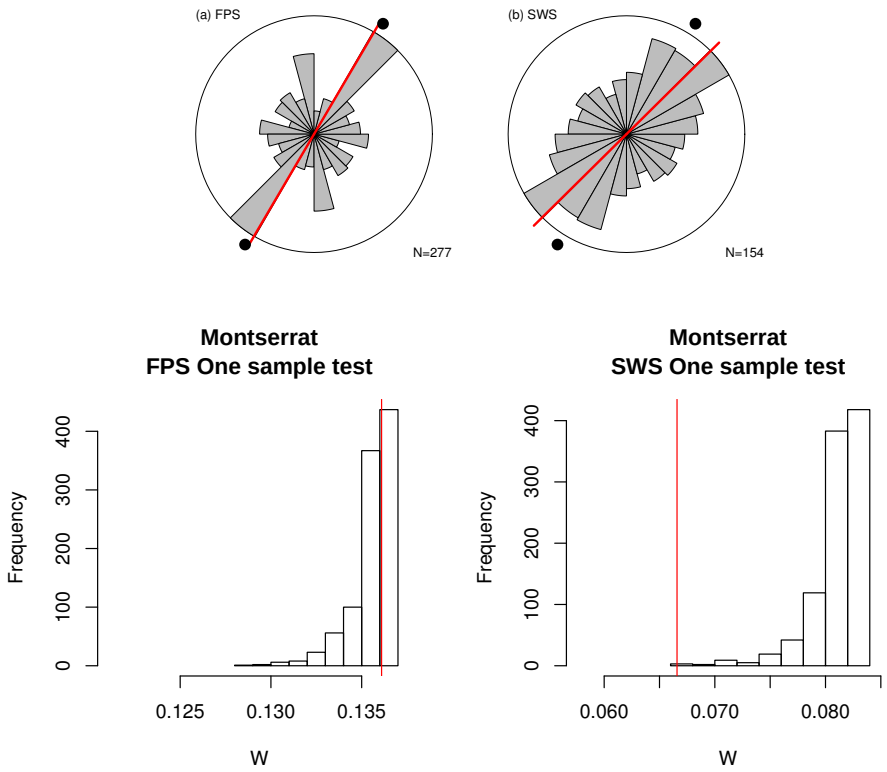

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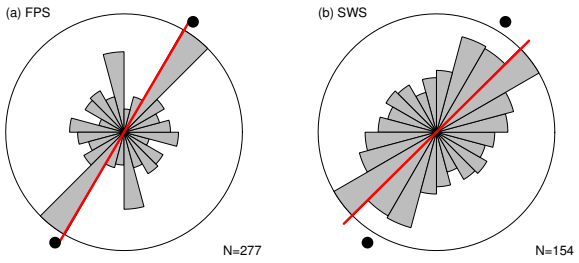

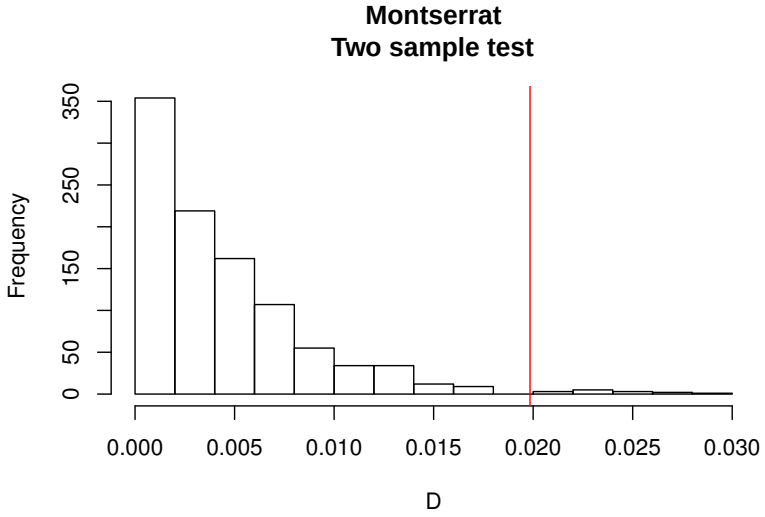

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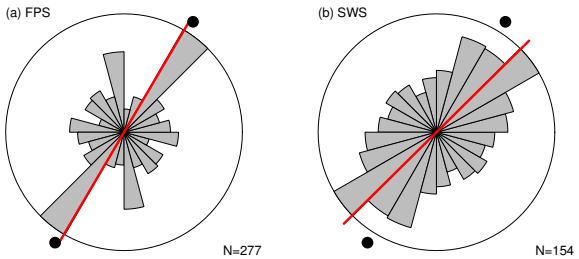

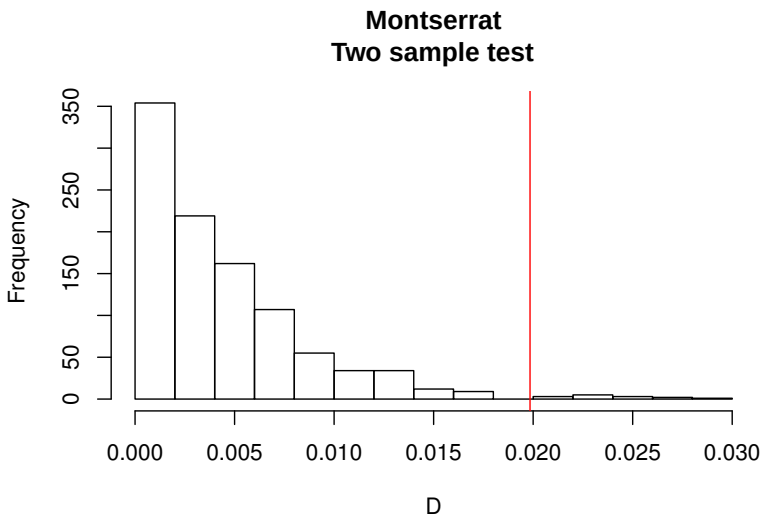

- Do the two methods agree?
  (non-parametric two sample randomisation test for common orientation)
  No: $D = ||\bar{t}_1 - \bar{t}_2||^2 = 0.0198$, p-value=0.014.

Orthogonal Axial Frames

Arnold & Jupp (2013) Statistics of Orthogonal Axial Frames, Biometrika, 100, 571-586

Three dimensions

Now extend to 3D, and beyond ...

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(2 axes equivalent to 3: $\mathbf{u}_3 = \mathbf{u}_1 \times \mathbf{u}_2$)

Three dimensions

Represent directions by angles

- 1 axis: (ϕ, θ): Unit vector

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

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- 3 axes: Euler angles (ϕ, θ, ψ): 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

$$
\begin{aligned}
t([U]) &= \mathbf{u}\mathbf{u}^T - \tfrac{1}{3} I_3 \\
&= \begin{bmatrix} \cos^2\phi\sin^2\theta - \frac{1}{3} & \sin\phi\cos\phi\sin^2\theta & \cos\phi\sin\theta\cos\theta \\ \sin\phi\cos\phi\sin^2\theta & \sin^2\phi\sin^2\theta - \frac{1}{3} & \sin\phi\sin\theta\cos\theta \\ \cos\phi\sin\theta\cos\theta & \sin\phi\sin\theta\cos\theta & \cos^2\theta - \frac{1}{3} \end{bmatrix}
\end{aligned}
$$

with scalar product

$$
\begin{aligned}
\langle t([U_1]), t([U_2])\rangle &= \mathrm{tr}\left(t([U_1])t([U_2])\right) \\
&= (\mathbf{u}_1^T\mathbf{u}_2)^2 - \tfrac{1}{3}
\end{aligned}
$$

and $||t||^2 = \frac{2}{3}$

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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

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Compute the average of the embedding matrices

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

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Sample dispersion

Combines the separate dispersions of the three axes

$$d = \sum_{j=1}^{3}\left[1 - \mathrm{tr}((\bar{t}_j + \tfrac{1}{3}I_3)^2)\right] \quad . \tag{2}$$

Test for Uniformity

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$$D = ||\bar{t}_1 - \bar{t}_2||^2$$

Inference

Frame Bingham distributions

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f([U]) &\propto \exp\left(\langle t([U]), (A_1, A_2, A_3)\rangle\right) \\
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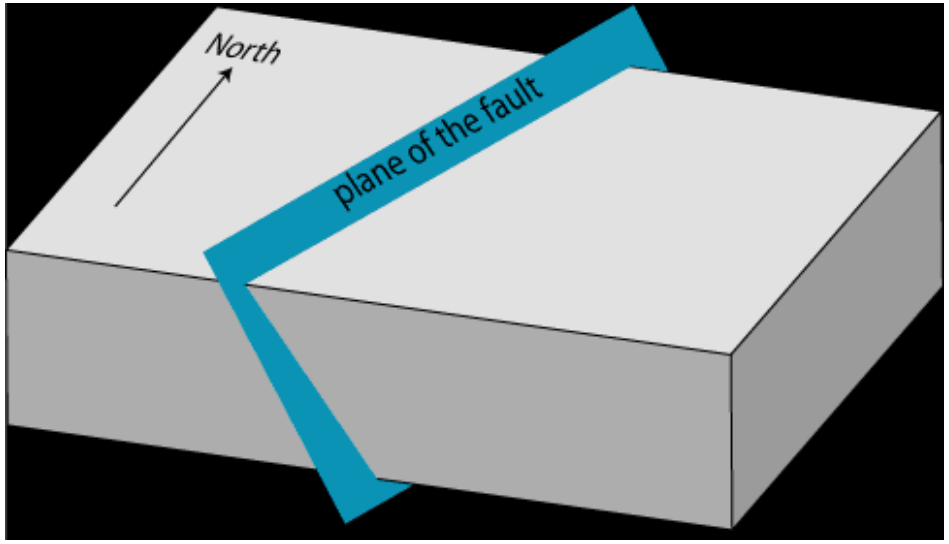
. . . a variety of parametric and non-parametric tests

Arnold & Jupp 2013

Application: Earthquake Focal Mechanisms

In an earthquake two blocks slide against each other



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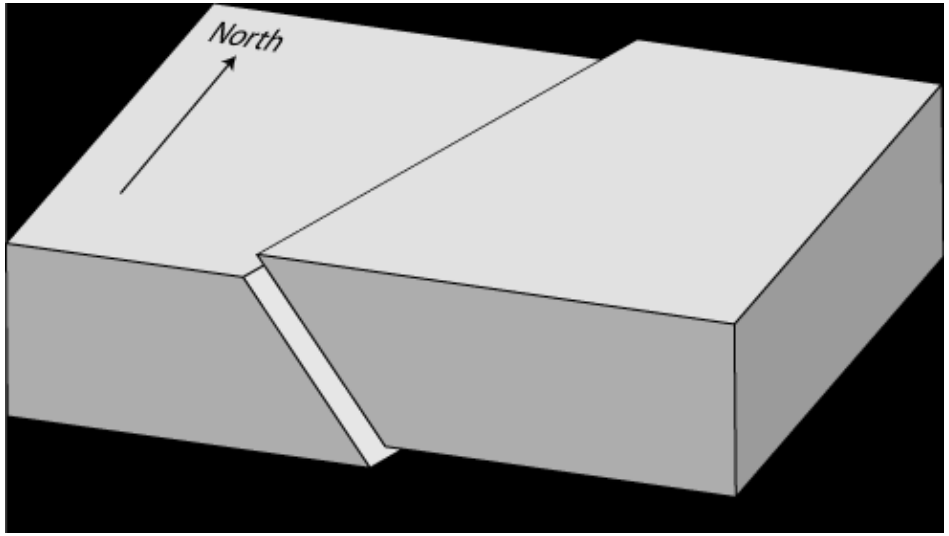

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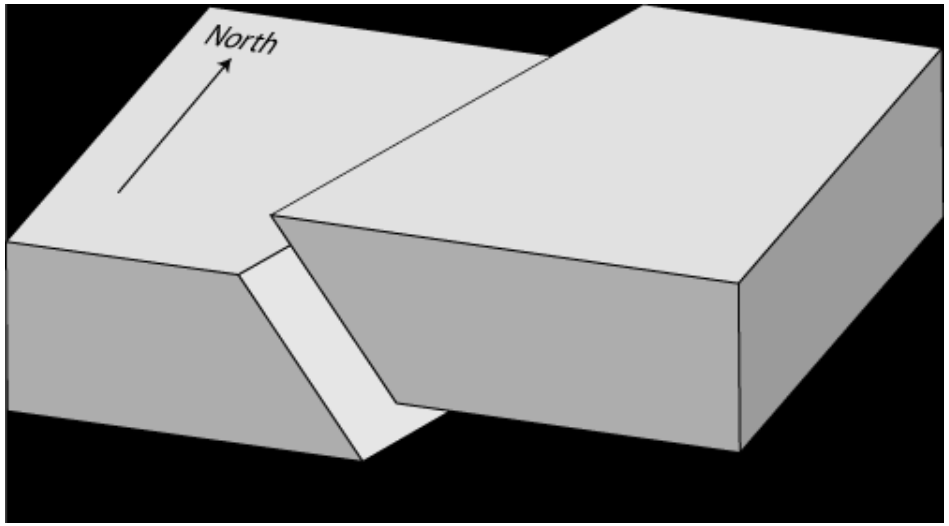

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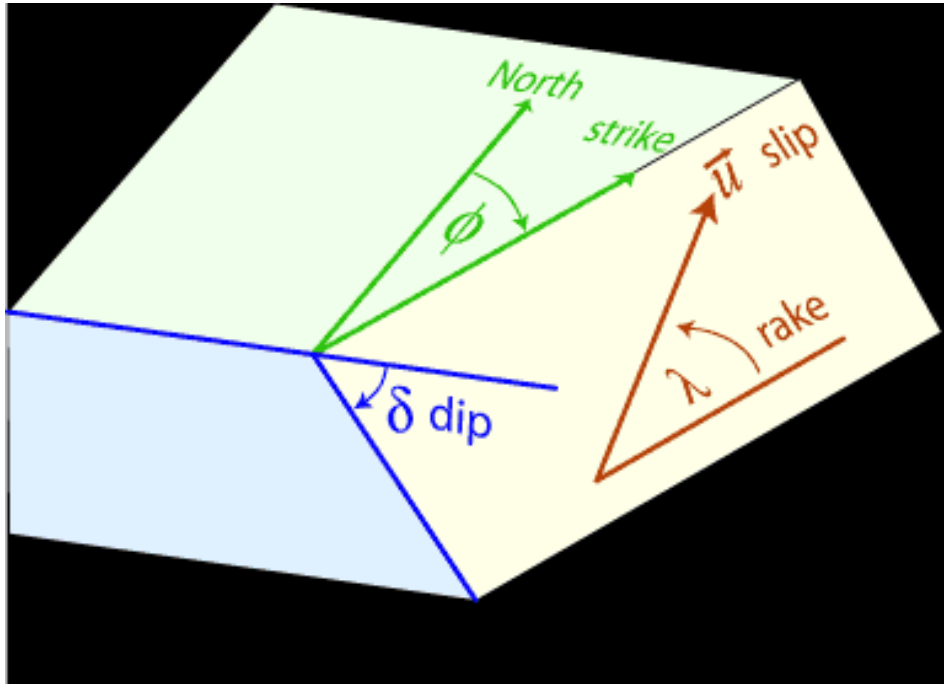
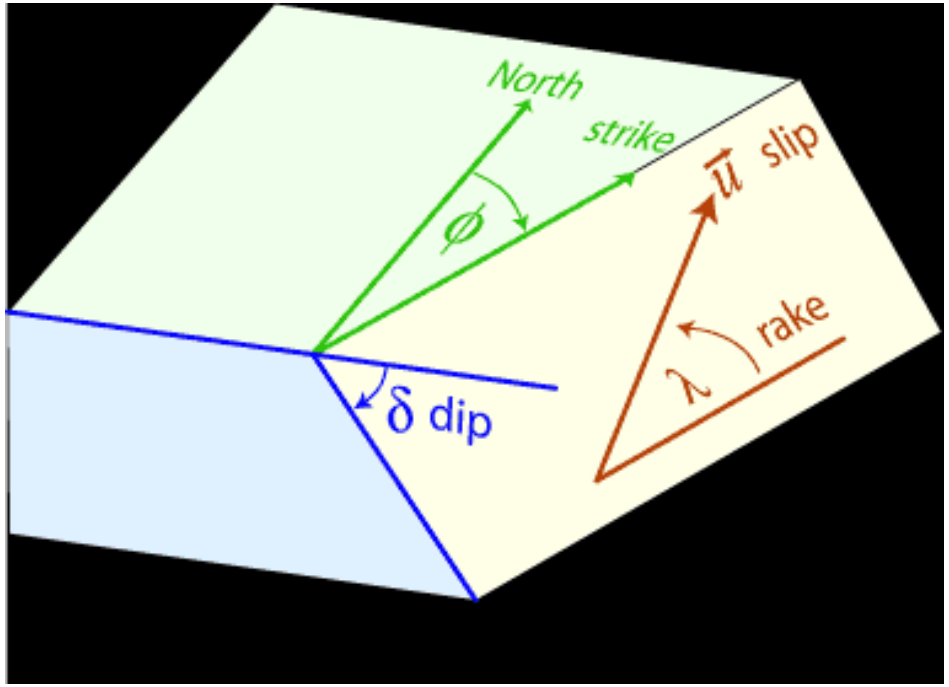


Summarise by three unit vectors

Earthquake Focal Mechanisms



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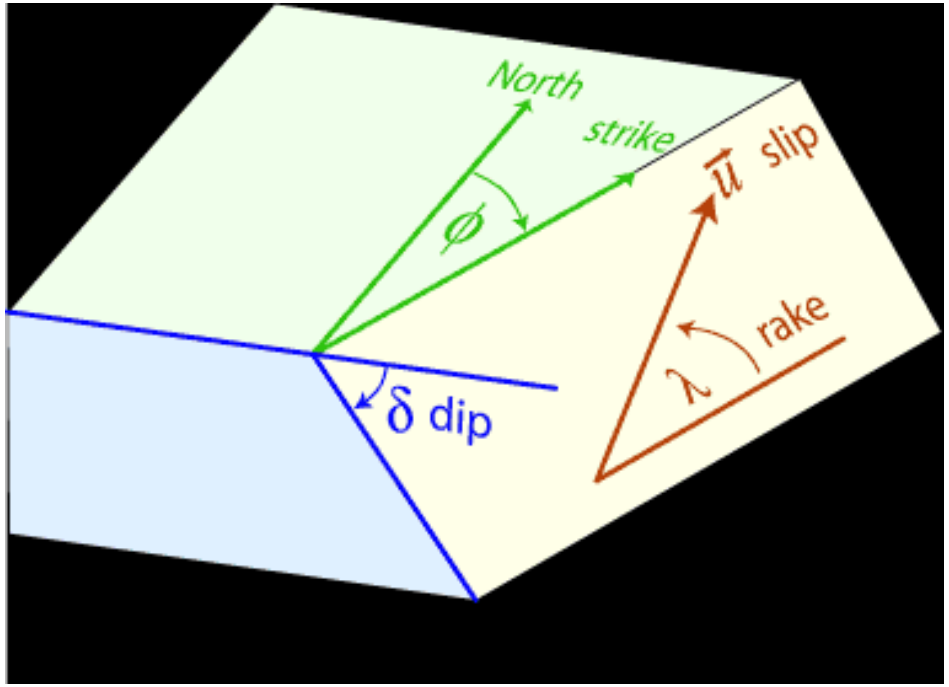
- Fault normal **n**

Earthquake Focal Mechanisms



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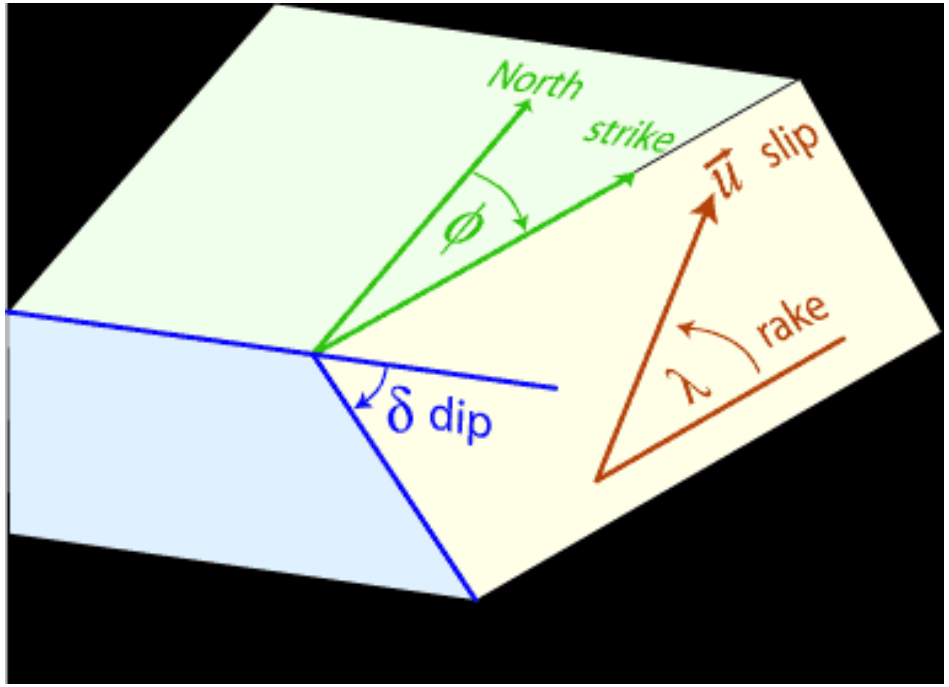

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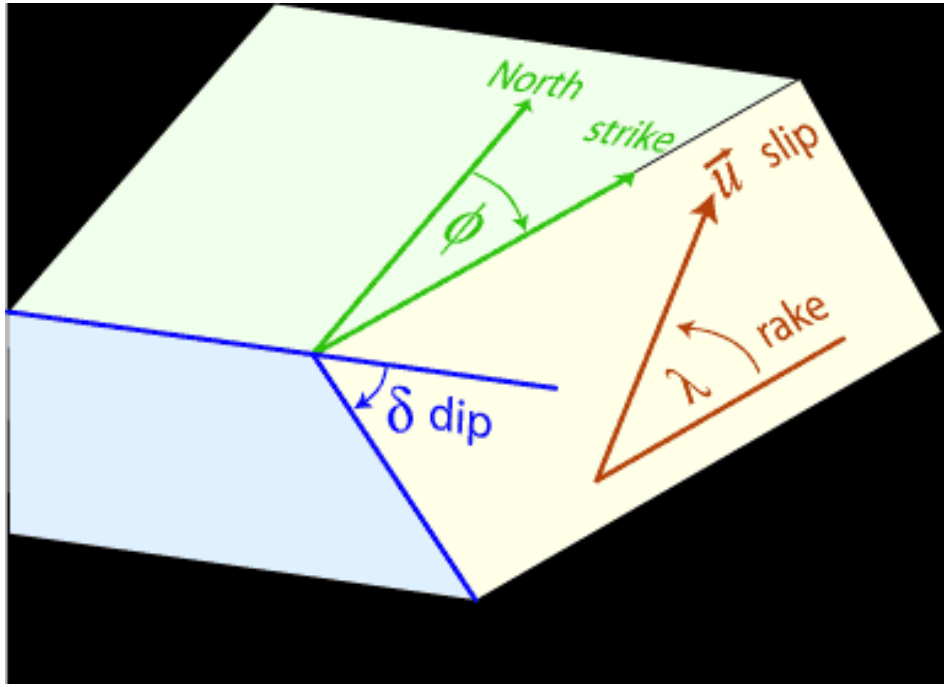

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$\Rightarrow$ Three axes: $\pm\mathbf{p} = \pm(\mathbf{n} - \mathbf{u})/\sqrt{2}$, $\pm\mathbf{t} = \pm(\mathbf{n} + \mathbf{u})/\sqrt{2}$, $\pm\mathbf{a} = \pm(\mathbf{p} \times \mathbf{t})$

Christchurch Earthquakes

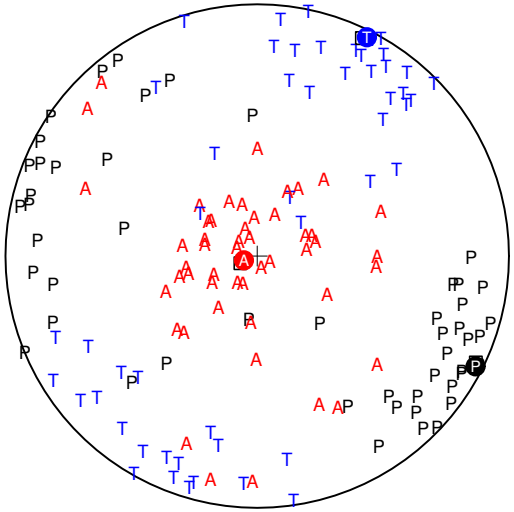
1904–2011

Christchurch Earthquakes

22 February 2011

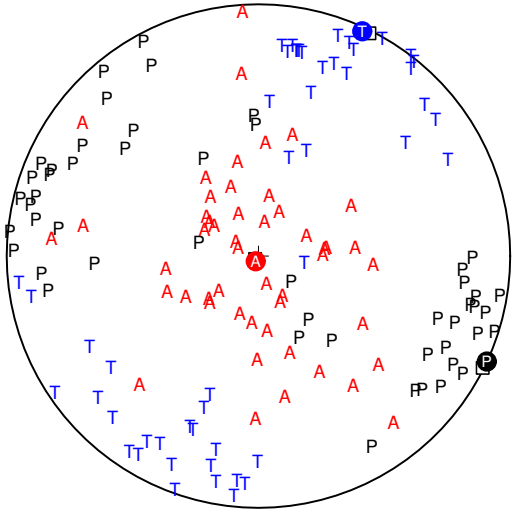
Example: 3D axes – oafs

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)

Example: 3D axes – oafs

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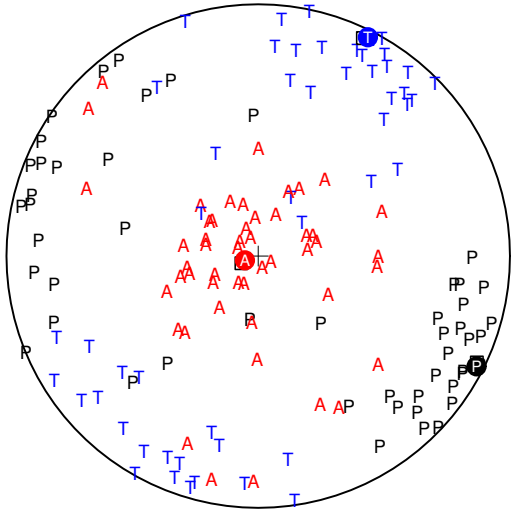

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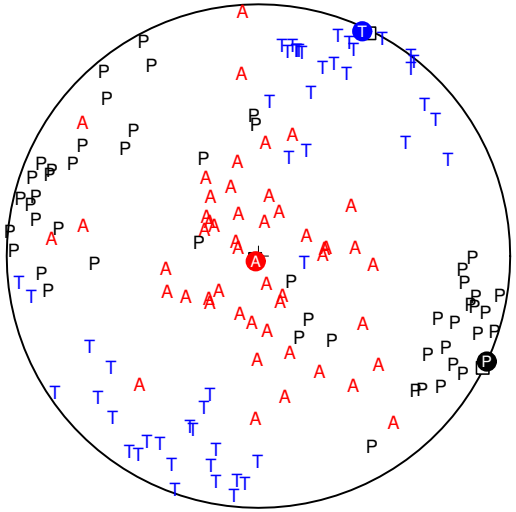

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  No: p-value 0.890

Ambiguous Rotations in 3D

Arnold, Jupp & Schaeben (2017) Statistics of Ambiguous Rotations J Multivariate Analysis, In press

Extending to more complex symmetries

Fluorite

Diopside

General Case in 3D

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**: (ϕ, θ, ψ)
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We have invariance under the action of a point symmetry group K

$$U \equiv UW_1 \equiv UW_2 \equiv \ldots \equiv UW_m \stackrel{def}{\equiv} [U]$$

We need **orientation representations** invariant under K: **symmetric frames**

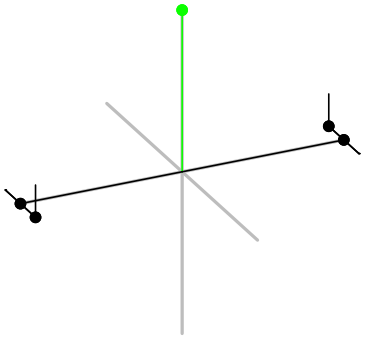
General Case in 3D

In crystallography, K is one of

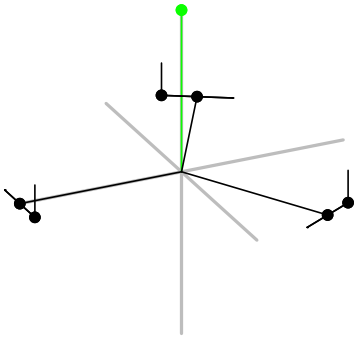
K		Examples	
C_r	cyclic	C_2	monoclinic crystals
D_r	dihedral	D_2	orthorhombic crystals
			(earthquake focal mechanisms)
		D_3	trigonal crystals
		D_4	tetragonal crystals
		D_6	hexagonal crystals
T	tetrahedral		
O	cubic		cubic crystals
Y	icosahedral		carboranes, viruses,
			quasi-crystals, liquid crystals
			radiolara

General Case in 3D

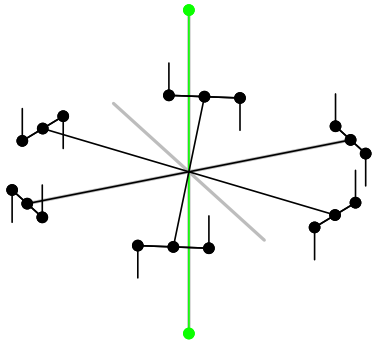
C_2=D_1



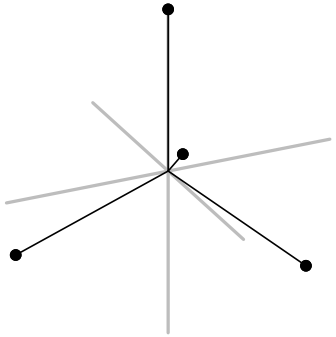
C_3



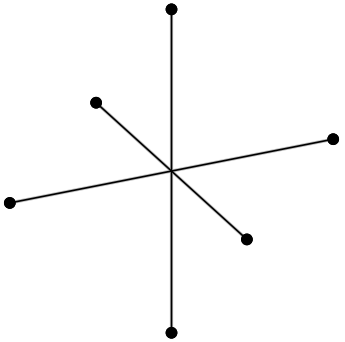
D_6



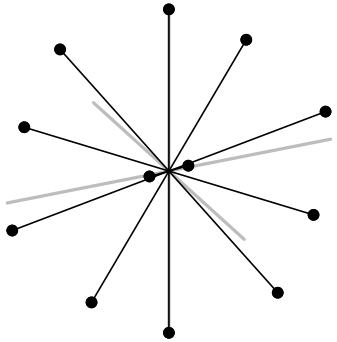
T



O



Y



Averaging approach

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

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

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Successful, but cumbersome

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Extend the single direction and single axis embedding approaches

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$$\begin{aligned} \mathbf{t} &= \mathbf{u} \\ \mathbf{t} &= \mathbf{u}\mathbf{u}^T - \tfrac{1}{2}\mathbf{I}_2 \quad = \quad \otimes^2\mathbf{u} - \tfrac{1}{2}\mathbf{I}_2 \end{aligned}$$

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$$\begin{aligned} (\otimes^r\mathbf{u})_{j_1 j_2 \ldots j_r} &= \prod_{k=1}^{r} u_{kj_k} \\ &= u_{1j_1}\, u_{2j_2} \ldots u_{rj_r} \end{aligned}$$

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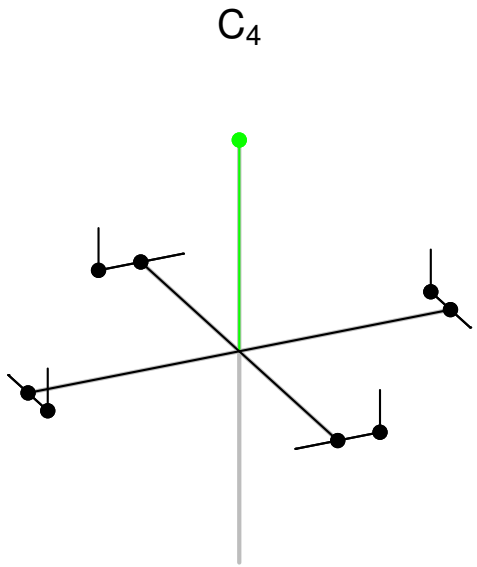
Gives the desired embedding.

Example: 4−fold axis C_4

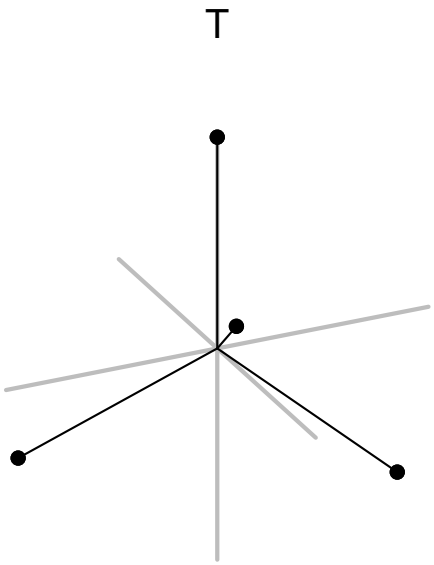
4 directions in a plane perpendicular to $\mathbf{u}_0$



Normal vector $\mathbf{u}_0$ and directions $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \mathbf{u}_4$

$$\mathbf{t} = (\mathbf{u}_0, \sum_{i=1}^{4} \otimes^4 \mathbf{u}_i - \tfrac{4}{5}\mathrm{symm}(\otimes^2 \mathbf{I}_3))$$

Example: Tetrahedral symmetry T



Directions $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \mathbf{u}_4$

$$\mathbf{t} = \sum_{i=1}^{4} \otimes^3 \mathbf{u}_i$$

Embedding

K	Frame	$t([U])$
C_1	$(\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3)$	$(\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3)$
C_2	$(\mathbf{u}_0, \pm\mathbf{u}_1)$	$(\mathbf{u}_0, \mathbf{u}_1\mathbf{u}_1^T - (1/3)I_3)$
C_r $(r \geq 3)$	$(\mathbf{u}_1, \ldots \mathbf{u}_r)$	$(\mathbf{u}_0, \sum_{i=1}^r \otimes^r \mathbf{u}_i - E[\cdot])$
D_2	$(\pm\mathbf{u}_1, \pm\mathbf{u}_2)$	$(\mathbf{u}_1\mathbf{u}_1^T - (1/3)I_3, \mathbf{u}_2\mathbf{u}_2^T - (1/3)I_3)$
D_r $(r \geq 3)$	$(\mathbf{u}_1, \ldots, \mathbf{u}_r)$	$\sum_{i=1}^r \otimes^r \mathbf{u}_i - E[\cdot]$
T	$(\mathbf{u}_1, \ldots, \mathbf{u}_4)$	$\sum_{i=1}^4 \otimes^3 \mathbf{u}_i$
O	$(\pm\mathbf{u}_1, \pm\mathbf{u}_2, \pm\mathbf{u}_3)$	$\sum_{i=1}^3 \otimes^4 \mathbf{u}_i - E[\cdot]$
Y	$(\pm\mathbf{u}_1, \ldots, \pm\mathbf{u}_6)$	$\sum_{i=1}^r \otimes^{10} \mathbf{u}_i - E[\cdot]$

Scalar Products

K	Frame	$\langle t([U]), t([V])\rangle$
C_1	$(\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3)$	$\mathbf{u}_1^T\mathbf{v}_1 + \mathbf{u}_2^T\mathbf{v}_2 + \mathbf{u}_3^T\mathbf{v}_3$
C_2	$(\mathbf{u}_0, \pm\mathbf{u}_1)$	$\mathbf{u}_0^T\mathbf{v}_0 + (\mathbf{u}_1^T\mathbf{v}_1)^2 - 1/3$
C_r $(r \geq 3)$	$(\mathbf{u}_1, \ldots \mathbf{u}_r)$	$\mathbf{u}_0^T\mathbf{v}_0 + \sum_{i=1}^r \sum_{j=1}^r (\mathbf{u}_i^T\mathbf{v}_j)^r - c_r$
D_2	$(\pm\mathbf{u}_1, \pm\mathbf{u}_2)$	$(\mathbf{u}_1^T\mathbf{v}_1)^2 + (\mathbf{u}_2^T\mathbf{v}_2)^2 - 2/3$
D_r $(r \geq 3)$	$(\mathbf{u}_1, \ldots, \mathbf{u}_r)$	$\sum_{i=1}^r \sum_{j=1}^r (\mathbf{u}_i^T\mathbf{v}_j)^r$
T	$(\mathbf{u}_1, \ldots, \mathbf{u}_4)$	$\sum_{i=1}^4 \sum_{j=1}^4 (\mathbf{u}_i^T\mathbf{v}_j)^3$
O	$(\pm\mathbf{u}_1, \pm\mathbf{u}_2, \pm\mathbf{u}_3)$	$\sum_{i=1}^3 \sum_{j=1}^3 (\mathbf{u}_i^T\mathbf{v}_j)^4 - 9/5$
Y	$(\pm\mathbf{u}_1, \ldots, \pm\mathbf{u}_6)$	$\sum_{i=1}^6 \sum_{j=1}^6 (\mathbf{u}_i^T\mathbf{v}_j)^{10} - 36/11$

Summary statistics

Normalisation

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Dispersion

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

Statistical tests

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Randomisation distribution reorients each sample element $[U_k]$ under the point group symmetry of $[M_0]$

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Two sample test:

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

Randomisation distribution permutes the sample labels of the observations $[U_{11}], \ldots, [U_{1n_1}], [U_{21}], \ldots, [U_{2n_2}]$

Probability Distributions

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$$f([U]|\kappa, [M]) = c(\kappa)^{-1} \exp\left\{\kappa\langle t([U]), t([M])\rangle\right\}$$

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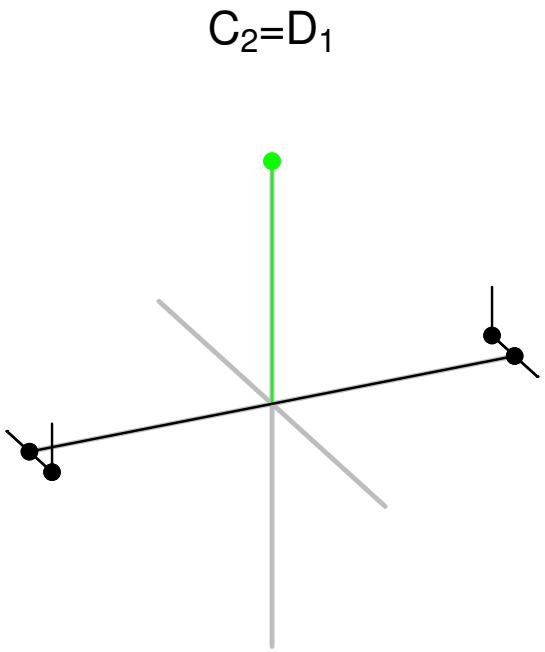
Generalisation of the von Mises and Fisher distributions.

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

wikipedia.org/Diopside

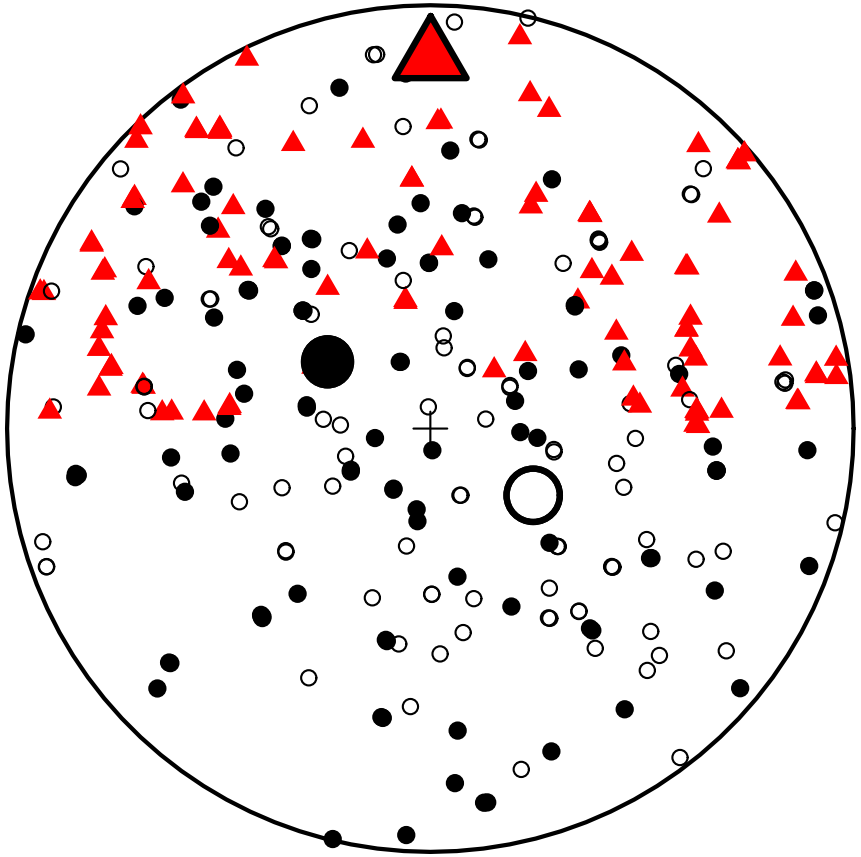


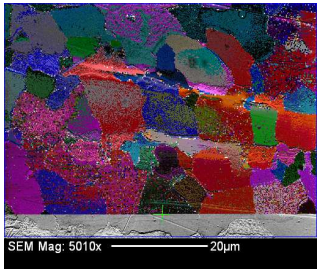
Symmetric under rotations of 180° about a single axis

Monoclinic

Diopside: C_2 symmetry

Observations from an Electron Backscattering Diffraction (EBSD) experiment





Orientations at 100 locations

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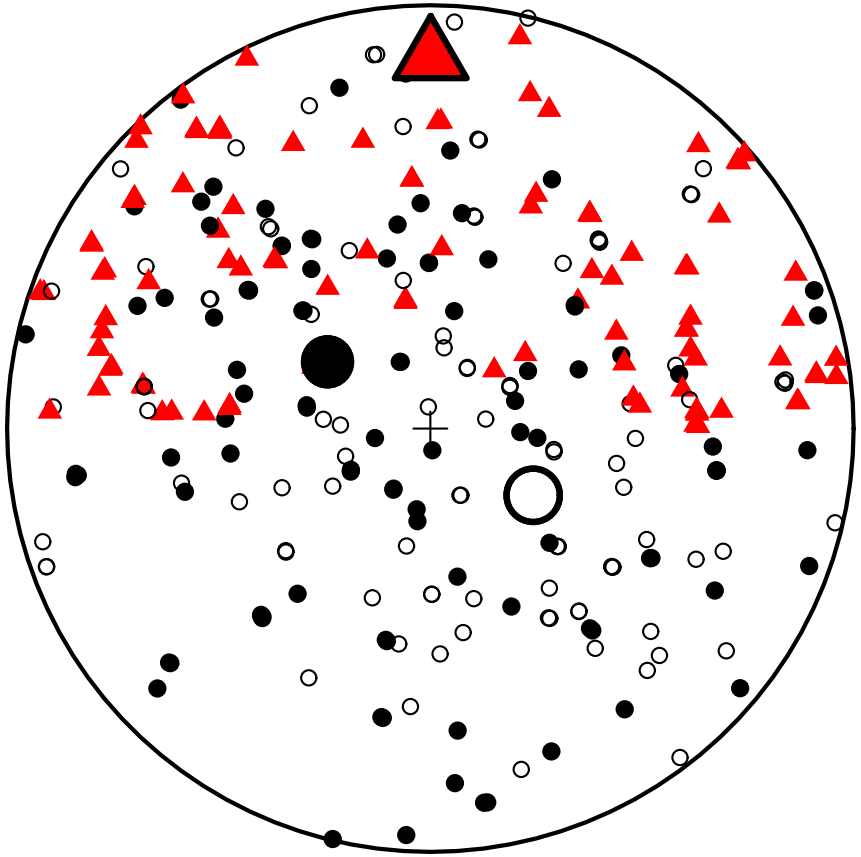

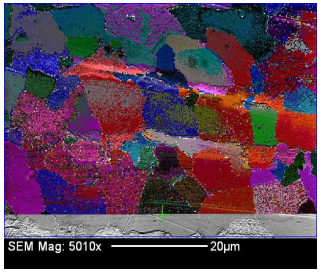

Orientations at 100 locations

$p-$value < 0.001 for a test of uniformity: not Uniform

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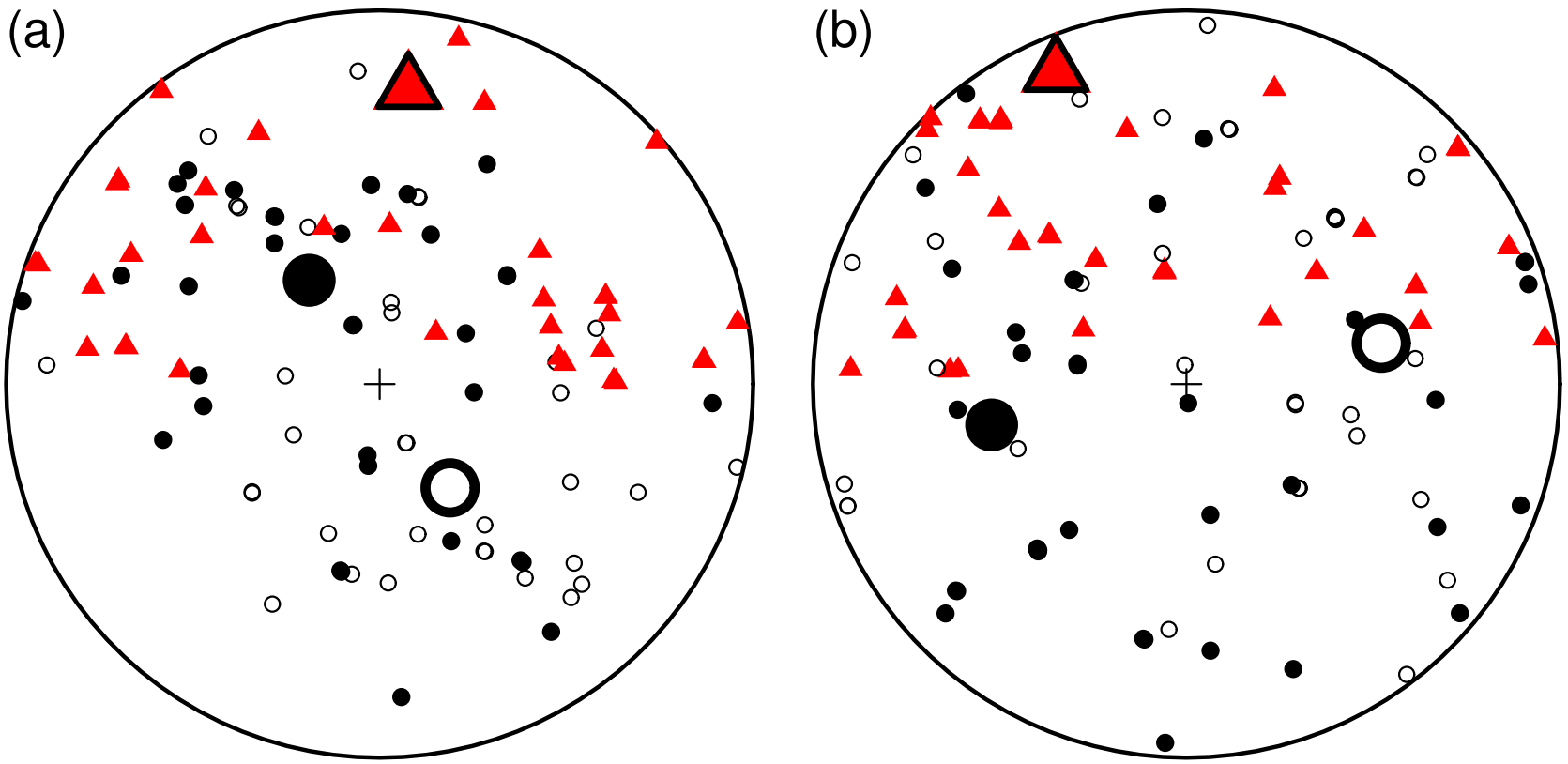
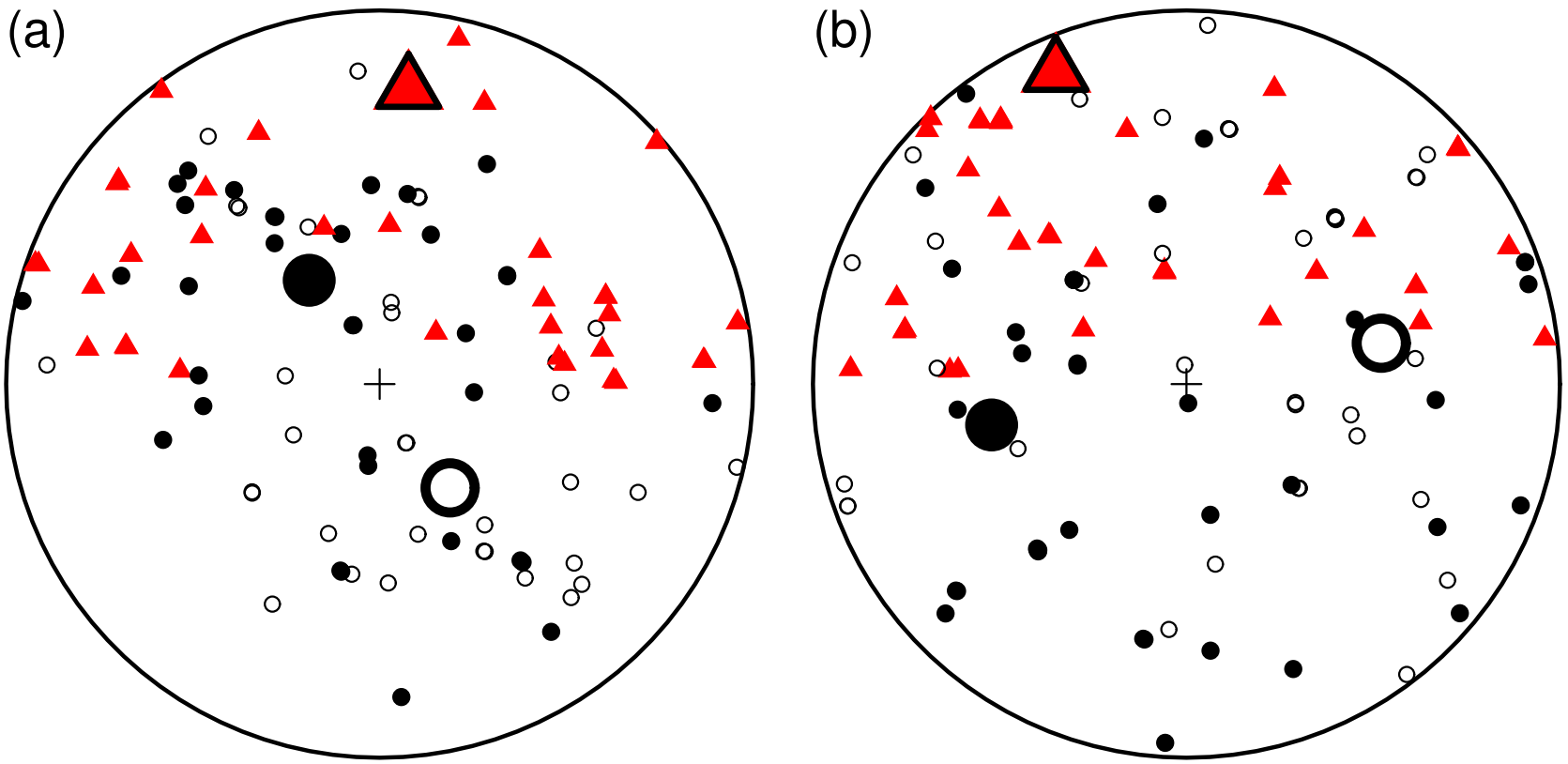


Orientations in two regions ($n_1 = 34$ and $n_2 = 37$).

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

The Future

- Misorientation and Regression relationships
- Phase transitions – solids undergoing a change of symmetry e.g. the Martensite transformation $O \to D_4$
- A whole lot of applications in seismology and crystallography

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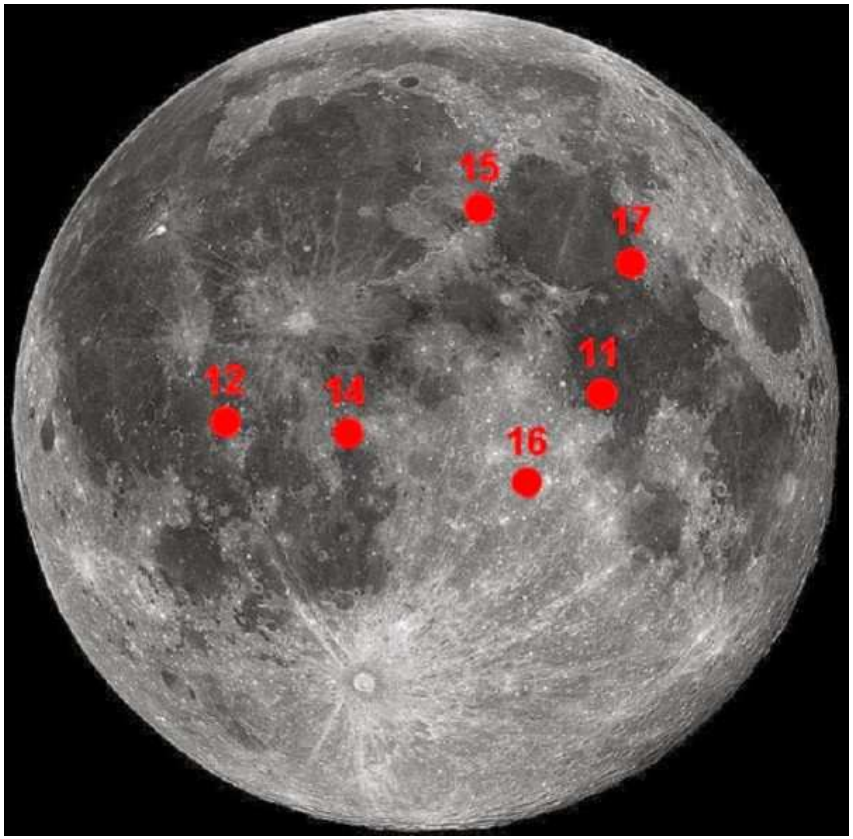
- and moon quakes ...

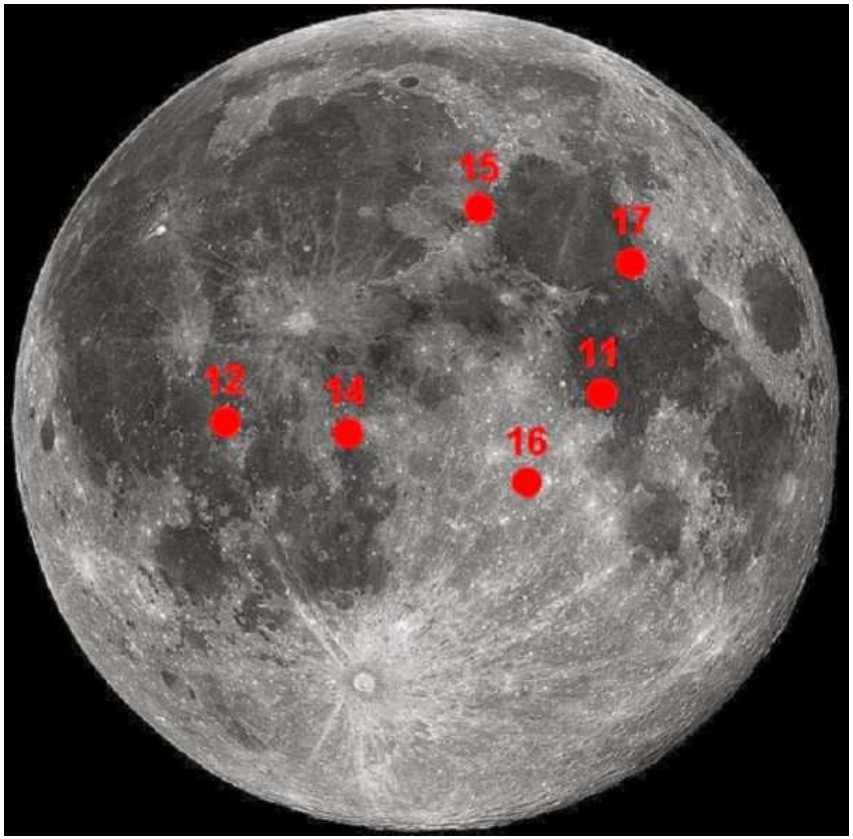
Moon Quakes



National Geographic

Seismometers deployed by Apollo missions
13000 moonquakes recorded between 1969-1977

Moon Quakes



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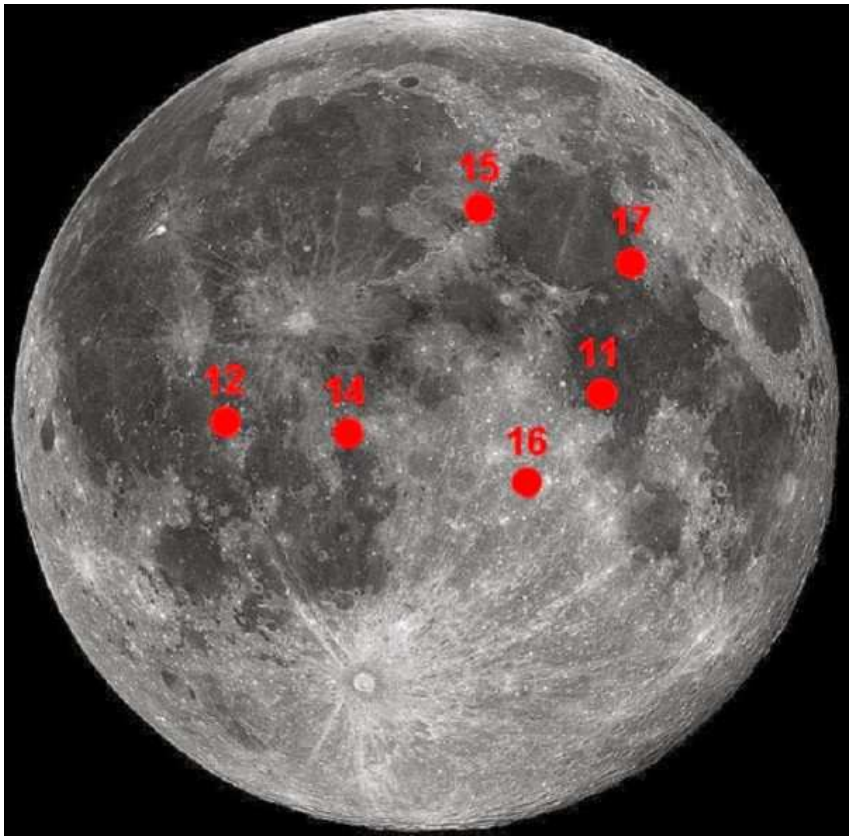

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Re-analyse using new methods

Thank You

Kia ora koutou