On the Central Limit Theorem for Fréchet Means: Theory and Applications

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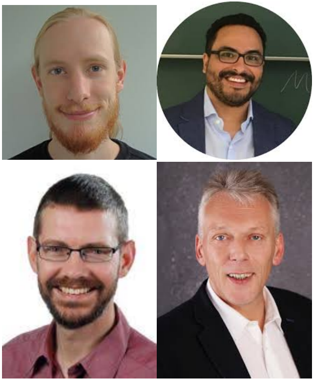
Outline

People Having Contributed to this Talk

- Benjamin Eltzner (Univ. of Göttingen)
- Fernando Galaz-García (Univ. of Karlsruhe)
- Thomas Hotz (Univ. of Ilmenau)
- Wilderich Tuschmann (Univ. of Karlsruhe)



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Here we do nonparametric asymptotics.

Euclidean Analog

Let i.i.d. $X, X_1, X_2, \ldots \in \mathbb{R}^D$ and $\bar{X}_n = \frac{X_1+\ldots+X_n}{n}$

Theorem (The Strong Law)

If $\mathbb{E}[X]$ exists then for $n \to \infty$

$$\bar{X}_n \to \mathbb{E}[X] \text{ a.s.}$$

Theorem (The Central Limit Theorem)

If $\mathbb{E}[\|X\|^2] < \infty$ then for $n \to \infty$

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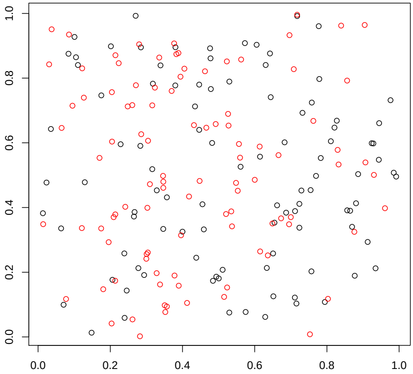
plugging in $\Sigma_n^X = \frac{1}{n-1}\sum_{j=1}^n (X_j - \bar{X}_n)(X_j - \bar{X}_n)^T$ for $\mathrm{cov}[X]$.

Test for Equality of Means

Two groups of random variables

$$X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} X \in \mathbb{R}^D \quad Y_1, \ldots, Y_m \overset{\text{i.i.d.}}{\sim} Y \in \mathbb{R}^D$$



Test H_0: $\mathbb{E}[X] = \mathbb{E}[Y]$

Hotelling Test for Equality of Means

- Under H_0 and either $\mathrm{cov}[X] = \mathrm{cov}[Y]$ or $n/m \to 1$,

$$T^2 := \frac{n+m-2}{\frac{1}{n}+\frac{1}{m}}(\bar{X}_n - \bar{Y}_m)^T (n\Sigma_n^X + m\Sigma_m^Y)^{-1}(\bar{X}_n - \bar{Y}_m)$$

$\stackrel{\mathcal{D}}{\to}$ explicitly known limit $(n, m \to \infty,\ 0 < \lim n/m < \infty)$

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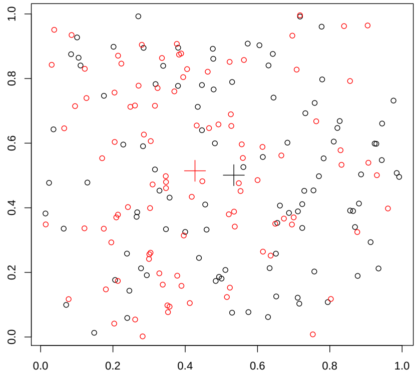
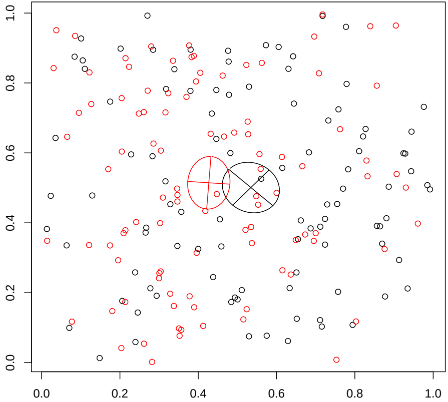


Reject H_0 with significance ($\alpha = 0.05$), not highly ($\alpha = 0.01$).

Principal Component Analysis (PCA)

Spectral decomposition $\mathrm{cov}[X] = \Gamma\Lambda\Gamma^T$.

- With eigenvectors $\Gamma = (\gamma_1, \ldots, \gamma_m) \in SO(m)$ to



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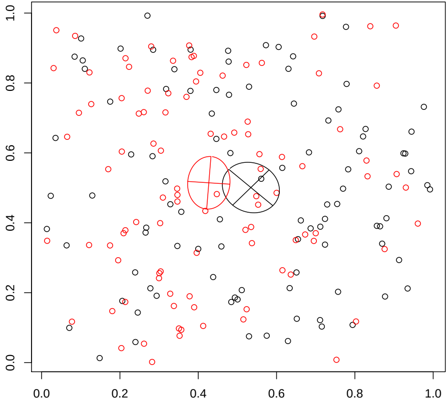

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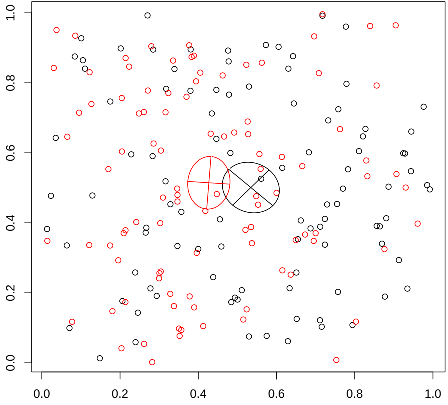

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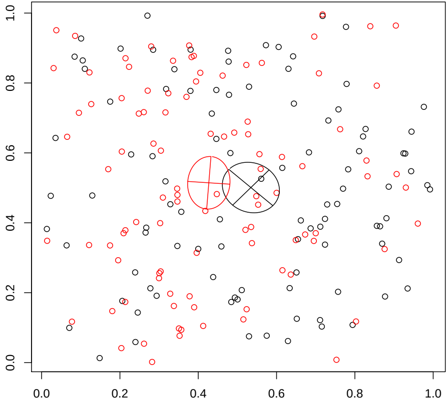
- giving main modes of variation $\to$ dimension reduction.
- Test for PCs γ_j ? Note, $\gamma_j \in \mathbb{S}^{m-1}$. Actually in $\mathbb{R}P^{m-1}$.



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Assumptions:

(A1) unique Fréchet mean $\mu \in \operatorname{argmin}_{p\in M} F(p)$ (difficult: Karcher (1977); Kendall (1990); Le (1998); Groisser (2005); Afsari (2011), not covered here),

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(A3) $\mu_n \stackrel{\mathbb{P}}{\to} \mu$ for a measurable selection of sample means

$$\mu_n \in \operatorname*{argmin}_{p \in M} F_n(p)$$

(guaranteed by Ziezold (1977); Bhattacharya and Patrangenaru (2003) under very general conditions).

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More assumptions:

(A4) $\exists G := \operatorname{cov}\left[\operatorname{grad}|_{x=\phi^{-1}(\mu)}\rho^2\big(X,\phi(x)\big)\right]$,

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Theorem (Bhattacharya and Patrangenaru (2005); Bhattacharya and Lin (2017))

Under Assumptions (A1) — (A6):

$$\sqrt{n}\left(\phi^{-1}(\mu_n) - \phi^{-1}(\mu)\right) \stackrel{\mathcal{D}}{\to} \mathcal{N}\left(0, H^{-1}GH^{-1}\right) .$$

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- Taylor expansion (with suitable $\widetilde{x}$ between 0 and x_0),

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- generalized weak law ($n \to \infty$ and $x_0 \to 0$)

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  (A6) $\Rightarrow$ $\mathbb{E}\left[\mathrm{Hess}|_{x=0}\rho(X,x)^2\right] > 0$

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  (A6) $\Rightarrow \mathbb{E}\left[\mathrm{Hess}|_{x=0}\rho(X,x)^2\right] > 0$
  $\Rightarrow$ BP-CLT.

(A2) Dissected: The Cut Locus

Corollary (2.3 from Bhattacharya and Lin (2017))

Instead of

(A2) *in a local chart* (U, ϕ), $\mu \in U \subseteq M$, $\phi^{-1}(U) = V \subseteq \mathbb{R}^D$,

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it suffices to require

(C) *there is a neighborhood* $W \subseteq M$ *of the cut locus* $\mathrm{Cut}(\mu)$ *of* μ *such that* $\mathbb{P}\{X \in W\} = 0$.

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Theorem (Le and Barden (2014))

$\mathbb{P}\{X \in \mathrm{Cut}(\mu)\} = 0$.

Stability of the Cut Locus

Let M be a complete, connected Riemannian D-manifold. We say that (the cut loci of) M is (are)

topologically stable if $\forall\, p \in M$, neighborhoods W of $\mathrm{Cut}(p)$, $\exists \delta = \delta_{W,p}$ such that $\mathrm{Cut}\big(B(p,\delta)\big) \subseteq W$;

geometrically stable if $\forall\, p \in M$, $\epsilon > 0$, $\exists \delta = \delta_{\epsilon,p}$ such that $\mathrm{Cut}\big(B(p,\delta)\big) \subseteq B\big(\mathrm{Cut}(p),\epsilon\big)$.

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Example (Eltzner et al. (2019))

1. The flat cylinder $M = \mathbb{S}^1 \times \mathbb{R}$ is metrically stable;
2. The Beltrami trumpet (pseudosphere) is not metrically stable.

What Else Can Go Wrong?

Consider (McKilliam et al. (2012), Hotz and H. 2015):

- $X_1, \dots, X_n \stackrel{\text{i.i.d.}}{\sim} X \in \mathbb{S}^1 = [-\pi, \pi]/\sim$
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Even $f(-\pi) = \frac{1}{2\pi}$ possible, $\lightning$(A6)

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- smeariness is measure dependent (!);
- smeariness, although only for nullset of the parameter space influences finite sample rates nearby.

Finite Sample Smeariness

Table 1.5 Orientations of 76 turtles after laying eggs (Gould's data cited by Stephens, 1969e)

Direction (in degrees) clockwise from north									
8	9	13	13	14	18	22	27	30	34
38	38	40	44	45	47	48	48	48	48
50	53	56	57	58	58	61	63	64	64
64	65	65	68	70	73	78	78	78	83
83	88	88	88	90	92	92	93	95	96
98	100	103	106	113	118	138	153	153	155
204	215	223	226	237	238	243	244	250	251
257	268	285	319	343	350				

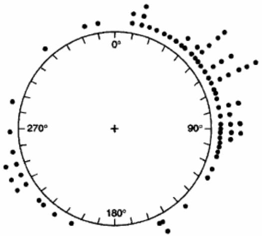
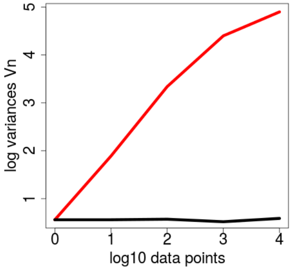


Figure 1.5 Circular plot of the turtle data of Table 1.5.

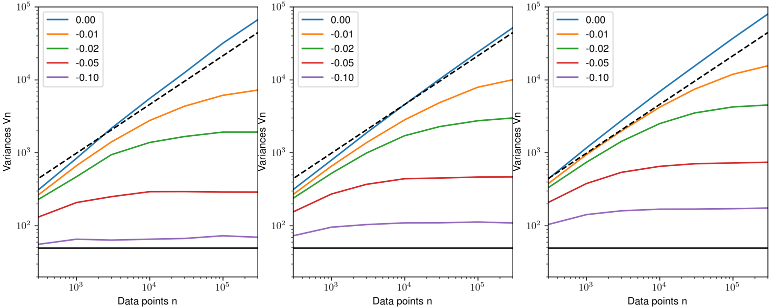
from Mardia and Jupp (2000).



Bootstrapped variance black = Euclidean in $[-\pi, \pi] \subset \mathbb{R}$, red = circular $\sim n^{2/3}$?

Two-Smeariness (Eltzner and H. 2018)

$r - 2 = 2$ smeary (dashed line)



On a sphere $\mathbb{S}^m$ with dimension (all derivatives $O(m^{-1/2})$)

$m = 2$ $m = 10$ $m = 100$

Separating Data from Descriptor Space

Generalized Fréchet Means (S.H 2011a,b):

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    - $\sqrt{n}\,(\phi(\hat{\gamma}) - \phi(\gamma)) \overset{\mathcal{D}}{\to} \mathcal{N}(0, \Sigma)$ by S.H. (2011a) if P is near γ a manifold with local chart ϕ, under regularity conditions adapted from (A1) – (A6).

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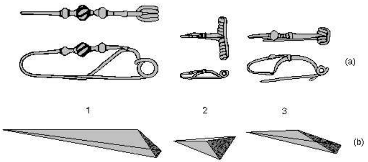
- Manifold stability for intrinsic means (singularities are repulsive for means) not for Procrustes means (!), cf. S.H. (2012). Open for GPCs.

Euclidean visualization of scores, o.g. projection onto GPCs (H. et al, 2010)

28 tetrahedral iron-age fibulae from a grave site in Münsingen, Switzerland (Hodson et al. (1966) and Small (1996)).



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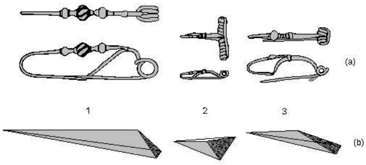

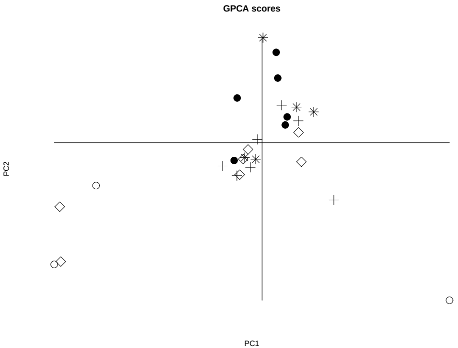

Groups from old to young: filled circles, stars, crosses, diamonds and circles.

PC2: Shape change; PC1: Stronger effect, diversification.

Two-Sample Descriptor Test

$$
\begin{array}{llcccll}
\text{Data:} & \underbrace{X_1,\ldots,X_n} & , & \underbrace{Y_1,\ldots,Y_m} & \in & Q \\
& \downarrow & & \downarrow & & \\
\text{Descriptors:} & p^X & & p^Y & \in & P \\
& \downarrow & \phi^{-1} & \downarrow & & \\
\text{Coordinates:} & Z^X & & Z^Y & \in & \mathbb{R}^D
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Under $H_0 : \mu^X = \mu^Y$,

$$\frac{nm}{n+m}(m+n-2)(Z^X - Z^Y)^T\left(n\,\widehat{\mathrm{cov}}[Z^X_{1\dots n}] + m\,\widehat{\mathrm{cov}}[Z^Y_{1\dots m}]\right)^{-1} \cdot (Z^X - Z^Y) \sim \mathcal{T}^2(k, n+m-2)$$

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But how to access $\widehat{\mathrm{cov}}[Z^X_{1\ldots n}]$ and $\widehat{\mathrm{cov}}[Z^Y_{1\ldots m}]$?

Bootstrapping

For $b = 1, \ldots, B$, resample:

- $X^*_{1,b}, \ldots, X^*_{n,b}$ from $X_1, \ldots, X_n$ gives $\widehat{\text{cov}}[Z^X_{1\ldots n}]$

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Again, for $b = 1, \ldots, B'$, resample:

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Then, the test

reject H_0 if $(Z^X - Z^Y)^T A^{-1} (Z^X - Z^Y) > c^*_{1-\alpha}$

has the asymptotic level α.

Improved Power

Recall, for $b = 1, \dots, B'$, resample:

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To improve the power, resample

- $X^{*,b}$ from $X_1, \dots, X_n$ and $Y^{*,b}$ from $Y_1, \dots, Y_m$

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Note:

- Euclidean PCA ist canonically nested.
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- or even small spheres,
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How about asymptotics of such nested random subspaces?

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is BNFD from P_m to P_j from the space

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$$T_{m,j} = \left\{ f = \{p^l\}_{l=m}^j : p^{l-1} \in S_{p^l}, l = j+1,\ldots,m \right\} ,$$

with projection along each descriptor

$$\pi_f = \pi_{p^{j+1},p^j} \circ \ldots \circ \pi_{p^m,p^{m-1}} : p^m \to p^j$$

Backward Nested Families of Descriptors

For another BNFD $f' = \{p'^l\}_{l=m}^j \in T_{m,j}$ set

$$d^j(f, f') = \sqrt{\sum_{l=m}^{j} d_j(p^l, p'^l)^2}\,.$$

Backward Nested Fréchet Means

Random elements $X_1, \dots, X_n \overset{\text{i.i.d.}}{\sim} X$ on a data space Q admitting BNFDs give rise to backward nested population and sample means (BN means) recursively defined via $f^m = \{Q\} = f_n^m$, i.e. $p^m = Q = p_n^m$ and for $j = m, \dots, 1$,

$$p^{j-1} \in \operatorname*{argmin}_{s \in S_{p^j}} \mathbb{E}[\rho_{p^j}(\pi_{f^j} \circ X, s)^2], \qquad f^{j-1} = (p^l)_{l=m}^{j-1}$$

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If all of the population minimizers are unique, we speak of unique BN means.

Strong Law

Theorem (S.H. and Eltzner (2018))

If the BN population means $f = (p^m, \dots, p^j)$ are unique and $f_n = (p_n^m, \dots, p_n^j)$ is a measurable selection of BN sample means then under "reasonable" assumptions

$$f_n \to f \text{ a.s.}$$

i.e. $\exists \Omega' \subseteq \Omega$ *m'ble with* $\mathbb{P}(\Omega') = 1$ *such that* $\forall \epsilon > 0$ *and* $\omega \in \Omega'$, $\exists N(\epsilon, \omega) \in \mathbb{N}$

$$d(f_n, f) < \epsilon \quad \forall n \geq N(\epsilon, \omega)\,.$$

The Joint CLT [S.H. and Eltzner (2018)]

With local chart $\eta \stackrel{\psi^{-1}}{\mapsto} f^{j-1} \mapsto \rho_{p^j}(\pi_{f^j} \circ X, p^{j-1})^2 := \tau^j(\eta, X)$:

$$\sqrt{n} H_\psi \big(\psi(f_n^{j-1}) - \psi({f'}^{j-1})\big) \quad \to \quad \mathcal{N}(0, B_\psi)\,.$$

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Idea of proof:

$$0 \quad = \quad \operatorname{grad}_\eta \sum_{k=1}^{n} \tau^j(\eta_n, X_k) + \sum_{l=j+1}^{m} \lambda_n^l \operatorname{grad}_\eta \sum_{k=1}^{n} \tau^l(\eta_n, X_k)$$

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$$\begin{aligned} 0 \quad = \quad & \frac{1}{\sqrt{n}} \operatorname{grad}_\eta \sum_{k=1}^{n} \tau^j(\eta', X_k) + \frac{1}{\sqrt{n}} \sum_{l=j+1}^{m} \lambda_n^l \operatorname{grad}_\eta \sum_{k=1}^{n} \tau^l(\eta', X_k) \\ & + \frac{1}{n} \left(\operatorname{Hess}_\eta \sum_{k=1}^{n} \tau^j(\widetilde{\eta}_n, X_k) + \sum_{l=j+1}^{m} \lambda_n^l \operatorname{Hess}_\eta \sum_{k=1}^{n} \tau^l(\widetilde{\eta}_n, X_k) \right) \\ & \cdot \sqrt{n}(\eta' - \eta_n) \end{aligned}$$

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The Joint Central Limit Theorem

With local chart $\eta \stackrel{\psi^{-1}}{\mapsto} f^{j-1} \mapsto \rho_{p^j}(\pi_{f^j} \circ X, p^{j-1})^2 := \tau^j(\eta, X)$:

$$\sqrt{n} H_\psi \left(\psi(f_n^{j-1}) - \psi(f'^{j-1})\right) \quad \to \quad \mathcal{N}(0, B_\psi)$$

and typical regularity conditions, where

$$H_\psi \quad = \quad \mathbb{E}\left[\mathrm{Hess}_\eta \tau^j(\eta', X) + \sum_{l=j+1}^{m} \lambda^l \, \mathrm{Hess}_\eta \tau^l(\eta', X)\right] \text{ and}$$

$$B_\psi \quad = \quad \mathrm{cov}\left[\mathrm{grad}_\eta \tau^j(\eta', X) + \sum_{l=j+1}^{m} \lambda^l \, \mathrm{grad}_\eta \tau^l(\eta', X)\right] .$$

and $\lambda_{j+1}, \dots \lambda_m \in \mathbb{R}$ are suitable such that

$$\mathrm{grad}_\eta \, \mathbb{E}\left[\tau^j(\eta, X)\right] + \sum_{l=j+1}^{m} \lambda^l \, \mathrm{grad}_\eta \, \mathbb{E}\left[\tau^l(\eta, X)\right]$$

vanishes at $\eta = \eta'$.

Factoring Charts

If the following diagram commutes we say the chart factors

$$\begin{array}{ccccccccc} T_{m,j-1} & \ni & f^{j-1} & = & (f^j, p^{j-1}) & \stackrel{\psi}{\to} & \eta & = & (\theta, \xi) \\ & & & & \downarrow \pi^{P_{j-1}} & & & & \downarrow \pi^{\mathbb{R}^{\dim(\theta)}} \\ P_{j-1} & \ni & & & p^{j-1} & \stackrel{\phi}{\to} & & & \theta \end{array}$$

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Then

$$\begin{array}{rcl} \eta = (\theta, \xi) \stackrel{\psi^{-1}}{\mapsto} f^{j-1} & \mapsto & \rho_{p^j}(\pi_{f^j} \circ X, p^{j-1})^2 \\ & = & \rho_{\pi^{P_j} \circ \psi_2^{-1}(\xi)} \left(\pi_{\psi_2^{-1}(\xi)} \circ X, \psi_1^{-1}(\theta) \right)^2 \\ & =: & \tau^j(\theta, \xi, X)\,, \end{array}$$

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&=: \quad \tau^j(\theta,\xi,X)\,,
\end{aligned}
$$

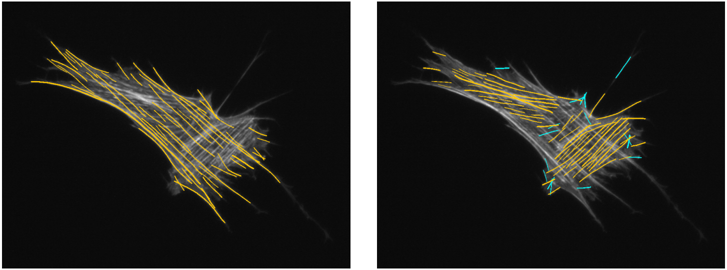
Taylor expansion at $\eta' = (\theta',\xi')$ gives a joint Gaussian CLT,

$$
\sqrt{n}H_\psi(\eta_n - \eta') = \sqrt{n}H_\psi \begin{pmatrix} \theta_n - \theta' \\ \xi_n - \xi' \end{pmatrix} \quad \to \quad \mathcal{N}(0, B_\psi)
$$

and projection to the θ coordinate preserves Gaussianity.

Application: Stem Cell Diversification (H. and Eltzner, 2018)

Actin-myosin structure of an adult stem cell after 16 hours.



Left: $m_1 =$ main orienation field filament pixels.
Right: $m_2 =$ smaller orienation field filament pixels,
Cyan: $m_3 =$ “rogue” filament pixels.

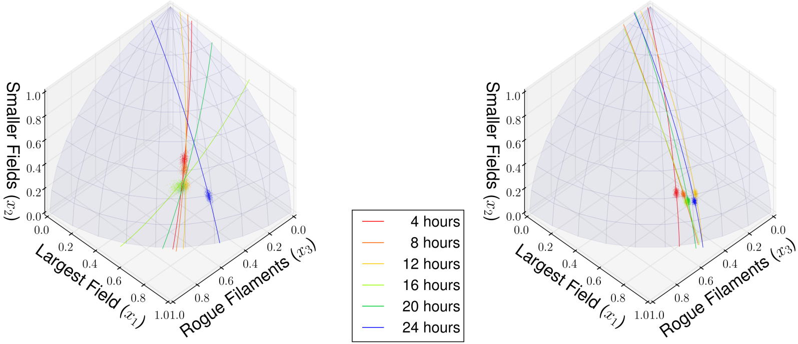
Composite data $m = m_1 + m_2 + m_3$ mapped to a sphere:

$$\left(\sqrt{\frac{m_1}{m}}, \sqrt{\frac{m_2}{m}}, \sqrt{\frac{m_3}{m}}\right)$$

Applying the Bootstrap Two-Sample Test

	nested mean		jointly great circle and nested mean	
Time	≤ 1 kPa	≥ 10 kPa	≤ 1 kPa	≥ 10 kPa
4h–8h	0.120	$< 10^{-3}$	0.308	$< 10^{-3}$
8h–12h	$< 10^{-3}$	$< 10^{-3}$	0.024	$< 10^{-3}$
12h–16h	0.126	$< 10^{-3}$	0.008	$< 10^{-3}$
16h–20h	0.468	0.626	0.494	0.462
20h–24h	$< 10^{-3}$	$< 10^{-3}$	$< 10^{-3}$	0.014

Visualization



Left: $\leq$ 1 kPa.

Right: $\geq$ 10 kPa

Wrap up and Outlook

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