Tutorial:
Geometric central limit theorems on singular spaces

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and Department of Statistical Science

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joint with Jonathan Mattingly (Duke)
Do Tran (Deutsche Bank (was: Göttingen))

`http://arxiv.org/abs/2311.09455`
`09454`
`09453`
`09451`

Interactions of Statistics and Geometry (ISAG) II

National University of Singapore

14 – 16 October 2024

Syllabus

1. overview (today)
2. geometry and measure on CAT(κ) spaces [`arXiv:...3, `§1-§2]
    - CAT(κ) spaces
    - angles and angular pairing
    - tangent cones
    - localized measures
    - escape and fluctuating cones
    - hulls
3. shadows and tangential collapse [`arXiv:...1`]
    - shadows [`arXiv:...3, `§3-§4]
    - radial transport
    - limit log
    - tangential collapse
4. convergence to Gaussian objects [`arXiv:...4`], [`arXiv:...5, `§6.1]
    - random tangent fields and their CLT
    - stratified Gaussians
5. central limit theorems via escape [`arXiv:...5, `§4-§6]
    - escape vectors
    - continuous mapping theorem

Outline

Linear Central Limit Theorem

Input

- vector space $\mathbb{R}^d$
- independent random variables $X_1, X_2, \ldots$
- distributed according to μ

Compare empirical mean $\bar{\mu}_n = \frac{1}{n}\sum_{i=1}^{n} X_i$

to population mean $\bar{\mu} = \int x\,\mu(dx)$

Law of Large Numbers (LLN): $\bar{\mu}_n \xrightarrow{n\to\infty} \bar{\mu}$ almost surely.

Central Limit Theorem (CLT): $\sqrt{n}\,(\bar{\mu}_n - \bar{\mu}) \xrightarrow{n\to\infty} N(0,\Sigma)$ in distribution, for random variable $N(0,\Sigma)$

- Gaussian
- centered at 0
- same covariance Σ as μ.

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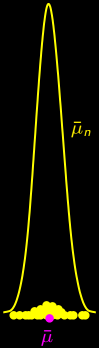

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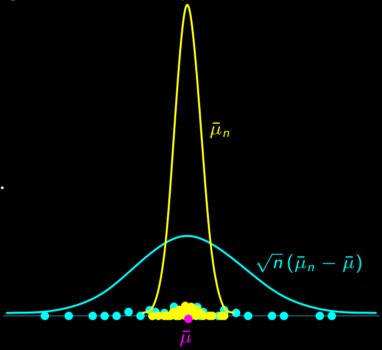

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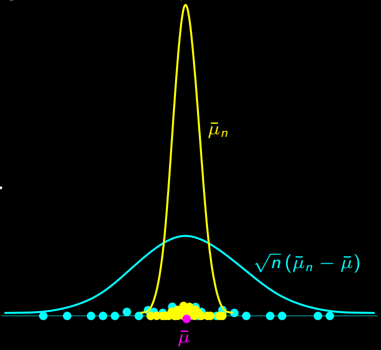

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Nonlinear data

Initial rationale: "Big Data" often sampled from nonlinear spaces.

Examples

- angles: points on a circle
  - wind direction
  - knee or elbow motion
- directions: points on a sphere
  - wrist or ankle motion
  - surface unit normal (e.g., medical imaging)
- shapes: points on a quotient of $d \times n$ matrices
- diffusion tensors: positive semidefinite matrices
- trees, e.g.:
  - phylogenetic tree space [Billera–Holmes–Vogtmann 2001],
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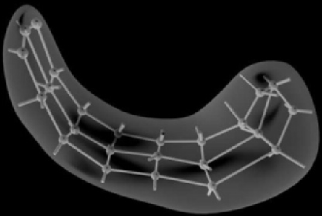
Hippocampus surfaces

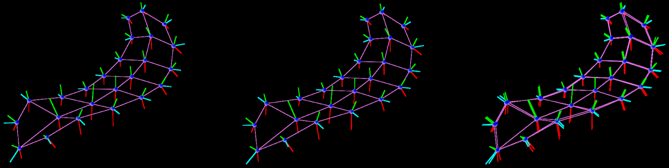
Skeletal representation



Fletcher, Pizer, and Joshi 2006

Dataset

276 skeleta of hippocampus surfaces:



courtesy S. Pizer

each datapoint $\in \mathbb{R}_+^{67} \times S^{68} \times (S^2)^{66}$, dim 267 in $\mathbb{R}^{334}$.

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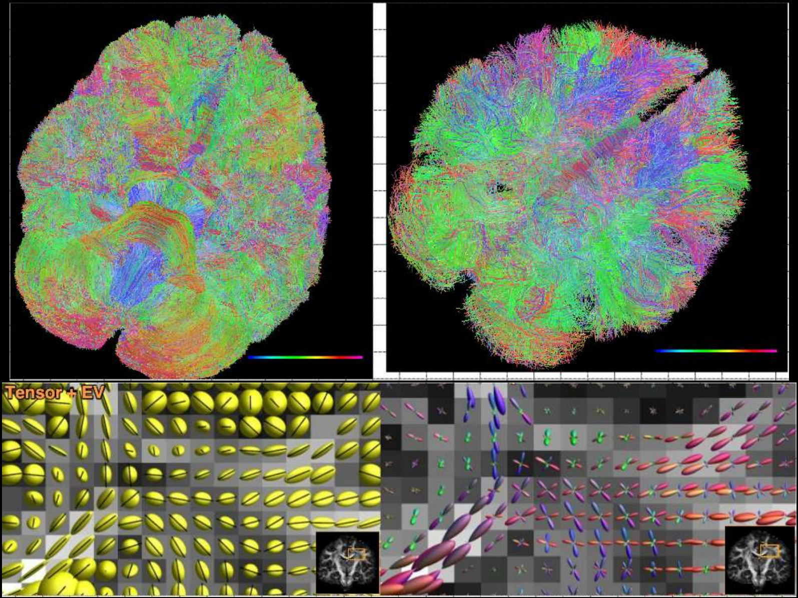
Streamlines from Diffusion Tensor Imaging



courtesy Zhengwu Zhang

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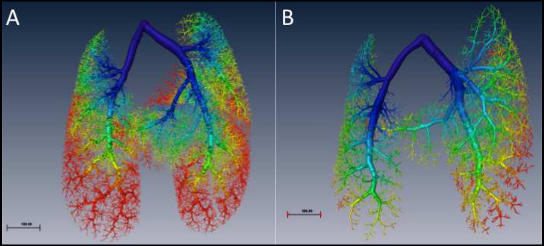
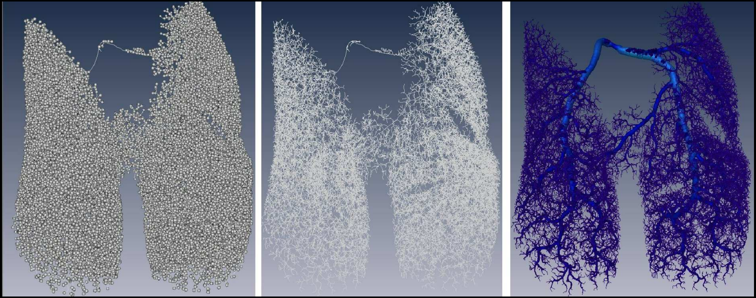
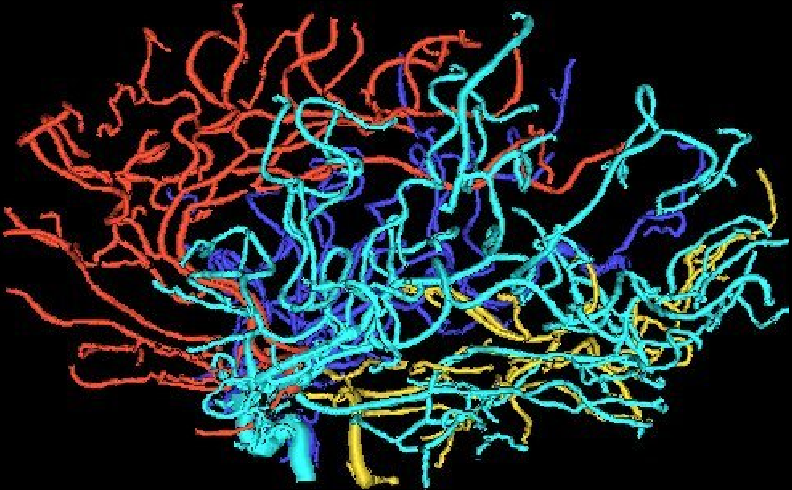
Lung vessels (CDH study)





courtesy Sean McLean

Brain arteries



[Bullitt and Aylward, 2002]

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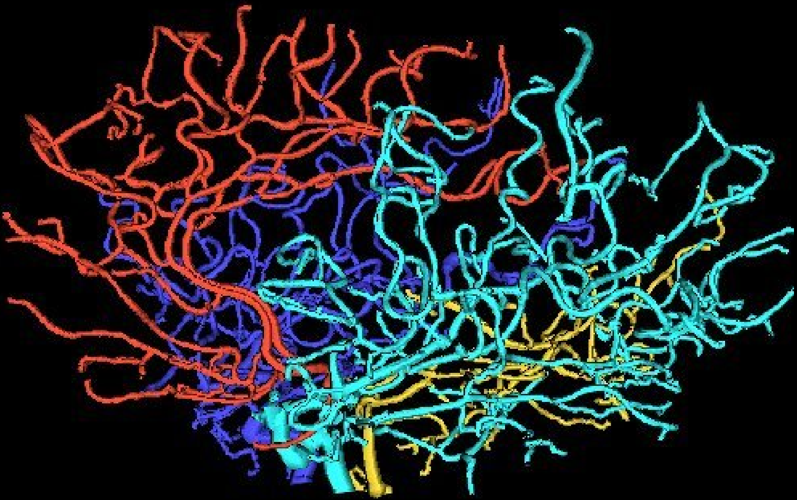

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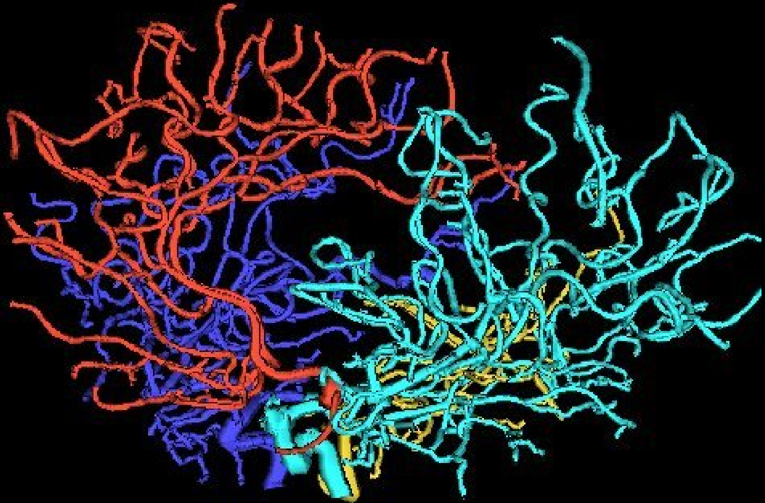

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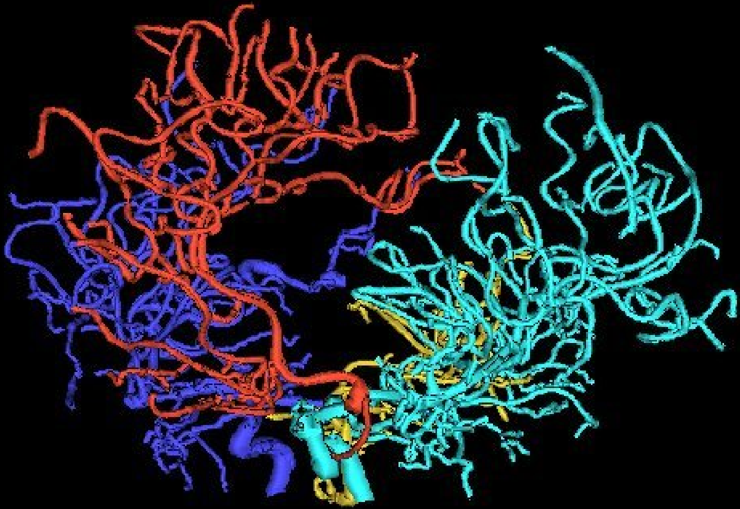

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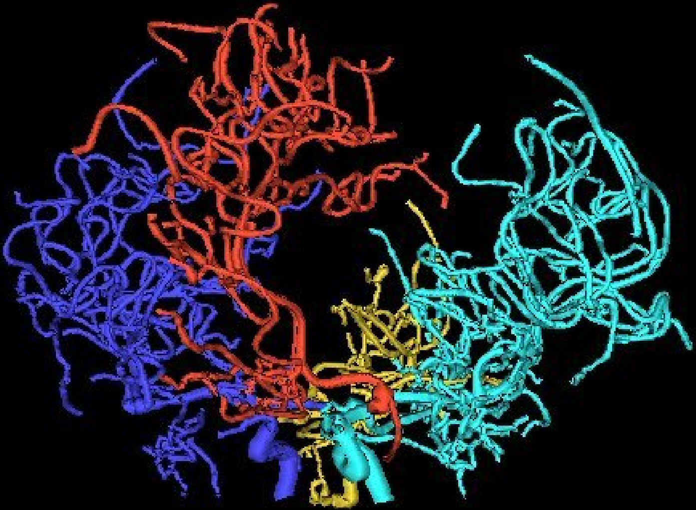

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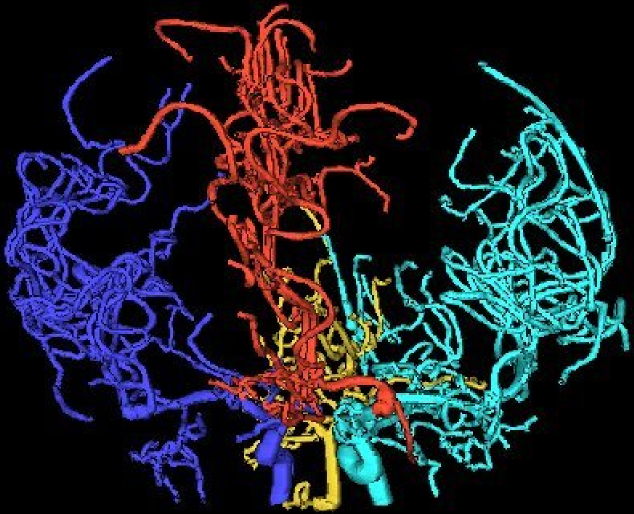

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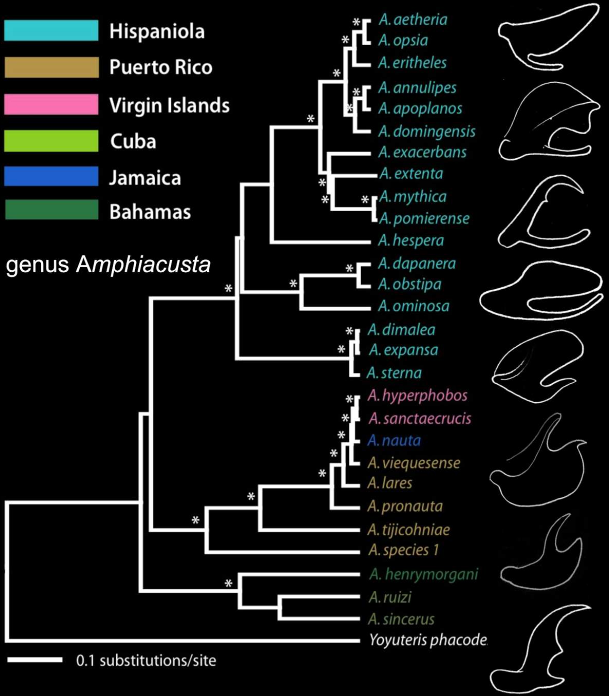
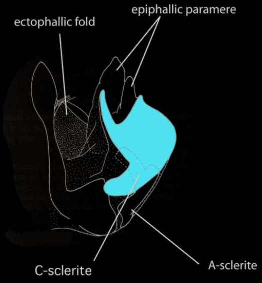
genus *Amphiacusta*





From Oneal, Otte & Knowles, 2010

Drawings by Dan Otte

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Phylogenetic trees

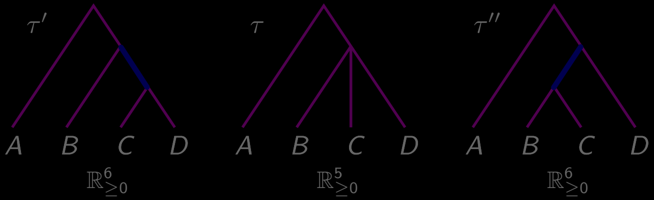
Def. A phylogenetic tree is a rooted metric tree with n labeled leaves

Distributions of trees come from

- tree reconstruction algorithms: LLN ⇒ sample mean → true tree
- evolutionary biology: “gene trees” from a “species tree”
- medical imaging: blood vessels, lungs, nerve cells, ...

Sample space $\mathcal{T}_n = \{\text{phylogenetic } n\text{-trees}\}$ is a union of polyhedral cones (orthants) [Billera–Holmes–Vogtmann 2001]

- $\mathcal{O}_\tau$ = trees with fixed topology $\tau \leftrightarrow \{\text{lists of edge lengths for } \tau\}$
  $= \text{orthant } \mathbb{R}^{E(\tau)}_{\geq 0}$



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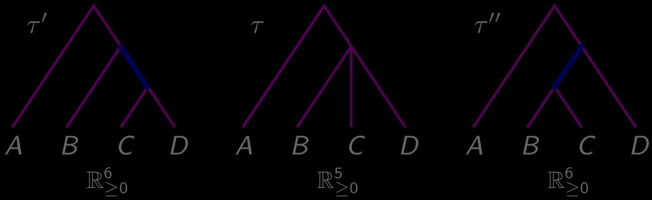

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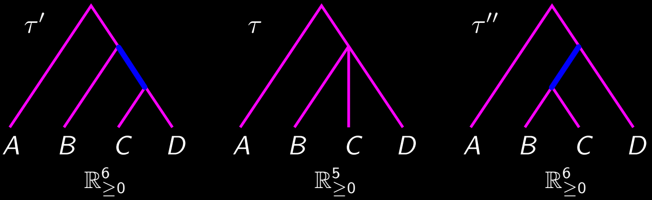

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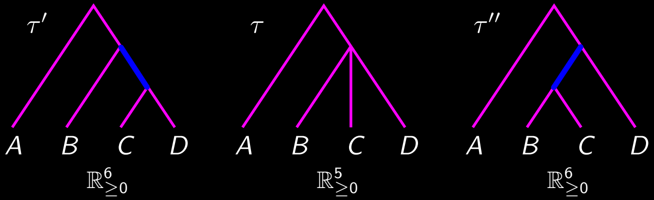

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Nonlinear data

Initial rationale: "Big Data" often sampled from nonlinear spaces.

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- angles: points on a circle
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- variance, PCA
- Law of Large Numbers (LLN), confidence intervals
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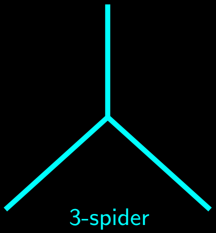

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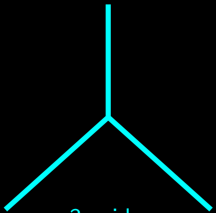

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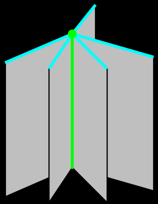

open book

$\mathbb{R}^d \times$ spider

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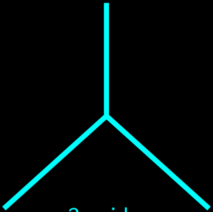

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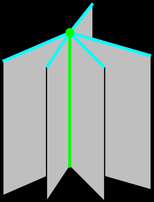

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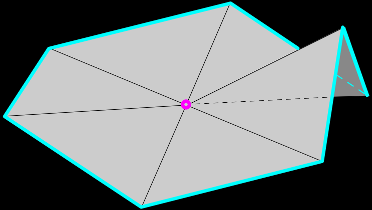

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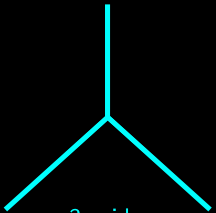

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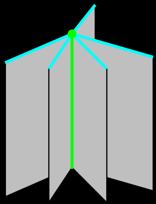

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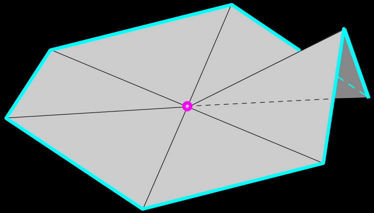

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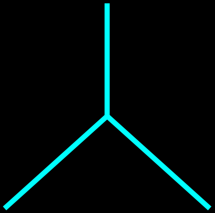
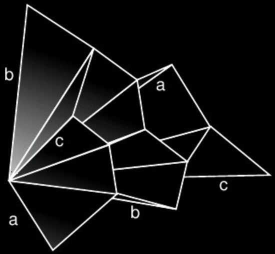


$\mathcal{T}_3$



$\mathcal{T}_4$

from [BHV 2001]

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Fréchet means

Sample space: Riemannian manifold M

What fails

1. sum or average of
   - $+$ points in M
   - $+$ random variables in M
2. “Gaussian” on M

Workarounds

1. **Def.** Probability distribution μ on any metric space M has Fréchet function

$$F_\mu(y) = \frac{1}{2}\int_M \underset{\substack{\uparrow\\ \text{square}\\ \text{distance}}}{d(x,y)^2}\,\underset{\substack{\uparrow\\ \text{measure}\\ \text{induced}\\ \text{by } \mu}}{\mu(dx)}$$

   and Fréchet mean $\bar{\mu} = \underset{y\in M}{\operatorname{argmin}}\, F_\mu(y)$.
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   - empirical mean $\bar{\mu}_n$ from empirical measure $\mu_n = \frac{1}{n}(\delta_{X_1} + \cdots + \delta_{X_n})$
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- as (moving) empirical mean converges
- to (fixed) population mean

⇒ limit is a random tangent vector
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Def. The logarithm map is

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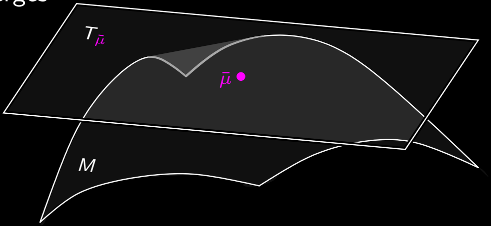

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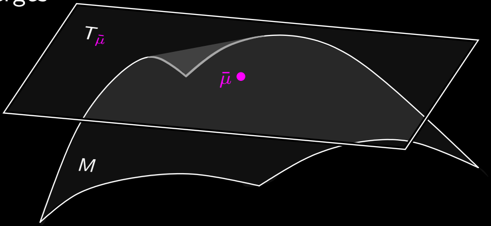

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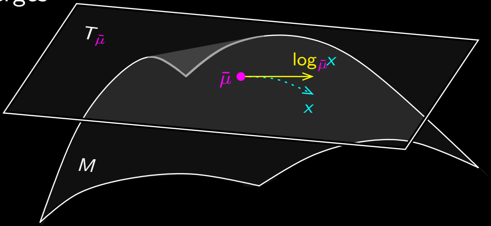

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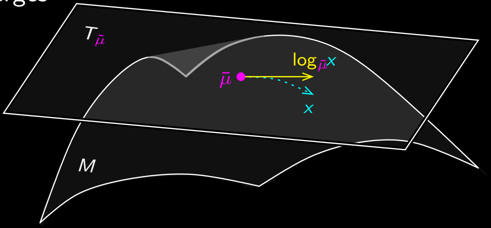

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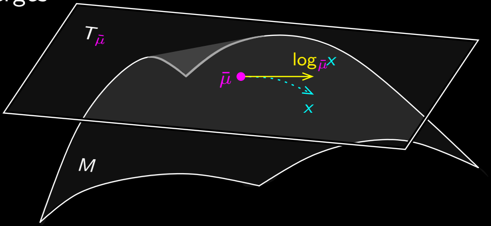

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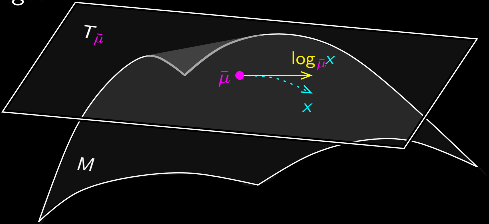

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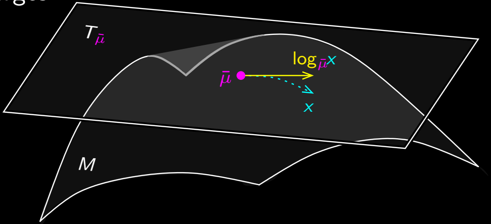

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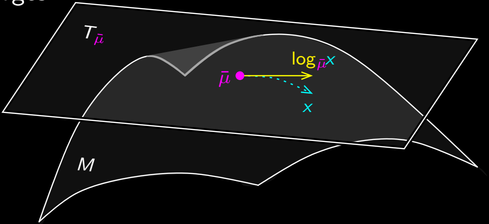
$\Rightarrow$ limit is a random tangent vector in tangent space $T_{\bar{\mu}}$



Def. The logarithm map is

$$\begin{aligned} \log_{\bar{\mu}} : M &\to T_{\bar{\mu}} M \\ x &\mapsto d(\bar{\mu}, x)\,V, \end{aligned}$$

where V = unit tangent to geodesic from $\bar{\mu}$ to x.

Back to linear setting

- μ on $M \rightsquigarrow \nu$ on $T_{\bar{\mu}} M$ for $\nu = \mu \circ \log_{\bar{\mu}}{}^{-1}$ Def. pushforward of μ to $T_{\bar{\mu}} M$
- linear CLT: $\sqrt{n}\,\bar{\nu}_n \xrightarrow{n\to\infty} N(0,\Sigma)$ in distribution

Question: Is this the manifold CLT? Not quite. . . .

Smooth manifold CLT

Def. The distortion map

$$\mathcal{H} : T_{\bar\mu}M \to T_{\bar\mu}M$$

is the inverse of the Hessian at $\bar\mu$ of the Fréchet function F_μ:

$$\mathcal{H} = (\nabla\nabla_{\bar\mu} F_\mu)^{-1}.$$

- $(M, \mu) \rightsquigarrow (T_{\bar\mu}M, \nu)$ forgets curvature of M
- e.g., rapidly spreading geodesics exiting $\bar\mu$ tug covariance of μ toward $\bar\mu$ as compared with ν around $0 \in T_{\bar\mu}M$

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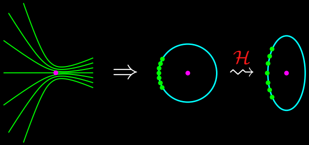

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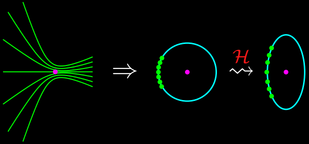

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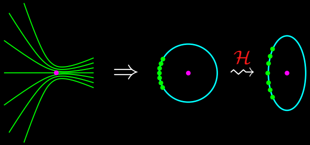

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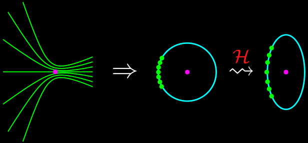

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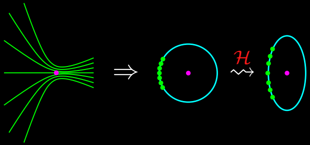

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Singular CLT

Problems: need appropriate

1. classes of spaces M and measures μ
2. analogues of Gaussian random variables as limiting distributions N
3. reflection of geometry ("curvature") of M in N

Solutions

1. - smoothly stratified metric space M of curvature bounded above
   - localized immured amenable probability measure μ on M
2. - reduce to linear case using extra step: tangential collapse $\mathcal{L} : T_{\bar{\mu}}M \to \mathbb{R}^m$

     so $$\begin{tikzcd} & \text{tangent cone: singular!} \arrow[d] & \\ M \arrow[r, "\log_{\bar{\mu}}"] & T_{\bar{\mu}}M \arrow[r, "\mathcal{L}"] & \mathbb{R}^m \end{tikzcd}$$
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Hypotheses

Hypotheses on M

- "nice" union of finitely many manifolds (strata)
- locally well defined exponential maps that are local homeomorphisms
  - essential for bringing asymptotics of sampling to $T_{\bar{\mu}}M$ and back to M
- curvature bounded above by κ: M is CAT(κ)
  - only really needed at $\bar{\mu}$
  - morally won't be infinitely curved anyway: Fréchet means would flee

Hypotheses on μ

- amenable: $d(x,-)^2$ has finite μ-expectation directional 2nd derivatives at $\bar{\mu}$
  - standard, mild, analytic sort of hypothesis on μ
  - allows differential and Taylor expansion techniques for optimization
- immured: $\log_{\bar{\mu}} \bar{\mu}_n \in$ convex cone generated by $\operatorname{supp}\mu$ when $\bar{\mu}_n$ is near $\bar{\mu}$
  - always if M is CAT(0) (e.g., $M = T_{\bar{\mu}}M$, such as $M = \mathcal{T}_n$ or open book)
  - always if $\operatorname{supp}\mu$ contains a neighborhood of $\bar{\mu}$
  - maybe always no matter what
- localized: unique Fréchet mean, locally convex F_μ, and $\log_{\bar{\mu}}$ defined a.s.
  - always if $\operatorname{supp}\mu \subseteq B(\bar{\mu}, \pi/\sqrt{\kappa})$
  - avoids cut locus and smeary issues
  - ensures pushforward of μ to $T_{\bar{\mu}}M$ is defined

Stratified spaces

Def [Mattingly, M–, Tran 2023]. M is smoothly stratified with distance $\mathbf{d}$ if

- M is a complete, locally compact, geodesic space
- $M = \bigsqcup_{j=0}^{d} M^j$ has disjoint locally closed strata M^j
- each stratum M^j
  - is a manifold with geodesic distance $\mathbf{d}|_{M^j}$
  - has closure $\overline{M^j} = \bigcup_{k \leq j} M^k$
- locally well defined exponential maps that are local homeomorphisms
- curvature bounded above by κ: M is $\mathrm{CAT}(\kappa)$

Examples

- graph (or network): strata are vertices and edges
- polyhedron: strata are (relatively open) faces
- real (semi)algebraic variety: strata ↔ equisingular loci

Actual examples

- fruit fly wings
- tree spaces
- shape spaces

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Examples

- graph (or network): strata are vertices and edges
- polyhedron: strata are (relatively open) faces
- real (semi)algebraic variety: strata $\leftrightarrow$ equisingular loci

Actual examples

- fruit fly wings
- tree spaces
- shape spaces

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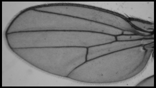

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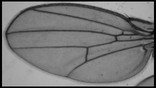

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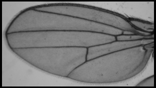

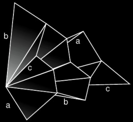

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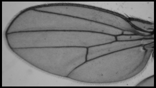

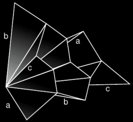

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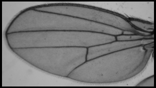

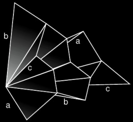

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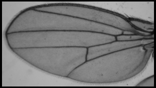

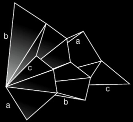

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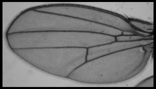

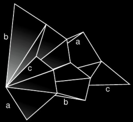

Hypotheses

Hypotheses on M

- "nice" union of finitely many manifolds (strata)
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Singular distortion

What can limiting distribution $\mathcal{H}_\sharp N(0, \Sigma)$ look like?

Example [Huckemann, Mattingly, M–, Nolen 2015]

- Isolated hyperbolic planar singularity: angle sum at apex is $\alpha > 2\pi$ (that is, circumference at radius 1 is α)

embedded in $\mathbb{R}^3$:

- Note: singularity of M is geometric, not topological
- Pushforward under distortion map $\mathcal{H}_\sharp$ is convex projection from tangent cone $T_{\bar{\mu}}M$ to fluctuating cone K.
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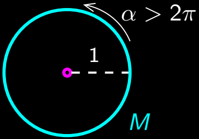

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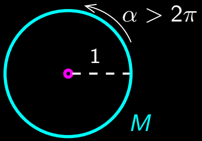

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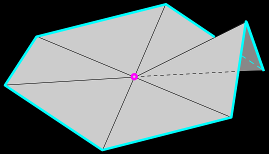

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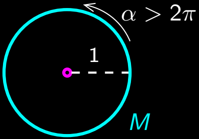

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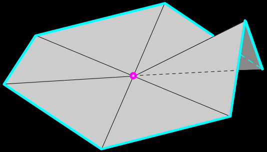

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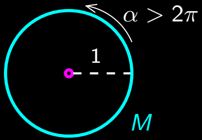
What can limiting distribution $\mathcal{H}_\sharp N(0, \Sigma)$ look like?

Example [Huckemann, Mattingly, M–, Nolen 2015]

- Isolated hyperbolic planar singularity: angle sum at apex is $\alpha > 2\pi$ (that is, circumference at radius 1 is α)



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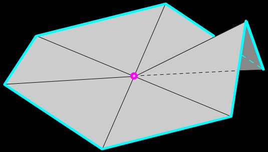

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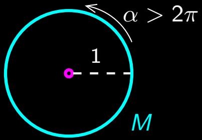

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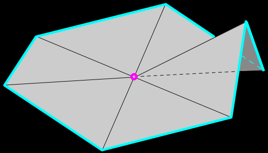

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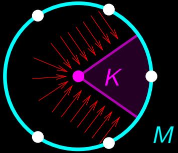

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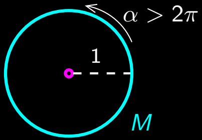

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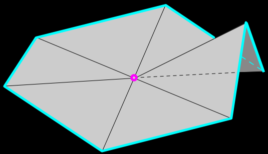

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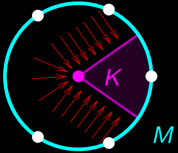

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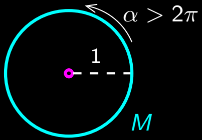

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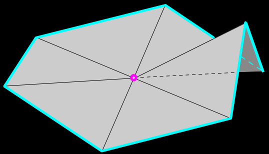

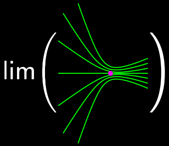

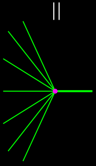

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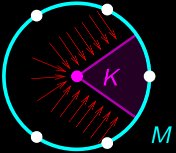

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Fundamental shifts in perspective via random fields or directional derivatives

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Summary of singular setting

1. shadow geometry at singular points of CAT(κ) spaces `[arXiv:2311.09451]`
   - CLT $\leftrightarrow$ variation of Fréchet means Lec 1
   - $\bar{\mu}$ can only escape in certain directions Z Lec 2
   - "shadow" directions beyond opposite Z, at angle $\geq \pi$, collapse to a ray Lec 3
   - directions within π of Z remain metrically intact ⋮
2. geometry of measures on smoothly stratified spaces `[arXiv:2311.09453]`
   - smooth setting: reduce to linear via $\log_{\bar{\mu}}$ Lec 1
   - singular setting: take log from infinitesimally nearby $\bar{\mu}$ Lec 3
   - miracle: this "limit log" isometrically preserves all escape directions ⋮
   - carefully iterating yields tangential collapse $\mathcal{L} : T_{\bar{\mu}}M \to \mathbb{R}^m$ ⋮
3. CLT for random tangent fields `[arXiv:2311.09454]`
   - spatial variation of $\bar{\mu}_n$ around $\bar{\mu}$ is too much to handle Lec 4
   - ask about variation along each ray separately ⋮
   - $\to$ Gaussian on that ray ⋮
   - multivariate Gaussian on any finite set of rays ⋮
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   - $\mathscr{E}(x)$: where does $\bar{\mu}$ go when mass is added at x? Lec 5
   - $\mathscr{E}$ linearizes #3 ⋮
   - CLT ↔ where does $\bar{\mu}$ go when Gaussian random mass Γ_μ is added? ⋮

Looking forward

Interpretations of Gaussian objects on singular spaces

- heat dissipation
- random walks
- infinite divisibility of probability distributions

Statistical developments

- convergence rates
- confidence regions
- geometric PCA, e.g., in the sense of [Marron, et al. since 2010s]
- smoothness/singularity testing
- learning stratified spaces
- singular influence functions

Infinite-dimensional singular settings

- persistence diagrams [Mileyko, Mukherjee, Harer 2011]
- spaces of measures [Lott 2006]

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Curvature invariants from distortion maps and tangential collapse

- generalize 2D angle deficit
- variation from point to point in M
- integrate to reflect topology of singular spaces?
- compare with singular homology or intersection cohomology
- how to construct measures with given Fréchet mean?

Functoriality and moduli

- distortion $\leftrightarrow$ how CLT transforms under morphism
- proposal for real or complex variety X:
  - take resolution of singularities $\widetilde{X} \to X$
  - push CLT on $\widetilde{X}$ forward to X
  - correction terms should involve local sheaf-theoretic data around $\bar{\mu}$
  - conj: results in well defined CLT on X
  - e.g.: compare pushforward CLT with singular CLT in smoothly stratified case
  - analogy: multiplier ideals
- asymptotics of sampling from moduli spaces
  - statistical invariants $\leftrightarrow$ typical or expected variation of algebraic structures
  - in neighborhoods of a fixed degeneration

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Next lecture: geometry and measure on CAT(κ) spaces