Geometric central limit theorems on non-smooth spaces

Ezra Miller

Duke University, Department of Mathematics
and Department of Statistical Science

ezra@math.duke.edu

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

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Duke University

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Outline

1. Linear Central Limit Theorem
2. Nonlinear data
3. History
4. Fréchet means
5. Logarithm maps
6. Smooth manifold CLT
7. Singular CLT
8. Singular distortion
9. New interpretations of CLTs
10. Future directions

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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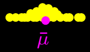

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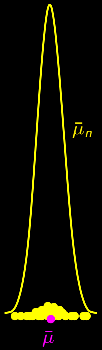

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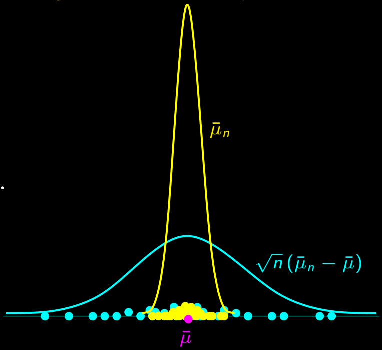

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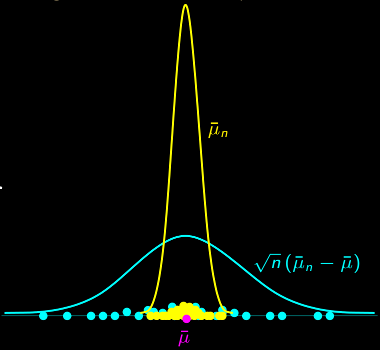

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Nonlinear data

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

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- 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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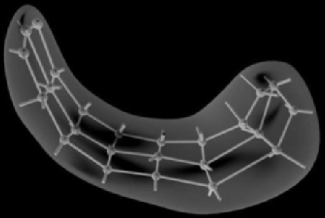
Hippocampus surfaces

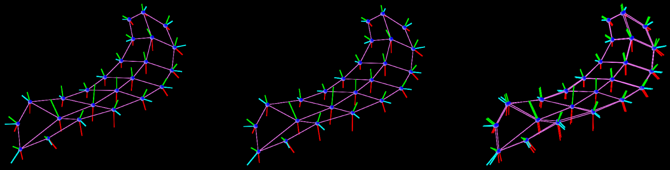
Medial axis representation



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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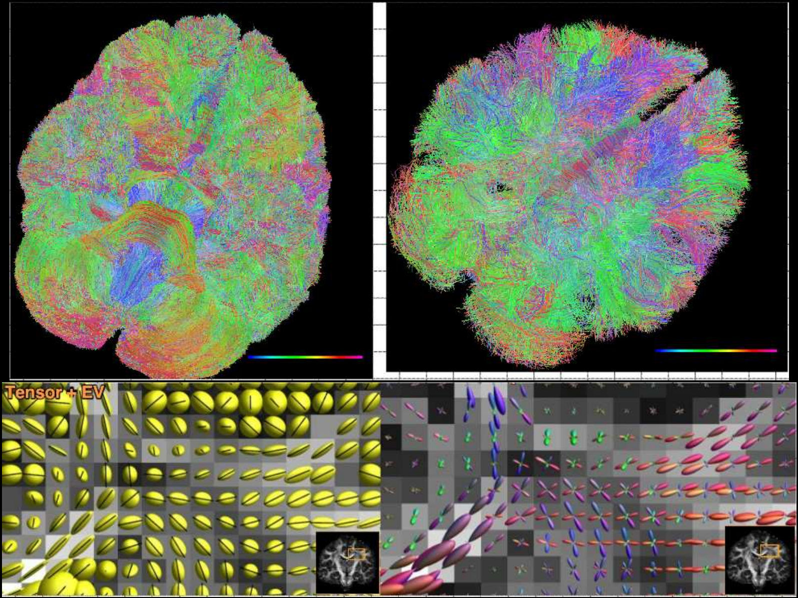
Streamlines from Diffusion Tensor Imaging



courtesy Zhengwu Zhang

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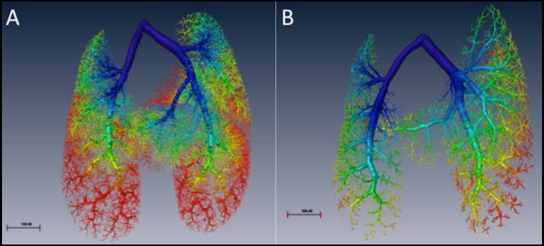
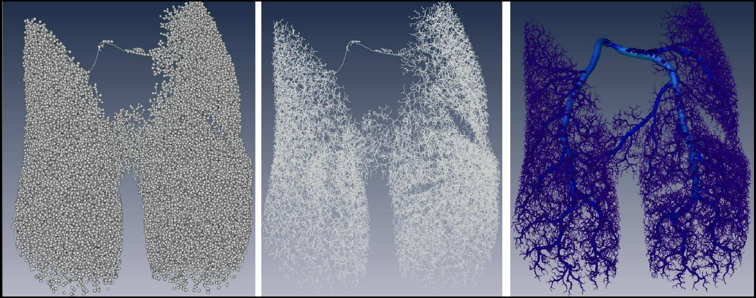
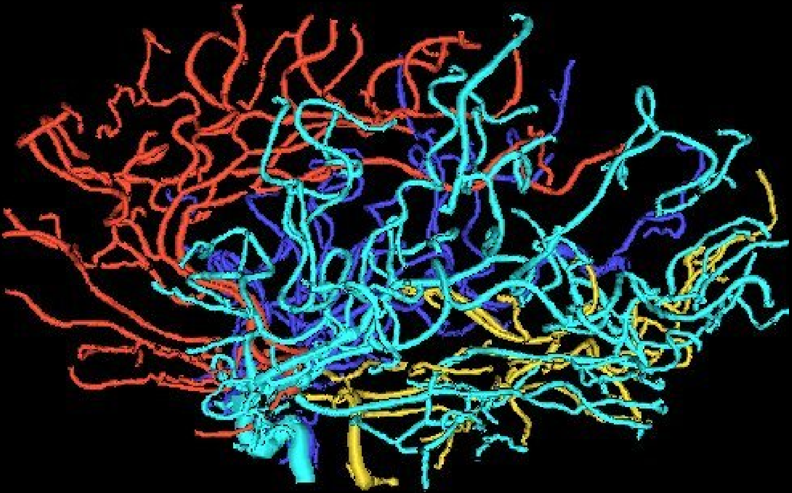
Lung vessels (CDH study)





courtesy Sean McLean

Brain arteries



[Bullitt and Aylward, 2002]

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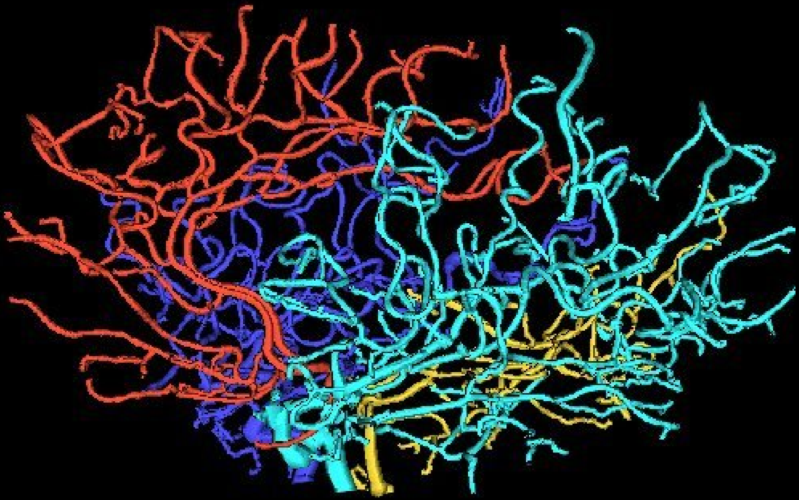

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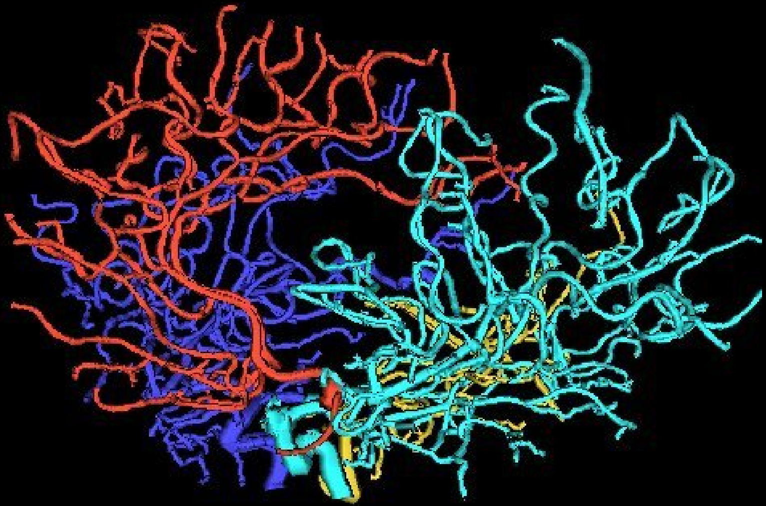

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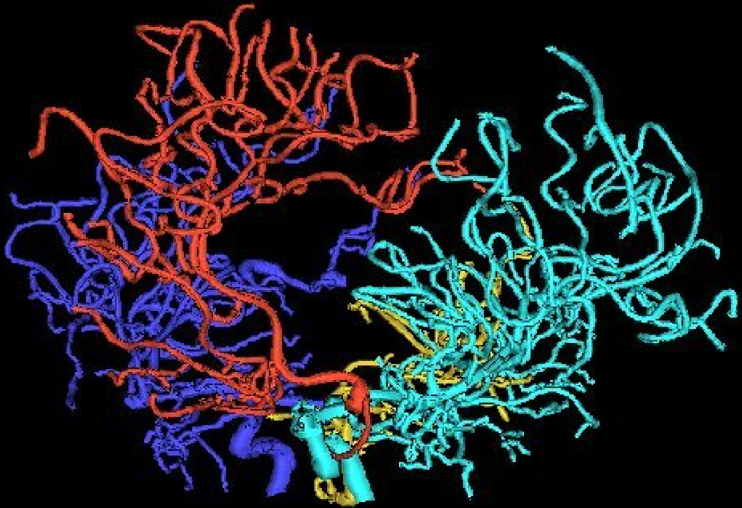

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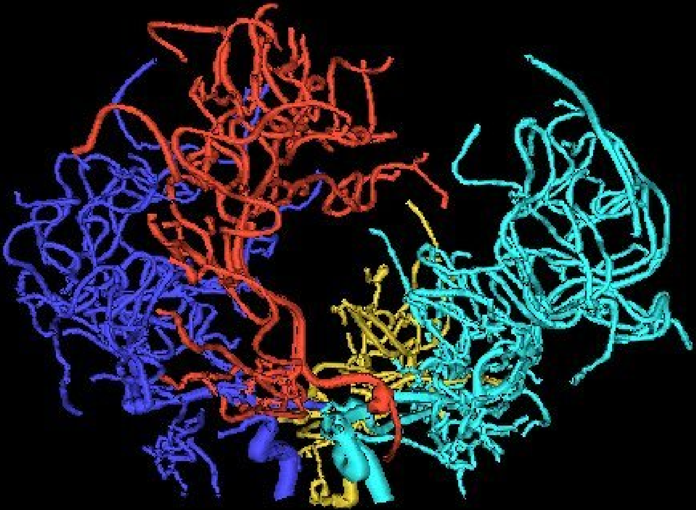

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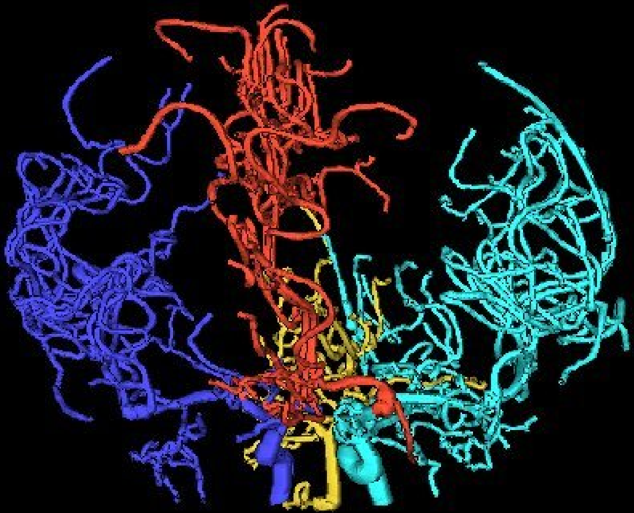

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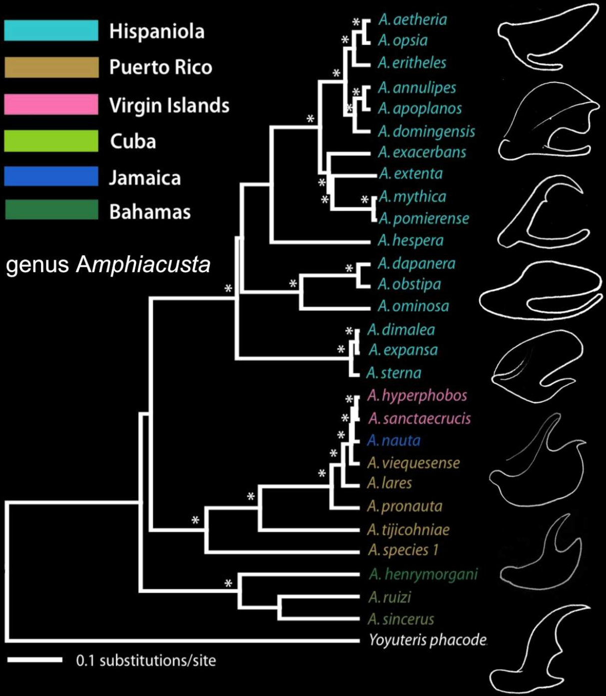

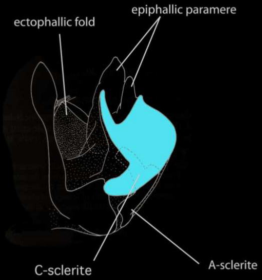

From Oneal, Otte & Knowles, 2010

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 $\Rightarrow$ sample mean $\to$ true tree
- evolutionary biology: "gene trees" from a "species tree"
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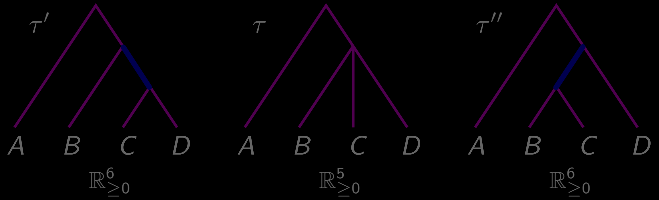
Sample space $\mathcal{T}_n = \{$phylogenetic n-trees$\}$ is a union of polyhedral cones (orthants) [Billera–Holmes–Vogtmann 2001]

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



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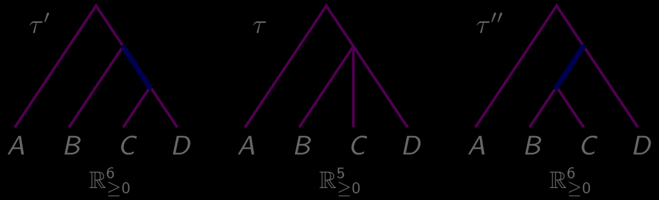

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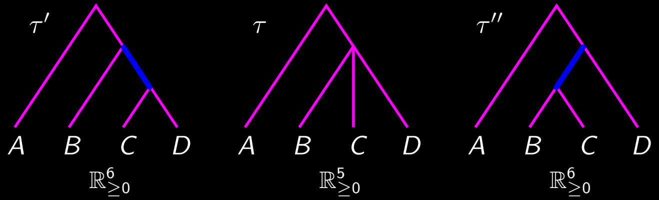

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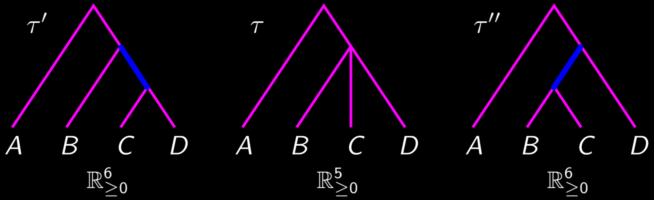

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Nonlinear data

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

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Mimic ordinary statistics: assume nonlinear M given; want

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- Law of Large Numbers (LLN), confidence intervals
- Central Limit Theorem (CLT)

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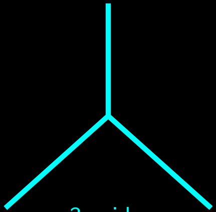

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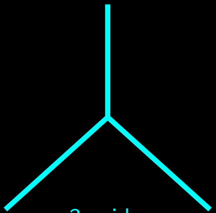

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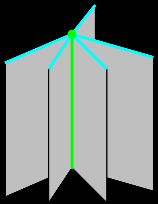

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$\mathbb{R}^d \times$ spider

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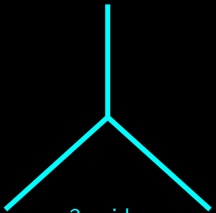

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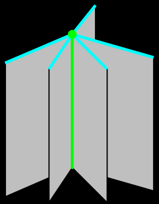

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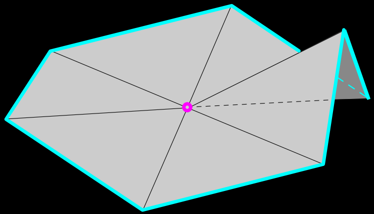

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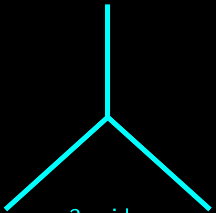

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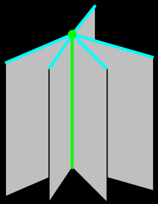

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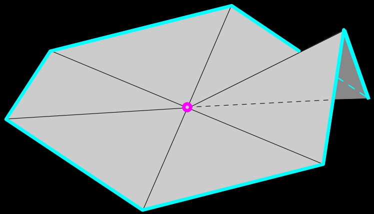

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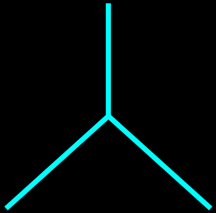
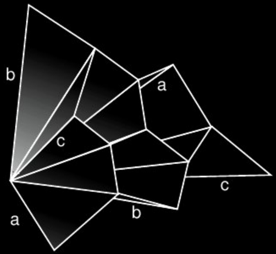


$\mathcal{T}_3$



$\mathcal{T}_4$

from [BHV 2001]

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Goal for today: CLT for general non-smooth spaces

Fréchet means

Sample space: Riemannian manifold M

What fails

1. sum or average of
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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 $\bar{\mu} = \operatorname*{argmin}_{y \in M} F_\mu(y)$.

   - "least squares approximation"
   - empirical mean $\bar{\mu}_n$ from empirical measure $\mu_n = \frac{1}{n}(\delta_{X_1} + \cdots + \delta_{X_n})$
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Recast CLT on manifold M

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- as (moving) empirical mean converges
- to (fixed) population mean

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

Def. The logarithm map is

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

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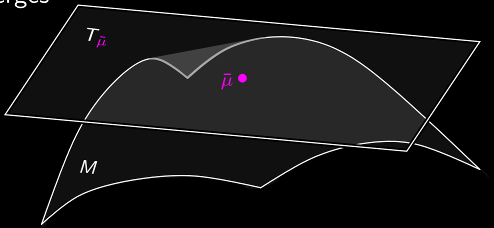

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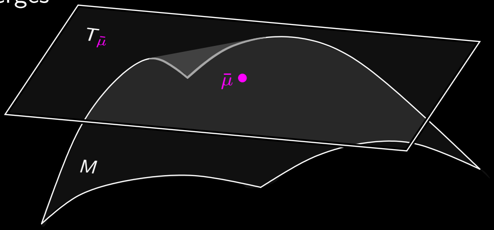

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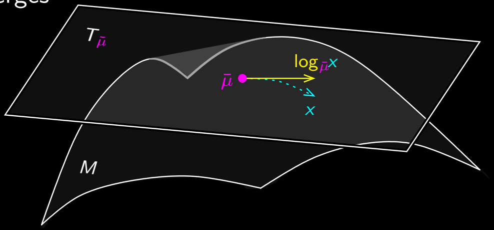

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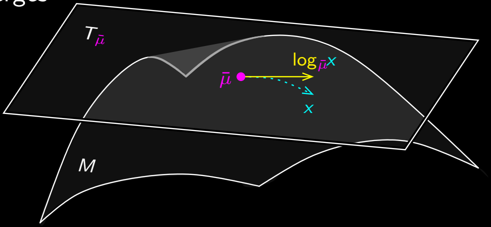

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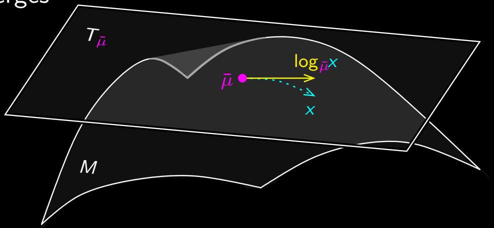

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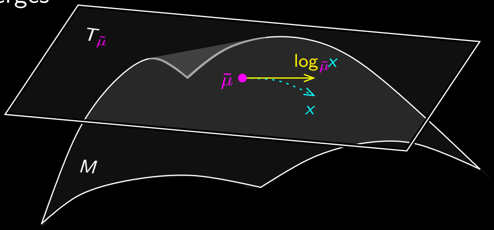

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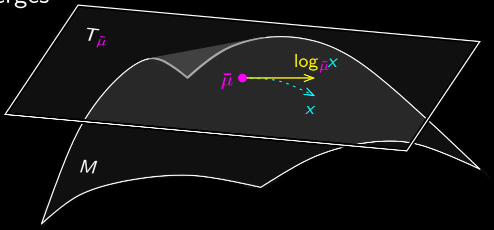

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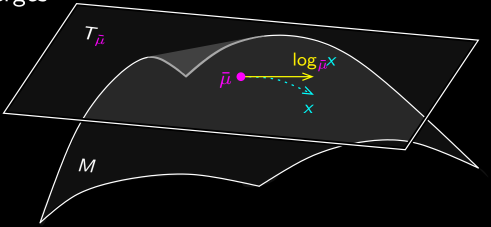

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Smooth manifold CLT

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 $\bar{\mu}$
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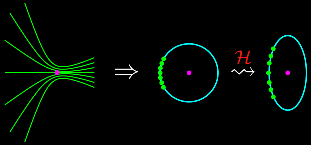

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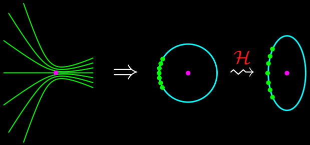

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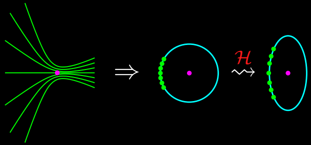

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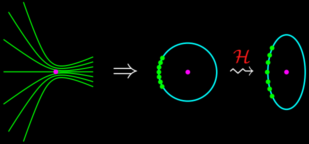

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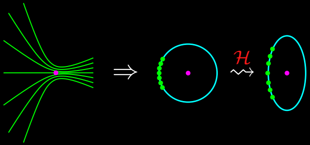

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Singular CLT

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

   tangent cone: singular!

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- "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 $\bar{\mu}$
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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 $\bar{\mu}$
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  - 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.
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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)

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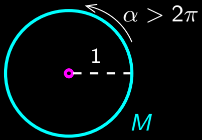

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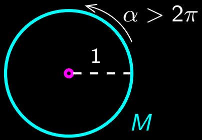

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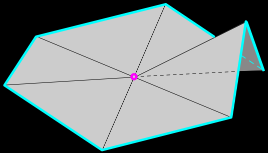

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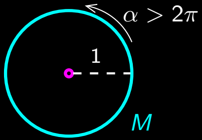

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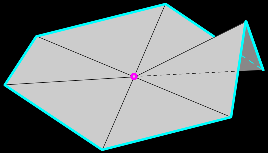

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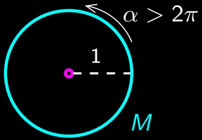

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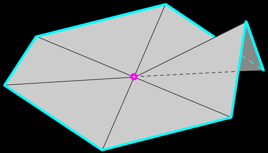

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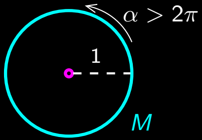

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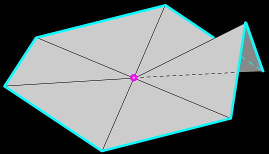

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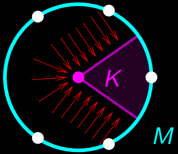

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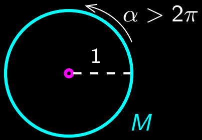

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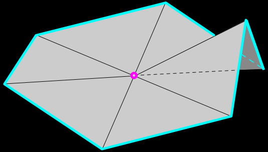

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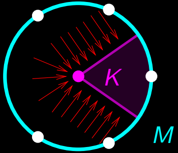

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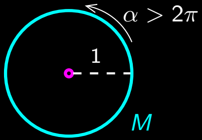

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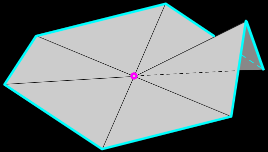

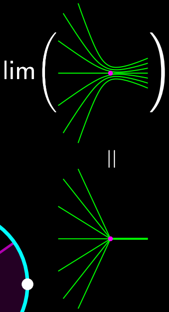

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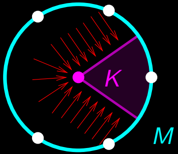

New interpretations of CLTs

Fundamental shifts in perspective via random fields or directional derivatives

CLT 2 [Mattingly, M–, Tran 2023]. Intrinsic, with Gaussian random field as limit:

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Fundamental shifts in perspective via random fields or directional derivatives

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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]
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- learning stratified spaces
- singular influence functions

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- persistence diagrams [Mileyko, Mukherjee, Harer 2011]
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- variation from point to point in M
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- compare with singular homology or intersection cohomology
- how to construct measures with given Fréchet mean?

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