What is a Gaussian on a singular space?

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

Geometric Sciences in Action:
from geometric statistics to shape analysis

CIRM Luminy

30 May 2024

Outline

Motivation and history

Mimic ordinary statistics: assume nonlinear M given; want

- averages: measure μ on $M \rightsquigarrow$ mean $\bar{\mu} \in M$
- variance, PCA
- Law of Large Numbers (LLN), confidence regions
- Central Limit Theorem (CLT)
  - smooth M [Bhattacharya and Patrangenaru 2003, 2005]
  - singular M
    - open books [SAMSI Working Group 2013]
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  - diffusion on metric spaces [Sturm 1998]

Goals for today

- Gaussians on singular spaces
- $\rightsquigarrow$ stratified CLT

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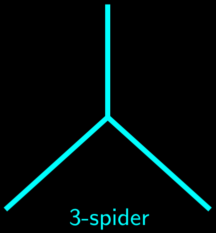

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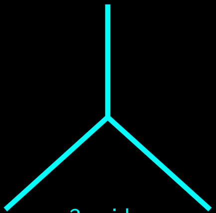

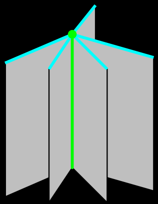

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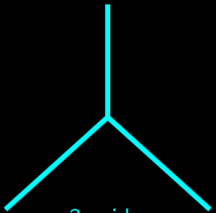
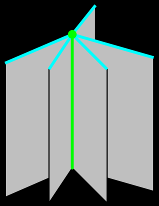
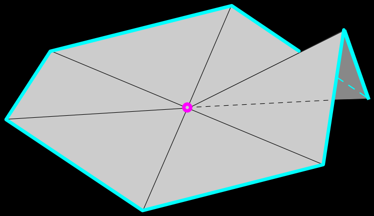


3-spider



open book

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



isolated hyperbolic planar singularity

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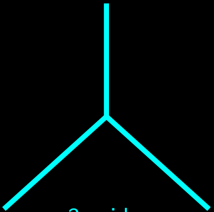

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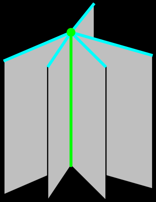

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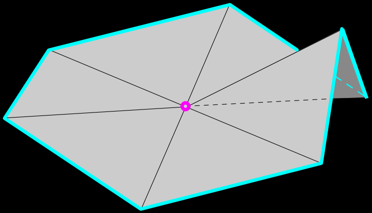

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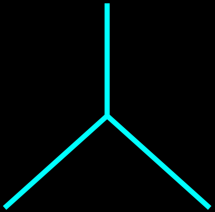
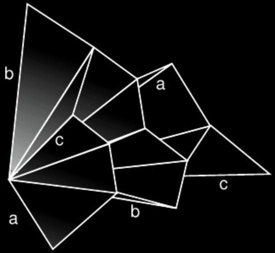


$\mathcal{T}_3$



$\mathcal{T}_4$

from [BHV 2001]

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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 $\overline{M^j} = \bigcup_{k \le j} M^k$
- 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 $\bar{\mu}$, which
  - morally won't be infinitely curved anyway: Fréchet means would flee

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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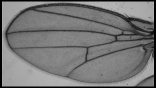

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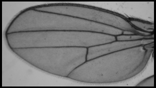

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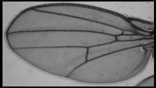

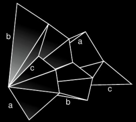

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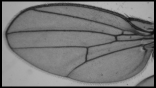

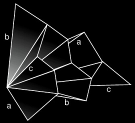

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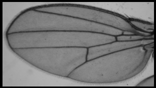

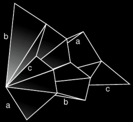

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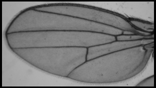

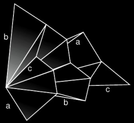

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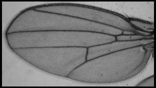

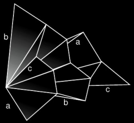

Fréchet means

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

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

and Fréchet mean $\bar{\mu} = \underset{y\in M}{\operatorname{argmin}}\, F_\mu(y)$.

Prop. M is CAT(κ)
$\Rightarrow$ M has tangent spaces (cones)

Def. The logarithm map is

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

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

Note. M singular at $\bar{\mu} \Leftrightarrow T_{\bar{\mu}}M \ncong \mathbb{R}^d$

Prop. M smoothly stratified
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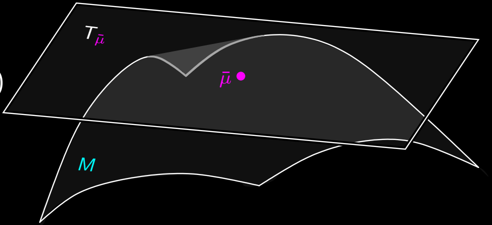

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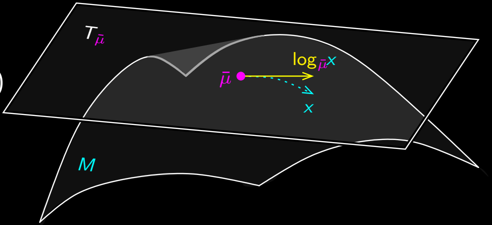

where V = unit tangent to geodesic from $\bar{\mu}$ to x.

Note. M singular at $\bar{\mu} \Leftrightarrow T_{\bar{\mu}}M \ncong \mathbb{R}^d$

Prop. M smoothly stratified
$\Rightarrow$ $T_{\bar{\mu}}M$ is a smoothly stratified CAT(0) cone.

Fréchet means

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

$$F_\mu(y) = \frac{1}{2}\int_M d(x,y)^2 \mu(dx)$$

($d(x,y)^2$ ↑ square distance; $\mu(dx)$ ↑ measure induced by μ)

and Fréchet mean $\bar{\mu} = \underset{y \in M}{\operatorname{argmin}} F_\mu(y)$.

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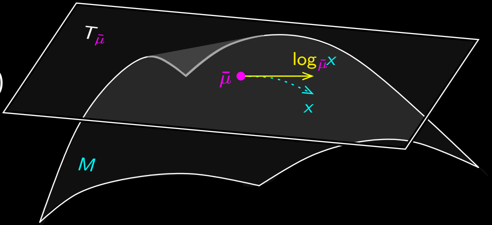

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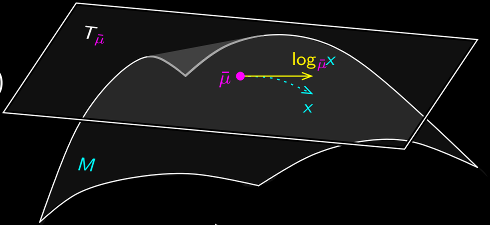

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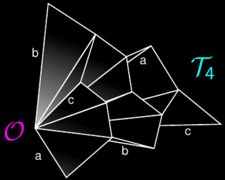

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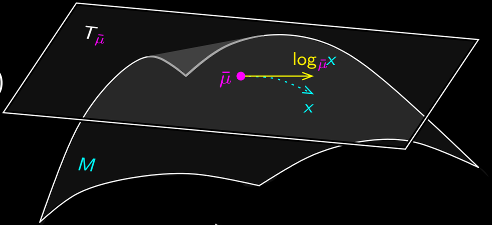

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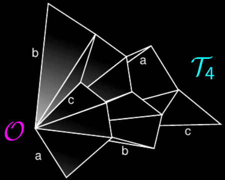

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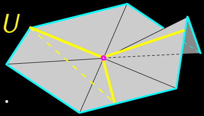

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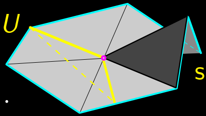

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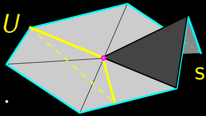

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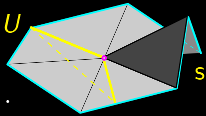

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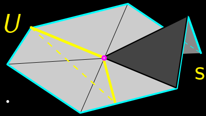

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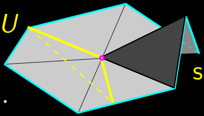

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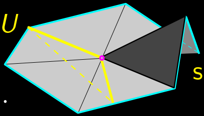

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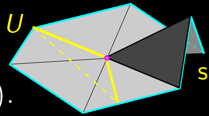

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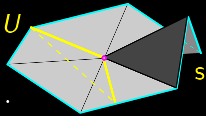

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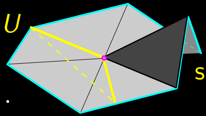

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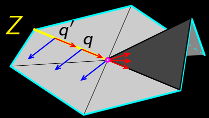

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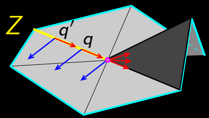

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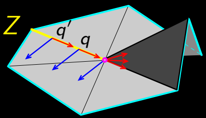

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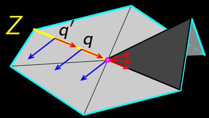

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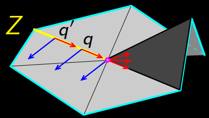

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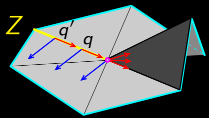

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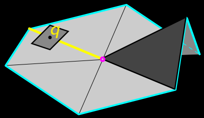

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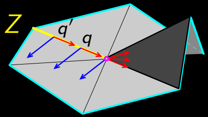

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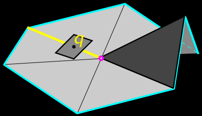

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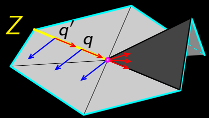

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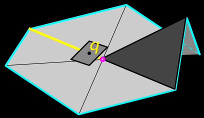

Idea. Z points out of stratum containing $\mathcal{O}$

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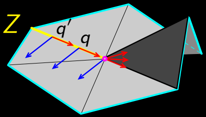

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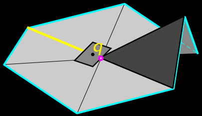

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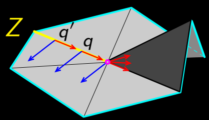

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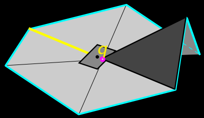

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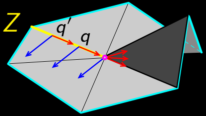

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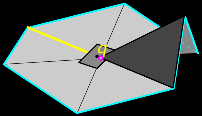

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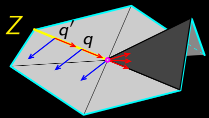

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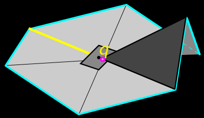

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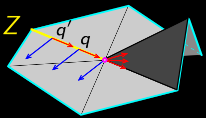

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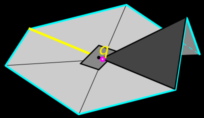

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Def. Localized μ on smoothly stratified M has fluctuating cone

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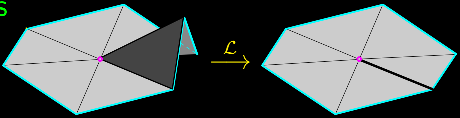
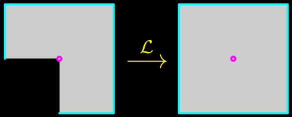
- kale: 

- nonconvex quadrants: 

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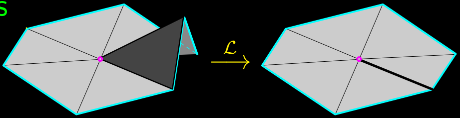
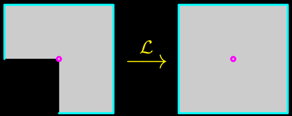
- kale: 

- nonconvex quadrants: 

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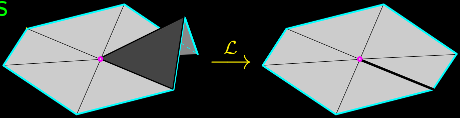
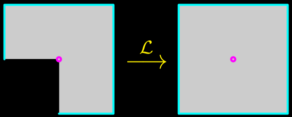
- kale: 

- nonconvex quadrants: 

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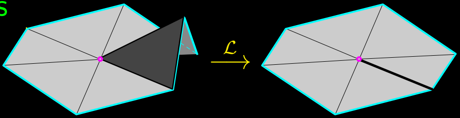

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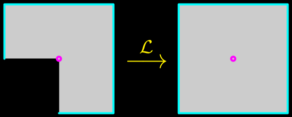

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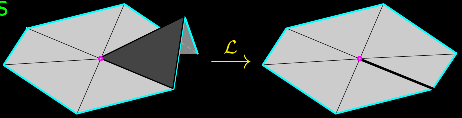

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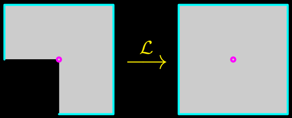

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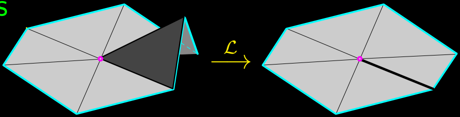
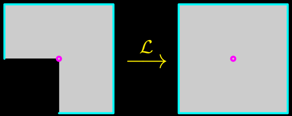
- kale: 

- nonconvex quadrants: 

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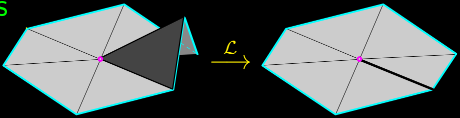

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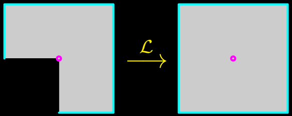

Stratified Gaussians

Smooth M: $T_{\bar\mu}M \cong \mathbb{R}^m$ already

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Lemma. The map $\mathcal{L}$ has a measurable section over $\mathbb{R}^\ell = \text{conv}(\text{image}\,\mathcal{L})$,

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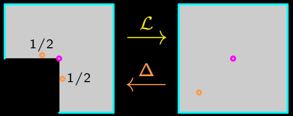
Example. 

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Perspective shift: continuous variation in Gaussians can come from redistributing weights on unmoving points rather than from spatial variation

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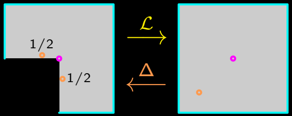
Example. 

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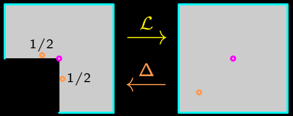

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Smooth M: $T_{\bar\mu}M \cong \mathbb{R}^m$ already

Singular M: use tangential collapse $T_{\bar\mu}M \xrightarrow{\mathcal{L}} \mathbb{R}^m$

Lemma. The map $\mathcal{L}$ has a measurable section over $\mathbb{R}^\ell = \mathrm{conv}(\mathrm{image}\,\mathcal{L})$,

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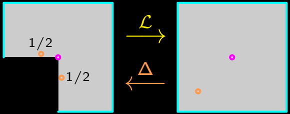

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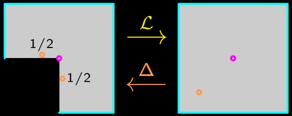
Example. 

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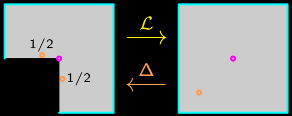
Example. 

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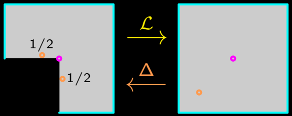
Example. 

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Central limit theorems

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Variational CLT in a space of measures

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Escape vectors

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

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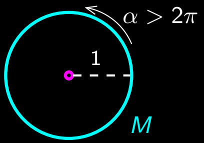

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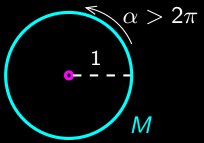

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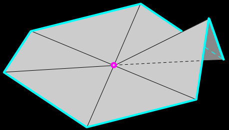
embedded in $\mathbb{R}^3$: 

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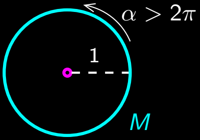

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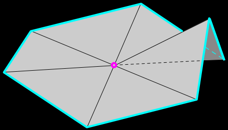
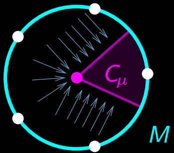
embedded in $\mathbb{R}^3$: 



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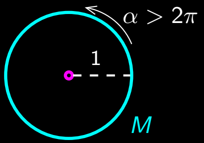

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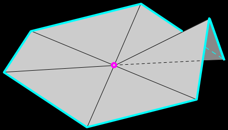

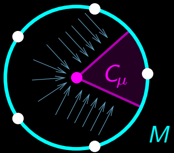

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- use G and Γ_μ to enable MCMC sampling
- heat dissipation and random walks: heat kernels
- infinite divisibility of probability distributions

Statistical developments

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

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- persistence diagrams [Mileyko, Mukherjee, Harer 2011]
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- 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]

Looking forward

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?

Algebraic singularities: 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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