

UC SANTA BARBARA

Introduction to ECE 594n

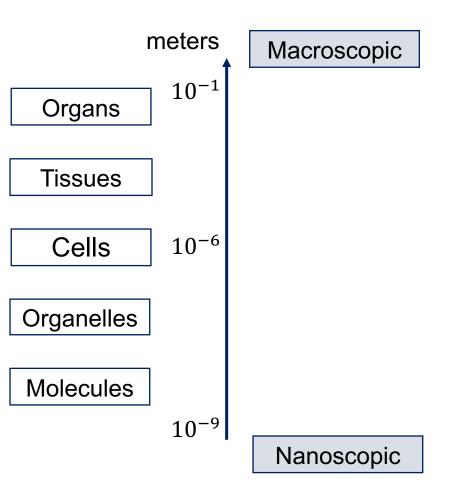
Geometric Machine Learning for Biomedical Imaging and Shape Analysis

Nina Miolane, Assistant Professor



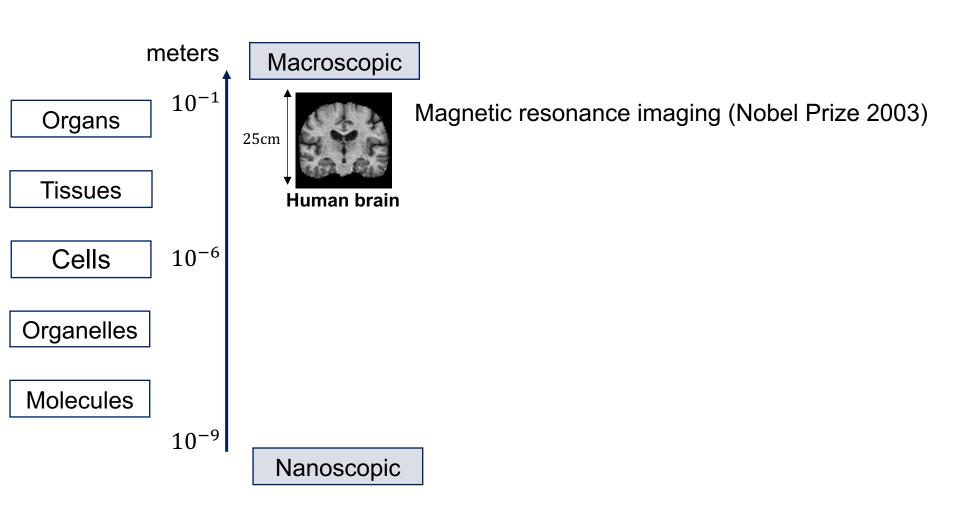
Bioimaging at Different Scales

Biomedical research: understand mechanisms of life.



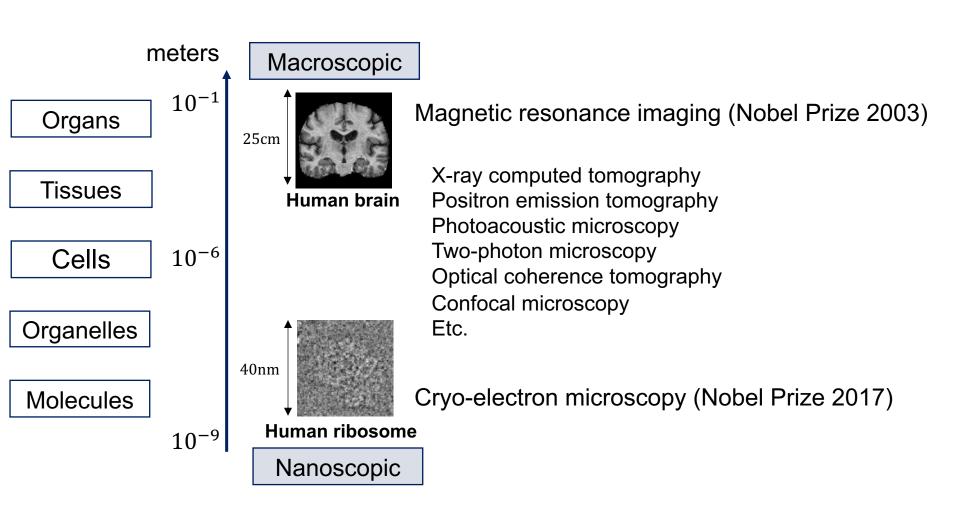
Bioimaging at Different Scales

Biomedical research: understand mechanisms of life.

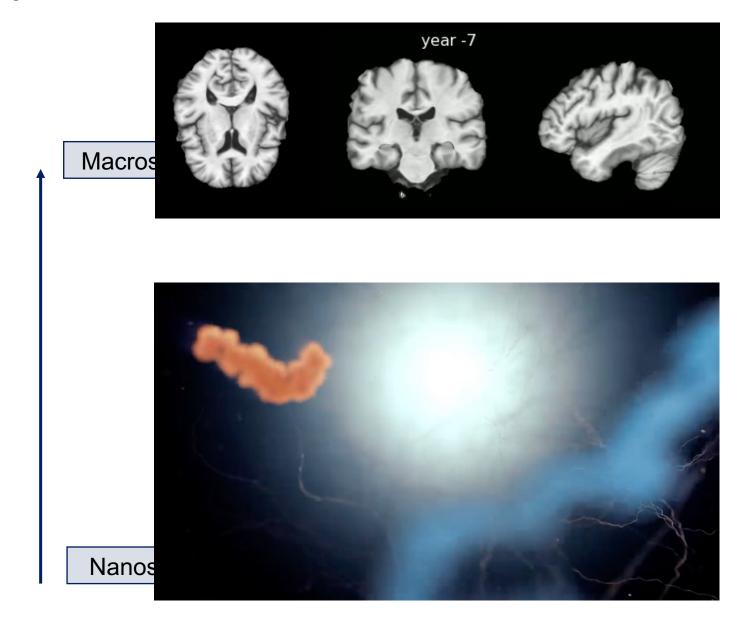


Bioimaging at Different Scales

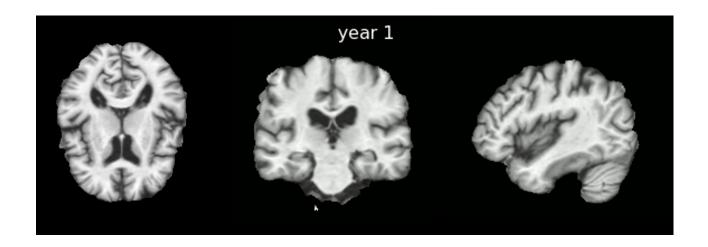
Biomedical research: understand mechanisms of life.



The Shapes Of You

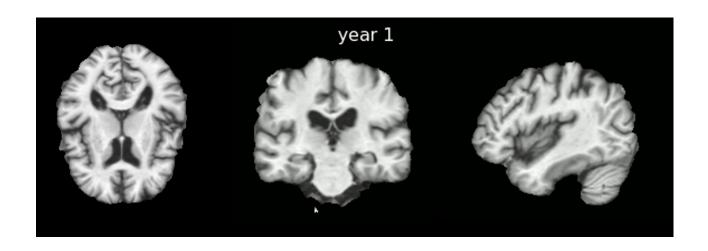


Simulation credits: Lorenzi, Ayache, Frisoni, Pennec (Inria). Video credits: US National Institute on Aging (NIH).



Function
Healthy/pathological state

→ Geometry



Function
Healthy/pathological state

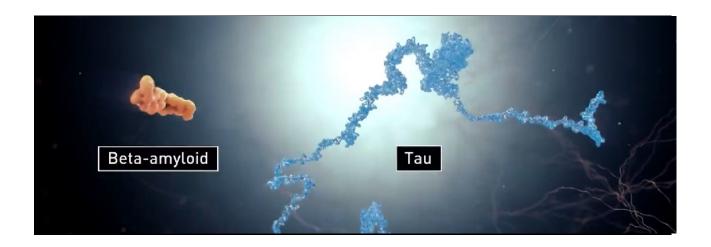
→ Geometry

Inverse model?

Biomedical discoveries

 \leftarrow

Geometry



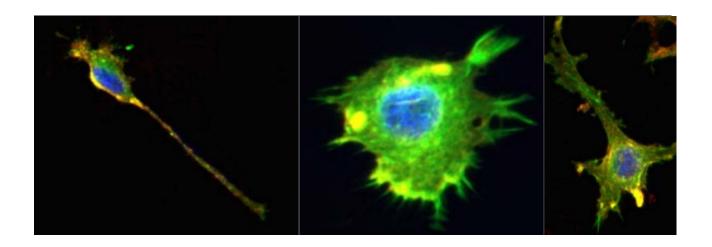
Function Healthy/pathological state

→ Geometry

Inverse model?

Biomedical discoveries

← Geometry



Function
Healthy/pathological state

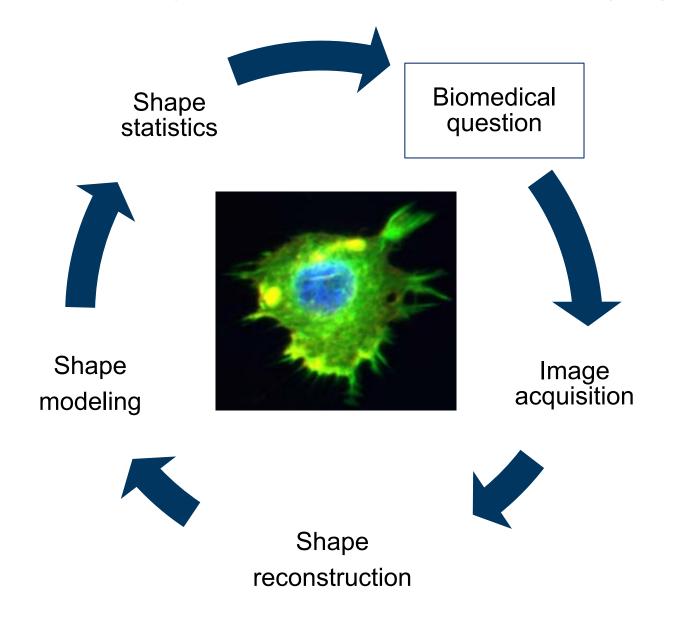
→ Geometry

Inverse model?

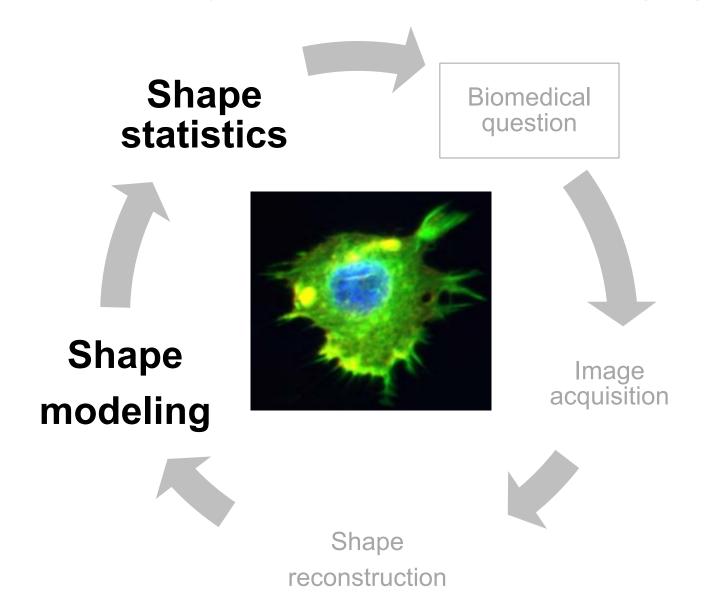
Biomedical discoveries

Geometry

Shape Analysis from Biomedical Imaging

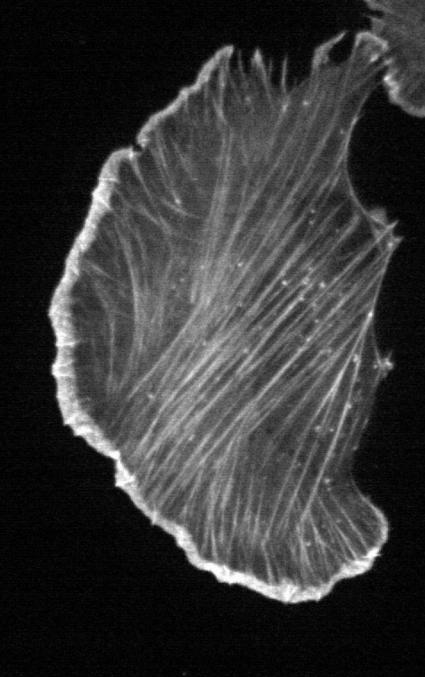


Shape Analysis from Biomedical Imaging

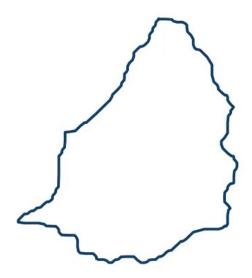


- Mathematical...
- Computational...
- Statistical...

...shape models



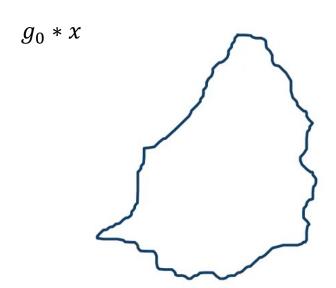
Translation



Shapes ↔ Equivalence classes

 G_0 Tran

Translation

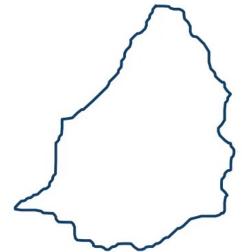


Shapes ↔ Equivalence classes

 G_0

Translation

 $g_0 * x$



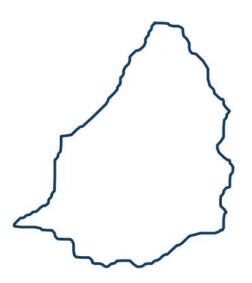
Shapes \leftrightarrow Equivalence classes = Elements of "Quotient space" Q

$$Q = \{[x] | x \in M\}$$
 where $[x] = \{y \in M \mid \exists g_0 \in G_0 \text{ s. t. } y = g_0 * x\}$

 G_0

Translation

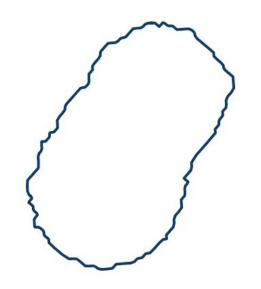
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Shapes ↔ Equivalence classes = Elements of "Quotient space" *Q*

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Smooth deformation

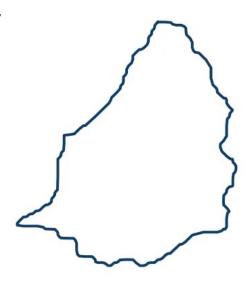


Shapes ↔ Deformations

 G_0

Translation

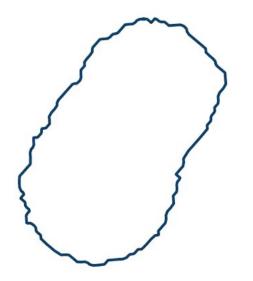
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Smooth deformation

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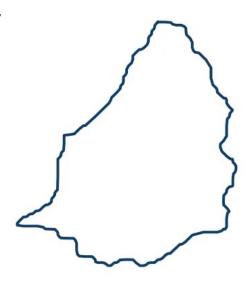
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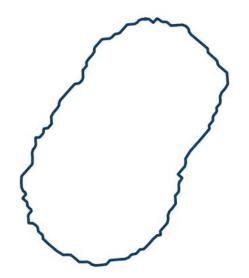
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Smooth deformation

g * x

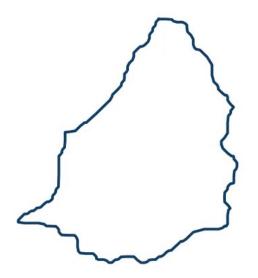


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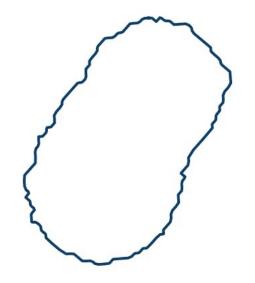
Shapes ↔ Deformations = Elements of "Lie group" *G*

Translation



Shapes ↔ Equivalence classes = Elements of "Quotient space" Q

Smooth deformation



Shapes ↔ Deformations = Elements of "Lie group" *G*

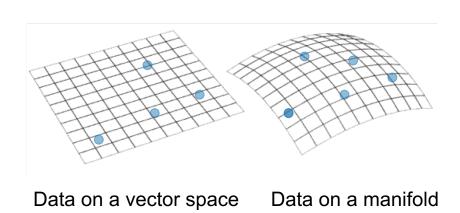
= Manifolds with additional geometric structures

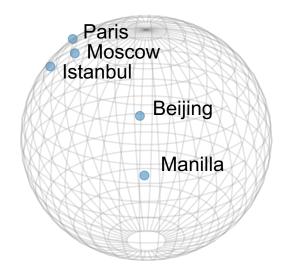
Quotients, Lie Groups = Manifolds

Generalize computing, statistics & (deep) learning to data on manifolds

Geographic data, e.g. coordinates of cities or earthquakes.

Example: Data on the sphere

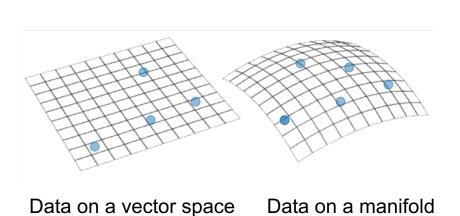


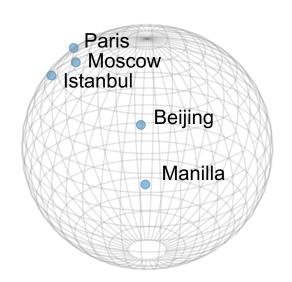


Quotients, Lie Groups = Manifolds

Generalize computing, statistics & (deep) learning to data on manifolds

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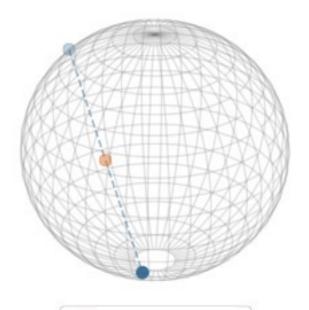


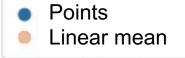
Example: Data on the sphere

Geomstats: Open-source Python package for Geometric Statistics

Why Geometric Statistics

- Mean: $\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i \rightarrow \text{linear}$
- Manifold → non-linear
- → Mean may not belong to the manifold





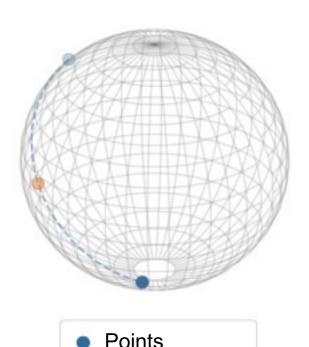
Why Geometric Statistics

- Fréchet mean $\bar{x} = \operatorname{argmin}_{x \in M} \sum_{i=1}^{n} \operatorname{dist}_{M(x,x_i)}^2$
- → Mean belongs to the manifold

```
from geomstats.learning.frechet_mean import \
FrechetMean
```

```
estimator = FrechetMean(metric=sphere.metric)
estimator.fit(points)
```

frechet_mean = estimator.estimate_



Fréchet mean

Why Geometric Statistics

- Fréchet mean $\bar{x} = \operatorname{argmin}_{x \in M} \sum_{i=1}^{n} \operatorname{dist}_{M(x,x_i)}^2$
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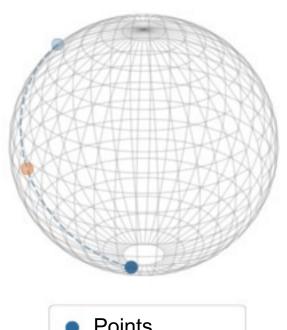
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Remarks:

- Whitney embedding theorem $M_m \subset \mathbb{R}^{2m}$
- Mean respecting additional geometries





Geomstats

Geomstats: Computing, statistics & (deep) learning for data on manifolds

- Backends: NumPy, Autograd, TensorFlow and PyTorch
- Instantiate manifold of interest

```
sphere = Hypersphere (dim=2)
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Apply estimation or learning method

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estimator = FrechetMean(metric=sphere.metric)
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Geomstats

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Geomstats Objectives:

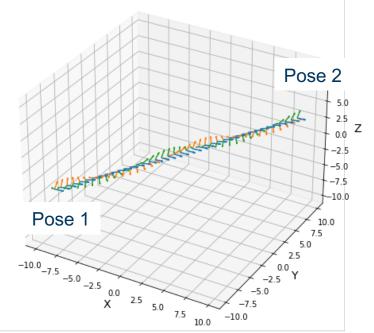
- Teach "hands-on" Geometric Statistics and Learning
- Democratize the use of Geometric Statistics and Learning
- Support research in Geometric Statistics and Learning
- → Compute with shape data

Basic Operations Coded on 20+ Manifolds

```
from geomstats.geometry.special_euclidean \
    import SpecialEuclidean

se3 = SpecialEuclidean(n=3, point_type='vector')
metric = se3.left_canonical_metric

initial_point = se3.identity
initial_tangent_vec = gs.array(
    [1.8, 0.2, 0.3, 3., 3., 1.])
geodesic = metric.geodesic(
    initial_point=initial_point,
    initial_tangent_vec=initial_tangent_vec)
```

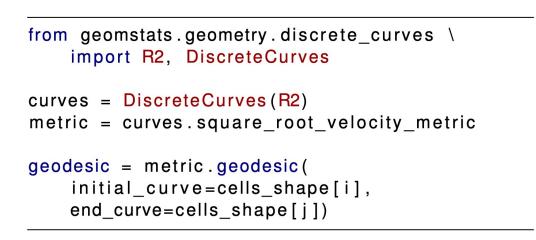


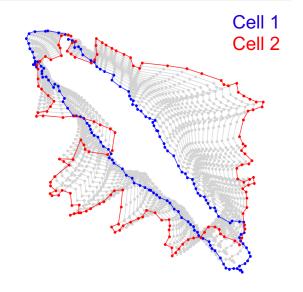
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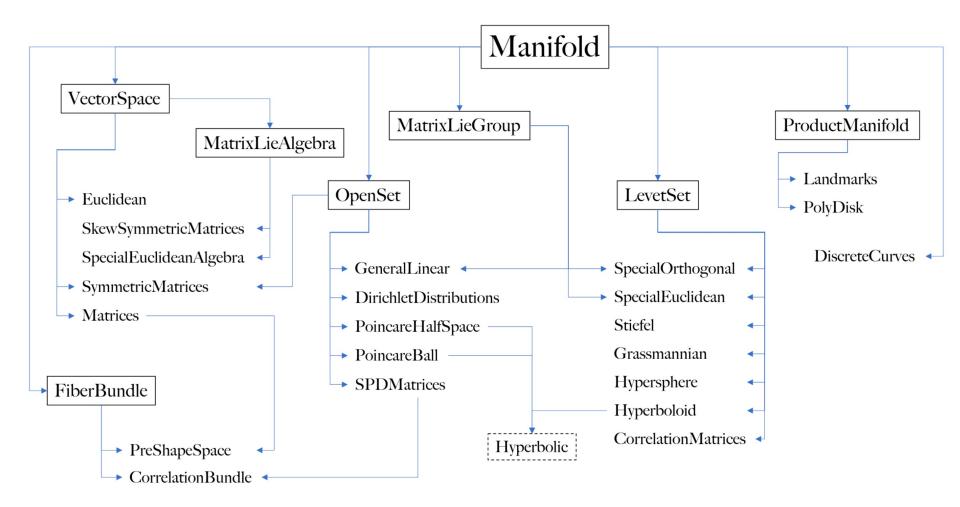
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Basic Operations Coded on 20+ Manifolds



Miolane et al. *Geomstats: a Python package for Riemannian geometry in machine learning.* Journal of Machine Learning Research (2020). **Miolane** et al. *Introduction to Geometric Learning with Geomstats.* SciPy International Conference (2020).

...Statistics and Learning

	Point estimation	Dimension Reduction	Stochastic processes	
Riemannian		(2019)		
Finsler				
Affine				
Stratified spaces	(2017-18)	(2020)		
Lie groups	(2015)			
Quotient spaces	(2017-21)			
Subriemannian			(2015)	

Miolane, Pennec: Computing bi-invariant pseudo-metrics on Lie groups for consistent statistics (2015).

Miolane, Pennec: A survey of mathematical structures for extending 2D neurogeometry to 3D image processing (2015).

Miolane, Holmes, Pennec: Template shape estimation: correcting an asymptotic bias (2017).

Miolane, Holmes, Pennec: Topologically constrained template (2018).

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Miolane, Poitevin, Lee, Holmes: Estimation of orientation and camera parameters in cryo-EM with autoencoders (2020).

Michel, Miolane et al. Cell morphometrics with the Riemannian elastic metric. (2021). In preparation.

Geometric..

...Statistics and Learning

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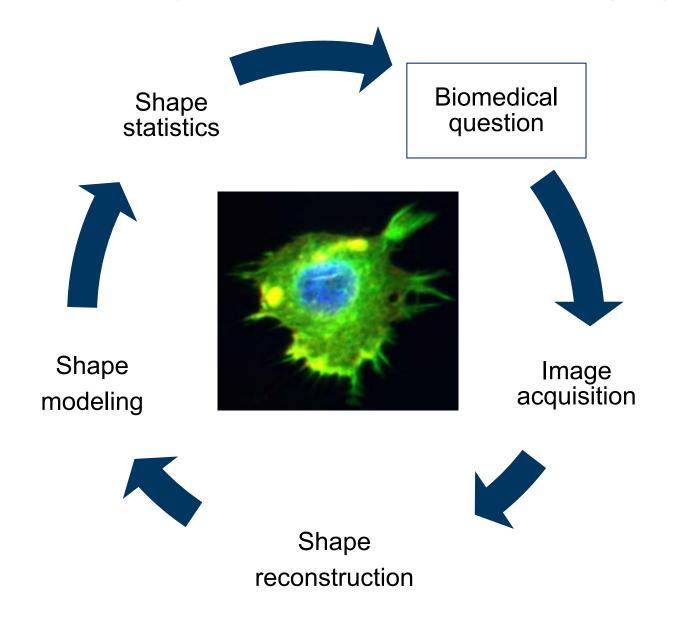
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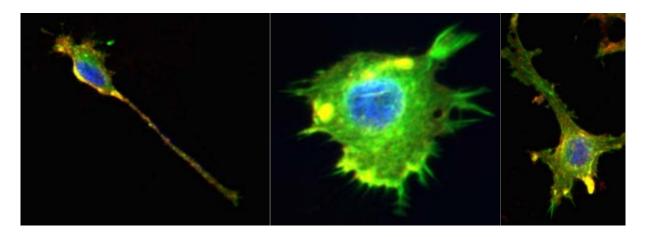
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Shape Analysis from Biomedical Imaging



Goal: Impact of Drug Treatment on Cancer Cell Shapes

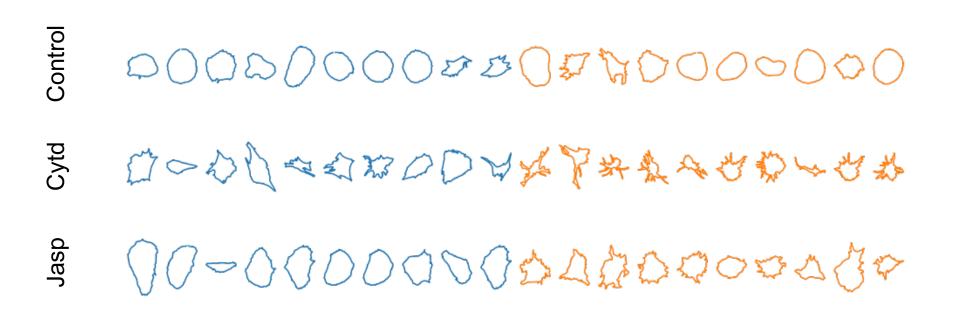
- Tumor grading → low accuracy and reproducibility [1]
- Cell morphometrics: cell state → cell shape
 - e.g. actin activity → irregular perimeter



- Questions:
 - How can we quantify differences in cell shapes?
 - How do cancer treatments affect cell?
- Collaborators: A. Prasad, K. Dao Duc, F. Michel, A. Le Brigant

Goal: Impact of Drug Treatment on Cancer Cell Shapes

curves, treatments, lines = geomstats.datasets.utils.load_cells()

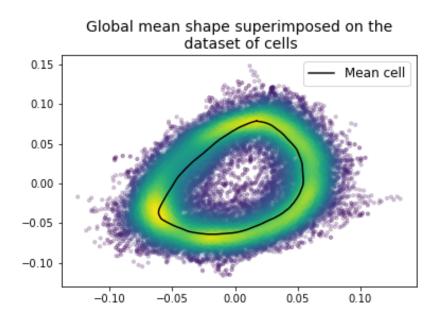


DLM8 DUNN

Computing the Mean Shape

```
curves = DiscreteCurves(R2)
mean =FrechetMean(metric=curves.square_root_velocity_metric)
mean.fit(cell_shapes)
```

mean_estimate = mean.estimate_



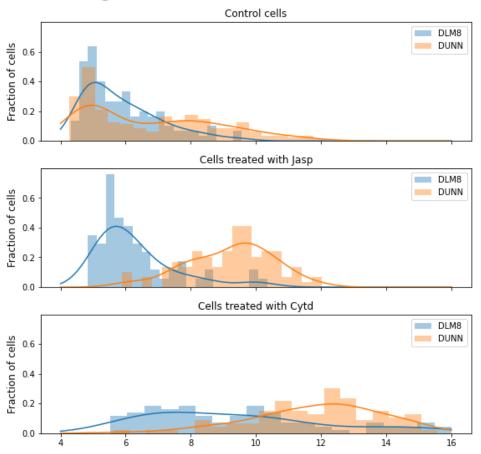
Hypothesis Testing on Shape Transformations

Dunn:

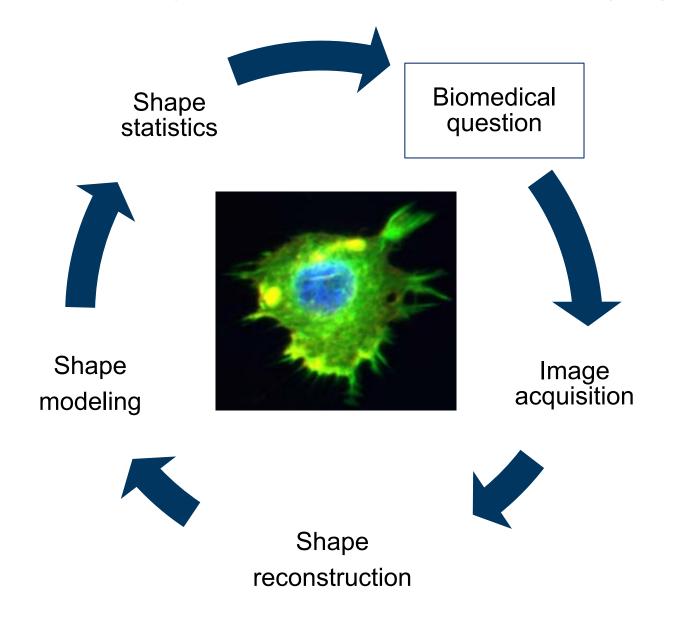
- higher variability in shapes
- further from mean shape
- Jasp treatment:
 - Effective on Dunn
 - Less effective on DLM8
- Cytd treatment:
 - Very effective on:
 - Dunn
 - DLM8

Statistically significant (p < 0.01)

Histograms of elastic distance to mean cell



Shape Analysis from Biomedical Imaging



...Statistics and Learning

	Point estimation	Dimension Reduction	Stochastic processes	Deep Learning
Riemannian				
Finsler				
Affine				
Stratified spaces				
Lie groups				
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Subriemannian				

Geometric Learning beyond shape modeling: equivariance, invariance properties



UC SANTA BARBARA

Exploring the Geometries of Life

Thank you for your attention.

