Geomstats:
A Python Package for Geometry in Machine Learning and Information Geometry

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Motivation

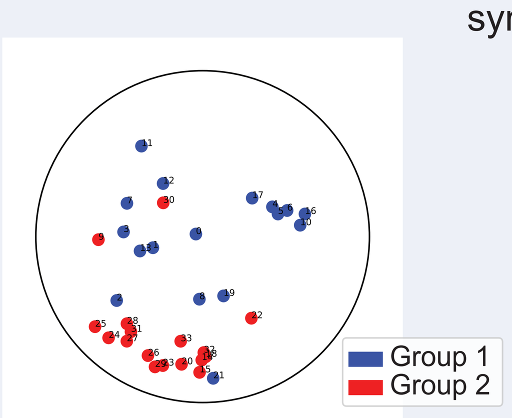
Data on manifolds:
- Geographic data,
- Interaction graphs,
- Correlation matrices,
- Rigid transformations, 3D frames, etc

Parameter Space as manifolds:
- Gaussian family: SPD(n)
- beta distributions: $\mathbb{R}^2_+$
- Hessian manifolds

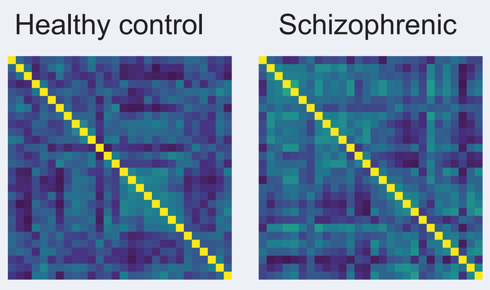
→ Learning that leverages the geometry of the data/parameter space

Cities coordinates
Data on the sphere

Karate Club Network
Data on the hyperbolic space



Brain connectomes
Data on the space of symmetric positive definite matrices



Objectives

- Teach "hands-on" Geometry, Learning and Information Geometry
- Democratize the use of Geometric Learning and Information Geometry in applications
- Support research in Geometric Learning and Information Geometry

Package Description

Geomstats is an open-source Python package for computations and statistics on nonlinear manifolds [Miolane et al., 2020]. geomstats relies on three different back-ends, `numpy`, `pytorch` and `tensorflow` with a generic common API

```
export GEOMSTATS_BACKEND=numpy
import geomstats.backend as gs
```

The package implements tools for over 15 manifolds, each endowed with one or many Riemannian metrics.
- Spaces of constant curvature (Hypersphere , Hyperbolic space with different representations)
- Symmetric Positive Definite matrices
- Lie Groups (Rotations, Rigid-body transformations)
- Linear Subspaces (Grassmannian, Stiefel)
- Curve spaces (Discrete curves, Landmark spaces)
- Probability Distributions (Gaussians, Beta)
- Products of the above

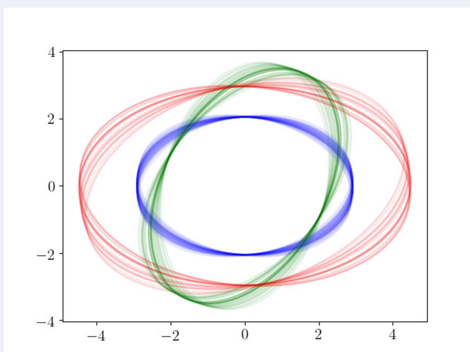


Figure 1: Random samples of SPD matrices from three classes.

Each module exposes methods to handle data that lie on the corresponding manifold, e.g. to sample random points, to check that a point indeed belongs to the manifold, to project vectors to tangent vectors to a point.

```
from geomstats.geometry.hypersphere import
  Hypersphere

sphere = Hypersphere(dim=2)
points = sphere.random_uniform(10)

print(sphere.belongs(points))
```

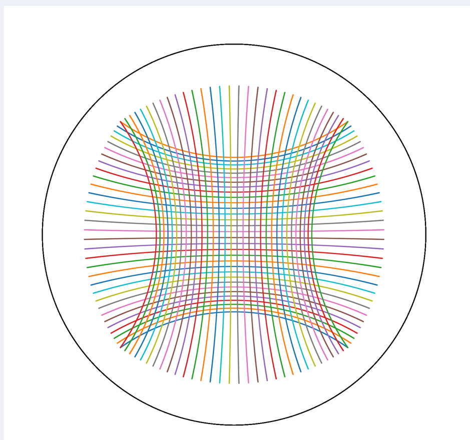


Figure 2: Geodesic grid on Poincaré disk.

Riemannian Metrics expose methods to compute inner-products, geodesics, exponential, logarithm and parallel transport maps. Numerical methods are used when no closed-form solution exist

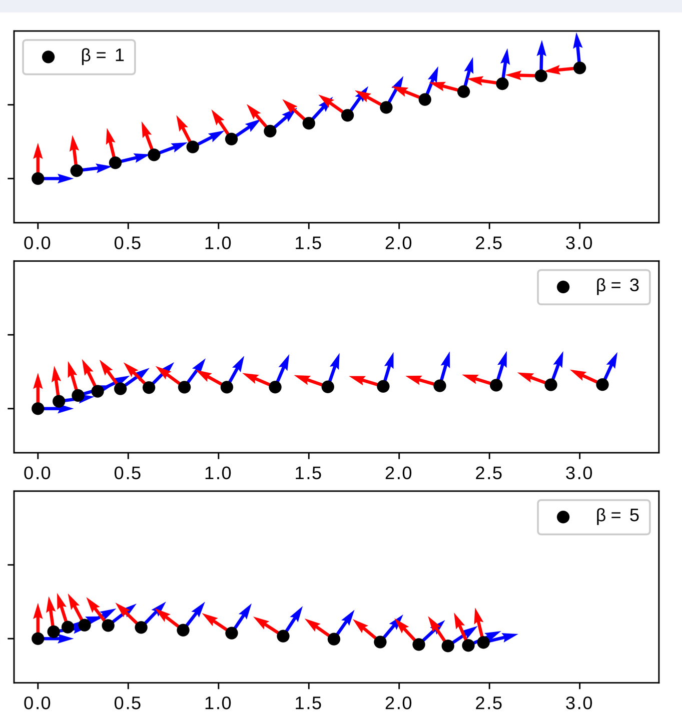


Figure 3: Geodesics in $SE(2)$ with different left-invariant metrics. β is an anisotropy coefficient of the metric. Automatic differentiation and gradient descent allow to compute logarithms by geodesic shooting

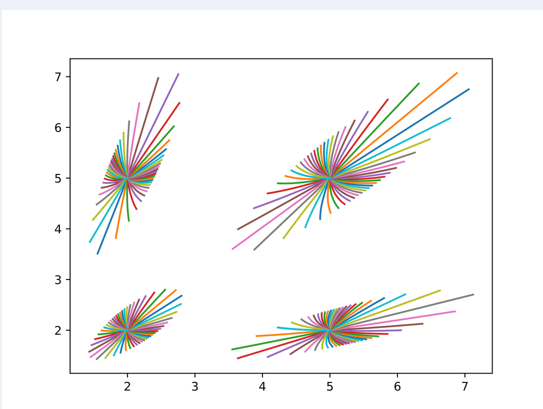


Figure 4: Geodesic balls on the manifold of Beta distributions with the Fisher metric

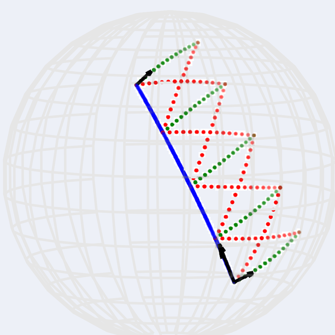


Figure 5: Schild's ladder: a numerical scheme to approach parallel transport [Guigui and Pennec, 2020]

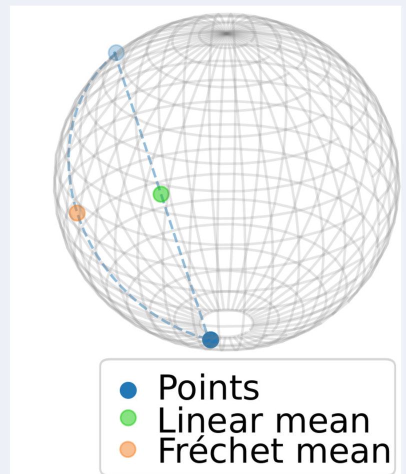
Fréchet Mean

- Generalized definition of the mean: $\bar{x} = \underset{x \in M}{\text{argmin}} \sum_{i=1}^n \text{dist}_M(x, x_i)^2$

→ Fréchet mean belongs to the manifold.

```
from geomstats.learning.frechet_mean import FrechetMean

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



From Logistic Regression to tangent Logistic Regression

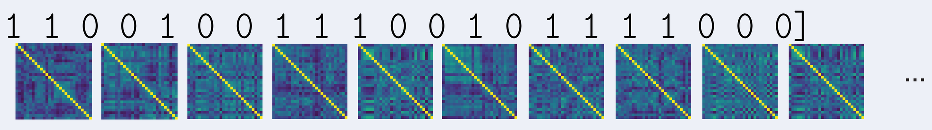
Use scikit-learn on the tangent space at the Fréchet mean

```
from geomstats.learning.preprocessing import ToTangentSpace
from sklearn.linear_model import LogisticRegression
from sklearn.pipeline import make_pipeline

data, patient_ids, labels = data_utils.load_connectomes()
X_train, X_test, y_train, y_test = train_test_split(data, labels, random_state=0)

metric_aff = SPDMetricAffine(n=28)
pipeline = make_pipeline(ToTangentSpace(geometry=metric_aff), LogisticRegression(C=2))
pipeline.fit(X_train, y_train)
pipeline.predict(X_test)
```

> [0 1 1 0 0 1 0 0 1 1 1 0 0 1 0 1 1 1 1 0 0 0]



From k-means to Riemannian k-means

Use Geomstats for unsupervised learning. Below an example of clustering on data from community network, embedded in the hyperbolic space [Gerald et al., 2020].

```
from geomstats.learning.kmeans import RiemannianKMeans

poincare_ball = PoincareBall(2)
karate_graph = data_utils.load_karate_graph()

hyperbolic_embedding = HyperbolicEmbedding()
embeddings = hyperbolic_embedding.embed(karate_graph)

kmeans = RiemannianKMeans(
    riemannian_metric=poincare_ball.metric,n_clusters=2,
    mean_method='frechet-poincare-ball')

centroids = kmeans.fit(X=embeddings, max_iter=100)
labels = kmeans.predict(X=embeddings)
```

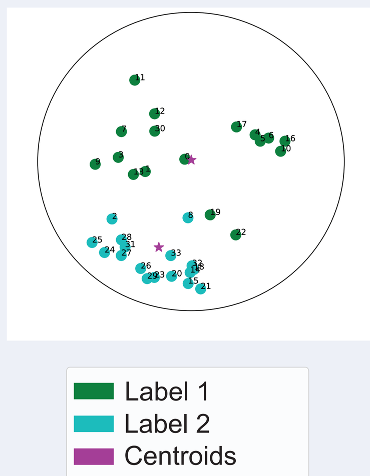


Figure 6: Riemannian k-means on the graph nodes after embedding in the Poincaré ball

Beta distributions to classify histograms

We use maximum likelihood to fit beta distributions to histograms of cortical thickness maps [Brigant et al., 2020]. The manifold of beta distributions endowed with the Fisher-Rao metric has negative curvature. Geodesic distances can be computed numerically to apply k-nearest neighbor or k-means algorithms.

```
from sklearn.neighbors import
  KNeighborsClassifier
from geomstats.geometry.beta_distributions
  import BetaDistributions

beta = BetaDistributions()
embeddings = beta.maximum_likelihood_fit(samples
  )

rnn = KNeighborsClassifier(n_neighbors=9, metric
  =beta.metric.dist)
rnn.fit(embeddings)
```

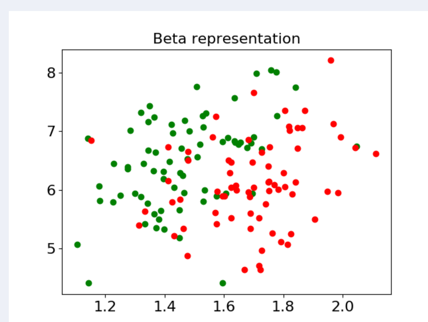


Figure 7: Embedding of the histograms in the 2d-manifold of beta distributions

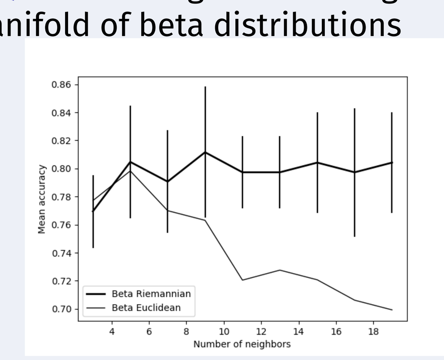


Figure 8: Mean accuracy of KNN classification on the cortical thickness data over 5-fold cross validation

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http://geomstats.ai