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Introduction to Riemannian Geometry and Geometric Statistics: From Basic Theory to Implementation with Geomstats

Nicolas Guigui
Université Côte d'Azur, Inria
nicolas.guigui@inria.fr

Nina Miolane
University of California Santa Barbara
ninamiolane@ucsb.edu

Xavier Pennec
Université Côte d'Azur, Inria
xavier.pennec@inria.fr

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Contents

Introduction to Riemannian Geometry and Geometric Statistics: From Basic Theory to Implementation with Geomstats

Nicolas Guigui[1], Nina Miolane[2] and Xavier Pennec[3]

[1] *Université Côte d'Azur, Inria, France; nicolas.guigui@inria.fr*
[2] *University of California Santa Barbara, USA; ninamiolane@ucsb.edu*
[3] *Université Côte d'Azur, Inria, France; xavier.pennec@inria.fr*

ABSTRACT

As data is a predominant resource in applications, Riemannian geometry is a natural framework to model and unify complex nonlinear sources of data. However, the development of computational tools from the basic theory of Riemannian geometry is laborious. The work presented here forms one of the main contributions to the open-source project geomstats, that consists of a Python package providing efficient implementations of the concepts of Riemannian geometry and geometric statistics, both for mathematicians and for applied scientists for whom most of the difficulties are hidden under high-level functions. The goal of this monograph is two-fold. First, we aim at giving a self-contained exposition of the basic concepts of Riemannian geometry, providing illustrations and examples at each step and adopting a computational point of view. The second goal is to

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demonstrate how these concepts are implemented in Geomstats, explaining the choices that were made and the conventions chosen. The general concepts are exposed and specific examples are detailed along the text. The culmination of this implementation is to be able to perform statistics and machine learning on manifolds, with as few lines of codes as in the wide-spread machine learning tool scikit-learn. We exemplify this with an introduction to geometric statistics.

1

Introduction

Since the formal axiomization of Euclid in his famous *Elements* (dated around 300 BC), geometry was considered as the properties of figures in the plane or in space. The abstract notion of space as a mathematical object emerged in 1827 with C. F. Gauss' *Theorema Egrerium* proving that curvature is an intrinsic quantity of a surface, i.e. that can be computed without reference to a "larger" embedding space. This notion was made precise by the cornerstone work of Riemann (1868)[1] built around the intuitive idea that a mathematical space results from varying a number of independent quantities, later identified as coordinates and formalized in the definition of a manifold by Whitney (1936). Riemannian Geometry (RG) is the study of such differentiable manifolds equipped with an inner product at each point that smoothly varies between points. This allows us to generalize the notions of angles, length and volumes, which can be integrated to global quantities highly coupled with the topology of the space.

Fruitful developments of these ideas allowed unifying previous examples of non-Euclidean geometries, that violate Euclid's parallel postulate (given a point and a straight-line, one and only one parallel straight-line

[1]See Riemann (1873), the English translation by W.K. Clifford

can be drawn through the point). These ideas echoed with the developments of Lagrangian and Hamiltonian mechanics, and were instrumental in formalizing the modern theories of Physics, and especially Einstein's general relativity. They also made profound impact on many areas of mathematics such as group theory, representation theory, analysis, and algebraic and differential topology.

At the intersection of Physics and geometry, groups represent symmetries and transformations between states, and from the modern point of view of Klein's Erlangen program, the study of geometry boils down to studying the action of groups on a space, and their invariants. The work of Elie Cartan enabled significant progress in this direction.

Riemannian geometry has thus become a vast subject that is not usually taught before graduate education in mathematics or physics, and that requires familiarity with many concepts from differential geometry. Hence, although some books on the topic cover most of the pre-requisites and fundamental results of Riemannian geometry, the entry cost for applied mathematicians, computer scientists and engineers is high.

Nowadays, as data is a predominant resource in applications, Riemannian geometry is a natural framework to model and unify complex nonlinear sources of data. However, the development of computational tools from the basic theory of Riemannian geometry is laborious due to often high dimensional and non-exhaustive coordinate systems, nonlinear and intractable differential equations, etc. This monograph aims at providing the computational tools to perform statistics and machine learning on Riemannian manifolds to the wider data science community. The work presented here forms one of the main contributions to the open-source project geomstats, that consists in a Python package providing efficient implementations of the concepts of Riemannian geometry and geometric statistics, both for mathematicians and for applied scientists for whom most of the difficulties are hidden under high-level functions.

Other Python packages do exist and mainly fall under one of two following categories. On the one hand, there are the packages that focus on a single application, for instance on optimization: `Pymanopt` (Townsend *et al.*, 2016), `Geoopt` (Becigneul and Ganea, 2019; Kochurov *et al.*, 2020), `TensorFlow RiemOpt` (Smirnov, 2021), and `McTorch` (Meghwanshi *et al.*, 2018) or on deep learning such as `PyG` (Fey and Lenssen, 2019), where, in this case the geometry is often restricted to graph and mesh spaces. On the other hand, there are packages dedicated to a single manifold: `PyRiemann` on SPD matrices (Barachant, 2015), `PyQuaternions` on 3D rotations (Wynn, 2014), and `PyGeometry` on spheres, tori, 3D rotations and translations (Censi, 2012). Some other packages, like `TheanoGeometry` (Kühnel and Sommer, 2017) are not actively maintained anymore. There is therefore a need for a unified open-source implementation of differential geometry and associated learning algorithms for manifold-valued data.

The goal of this monograph is two-fold. First, we aim at giving a self-contained exposition of the basic concepts of Riemannian geometry, providing illustrations and examples at each step and adopting a computational point of view. We cover the basics of differentiable manifolds (Section 2), Riemannian manifolds (Section 3) and Lie groups (Section 4). Then we delve into more complex structures defined by invariance properties, in particular quotient metrics, and metrics on homogeneous and symmetric spaces (Section 5). Most proofs are omitted for brevity, but references to the proof of each statement are given. The interested reader may refer to the textbooks Lafontaine *et al.* (2004), Gallier and Quaintance (2020), Boumal (2023), and Lee (2003) for more details. Some mathematical definitions from the prerequisites can be found in the lexicon in Appendix A. The second goal is to demonstrate how these concepts are implemented in geomstats, explaining the choices that were made and the conventions chosen. The general concepts are exposed in Section 2.2, and detailed along the text and examples. The culmination of this implementation is to be able to perform statistics and machine learning on manifolds, with as few lines of codes as in the wide-spread machine learning tool `scikit-learn`. We exemplify this in Section 6 with a brief introduction to geometric statistics.

Updates This monograph was written for geomstats version `2.5.0` released in April 2022. There are two categories of code snippets in this monograph: those from the core of the package, that explain how it is implemented, and those for examples and figures. For updates on the former, we invite the interested reader to check the current master branch of the main geomstats repository[2]. In order to ensure compatibility of the latter with future releases of the package, we maintain a companion repository on Github[3].

[2]https://github.com/geomstats/geomstats
[3]https://github.com/geomstats/ftmal-paper

Appendices

A

Lexicon

Definition A.1 (Topology). Let M be a set and $\mathcal{P}(M)$ the set of subsets of M. Then a *topology* on M is a set $\Theta \in \mathcal{P}(M)$ such that

- $\emptyset \in \Theta$ and $M \in \Theta$
- $\forall U, V \in \Theta, U \cap V \in \Theta$
- $C \subseteq \Theta \implies \bigcup_{U \in C} U \in \Theta$

The sets in Θ are called *open* sets, and a set S is said to be *closed* if and only if $M \setminus S \in \Theta$. Such a pair (M, Θ) is called a topological space.

Definition A.2 (Hausdorff). A topological space (M, Θ) is said to be *Hausdorff* if, for any two distinct points $p, q \in M$, there exist open neighborhoods of p and q with empty intersection.

Definition A.3. A topological space (M, Θ) is second-countable if there exists some countable collection $\mathcal{A} = \{U_i\}_{i \in \mathbb{N}}$ of open sets of M such that any open set can be written as a union of elements of $\mathcal{A}$

Definition A.4 (Connected). A topological space (M, Θ) is said to be *connected* unless there exist two non empty open sets $A, B \in \Theta$ such that $A \cap B \neq 0$ and $M = A \cup B$.

Equivalently, M is connected if and only if the only subsets that are both open and closed are M itself and the empty set $\emptyset$.

Definition A.5 (Group). A *group* is a couple $(G, \cdot)$ where G is a nonempty set, and $\cdot : G \times G \to G$ is a map such that

- $\exists e \in G, \forall g \in G,\ e \cdot g = g \cdot e = g$,
- $\forall g \in G, \exists h,\ g \cdot h = h \cdot g = e$. We define the inverse of g for $\cdot$ as $g^{-1} = h$ in this case.

Definition A.6 (Homomorphism). Les $(G, \cdot)$ and $(H, \bullet)$ be two groups, and $f : G \to H$ be a map. Then f is a *homomorphism* if for any $x, y \in G$, $f(x \cdot y) = f(x) \bullet f(y)$.

Definition A.7 (Algebra). An *algebra* over a field K is a vector space $(A, +, \cdot)$ over K equipped with a bilinear multiplicative law $\otimes : A \times A \to A$ such that

- (distributivity) $\forall x, y, z \in A$, $(x + y) \otimes z = x \otimes z + y \otimes z$ and $z \otimes (x + y) = z \otimes x + z \otimes y$
- (compatibility with scalars) $\forall a, b \in K, \forall x, y \in A$, $(ax) \otimes (by) = (ab)x \otimes y$.

Definition A.8 (Injective-Surjective-Bijective map). Let E, F be two sets and $f : E \to F$ a map between E and F. Then we say that

- f is *injective* if for every $x, x' \in E$, $x \neq x' \implies f(x) \neq f(x')$,
- f is *surjective* if for every $y \in F$, there exists $x \in E$ such that $y = f(x)$,
- f is *bijective* if it is both injective and surjective.

Definition A.9 (Continuous map). Let E, F be two topological spaces. $f : E \to F$ is *continuous* of C^0 if for every open set $U \subset F$, its preimage $f^{-1}(U)$ by f is an open set of E.

Definition A.10 (Homeomorphism). Let $f : E \to F$ be a map between two topological spaces. f is called a *homeomorphism* if it has the following properties:

- f is a bijection,
- f is continuous,
- the inverse f^{-1} of f is continuous.

Definition A.11 (Differential map). Let $p, n \in \mathbb{N}$, $f : U \subset \mathbb{R}^n \to \mathbb{R}^p$ a map defined on an open set U, and $x_0 \in U$. We say that f is *differentiable* at x_0 if there exists a linear map L defined in $\mathbb{R}^n$ such that

$$\forall h, \quad f(x_0 + h) = f(x_0) + L(h) + o(\|h\|).$$

In that case, L is unique and is called the differential of f at x_0, and written df_{x_0}.

Definition A.12 (Class C^k). Let $p, n \in \mathbb{N}$, $f : U \subset \mathbb{R}^n \to R^p$ a map defined on an open set U. f is C^1 if it is differentiable on U and the map $x \mapsto df_x$ is continuous on U. Similarly we say that f is C^k or of class C^k for $k \in \mathbb{N} \cup \{\infty\}$ if f is k-times differentiable.

Definition A.13 (C^k-diffeomorphism). Let $k \in (\mathbb{N} \setminus \{0\}) \cup \{\infty\}$ and let $f : U \to V$ be a map between two open sets of $\mathbb{R}^n$. f is called a *diffeomorphism* of class C^k if it has the following properties:

- f is a bijection,
- f is of class C^k,
- the inverse f^{-1} of f is C^k.

Definition A.14 (Inner product). Let E be a real vector space. An inner product is a symmetric positive-definite bilinear map $\langle \cdot, \cdot \rangle : E \times E \to \mathbb{R}$, i.e. $\forall x, y \in E, \langle x, y \rangle = \langle y, x \rangle$ and $\langle x, x \langle > 0 \iff x \neq 0$.

Definition A.15 (σ-algebra). Let M be a set and $\mathcal{P}(M)$ the set of subsets of M. A subset $\Sigma \subseteq \mathcal{P}(M)$ is called σ-*algebra* if it has the three following properties:

- It is closed under complementation: for any set $S \in \Sigma$, $M \setminus S \in \Sigma$;
- M is an element of Σ: $M \in \Sigma$;
- Σ is closed under countable unions: $\forall (S_i)_{i \in \mathbb{N}}$, $\bigcup_i S_i \in \Sigma$.

Definition A.16 (Borel σ-algebra). Let M be a topological set. The *Borel* σ-algebra $\mathcal{B}(M)$ on M is the smallest σ-algebra that contains all the open sets of M.

Definition A.17 (Probability measure). Let $\mathcal{F}$ be a σ-algebra over a set Ω. A probability measure Pr is a function $\Pr : \mathcal{F} \to [0, 1]$ such that:

- Pr is σ-additive: $\forall (S_i)_{i \in \mathbb{N}}$, $\Pr(\bigcup_i S_i) \in \Sigma_i \Pr(S_i)$.
- Pr has unit mass: $\Pr(\Omega) = 1$

B

$SE(n)$ with an anisotropic metric

B.1 Geodesics

Below is the code to plot geodesics of $SE(n)$ with the anisotropic metric described in Example 4.14. The code will be updated on the dedicated Github repository[1].

```
import matplotlib.pyplot as plt

import geomstats.backend as gs
import geomstats.visualization as visualization
from geomstats.algebra_utils import from_vector_to_diagonal_matrix
from geomstats.geometry.invariant_metric import InvariantMetric
from geomstats.geometry.special_euclidean import SpecialEuclidean

SE2_GROUP = SpecialEuclidean(n=2, point_type='matrix')
N_STEPS = 15


def main():
    """Plot geodesics on SE(2) with different structures."""
    theta = gs.pi / 4
    initial_tangent_vec = gs.array([
        [0., - theta, 1],
        [theta, 0., 1],
        [0., 0., 0.]])
    t = gs.linspace(0, 1., N_STEPS + 1)
    tangent_vec = gs.einsum('t,ij->tij', t, initial_tangent_vec)

    fig = plt.figure(figsize=(10, 10))
```

[1] https://github.com/geomstats/ftmal-paper

```
    maxs_x = []
    mins_y = []
    maxs = []
    for i, beta in enumerate([1., 2., 3., 5.]):
        ax = plt.subplot(2, 2, i + 1)
        metric_mat = from_vector_to_diagonal_matrix(gs.array([1, beta, 1.]))
        metric = InvariantMetric(SE2_GROUP, metric_mat, point_type='matrix')
        points = metric.exp(tangent_vec, base_point=SE2_GROUP.identity)
        ax = visualization.plot(
            points, ax=ax, space='SE2_GROUP', color='black',
            label=r'$\beta={}$'.format(beta))
        mins_y.append(min(points[:, 1, 2]))
        maxs.append(max(points[:, 1, 2]))
        maxs_x.append(max(points[:, 0, 2]))
        plt.legend(loc='best')

    for ax in fig.axes:
        x_lim_inf, _ = plt.xlim()
        x_lims = [x_lim_inf, 1.1 * max(maxs_x)]
        y_lims = [min(mins_y) - .1, max(maxs) + .1]
        ax.set_ylim(y_lims)
        ax.set_xlim(x_lims)
        ax.set_aspect('equal')
    plt.savefig('../figures/geo-se2.eps', bbox_inches='tight', pad_inches=0)
    plt.show()


if __name__ == '__main__':
    main()
```

B.2 Curvature

This metric is used already in Example 4.13. From the structure constants and Equation (4.4), we can compute the associated Christoffel symbols at identity for the frame $(\tilde{e_1}, \dots \tilde{e_6})$. Let $\tau = (\sqrt{\beta} + \frac{1}{\sqrt{\beta}})$. We obtain

$$\Gamma_{ij}^{k} = \frac{1}{2\sqrt{2}} \quad \text{if } \; ijk \; \text{ is a cycle of } [1,2,3], \tag{B.1}$$

$$\Gamma_{15}^{6} = -\Gamma_{16}^{5} = -\frac{2}{\tau}\Gamma_{24}^{6} = \frac{2}{\tau}\Gamma_{26}^{4} = \frac{2}{\tau}\Gamma_{34}^{5} = -\frac{2}{\tau}\Gamma_{35}^{4} = \frac{1}{\sqrt{2}}, \tag{B.2}$$

and all the others are null.

Lemma B.1. $(SE(3), g)$ is locally symmetric, i.e. $\nabla R = 0$, if and only if $\beta = 1$.

We can now prove Lemma B.1, formulated as: $(SE(3), g)$ is locally symmetric, i.e. $\nabla R = 0$, if and only if $\beta = 1$. This is valid for any dimension $d \geq 2$ provided that the metric matrix G is diagonal, of size $d(d+1)/2$, with ones everywhere except one coefficient of the translation part.

Proof. For $\beta = 1$, $(SE(d), g)$ is isometric to $(SO(d) \times \mathbb{R}^d, g_{rot} \oplus g_{trans})$. As the product of two symmetric spaces is again symmetric, $(SE(d), g)$ is symmetric.

We prove the contraposition of the necessary condition. Let $\beta \neq 1$. We give i, j, k, l s.t. $(\nabla_{e_i} R)(e_j, e_k)e_l \neq 0$:

$$\begin{aligned}(\nabla_{e_3} R)(e_3, e_2)e_4 &= \nabla_{e_3}(R(e_3, e_2)e_4) - R(e_3, \nabla_{e_3} e_2)e_4 - R(e_3, e_2)\nabla_{e_3} e_4 \\ &= \nabla_{e_3}(R(e_3, e_2)e_4) + \frac{1}{\sqrt{2}} R(e_3, e_1)e_4 - \frac{\tau}{2\sqrt{2}} R(e_3, e_2)e_5.\end{aligned}$$

And from the above

$$\begin{aligned}R(e_3, e_2)e_4 &= \nabla_{e_3}\nabla_{e_2} e_4 - \nabla_{e_2}\nabla_{e_3} e_4 - \nabla_{[e_3,e_2]} e_4 \\ &= -\frac{\tau}{2\sqrt{2}} \nabla_{e_3} e_6 - \nabla_{e_2} e_5 + \frac{1}{\sqrt{2}} \nabla_{e_1} e_4 \\ &= 0. \\ R(e_3, e_1)e_4 &= \nabla_{e_3}\nabla_{e_1} e_4 - \nabla_{e_1}\nabla_{e_3} e_4 - \nabla_{[e_3,e_1]} e_4 \\ &= -\frac{\tau}{2\sqrt{2}} \nabla_{e_1} e_5 - \frac{1}{\sqrt{2}} \nabla_{e_2} e_4 \\ &= -\frac{\tau}{4} e_6 + \frac{\tau}{4} e_6 = 0. \\ R(e_3, e_2)e_5 &= \nabla_{e_3}\nabla_{e_2} e_5 - \nabla_{e_2}\nabla_{e_3} e_5 - \nabla_{[e_3,e_2]} e_5 \\ &= \frac{\tau}{2\sqrt{2}} \nabla_{e_2} e_4 + \frac{1}{\sqrt{2}} \nabla_{e_1} e_5 \\ &= -\frac{\tau^2}{8} e_6 + \frac{1}{2} e_6 = \frac{1}{2}(1 - \frac{\tau^2}{4}) e_6.\end{aligned}$$

And therefore

$$\begin{aligned}\beta \neq 1 &\implies \tau = (\sqrt{\beta} + \frac{1}{\sqrt{\beta}}) \neq 2 \\ &\implies (\nabla_{e_3} R)(e_3, e_1)e_4 = -\frac{\tau}{4\sqrt{2}}(1 - \frac{\tau^2}{4}) e_6 \neq 0,\end{aligned}$$

which proves Lemma B.1. □

B.3 One parameter subgroups

Note that these don't depend on the choice of the metric.

```
import matplotlib.pyplot as plt

import geomstats.backend as gs
import geomstats.visualization as visualization
from geomstats.geometry.special_euclidean import SpecialEuclidean

SE2_GROUP = SpecialEuclidean(n=2, point_type='matrix')
N_STEPS = 30
end_time = 2.7

theta = gs.pi / 3
initial_tangent_vecs = gs.array([
    [[0., - theta, 2], [theta, 0., 2], [0., 0., 0.]],
    [[0., - theta, 1.2], [theta, 0., 1.2], [0., 0., 0.]],
    [[0., - theta, 1.6], [theta, 0., 1.6], [0., 0., 0.]]])
t = gs.linspace(-end_time, end_time, N_STEPS + 1)

fig = plt.figure(figsize=(6, 6))
for tv, col in zip(initial_tangent_vecs, ['black', 'y', 'g']):
    tangent_vec = gs.einsum('t,ij->tij', t, tv)
    group_geo_points = SE2_GROUP.exp(tangent_vec)
    ax = visualization.plot(
        group_geo_points, space='SE2_GROUP', color=col)
ax = visualization.plot(
    gs.eye(3)[None, :, :], space='SE2_GROUP', color='slategray')
ax.set_aspect('equal')
ax.axis("off")
plt.savefig('../figures/exponential_se2.eps')
plt.show()
```

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