"Algorithms for data fitting on some common homogeneous spaces"

Rentmeesters, Quentin

ABSTRACT

In signal processing, we have often to deal with data that belong to non-linear spaces, or manifolds. We can think about the rotation group in pose estimation, the diffusion tensors in image processing, or the Grassmann manifold in subspace tracking techniques. The goal of this thesis is to design algorithms to analyze this kind of data. We first consider averaging problems on Riemannian manifolds. In particular, we study gradient and Newton methods to compute the Karcher mean of rotation matrices and symmetric positive definite matrices. Then, we design a gradient method to compute a geodesic that best fits a set of time-labeled data points. We describe the approach on different symmetric spaces of interest in practical applications. Finally, on some Riemannian manifolds, there is no known algorithm to compute the Riemannian distance between two points. This is the case for the Stiefel manifold, the general linear group, or the symplectic group. We address these problems by developing some optimization schemes that enable us to compute this distance in some cases.

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Rentmeesters, Quentin. Algorithms for data fitting on some common homogeneous spaces. Prom. : Van Dooren, Paul ; Absil, Pierre-Antoine http://hdl.handle.net/2078.1/132587

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Algorithms for data fitting on some common homogeneous spaces

Quentin Rentmeesters

Thesis submitted in partial fulfillment of the requirements for the degree of Docteur en sciences de l’ingénieur

Dissertation committee:
Paul Van Dooren (UCL, Advisor)
Pierre-Antoine Absil (UCL, Advisor)
Philippe Lefèvre (UCL, Chair)
Chafik Samir (Université d’Auvergne, France)
Jean-Charles Delvenne (UCL)
Raf Vandebril (Katholieke Universiteit Leuven, Belgium)
Acknowledgements
First of all, I would like to thank my thesis supervisors Paul Van Dooren and Pierre-Antoine Absil for all their support. I’m thankful to all the members of my thesis committee for all the time they have spent on reading and commenting this manuscript. I’m thankful to Isabelle and Nathalie for all the administrative tasks they did with a lot of patient and efficiency. I’m grateful to all my colleagues in Euler. I have really enjoyed being a PhD student there. I also thank Stephane and Olivier for the nice discussions we had. Last but not least, I would like to thank all my friends and my family for their constant support.
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Chapter 1

Introduction

Analysing data that belong to non-linear spaces, or manifolds, has become a very popular task in recent years. Such kind of data are extremely widespread in many areas of engineering. For instance, the wind directions are represented by points on the circle in orientation statistics. In mechanics, the position of a rigid body in the 3-dimensional space can be represented by the 3 coordinates of its centre of mass and a rotation, which defines the orientation of the rigid body with respect to a reference frame. This space, whose points represent a position and an orientation, is the special Euclidean group $SE(3)$, see [38] for an application in filtering. In medical imaging, one wants to study the structure of the white matter of the brain by analysing the diffusion of water at each voxel. The diffusion of water at one voxel being represented by a 3-dimensional diffusion tensor, i.e. a 3-dimensional symmetric positive definite matrix, specific tools to handle these kind of data are in need, see [18, 43].

In image processing, the shape of an object can be represented as a point on a manifold, called a shape space, which is the set of closed curves in the plane $\mathbb{R}^2$ modulo translation, scaling, rotation and reflection, see [65] and [37] for an overview. In array signal processing, one needs to identify the subspace spanned by the measurements to recover the angles of arrival of a set of sources. This subspace can be seen as a point on the Grassmann manifold. Using this approach, a Bayesian subspace tracking method has been proposed in [55].

An important effort of research has been done in the engineering community, to extend the classical data analysis techniques at our disposal in the Euclidean space $\mathbb{R}^n$ to manifolds. Actually, to Riemannian manifolds, which are manifolds where each tangent space is equipped with an inner product that varies smoothly. They are thus natural extensions of Euclidean spaces. The induced notion of distance is called the Riemannian distance. And, with this notion of distance, most of the data processing techniques at our disposal in $\mathbb{R}^n$ can be extended to the manifold setting. In [43, 58], the authors compute the mean and the variance of a set of points. An extension of linear regression to manifold data using geodesic curves, and even other kind of curves is proposed [36],
and see also [50]. Since these problems do not admit a closed form solution in general, and since most of them have a variational description, the numerical methods designed to solve them often rely on optimization techniques. Optimization on Riemannian manifolds has become more and more popular in the last few decades, see [19] for gradient methods along geodesic curves, [59] for a nice introduction to Riemannian optimization theory on manifolds, and [2, 14], for applications to some classical problems in linear algebra.

Most of the manifolds appearing in practical applications have actually more structure than the Riemannian manifold structure. Some of them have a group structure like the set of rotations in \( \mathbb{R}^3 \) or the special Euclidean group \( SE(3) \). Others, like the Grassmann manifold or the Stiefel manifold are homogeneous in the sense that they look the same at every point. These extra structures are of crucial importance in the design of algorithms tailored to manifold data processing, and, in particular, when the Riemannian structure is compatible with the homogeneous space structure or the group structure.

One of the most basic computational task that one would like to achieve on these non-linear spaces consists in computing the mean of a set of points. Many different notions of mean exist, but in this thesis, we will only consider the so-called Riemannian means or Karcher means. They are defined as the points on the manifold that locally minimize the sum of the squared Riemannian distances between these points and the data points. Observe that, when this definition is particularized to the Euclidean space \( \mathbb{R}^n \), it yields classical notion of (arithmetic) mean obtained by adding all the data points and dividing the result by the number of data points. Unfortunately, as opposed to the Euclidean space \( \mathbb{R}^n \), uniqueness is not guaranteed anymore, and, in general, there is no simple formula to compute these means. Thus, it is often necessary to rely on numerical approximations. In Chapter 3, Newton and gradient methods are compared to compute the Karcher mean of rotation matrices. A gradient method with a step size selection rule that ensures the convergence is also proposed to compute the Karcher mean of a set of symmetric positive definite matrices, and it is also shown that using a Newton method can be advantageous in some cases. Finally, it is shown how to take advantage of the structure of some structured covariance matrices to compute their Karcher mean.

A little more advanced task consists in approximating a set of time labeled data points by a geodesic curve, i.e. a curve that generalizes the notion of straight line. This problem and some of its generalizations to other kind of curves has received much attention in recent years. In Chapter 4, we propose an optimization scheme based on the parametrization of the geodesic curves using their starting point and velocity. To determine the gradient, we use the nice theory of Jacobi fields and show how they can be computed on some Riemannian symmetric spaces like the sphere embedded in \( \mathbb{R}^3 \), the rotation group \( SO(3) \), the set of symmetric positive definite matrices and the Grassmann manifold.

On some spaces, like the Stiefel manifold, despite the fact that its geometry has been well studied [14], computing the distance between two points is not an easy task. Since it is important in Karcher mean computation, in Bayesian
filtering [57], and in clustering [21], we propose a simple numerical scheme to compute this distance and we study under which conditions it converges in Chapter 5. Finally, in Chapter 6, the same problem is also studied on the general linear group $GL(n)$ equipped with a left invariant Riemannian metric [5], and the approach is illustrated on the symplectic group where averaging problems are in need, see [17].

1.1 Related publications/conferences


- 20th International Symposium on Mathematical Theory of Networks and Systems (MTNS), Melbourne Australia. Talk entitled: *Computing the Riemannian log map on the Stiefel manifold.*

- In preparation: Newton and gradient methods for Karcher mean computation of symmetric positive definite matrices.
Chapter 2
Basics on differential geometry

This chapter is a short introduction to differential geometry and Riemannian geometry. Some more specific subjects like Lie groups, homogeneous spaces and symmetric spaces are also covered. This section can be readily skipped by readers who have already a basic background on these subjects. This Chapter is mainly based on [10, 20, 26, 34, 53].

2.1 Manifolds theory

A set $\mathcal{M}$ is a manifold if it locally looks like $\mathbb{R}^n$. To make that precise, let us introduce some definitions.

**Definition 1** (Local coordinate map or chart). *Let $\mathcal{M}$ be a topological space, a local coordinate map is a pair $(U, \phi)$ such that $U$ is an open subset of $\mathcal{M}$ and $\phi$ is a homeomorphism onto a subset of $\mathbb{R}^n$. We say that $(U, \phi)$ is a local coordinate map at $p$ if $p \in U$.***
Definition 2 (Atlas of class $C^k$ ($k \geq 1$)). Let $\mathcal{M}$ be a topological space, an atlas of class $C^k$ on $\mathcal{M}$ is a family of charts

$$\mathcal{A} = \{(U_i, \phi_i)|i \in I\}$$

such that

- $\phi_i(U_i) \subseteq \mathbb{R}^n$ ($n$ is constant for all $i \in I$),
- the $U_i$’s cover $\mathcal{M}$: $\mathcal{M} = \bigcup U_i$,
- if $U_i \cap U_j \neq \emptyset$ then the transition map:

$$\phi_i \circ \phi_j^{-1} : \phi_j(U_i \cap U_j) \subseteq \mathbb{R}^n \to \phi_i(U_i \cap U_j) \subseteq \mathbb{R}^n$$

is a $C^k$-diffeomorphism.

With this atlas $\mathcal{A}$, often called a differentiable structure, it is possible to talk about differentiable real-valued functions on $\mathcal{M}$: $f : \mathcal{M} \to \mathbb{R}$ is differentiable if $f \circ \phi^{-1} : \mathbb{R}^n \to \mathbb{R}$ is differentiable. The set of $r$-differentiable real-valued functions on $(\mathcal{M}, \mathcal{A})$ is denoted by $C^r(\mathcal{M})$.

Different atlases can define the same differentiable structure, i.e. the corresponding set of differentiable real-valued functions will be the same. To circumvent this issue, we can define a maximal atlas $\hat{\mathcal{A}}$ from $\mathcal{A}$ by adding to $\mathcal{A}$, all the charts that are compatible with $\mathcal{A}$. By compatible, we mean that the charts must satisfy Definition 2.

Definition 3 (Manifold). A set $\mathcal{M}$ is a manifold if it is a topological space and it has a differentiable structure.
Remark: Notice that \((U, \phi^{-1})\) is a local parametrization. The co-domain of \(\phi\) is \(\mathbb{R}^n\) and its image must be an open set of \(\mathbb{R}^n\) since we have required that \(\phi\) is an homeomorphism. By requiring this, we induce a topology on \(\mathcal{M}\) if the set \(\mathcal{M}\) does not come equipped with a topology. The open sets in \(\mathcal{M}\) will be the reverse image of the open sets of \(\mathbb{R}^n\). A basis for the topology on \(\mathcal{M}\) is given by the \(U_i\)'s of the maximal atlas, i.e. the open sets in \(\mathcal{M}\) are arbitrary unions of \(U_i\)'s. This topology can be also defined using one atlas \(\mathcal{A}\): \(U\) is open if \(\phi_i(U \cap U_i)\) is open for every chart \((U_i, \phi_i) \in \mathcal{A}\). The topology is often required to be Hausdorff (separable) and second countable. The topology induced from the charts does not necessarily satisfy these two properties.

In this thesis, we only consider smooth manifolds.

### 2.2 Tangent vectors and tangent spaces

Let \(G(p)\) be the ring of real-valued smooth functions locally defined at \(p \in \mathcal{M}\), we have the following definition:

**Definition 4.** A tangent vector at a point \(p \in \mathcal{M}\) is a derivation, i.e. a map \(X_p : G(p) \to \mathbb{R}\) such that

- \(X_p(\alpha f + \beta g) = \alpha X_p(f) + \beta X_p(g)\) Linearity,
- \(X_p(fg) = X_p(f)g(p) + f(p)X_p(g)\) Leibniz rule,

for all \(\alpha, \beta \in \mathbb{R}\) and \(f, g \in C^\infty(\mathcal{M})\).

The set of derivations at \(p\) denoted by \(T_p \mathcal{M}\) has a natural vector space structure, and it is the tangent space at \(p\). Observe that there exists many ways to represent a tangent vector at \(p\) using some vector space isomorphisms. Indeed, let \((U, \phi)\) be a chart around \(p\), and let \(t \mapsto \gamma(t)\) be a curve in \(\mathcal{M}\) such that \(\gamma(0) = p\). The image of this curve in the chart \((U, \phi)\) is denoted by \(\hat{\gamma}(t) = \phi(\gamma(t))\). Let \(v = \dot{\gamma}(0) \in \mathbb{R}^n\); it can be shown that

\[
X_p(f) = \frac{d}{dt}f(\gamma(t))|_{t=0} = \frac{d}{dt}f(\phi^{-1}(\hat{\gamma}(t)))|_{t=0} = \frac{d}{dt}f(\phi^{-1}(\phi(p) + tv))|_{t=0}.
\]

Thus, there is a vector space isomorphism between: the equivalence classes of curves that agree with \(\hat{\gamma}\) up to first order \([\gamma]\), the vectors \(v \in \mathbb{R}^n\), and the induced equivalence classes of curves \([\gamma] = [\phi^{-1}(\hat{\gamma})]\).

#### 2.2.1 Differentiable maps between manifolds

A map \(F : \mathcal{M}_1 \to \mathcal{M}_2\) is smooth if its expression on charts is smooth, i.e. if \(p \in \mathcal{M}_1\),

\[
\phi_2 \circ F \circ \phi_1^{-1} : \phi_1(U_1) \to \phi_2(U_2)
\]

is a smooth map.
The differential of a smooth map $F$ at $p$ is a linear map:

$$DF_p : T_p M \to T_{F(p)} M,$$

i.e. it associates a derivation at $p$ to a derivation at $F(p)$, and it is defined by

$$(DF(X_p))_{F(p)}(f) = X_p(f \circ F).$$

The differential $DF_p$ is also denoted by $F^*_p$. If we work in some coordinate system and represent $T_p M$ using $T_{\phi_1(p)} \mathbb{R}^n$, the differential of the map (2.1) is a map from $T_{\phi_1(p)} \mathbb{R}^n$ to $T_{\phi_2(F(p))} \mathbb{R}^n$.

**Definition 5.** Two differentiable structures on the same topological space are different if the identity map is not a diffeomorphism. Two manifolds $M_1$ and $M_2$ are diffeomorphic if there exists a diffeomorphism between them.

**Example 1** (Different differentiable structures on the real line). Let us consider the real line with two manifold structures $M_1$ and $M_2$ defined by the following atlases:

$$\phi_1 : \mathbb{R} \to \mathbb{R}, x \mapsto x,$$

$$\phi_2 : \mathbb{R} \to \mathbb{R}, x \mapsto x^3.$$

These two atlases define two different manifolds since the differentiable structures are different: the identity map between these two manifolds in the natural
coordinates is given by $x \mapsto x^3$, which is not a diffeomorphism. In particular, the function $f(x) = x$ is smooth in $M_1$ since $f \circ \phi_1^{-1}(x) = x$ is a smooth function but it is not smooth in $M_2$ since $f \circ \phi_2^{-1}(x) = x^{1/3}$ is not smooth (its first derivative does not exist at 0). But $M_1$ and $M_2$ are diffeomorphic since the map:

$$M_1 \to M_2 : x \mapsto x^{1/3}$$

is a diffeomorphism. Indeed, its expression on the chart is $x \mapsto x$, which is a diffeomorphism.

Here are some specific maps between manifolds that are important to define submanifolds, quotient manifolds,...

- When the differential of $F$ is injective at each point (it is a map of constant rank), $F$ is an immersion.

- We say that $(M_1, F)$ is a submanifold of $M_2$ if $F$ is an injective immersion. In that case, $F$ is called an inclusion map. The following theorem is useful to build submanifolds.

**Theorem 1** ([61, Theorem 1.38]). Let $M$ and $N$ be two smooth manifolds of dimension $m$ and $n$, respectively. Assume that $F : M \to N$ is a smooth map, that $q$ is a point of $N$, that $P = F^{-1}(q)$ is a non-empty set, and that $dF : T_pM \to T_{F(p)}N$ is surjective for all $p \in P$. Then $P$ has a unique manifold structure such that $(P, i)$ is a submanifold of $M$ ($i$ is the inclusion map). Moreover, $i : P \to M$ is actually an embedding (see the item below), and the dimension of $P$ is $m - n$.

This theorem can be used to show that the sphere $S^2$ is an embedded submanifold of $\mathbb{R}^3$. Indeed, the sphere is the pre-image of 1 by the smooth map $F : \mathbb{R}^3 \to \mathbb{R}$, $(x, y, z) \mapsto x^2 + y^2 + z^2$. Since $DF(x, y, z) = 2xdx + 2ydy + 2zdz$, $DF(x, y, z)$ is surjective (of rank 1) when $(x, y, z) \in S^2$. Consequently, $S^2$ is a 2-dimensional embedded submanifold of $\mathbb{R}^3$.

Furthermore, the tangent plane of the sphere seen as a surface in $\mathbb{R}^3$ at a point $p$, is given by $p + \ker(DF)$.

- An immersion which is a homeomorphism onto its image $F(M_1)$ (with respect to the relative topology or subspace topology on $F(M_1)$, i.e. the open sets are the intersections of the open sets of $M_2$ with $F(M_1)$ ) is an embedding or (imbedding). The dimension of $M_2$ must be greater or equal to the dimension of $M_1$. One simple example of embedding is the inclusion map $i : \mathbb{R}^2 \to \mathbb{R}^3, (x_1, x_2) \mapsto (x_1, x_2, 0)$. The following theorem ensures that any differentiable manifold can be embedded into $\mathbb{R}^n$:

**Theorem 2** (Whitney, 1936). If $M$ is an $n$-dimensional $C^k$-manifold for $1 \leq k \leq \infty$ then there exists a $C^k$-embedding $F : M \to \mathbb{R}^{2n+1}$.
• An immersion from an open subset $U$ of $\mathbb{R}^n$ to $\mathcal{M}$ is a local parameterization of $\mathcal{M}$. If $(U, \phi)$ is a chart of $\mathcal{M}$ then $\phi^{-1}$ is a local parameterization of $\mathcal{M}$.

• $F$ is a diffeomorphism if $F$ is a bijection (one-to-one and onto) and $F^{-1}$ is smooth.

• $F$ is a submersion if its differential is surjective at each point. A surjective submersion is called a quotient map. The canonical example of a submersion is the projection map

$$\pi : \mathbb{R}^3 \to \mathbb{R}^2, (x_1, x_2, x_3) \mapsto (x_1, x_2).$$

It is also a quotient map.

2.2.2 The tangent bundle and vector fields

The tangent bundle is the disjoint union of the tangent spaces of $\mathcal{M}$,

$$T\mathcal{M} = \bigcup_{p \in \mathcal{M}} T_p \mathcal{M} \triangleq \bigcup_{p \in \mathcal{M}} \{(p, v) | v \in T_p \mathcal{M}\},$$

$$= \{(p, v) | p \in \mathcal{M}, v \in T_p \mathcal{M}\}.$$  

It is important to keep track of which tangent spaces the vector $v$ belongs to. That is why the disjoint union is taken. Notice that we can write $(p, X_p) \in T\mathcal{M}$ but also $X_p \in T\mathcal{M}$ by identifying $X_p$ with $(p, X_p)$. Let us denote by $\pi$, the canonical projection:

$$\pi : T\mathcal{M} \to \mathcal{M}, \pi(p, v) = p.$$  

So we have $\pi^{-1}(p) = T_p \mathcal{M}$.

A differentiable map $\sigma : \mathcal{M} \to T\mathcal{M}$ is called a section of the tangent bundle if

$$\pi(\sigma(p)) = p \quad \forall p \in \mathcal{M},$$

i.e., the map $\sigma$ must associate the point $p$ to an element of the fiber $F_p = T_p \mathcal{M}$ containing it. A section of the tangent bundle is a vector field on $\mathcal{M}$ (not necessarily a smooth vector field).

**Theorem 3.** The tangent bundle $T\mathcal{M}$ admits a $(2n\text{-dimensional})$ smooth manifold structure such that $\pi : T\mathcal{M} \to \mathcal{M}$ is a smooth map.

Let $(U, \phi)$ be a chart around $p$ and let us define the basis $(E_1, ..., E_n)$ of the tangent space at $p$ using $E_i : f \mapsto \frac{d}{ds}(f \circ \phi^{-1})(\phi(p) + s e_i)|_{s=0}$, where $(e_1, ..., e_n)$ is the standard basis of $\mathbb{R}^n$. A smooth structure is given by charts of the following form (built from the charts of $\mathcal{M}$):

$$\tilde{\phi}(p, \sum_{i=1}^n v^i E_i) = (\phi(p), v^1, ..., v^n) \in \mathbb{R}^{2n}.$$
Definition 6. Let \( M \) be a smooth manifold, a smooth section of the tangent bundle \((TM, M, \pi)\):

\[
X : M \to TM,
\]
is called a smooth vector field.

The real vector space of smooth vector fields on \( M \) is denoted by \( \mathcal{Y}(M) \).

A more algebraic definition of a vector field is the following:

**Definition 7.** A vector field can also be seen as a linear map \( X : C^\infty(M) \to C^\infty(M) \), which satisfies

\[
X(fg) = f(X(g)) + g(X(f)).
\]

The following construction will be useful in the study of Lie groups. If we take the commutator of two vector fields, we get a vector field. This is not true if we take a simple composition since the composition will not satisfy the Leibniz rule.

**Definition 8.** The Lie bracket of two vector fields \( X, Y \in \mathcal{Y}(M) \) is

\[
[X, Y](f) = X \circ Y(f) - Y \circ X(f).
\]

The commutator is a derivation and so a smooth section. It is obviously linear and it satisfies the Leibniz rule. Indeed, using the Leibniz rule, one obtains:

\[
X \circ Y(fg) = X(Y(f)g + fY(g)) = X \circ Y(f)g + Y(f)X(g) + X(f)Y(g) + fX \circ Y(g),
\]

and

\[
Y \circ X(fg) = Y(X(f)g + fX(g)) = Y \circ X(f)g + X(f)Y(g) + Y(f)X(g) + fY \circ X(g).
\]

Subtracting the latter to the former yields the result. Equipped with this bilinear map, called a Lie bracket, the set of smooth vector fields becomes an infinite dimensional Lie algebra.

**Definition 9.** A Lie algebra is a vector space \( V \) with a binary operation \([.,.]\) called the Lie bracket, that satisfies the following properties:

- **Bi-linearity,**
- **Skew-symmetry:** \([x,y] = -[y,x] \forall x, y \in V,\)
- **Jacobi identity:** \([[[x,y],z] + [[z,x],y] + [[y,z],x] = 0 \forall x, y, z \in V.\)

Let \( \phi : M \to N \) be a smooth map and let \( V \in \mathcal{Y}(M) \) and \( W \in \mathcal{Y}(N) \), we say that these two vector fields are \( \phi \)-related if

\[
W_{\phi(p)} = D\phi(p)[V_p] \forall p \in M,
\]
or equivalently \( W_{\phi(p)}f = V_p(f \circ \phi) \) for any real-valued smooth function \( f \) on \( N \). Note that in this definition, \( V \) and \( W \) are required to be smooth.
Theorem 4 (Proposition 4.10 in [35]). Let $\phi : \mathcal{M} \rightarrow \mathcal{N}$ be a diffeomorphism, and let $V$ be a smooth vector field on $\mathcal{M}$, then the vector field defined pointwise by $W_{\phi(p)} = D\phi(p)[V_p]$ is a smooth vector field.

Let $\phi : \mathcal{M} \rightarrow \mathcal{N}$ be a smooth map, $X, Y \in \mathcal{T}(\mathcal{M})$, $\bar{X}, \bar{Y} \in \mathcal{T}(\mathcal{N})$ such that $X$ is $\phi$-related to $\bar{X}$ and $Y$ is $\phi$-related to $\bar{Y}$, then $[X,Y]$ and $[\bar{X},\bar{Y}]$ are $\phi$-related, i.e.

$$D\phi[X,Y] = [X,Y]_{\phi(p)}.$$

Indeed, we have for any smooth function on $\mathcal{N}$:

$$(D\phi[X,Y])_p f = [X,Y]_p (f \circ \phi),$$

$$= X_p Y(f \circ \phi) - Y_p X (f \circ \phi),$$

$$= X_p ((D\phi Y)(f \circ \phi)) - Y_p ((D\phi X)(f \circ \phi)),$$

$$= X_p (\bar{Y} f \circ \phi) - Y_p (\bar{X} f \circ \phi),$$

$$= (D\phi X)_{\phi(p)} \bar{Y} f - (D\phi Y)_{\phi(p)} \bar{X} f,$$

$$= \bar{X}_{\phi(p)} \bar{Y} f - \bar{Y}_{\phi(p)} \bar{X} f,$$

$$= [\bar{X}, \bar{Y}]_{\phi(p)} f.$$

The Lie derivative is defined using the flow of the vector field $X$ that exists on a neighbourhood of any point. Let $t \mapsto \phi^t(p)$ denote the flow of $X$ starting at $p$. We have

$$\mathcal{L}_X f|_p = \frac{d}{dt} f(\phi^t(p))|_{t=0} = X_p(f),$$

$$\mathcal{L}_X Y = [X,Y],$$

$$X g(Y,Z) = \mathcal{L}_X g(Y,Z) = \frac{d}{dt} g(\phi^t(p)(X(\phi^t(p))), Y(\phi^t(p)))$$

$$= \mathcal{L}_X g(Y,Z) + g(\mathcal{L}_X Y, Z) + g(X, \mathcal{L}_X Z),$$

where $g$ is a smooth 2-form, and $X,Y$ are two smooth vector fields. By smooth 2-form, one means that the smooth real-valued function:

$$p \mapsto g_p(X_p, Y_p),$$

is smooth. The term $X g(Y,Z)$ simply denotes the derivative of this function in the direction $X$. Note that the last relation implicitly defines $\mathcal{L}_X(g)$, the Lie derivative of the 2-form $g$.

### 2.3 Riemannian manifolds, metrics and isometries

A Riemannian manifold is a generalization of the Euclidean space $(\mathbb{R}^n, g_E)$ where $g_E$ is the canonical inner product. The main idea is to specify an inner
product \( g \) (i.e., a symmetric positive definite bi-linear 2-form) on each tangent space such that the function \( p \mapsto g_p(X_p, Y_p) \) is a smooth function for all \( X, Y \in \mathcal{T}(\mathcal{M}) \). Equipped with this structure, a manifold \( \mathcal{M} \) is called a Riemannian manifold. In particular, the metric enables us to define geodesics (a generalization of the notion of straight lines), the distance between two points, and the notion of sectional curvature.

**Definition 10** (Riemannian metric). A Riemannian metric \( g \) is a smooth bi-linear 2-form such that \( g_p \) is an inner product, i.e. \( g_p \) is symmetric positive definite.

**Definition 11** (Isometry [13, p. 38]). Let \((\mathcal{M}_1, g_1)\) and \((\mathcal{M}_2, g_2)\) be two Riemannian manifolds, a diffeomorphism \( \phi : \mathcal{M}_1 \rightarrow \mathcal{M}_2 \) is called an isometry if:

\[
g_{\phi(p)}(X, Y) = g_p(D\phi_p(X), D\phi_p(Y)), \quad \forall p \in \mathcal{M}_1, \forall X, Y \in T_p\mathcal{M}_1.
\]

We say that \( \phi \) is a local isometry if each point \( p \in \mathcal{M}_1 \) has a neighborhood \( U \) such that the restriction \( \phi_U \) is an isometry onto an open subset of \( \mathcal{M}_2 \). An isometry \( \phi : (\mathcal{M}_1, g_1) \rightarrow (\mathcal{M}_2, g_2) \) is called an isometry of \( \mathcal{M} \). A composition of isometries and the inverse of an isometry are again isometries, so the set of isometries of \( \mathcal{M} \) is a group, called the isometry group of \( \mathcal{M} \); it is denoted by \( I(\mathcal{M}) \). (It can be shown that the isometry group is always a finite-dimensional Lie group acting smoothly on \( \mathcal{M} \); see, for example, [31, Vol 1]).

### 2.4 Connections, geodesics, sectional curvature and Jacobi fields

An affine connection defines a way to differentiate smooth vector fields.

**Definition 12** (Affine connection). An affine connection is a \( \mathbb{R} \)-bilinear map \( \nabla : \mathcal{T}(\mathcal{M}) \times \mathcal{T}(\mathcal{M}) \rightarrow \mathcal{T}(\mathcal{M}) \) that satisfies the following properties

\[
\begin{align*}
\nabla_X f Y &= f \nabla_X Y \quad \text{\( C^\infty(\mathcal{M}) \)-linearity in \( X \)} \\
\nabla_X f Y &= (\nabla_X f) Y + f \nabla_X Y \quad \text{Leibniz rule}
\end{align*}
\]

for all \( X, Y \in \mathcal{T}(\mathcal{M}) \) and \( f \in C^\infty(\mathcal{M}) \).

Associated to a connection are its torsion tensor:

\[
T(X, Y) = \nabla_X Y - \nabla_Y X - [X, Y],
\]

and its curvature endomorphism:

\[
R(X, Y) Z = \nabla_X \nabla_Y Z - \nabla_Y \nabla_X Z - \nabla_{[X, Y]} Z.
\]
There exist many affine connections on a manifold. But it is possible to single out one. Let $\mathcal{M}$ be an embedded Riemannian submanifold manifold of the Euclidean space $\mathbb{R}^n$ with the induced metric $g_E|_{\mathcal{T}_p\mathcal{M}}$. There exists a specific connection called the tangential connection that is given by

$$\nabla_X Y|_p = P_{\mathcal{T}_p\mathcal{M}} \frac{d}{dt} Y(p + tX)|_{t=0},$$

where $P_{\mathcal{T}_p\mathcal{M}}$ is the orthogonal projection on the tangent space at $p$ and $\frac{d}{dt} Y(p + tX)|_{t=0}$ is the Euclidean connection or the classical differential of a vector field. It turns out that this connection satisfies two additional properties: it is compatible with the metric, and it is symmetric, see below. We have the following theorem:

**Theorem 5** (Fundamental theorem of Riemannian geometry). There is a unique affine connection such that:

- $Xg(Y, Z) = g(\nabla_X Y, Z) + g(Y, \nabla_X Z)$ compatibility with the metric,
- $[X, Y] = \nabla_X Y - \nabla_Y X$ symmetry or torsion free.

This connection is called the Riemannian connection or the Levi-Civita connection and it can be computed using the Koszul formula:

$$2g(\nabla_X Y, Z) = Xg(Y, Z) + Yg(X, Z) - Zg(X, Y) + g([X, Y], Z) - g([X, Z], Y) - g([Y, Z], X).$$

Using the connection we can define the notion of geodesic curve and parallel vector field along a curve. Let $t \mapsto \gamma(t)$ be a curve in $\mathcal{M}$, $\nabla$ defines a unique operator acting on smooth vector fields along $\gamma$ $D_t : \mathcal{T}(\gamma) \to \mathcal{T}(\gamma)$ which is $\mathbb{R}$-linear, satisfies

$$D_t(fV) = \frac{df}{dt} V + fD_t V \quad \forall f \in C^\infty(\mathcal{M}),$$

and when $V$ is extendible to a smooth vector field $\tilde{V}$ on $\mathcal{M},$

$$D_t V = \nabla_{\dot{\gamma}} \tilde{V}.$$  

**Definition 13** (Geodesic). Let $\gamma : U \subset \mathbb{R} \to \mathcal{M}$, $t \mapsto \gamma(t)$ be a smooth curve in $\mathcal{M}$, it is a geodesic if $D_t\dot{\gamma}(t) = 0 \quad \forall t \in U.$

**Definition 14** (Parallel vector field). A vector field $Y \in \mathcal{T}(\mathcal{M})$ is said to be parallel along a curve $t \mapsto \gamma(t)$ if

$$D_t Y(t) = 0.$$
In this case, we write $Y(t) = \Gamma^{0\to t}_{t\to \gamma(t)} Y(0)$. Since in this thesis, the parallel transport is always along a geodesic curve, we will simply write $Y(t) = \Gamma^{\gamma(0)\to \gamma(t)} Y(0)$.

A geodesic is thus a curve whose tangent vector is parallel, or a curve of acceleration zero. In the Euclidean space $\mathbb{R}^n$ (equipped with the Euclidean connection), the image of geodesics are straight lines.

The following results show that an isometry $\phi$ preserves the Riemannian connection, and the Riemannian curvature endomorphism.

**Theorem 6** (Naturality of the Riemannian Connection [34, Prop. 5.6., p. 71]). Suppose $\phi : (\mathcal{M}_1, g_1) \to (\mathcal{M}_2, g_2)$ is an isometry.

1. $\phi$ takes the Riemannian connection $\nabla^1$ of $g_1$ to the Riemannian connection $\nabla^2$ of $g_2$, in the sense that
   $\phi^*(\nabla^1_X Y) = \nabla^2_{\phi^*X} \phi^*Y$.

2. If $t \mapsto \gamma(t)$ is a curve in $\mathcal{M}$ and $V$ is a vector field along $\gamma$, then
   $\phi^* D_t V = D_t(\phi^* V)$.

3. $\phi$ takes geodesics to geodesics: if $t \mapsto \gamma(t)$ is the geodesic in $\mathcal{M}$ with initial point $p$ and initial velocity $V$, then $\phi \circ \gamma$ is the geodesic in $\mathcal{M}$ with initial point $\phi(p)$ and initial velocity $\phi^* V$.

**Theorem 7** (Lemma 7.2. [34, p. 119]). The Riemannian curvature endomorphism is local isometry invariant. More precisely, if $\phi : (\mathcal{M}_1, g_1) \to (\mathcal{M}_2, g_2)$ is a local isometry, then

$$R^2(\phi^* X, \phi^* Y) \phi^* Z = \phi^*(R^1(X, Y)Z).$$

Let $t \mapsto \gamma(t)$ be a geodesic curve such that $\gamma(0) = p$ and $\dot{\gamma}(0) = V$, the exponential map is given by

$$\exp_p(V) = \gamma(1),$$

and thus $\gamma(t) = \exp_p(tV)$. Note that the exponential map defines a local diffeomorphism from an open subset $U$ of $T_p\mathcal{M}$ containing 0 to $\exp_p(U) \subset \mathcal{M}$. Thus, we can use the inverse of the exponential map, defined locally around $p$, to build a chart $(\exp(U), \exp^{-1}_p)$. This set of coordinates are called normal coordinates. Let $c : [a, b] \to \mathcal{M}$ be a piecewise regular ($\dot{c}(t) \neq 0 \forall t \in [a, b]$) smooth curve on a connected Riemannian manifold $(\mathcal{M}, g)$, its length is defined by

$$L(c) = \int_a^b \sqrt{g(\dot{c}(t), \dot{c}(t))} dt.$$
Note that this integral does not depend on the parameterization of \( c \), i.e., \( L(c) = L(c \circ \alpha) \) for any diffeomorphism \( \alpha : [c, d] \to [a, b] \). The connected Riemannian manifold \((\mathcal{M}, g)\) becomes a metric space with the distance:

\[
d(p, q) = \inf\{ c \text{ is a piecewise regular smooth curve} | c(0) = p, \ c(1) = q \}.
\]

The following theorem relates a property of the exponential map and the completeness of the metric space \((\mathcal{M}, d)\).

**Theorem 8** (Hopf-Rinow Theorem, see [10]). Let \( \mathcal{M} \) be a connected Riemannian manifold. The following conditions are equivalent:

1. \( \mathcal{M} \) is a complete metric space where the distance from \( p \) to \( q \) in \( \mathcal{M} \) is defined as the minimum length of all curves from \( p \) to \( q \).
2. For some \( p \in \mathcal{M} \), the exponential map \( \exp_p \) is defined on all of \( T_p \mathcal{M} \).
3. For all \( p \in \mathcal{M} \), the exponential map \( \exp_p \) is defined on all of \( T_p \mathcal{M} \).

Any of these conditions imply:

4. Any two points \( p \) and \( q \) of \( \mathcal{M} \) can be joined by a geodesic whose length is the distance from \( p \) to \( q \).

Let \( \mathcal{M} \) be a complete Riemannian manifold, and thus by Hopf-Rinow, the exponential map is defined for all time \( t \) and it is thus surjective. Let \( t \mapsto \gamma(t) \) be a geodesic curve such that \( \gamma(0) = p \). We say that \( \gamma(t_c) \) is a cut point of this geodesic when the geodesic \( t \mapsto \gamma(t) \) stops to be minimizing after \( t_c \). Notice that \( t_c > 0 \) since \( \exp_p \) is a local diffeomorphism on a sufficiently small ball in \( T_p \mathcal{M} \). The union of the cut points of all geodesics that start at \( p \) is called the cut locus at \( p \) and it is denoted by \( C(p) \). We can also look at \( C(p) \) in the tangent space at \( p \). Let

\[
\mathcal{B}_p = \{ V \in T_p \mathcal{M} \mid d(\exp_p(V), p) = \|V\| \},
\]

the boundary of \( \mathcal{B}_p \) is called the cut locus in \( T_p \mathcal{M} \). The injectivity radius is defined by:

\[
\text{inj}(\mathcal{M}) = \min\{\|V\| \mid p \in \mathcal{M}, \ V \in \partial \mathcal{B}_p \},
\]

i.e. it is the largest \( r \) such that \( \exp_p \), restricted to the open ball of radius \( r \) is an embedding. We also use the notation \( \text{inj}(p) \) when the \( \min \) is not taken over any \( p \in \mathcal{M} \). Let

\[
\mathcal{D}_p = \{ q \in \mathcal{M} \mid d(p, q) < \text{inj}(p) \}.
\]

on \( \mathcal{D}_p \), we can define the inverse of the exponential map called the Riemannian log-mapping and denoted by \( \exp_p^{-1} : \mathcal{D}_p \to T_p \mathcal{M} \). In this thesis, we will consider a broader definition. Let

\[
\mathcal{L}_p(q) = \{ V \in T_p \mathcal{M} \mid \gamma_V(1) = q \},
\]

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where $t \mapsto \gamma_V(t)$ is a geodesic curve starting at $p$ and such that $\dot{\gamma}(0) = V$. Any element of the set $\mathcal{L}_p(q)$ will be called a log-mapping. Note that the element(s) of $\mathcal{L}_p(q)$ of smallest norm correspond(s) to a minimizing geodesic $t \mapsto \gamma_V(t)$. This definition is used in Chapter 5 and in Chapter 6.

The sectional curvature of a section $s$ of the tangent space $T_p\mathcal{M}$ is defined by

$$\kappa(X,Y) = \frac{g(R(X,Y)Y,X)}{g(X,X)g(Y,Y) - g(X,Y)^2},$$

where $X$ and $Y$ form a basis of $s$. Since $\kappa$ depends only on span$(X,Y)$, this is well defined.

**Definition 15** (Jacobi field). Let $\gamma : [0,a] \to \mathcal{M}$, $t \mapsto \gamma(t)$ be a geodesic curve. A vector field $t \mapsto J(t)$ is a Jacobi field along $\gamma$ if it satisfies the following equation:

$$D_t^2 J + R(J,\dot{\gamma}(t))\dot{\gamma}(t) = 0. \quad (2.2)$$

Since this last equation is a second order linear differential equation, every Jacobi field is uniquely determined by choosing two boundary conditions. For instance, we can fix $J(t^*)$ and $\dot{J}(t^*)$ at $t^*$ or fix $J(0)$ and $J(a)$.

A variation through geodesics, also called a 1-parameter family of geodesics, is a smooth map $\Omega : [-\epsilon,\epsilon] \times [0,a] \to \mathcal{M}$, such that, for any fixed $s$, $t \mapsto \Omega(s,t)$ is a geodesic curve. It can be shown that every Jacobi field arises as the variational vector field of a variation through geodesics, see, e.g., [10]. More precisely, $t \mapsto J(t)$ is a Jacobi field if and only if $J(t) = \partial_s\Omega(s,t)|_{s=0}$ for some variation through geodesics $\Omega$.

Indeed, let us define the two following vector fields along $\Omega$:

$$T(s,t) = \partial_t\Omega(s,t), \quad S(s,t) = \partial_s\Omega(s,t).$$

Since $\Omega$ is smooth, we have

$$[T,S] = [D\Omega[\partial_t], D\Omega[\partial_s]] = D\Omega[[\partial_s, \partial_t]] = 0,$$

since $[\partial_s, \partial_t] = 0$ (for any smooth function $f$, $[\partial_s, \partial_t]f = 0$). Using the definition of the Riemannian curvature endomorphism, one obtains:

$$R(S,T)T = \nabla_S\nabla_T T - \nabla_T\nabla_S T - \nabla_{[S,T]} T = -\nabla_T \nabla_S T, \quad (2.3)$$

since $[S,T] = 0$, and $\nabla_T T = 0$ since $\Omega$ is a variation through geodesics. Using the torsion free property of the Riemannian connection, one obtains

$$\nabla_T \nabla_S T - \nabla_S \nabla T = [S,T] = 0,$$

and we can replace $\nabla_S T$ by $\nabla_T S$ in (2.3), which yields:

$$\nabla_T \nabla_T S + R(S,T)T = 0.$$
Setting \( s = 0 \), yields the Jacobi equation (2.2).

The Jacobi field equation (2.2) is particularly easy to solve on Riemannian symmetric spaces. Indeed, on these spaces, the Riemannian curvature endomorphism is parallel, i.e. \( \nabla R = 0 \). This means that \( \nabla_W R = 0 \forall W \in \mathfrak{X}(\mathcal{M}) \) where the covariant derivative of a tensor is defined by

\[
(\nabla_W R)(X, Y, Z) = \nabla_W(R(X, Y)Z) - R(\nabla_W X, Y)Z - R(X, \nabla_W Y)Z - R(X, Y)\nabla_W Z,
\]

for any smooth vector fields \( X, Y, Z, W \). So if \( X \) is a vector field along \( \gamma \), we obtain

\[
D_t R(X, \dot{\gamma}(t))\dot{\gamma}(t) = R(D_t X, \dot{\gamma}(t))\dot{\gamma}(t).
\]

Thus, if \( X \) is parallel along \( \gamma \), \( R(X, \dot{\gamma}(t))\dot{\gamma}(t) \) is also parallel along \( \gamma \). Consequently, by choosing a parallel frame \((E_1(t), \ldots, E_n(t))\) along \( \gamma \), we obtain a second order constant coefficients differential equation. More precisely, let \( J(t) = \sum_{i=1}^{n} J_i(t) E_i(t) \), the equation (2.2) becomes

\[
\sum_{i=1}^{n} \dot{J}_i(t) E_i(t) = \sum_{i=1}^{n} J_i(t) R(E_i(t), \dot{\gamma}(t))\dot{\gamma}(t),
\]

\[
= \sum_{i=1}^{n} J_i(t) \sum_{j=1}^{n} r_{ij} E_j(t),
\]

where the \( r_{ij} \)'s for \( 1 \leq j \leq n \) denote the components of \( R(E_i(t), \dot{\gamma}(t))\dot{\gamma}(t) \) in the frame, and the \( r_{ij} \)'s do not depend on the time since \( R(E_i(t), \dot{\gamma}(t))\dot{\gamma}(t) \) is parallel along \( \gamma \). In this thesis, Jacobi fields are used to derive explicit expressions for the Hessian of the squared Riemannian distance function in Chapter 3, and also to compute the differential of the map: \( h : T\mathcal{M} \to \mathcal{M}, (p, v) \mapsto \exp_p(v) \) in Chapter 4.

### 2.5 Lie groups

Since most of the manifolds encountered in engineering and physics are homogeneous spaces, this topic deserves at least a small introduction. Homogeneous spaces are spaces that look the same everywhere. In order to describe what we mean by "looking the same everywhere", we first need to study the theory of Lie groups and their actions on manifolds. The theory of homogeneous spaces has been well studied, see, e.g., [31]. When the homogeneous structure is compatible with the Riemannian structure, there exist algebraic expressions for geodesics, curvature endomorphisms, and even parallel transports. They are thus particularly suited to derive numerical algorithms. This section is mainly based on [1, 9, 34, 35].
2.5.1 Lie groups

A Lie group is a group that has also a manifold structure such that the group operation is smooth. Let us first introduce some definitions.

**Definition 16** (Group). A group is a set $G$ with an operation called the group operation denoted multiplicatively

$$
\mu : G \times G \to G, \ (g_1, g_2) \mapsto g_1g_2
$$

such that:

1. **Closedness**
   $$
   \forall g_1, g_2 \in G, \ g_1g_2 \in G
   $$

2. **Associativity**
   $$
   \forall g_1, g_2, g_3 \in G \ (g_1g_2)g_3 = g_1(g_2g_3)
   $$

3. There exists a neutral element
   $$
   \exists e \in G \ s.t. \ \forall g \in G ge = eg = g
   $$

4. Each element has an inverse
   $$
   \forall g \in G \ \exists g^{-1} \ s.t. \ gg^{-1} = e
   $$

When the operation is commutative the group is called abelian. It can be shown that the identity element $e$ is unique and that the inverse on the right is also the inverse on the left and it is unique.

**Definition 17** (Lie group). A lie group $G$ is a group such that the group operation $\mu : G \times G \to G$ is a smooth map ($C^\infty$).

Let us define the two following smooth maps $G \to G$:

$$
L_h(g) = hg \text{ and } R_h(g) = gh,
$$
called the left and right actions, respectively.

**Theorem 9.**

1. $L_h$ and $R_h$ are diffeomorphisms.

2. The group operation $\mu : G \times G \to G$ is a submersion.

3. The inverse map $\text{Inv} : G \to G, \ g \mapsto g^{-1}$ is a diffeomorphism.

**Example 2** (Example: the set $SO(2)$ of rotations in $\mathbb{R}^2$). It is a 1-dimensional manifold and it has a group structure. Rotations are in 1 to 1 correspondence with the circle $S^1$. 

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Let \( g \) be a rotation in \( \mathbb{R}^2 \). A rotation can be represented as a linear map \( g : \mathbb{R}^2 \to \mathbb{R}^2 \). On an orthonormal basis of \( \mathbb{R}^2 \), this linear map admits the following matrix representation:

\[
R = \begin{bmatrix}
cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{bmatrix} = \exp \begin{bmatrix} 0 & -\theta \\ \theta & 0 \end{bmatrix},
\]

which corresponds to a rotation around the origin of an angle \( \theta \) anti-clockwise if \( \theta > 0 \). We also have

\[
\begin{bmatrix}
cos(\alpha) & -\sin(\alpha) \\
\sin(\alpha) & \cos(\alpha)
\end{bmatrix}_{g_{\alpha}} \begin{bmatrix}
cos(\beta) & -\sin(\beta) \\
\sin(\beta) & \cos(\beta)
\end{bmatrix}_{g_{\beta}} = \begin{bmatrix}
cos(\alpha + \beta) & -\sin(\alpha + \beta) \\
\sin(\alpha + \beta) & \cos(\alpha + \beta)
\end{bmatrix}_{g_{\alpha + \beta}}.
\]

So \( SO(2) \) is isomorphic to \((S^1, +)\).

The following example is very important since many manifolds appearing in practical applications can be seen as Lie subgroups of the general linear group. **Example 3** (The general linear group \( GL(n, \mathbb{R}) \) or simply \( GL(n) \) is the set of non-singular \( n \times n \) real matrices \( \mathbb{R}^{n \times n} \)).

\[
GL(n) : \{ A \in \mathbb{R}^{n \times n} \mid \det A \neq 0 \}.
\]

The function \( A \mapsto \det A \) is a polynomial function of the entries of the matrix \( A \) and so it is a smooth function. Since \( \mathbb{R}/0 \) is an open set, its reverse image will be an open set. Hence, \( GL(n) \) is an open subset of \( \mathbb{R}^{n \times n} \cong \mathbb{R}^{n^2} \) and thus a manifold. Let \( A_1, A_2 \in \mathbb{R}^{n \times n} \) and \( A_3 = A_1A_2 \), the entries of \( A_3 \) are polynomial functions of the entries of \( A_1 \) and \( A_2 \) and so the product operation is smooth. Notice that the map \( A \mapsto A^{-1} \) is also smooth. Indeed, using the Cramer rule, the entries of \( A^{-1} \) are rational functions of the entries of \( A \) whose denominator is different of 0, so there are smooth functions. The general linear group has two connected components: the matrices of positive determinant (this is the identity component denoted by \( GL^+(n) \)), and the matrices of negative determinant.

**Example 4** (The isometry group of a Riemannian manifold \( I(M) \)). It is always finite dimensional.

**Definition 18** (Homomorphism of Lie groups). An homomorphism is a map that preserves the structure. Hence, for a Lie group, it is a smooth map \( F : G \to H \) (with respect to the smooth structure of \( G \) and \( F \)) that satisfies:

\[
F(g_1g_2) = F(g_1)F(g_2) \quad \forall g_1, g_2 \in G.
\]

Let \( e_G \) be the identity element in \( G \), we have \( F(e_G) = F(e_G)^2 \) which by multiplying both sides by \( F(e_G)^{-1} \) implies \( F(e_G) = e_H \). So the identity element in \( G \) is necessarily mapped to the identity element in \( H \). Furthermore, we have

\[
F(e_G) = F(gg^{-1}) = e_H = F(g)F(g^{-1}),
\]

which implies that \( F(g^{-1}) = F(g)^{-1} \).
**Definition 19** (Lie subgroups). $H$ is a Lie subgroup of $G$ if $H$ is a subgroup of $G$ and a submanifold of $G$.

**Theorem 10** (Cartan’s theorem). A closed subgroup of $G$ admits a unique smooth structure which makes it an embedded Lie subgroup of $G$, i.e., a Lie subgroup such that the inclusion map is a smooth embedding.

**Definition 20.** A matrix Lie group is a Lie subgroup of $GL(n)$.

Cartan’s Theorem is useful to generate Lie subgroups of $GL(n)$ by adding some polynomial constraints.

**Special linear group**

$$SL(n) = \{ A \in GL(n) \mid \det(A) = 1 \}$$

**Orthogonal group**

$$O(n) = \{ A \in GL(n) \mid A^\top A = I_n \}$$

Notice that any $A \in O(n)$ preserves the euclidean inner product in $\mathbb{R}^n$: $g_E(x, y) = x^\top y$. This group is composed of two connected components: $\{ A \in O(n) \mid \det(A) = 1 \}$ and $\{ A \in O(n) \mid \det(A) = -1 \}$.

**Special orthogonal group**

$$SO(n) = \{ A \in O(n) \mid \det(A) = 1 \}$$

The general linear group plays a very important role in the theory of Lie groups mainly because any connected Lie group $G$ admits an almost faithful (i.e. one-to-one or injective) representation, i.e., a smooth map and a group homomorphism

$$F : G \to GL(V),$$

where $GL(V)$ is the set of invertible linear maps from a vector space $V$ to itself. The term almost faithful means here that the kernel: $\ker(F) = \{ g \in G \mid F(g) = e \}$ is of measure zero.

### 2.5.2 Lie algebras and left invariant vector fields

**Definition 21.** A left invariant vector field (l.i.v.f.) on a Lie group $G$ is a vector field $p \mapsto X(p)$ which satisfies

$$DL_g(X(p)) = X(gp).$$

To uniquely define a left invariant vector field, it suffices to specify it at a point, the identity $e$ for example, and then to extend it at any $g$ using the isomorphism $DL_g$. The set of left invariant vector fields is called the Lie algebra of $G$, and it is denoted by a lower case gothic letter $\mathfrak{g}$. 

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Theorem 11 (Proposition 3.7 in [61]). Let $G$ be a Lie group and $\mathfrak{g}$ its set of left invariant vector fields.

- $\mathfrak{g}$ is a real vector space, and the map $\alpha : G \to T_e G$ defined by $\alpha(X) = X(e)$ is an isomorphism of $\mathfrak{g}$ with the tangent space $T_e G$. Thus, $\dim(\mathfrak{g}) = \dim(G)$.
- Left invariant vector fields are smooth.

Observe that $\mathfrak{g}$ is a Lie algebra in the sense of definition 9 where the bracket operation is given by the commutator of smooth left invariant vector fields. Since the set of l.i.v.f’s $\mathfrak{g}$ is isomorphic to the vector space $T_e G$, the Lie bracket must have a simple representation on $T_e G$. Here are two examples:

- The Lie algebra $\mathbb{R}^3$ with the vector product $[u, v] = u \times v$, see Table 2.1 is one representation of the Lie algebra of the special orthogonal group $SO(3)$.
- $\mathbb{R}^{n \times n}$ is the Lie algebra of the general linear group $GL(n)$ with the matrix commutator $[A, B] = AB - BA$ as Lie bracket.

Here are Lie algebras of some Lie subgroups of the general linear group:

**General linear group**

\[ \mathfrak{gl}(n) = \mathbb{R}^{n \times n}, \]

**Special linear group**

\[ \mathfrak{sl}(n) = \{ A \in \mathbb{R}^{n \times n} \mid \text{tr}(A) = 0 \}, \]

**Orthogonal group and special orthogonal group**

\[ \mathfrak{o}(n) = \mathfrak{so}(n) = \{ A \in \mathbb{R}^{n \times n} \mid A = A^\top \}. \]

They are all equipped with the matrix commutator as Lie bracket. Left invariant vector fields can be used to show that the tangent bundle of any Lie group is trivial, i.e. $TG \cong G \times T_e G$. Indeed, we can build the following tangent bundle isomorphism:

\[ G \times T_e G \to TG \quad (g, v) \mapsto (g, DL_g v), \quad v \in T_e G \quad (2.4) \]

Or equivalently, let $(E_1, \ldots, E_n)$ be a basis of the tangent space $T_e G$, since $DL_g$ is an isomorphism, $(DL_g[E_1], \ldots, DL_g[E_n])$ is a basis of $T_g G$. Thus, $g \mapsto (DL_g[E_1], \ldots, DL_g[E_n])$ defines a smooth basis, called a frame, on $G$.

**Theorem 12.** Left invariant vector fields are complete, i.e., the flow $\phi^t(I)$ of a l.i.v.f $V$ has domain $\mathbb{R} \times G$. 

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\[ \tilde{v} = (v_1, v_2, v_3) \in \mathbb{R}^3 \]\[ v = \begin{bmatrix} 0 & -v_3 & v_2 \\ v_3 & 0 & -v_1 \\ -v_2 & v_1 & 0 \end{bmatrix} \]
\[ g_p(\tilde{v}, \tilde{v}) = \|\tilde{v}\|_2^2 \]
\[ [\tilde{v}, \tilde{w}] = \tilde{v} \times \tilde{w} \]
\[ [v, w] = vw - wv \]

Table 2.1: Representation of \text{so}(3)

On the general linear group, this flow is the solution of \( \frac{d}{dt} \phi^t(I) = DL_{\phi^t(I)}v \), which yields
\[ \phi^t(I) = e^{tV} , \]
where \( e^{tV} \) stands for the matrix exponential defined by
\[ e^{tV} = \sum_{k=0}^{\infty} \frac{(tV)^k}{k!} \].

**Definition 22** (Lie group exponential map). Let \( t \mapsto \gamma(t) \) be an integral curve of the left invariant vector field \( v \in \mathfrak{g} \), i.e. \( \dot{\gamma}(0) = v \) and \( \dot{\gamma}(t) = L_{\gamma(t)}v \) such that \( \gamma(0) = e \). The Lie group exponential map is defined by:
\[ \exp : \mathfrak{g} \to G, \ v \mapsto \gamma(1) \].

It can be shown that every Lie group homomorphism from \((\mathbb{R}, +)\) to \( G \), i.e. a one-parameter subgroup of \( G \) is of the form \( t \mapsto \gamma(t) \in G \) where \( \gamma \) is defined as above.

### 2.5.3 Adjoint representations

Let us define the following mapping:
\[ C_g(h) = ghg^{-1} , \]
called a conjugation by \( g \). Notice that the fixed points \( p \) of \( C_g \) are the elements of \( G \) that commute with \( g \). The conjugation by \( g \) defines a homomorphism of group since
\[ C_g(h_1h_2) = C_g(h_1)C_g(h_2) , \]
which implies \( C_g(e) = e \) and \( C_g(h^{-1}) = C_g(h)^{-1} \).

The differential of the conjugation at the identity element \( e \):
\[ DC_g(e) : T_eG \to T_{C_g(e)=e}G \]
defines a linear map on the Lie algebra:
\[ Ad_g = DC_g(e) : \mathfrak{g} \to \mathfrak{g} \].

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Theorem 13. The adjoint mapping:

\[ Ad : G \rightarrow GL(g), \]

is a linear representation, i.e. a smooth homomorphism.

If \( G \) is a matrix Lie group (i.e. a closed subgroup of \( GL(n, \mathbb{R}) \)), then its Lie algebra is a Lie sub-algebra of \( \mathfrak{gl}_n(\mathbb{R}) \), i.e. a sub-vector space of \( \mathfrak{gl}_n(\mathbb{R}) \) that is closed under the Lie bracket operation. In this case, the adjoint map is given by \( Ad_g(x) = \frac{d}{dt} ge^{tx} g^{-1} \big|_{t=0} = gxg^{-1} \).

2.6 Homogeneous spaces

In this section, we consider Lie groups as transformation groups acting on manifolds. These transformation groups often represent the transformations that leave invariant some extra structures. For instance, the group of diffeomorphisms of \( M \) that preserve the Riemannian metric. This group is called the isometry group, and when it is sufficiently large, it is useful to derive expressions for the geodesic curves. In this section, we introduce the basic definitions and mention two theorems that are useful to generate most of the manifolds encountered in practical applications.

Definition 23. Let \( G \) be a Lie group and \( M \) be a smooth manifold. A left action of \( G \) on \( M \) is a smooth mapping:

\[ \lambda : G \times M \rightarrow M, \]

which satisfies

\[ \lambda(e, m) = m, \]

where \( e \) is the identity element of \( G \) and

\[ \lambda(g_1g_2, m) = \lambda(g_1, \lambda(g_2, m)). \]

A very common shorthand notation for the left action is the following:

\[ \lambda(g, m) = g \cdot m. \]

We could also define a right action: \((g, m) \mapsto m \cdot g\). Since we have

\[ m \cdot (g_1g_2) = (m \cdot g_1) \cdot g_2, \]

the right action of a group element \( g_1g_2 \) consists in applying first \( g_1 \) and then \( g_2 \). For the left action, that is the contrary. We will only consider left actions. This is without loss of generality, since the following map: \((g, m) \mapsto g^{-1} \cdot m\), where the action (on the left) is actually a right action.

Let us now introduce some properties of the left action.
**Definition 24.** A left action is effective or faithful if:

\[ g \cdot p = p \quad \forall p \in M \Rightarrow g = e. \]

Note that, by definition we have \( e \cdot p = p \). The effective condition implies that the group \( G \) cannot be too big, i.e. the only element of the group that acts as the identity map on the whole of \( M \) is the identity \( e \).

Of course, for a specific \( p \in M \) it could be that there exist many elements of the group that fix \( p \). These elements form a group called the isotropy group.

**Definition 25.** Isotropy group or the stabilizer at \( p \):

\[ G_p = \text{Iso}_p = \{ g \in G \mid g \cdot p = p \} \subseteq G. \]

This group is a subgroup of \( G \).

**Definition 26.** The orbit of a point \( p \in M \) is

\[ O_p = G \cdot p = \{ g \cdot p \mid g \in G \} \subseteq M. \]

In some cases, the orbit of any point of \( M \) is the whole \( M \), i.e. \( O(p) = M \).

**Definition 27.** An action is transitive if

\[ \forall p_1, p_2 \in M \exists g \in G \text{ s.t. } g : p_1 = p_2. \]

Notice that it is sufficient to require that the action is transitive with respect to a specific point \( o \in M \), i.e.,

\[ \forall p \in M \exists g \in G \text{ s.t. } g \cdot o = p. \]

Indeed, let us assume that \( g_1 \cdot o = p_1 \) and \( g_2 \cdot o = p_2 \), by taking the action related to \( g_1^{-1} \) we have \( o = g_1^{-1} \cdot p_1 \), and thus \( g_2 \cdot (g_1^{-1} \cdot p_1) = p_2 \). So the action is transitive. To be transitive the group \( G \) must be big enough.

Let us consider three simple examples: the plane \( \mathbb{R}^2 \), the sphere \( S^2 \), and a Lie group \( G \).

**Example 5.** Let \( G = (\mathbb{R}^2, +) \) and \( M \) be the plane. If we specify a coordinate system in the 2-dimensional plane we can represent a point by its coordinates \( m \), then a left action is given by:

\[ \lambda(g, m) = g \cdot m = g + m. \]

It is simply a translation. Notice that \( G \) is abelian and left and right actions are equivalent in this case. The only translation that fixes a point in the plane is the zero translation (the identity) so the isotropy group is \( \{ e \} \) and we say that the action is free and it is thus also effective. The orbit of any point in the plane is the whole plane since the action is transitive.
Example 6. The set of rotations in $\mathbb{R}^3$, i.e. $SO(3)$ acts on the sphere $S^2$. To represent this action, let us identify the points on the sphere with the unit norm vectors in $\mathbb{R}^3$. The left action is then simply given by

$$\lambda(g, m) = g \cdot m = gm,$$

where in the right-hand side, we have used the matrix vector product. This action is smooth, transitive and effective but not free. Indeed, for any point $p$ in $S^2$, let $H$ be the set of rotations of principal axis $p$. Each element of $H$ fixes the point $p$ and all the other rotations move the point $p$. Hence, $H$ is the isotropy group at $p$.

Example 7. A Lie group $G$ acts on itself via $\lambda(g, p) = L_g(p)$. This action is free and transitive.

The isotropy groups at two different points are related. Indeed, let $g$ such that $g \cdot p_1 = p_2$. We have that

$$G_{p_2} = gG_{p_1}g^{-1},$$

since $gG_{p_1}g^{-1} \cdot p_2 = gG_{p_1}g^{-1}(g \cdot p_1) = p_2$. So the isotropy groups are conjugate subgroups.

The next three theorems are the main three results about homogeneous spaces.

Theorem 14. Let $G$ be a Lie group and $\lambda : G \times M \to M$ be a left action on a smooth manifold $M$. Then, for all $m \in M$,

- the isotropy group $G_m$ of the point $m$ is a closed Lie subgroup of $G$,
- the orbit $G \cdot m \subseteq M$ can be given the structure of a smooth submanifold of $M$ such that the map

$$\lambda(., m) : G \to G \cdot m, \ g \mapsto \lambda(g, m),$$

is a smooth submersion.

Theorem 15. Let $H$ be a closed subgroup of a Lie group $G$. (This implies that $H$ is a Lie subgroup, i.e. a subgroup and a submanifold of $G$). Then there exists a unique smooth structure on the set of left cosets $G/H$ such that the quotient map (or the coset map) $\pi : G \to G/H$ is a smooth submersion. Moreover, with this smooth structure, the left action:

$$\lambda : G \times G/H \to G/H, \ (p, gH) \mapsto pgh,$$

is a transitive smooth left action.

Theorem 16. Let $\lambda : G \times G \cdot m \to G \cdot m$ be a transitive action of the Lie group $G$ on $G \cdot m$ and let $H$ be the isotropy group of $m$. The mapping

$$\phi : G/H \to G \cdot m : \phi(gH) \mapsto \lambda(g, m),$$

is a diffeomorphism.
Figure 2.3: There are actually different ways to go through this picture. We can start from a Lie group, let say the general linear group, for which we have a concrete representation using matrices. Then, we can quotient this group by some closed subgroup \( H \) and we will get a homogeneous spaces. The other way (bottom-up) consists in starting from the manifold \( G \cdot m \), then finding a group \( G \) that acts transitively on \( G \cdot m \) and the isotropy group \( H \) at a point \( m \).

For proofs, see [8, 9, 61].

Theorem 14 is useful to show that some subsets of \( \mathbb{R}^n \) have a submanifold structure. For instance, the action of \( \text{SO}(3) \) on \( \mathbb{R}^3 \) (by matrix-vector multiplication) is smooth. Let \( N = [0 \ 0 \ 1]^T \in \mathbb{R}^3 \), the sphere \( S^2 \) embedded in \( \mathbb{R}^3 \) can be seen as the orbit \( \text{SO}(3) \cdot N \). Thus, this gives another way, to show that the sphere \( S^2 \), can be seen as a submanifold of \( \mathbb{R}^3 \). We also know that the isotropy group of \( N \) is a closed subgroup of \( \text{SO}(3) \) (since it is the reverse image of the point \( N \) by the continuous action \( \lambda(.,N) \)). This isotropy group corresponds to the rotations whose axis of rotation is \( N \), and it is thus isomorphic to \( \text{SO}(2) \). Then, using Theorem 15, \( S^2 \) can be also regarded as the set of left cosets \( \text{SO}(3)/\text{SO}(2) \).

Looking at \( \mathcal{M} \) as an homogeneous space \( \mathcal{M} = G/H \) gives us a representation for the tangent space at any point \( m \) of the homogeneous space. Indeed, we have the following vector space isomorphism:

\[
\frac{\mathfrak{g}}{\mathfrak{h}} \cong T_m G \cdot m, \quad V \mapsto V_m(f) = \frac{d}{dt} f(\exp(tV) \cdot m)|_{t=0}.
\]

**Definition 28.** A homogeneous space \( G/H \), on which the connected group \( G \) acts transitively and effectively, is reductive if the Lie algebra \( \mathfrak{g} \) of \( G \) can be decomposed as the direct sum

\[
\mathfrak{g} = \mathfrak{h} \oplus \mathfrak{m} \text{ with } Ad_H \mathfrak{m} \subset \mathfrak{m}.
\]

The last condition implies \( [\mathfrak{h},\mathfrak{m}] \subset \mathfrak{m} \) and it is equivalent to it when \( H \) is connected.

On a reductive homogeneous space, there is a one to one correspondence (bijection) between \( Ad_H \)-invariant inner products on \( \mathfrak{m} \) and \( G \)-invariant Riemannian metrics \( g \) on \( G/H \). If the metric \( g \) is \( G \)-invariant, we say that \( G \) is a reductive homogeneous space.

\((\mathfrak{g},+)^1\) the set of left cosets in the group \( (\mathfrak{g},+) \)
acts on $G/H$ by isometries, and $(G/H, g)$ is called a Riemannian homogeneous space. All the Riemannian manifolds considered in this thesis are reductive homogeneous spaces equipped with an $Ad_H$-invariant inner product. A particular class of such spaces, called Riemannian globally symmetric spaces is considered in the next section.

### 2.7 Riemannian symmetric spaces

The goal of this section is to introduce some definitions and properties of Riemannian symmetric spaces. Our main interest in these spaces is that it is relatively easy to compute their curvature endomorphism, geodesics and parallel transports. They have a parallel curvature tensor which leads to explicit expressions for the Jacobi fields. This fact is used extensively in Chapter 4.

The symmetric spaces and locally symmetric spaces are studied extensively
in [8, 10, 23, 42] provide a good introduction.

**Definition 29** (Riemannian symmetric spaces). A (Riemannian) symmetric space $\mathcal{M}$ is a Riemannian manifold $\mathcal{M}$ such that for any $p \in \mathcal{M}$, the geodesic symmetry at $p$:

$$s_p : \mathcal{M} \rightarrow \mathcal{M}, \gamma(t) \mapsto \gamma(-t),$$

where $t \mapsto \gamma(t)$ is a geodesic starting at $p$, is an isometry.

In our case, we will only consider Riemannian symmetric spaces. For more details about non Riemannian symmetric spaces, see [42].

As an example, we can think of the central symmetry in the Euclidean space $\mathbb{R}^2$. In this case, the symmetry $s$ has only one global fixed point. On the circle $S^1$, parametrized by an angle $\theta \in [0, 2\pi]$, a symmetry is given by

$$s_\theta(q) = \theta - (q - \theta) = 2\theta - q.$$

It is simply the angular symmetry. Notice that here, the symmetry at any point $p$ admits also its antipodal point as a fixed point.

Another interesting property for symmetric spaces is that they have parallel curvature tensor. This is because the symmetry $s_p$ leaves the curvature endomorphism and its covariant derivative invariant. Indeed, we have

$$Ds_p((\nabla X R)(Y, Z)W) = \nabla_{Ds_p X}R(Ds_p Y, Ds_p Z)Ds_p W,$$

which, at $p$, implies


Thus, $\nabla R = 0$. This almost characterizes symmetric spaces and motivates the following definition.

**Definition 30** (Locally symmetric spaces). A locally symmetric space is a Riemannian manifold whose curvature tensor is parallel, i.e. $\nabla R = 0$.

This condition is equivalent to say that at each point $p \in \mathcal{M}$, the geodesic reflection or the reflection through the origin in normal coordinates is an isometry but only on some ball centred at $p$. The isometry property is then only local and not global as in the definition 29.

The following theorem, [10, Prop. 3.37] makes the link between the Riemannian symmetric space structure of a manifold $\mathcal{M}$ and its homogeneous space structure $\mathcal{M} = G/H$ where $G$ is the isometry group of $\mathcal{M}$ and $H$ is the isotropy group of some point $m \in \mathcal{M}$.

**Theorem 17** ([10, Prop. 3.36]).

1. $\mathcal{M}$ simply connected complete (the geodesic curves are defined for all $t$ ) and locally symmetric implies $\mathcal{M}$ symmetric.

2. $\mathcal{M}$ symmetric implies $\mathcal{M}$ Riemannian homogeneous. It is possible to write $\mathcal{M} = G/H$ where $G$ is the isometry group of $\mathcal{M}$ and $H$ is the isotropy group of some point $o \in \mathcal{M}$.
3. Let $\mathcal{M} = G/H$ be symmetric with $G$ the isometry group of $\mathcal{M}$ and $H$ the isotropy group of $o \in \mathcal{M}$. Let $s_o : \mathcal{M} \to \mathcal{M}$ be the symmetry at $o$. Then, the map

$$\sigma : G \to G, \ g \mapsto s_og s_o,$$

is an involutive automorphism (a map from $G$ to $G$ that preserves the group structure, is a bijection and such that $\sigma^2 = I_d$) of the group $G$. The set $F$ of fixed points of $\sigma$ is a closed subgroup containing the isotropy group $H$. We have actually $F_c \subset H \subset F$ where $F_c$ is the identity component of $H$.

4. Conversely, let $G$ be a Lie group, $\sigma$ an automorphism involutive, and let $F$ be the set of fixed points of $\sigma$ and $\langle \cdot, \cdot \rangle$ a left invariant metric on $G/F$. The relation $\sigma(gf) = \sigma(g)\sigma(f) = \sigma(g)f$ shows that $\sigma$ induces a diffeomorphism of $G/F$. If this diffeomorphism preserves the metric $\langle \cdot, \cdot \rangle$, then $G/F$ is a symmetric space.

5. A simply connected Lie group $G$ possesses an automorphism $\sigma$ such that $\sigma^2 = I$ if and only if there exist a decomposition of the Lie algebra $\mathfrak{g} = \mathfrak{m} \oplus \mathfrak{h}$ with

$$[\mathfrak{h}, \mathfrak{h}] \subset \mathfrak{h} \quad [\mathfrak{h}, \mathfrak{m}] \subset \mathfrak{m} \quad [\mathfrak{m}, \mathfrak{m}] \subset \mathfrak{h}. \quad (2.5)$$

In case $G/F$ admits a $\sigma$-invariant Riemannian metric, $G/F$ is a globally symmetric space.

If the condition (2.5) is not satisfied, there exists no automorphism $\sigma$ and so using point (3), the space is not symmetric. The points (4) and (3), in this theorem are particularly useful to characterize Riemannian symmetric spaces, see also [23] for more details.

The following theorem gives very useful results to obtain explicit expressions for curvature endomorphisms, geodesics, and parallel transports on symmetric spaces.

**Theorem 18** ([31, Theorem 3.2 p.231 II]). Let $\mathcal{M} = G/H$ be a Riemannian symmetric space with $\mathfrak{m}$ and $\mathfrak{g}$ defined as in (2.5):

- the Riemannian curvature endomorphism is parallel, i.e., $\nabla R = 0$,
- for each $S \in \mathfrak{m}$, $\lambda(\exp(tS), m)$ is a geodesic starting at $m$ and, conversely, every geodesic starting at $m$ is of this form,
- the curvature endomorphism at the identity is given by $R_1(X,Y)Z = -[[X,Y],Z]$ for $X,Y,Z \in \mathfrak{m}$.

**Theorem 19** (Parallel transport on symmetric space). The parallel transport along a geodesic $\gamma : \Gamma_{\gamma(0)} \to \Gamma_{\gamma(t)} : T_{\gamma(0)}\mathcal{M} \to T_{\gamma(t)}\mathcal{M}$ can be realized by $Ds_{\gamma(t)} \circ Ds_{\gamma(t/2)}$ or by $Ds_{\gamma(t/2)} \circ Ds_{\gamma(0)}$. 

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2.7.1 Examples

Euclidean Space \( \mathbb{R}^n \)

The Lie group \((\mathbb{R}^n, +)\) acts on \(\mathbb{R}^n\) by isometries. The symmetry is given by \(s_p(q) = 2p - q\), and it is an isometry.

The rotation group \(SO(n)\)

By introducing the following inner product on \(\mathfrak{so}(n)\)

\[
g(X, Y) = \frac{1}{2} \text{tr}(X^T Y),
\]

we turn \(SO(n)\) into a Riemannian manifold. This inner product is bi-invariant (on the left and on the right) to the action of the special orthogonal group. Since the metric is bi-invariant, the geodesics are one parameter subgroups, i.e. the Lie group exponential map corresponds to the Riemannian exponential map. The geodesic curve starting at \(p\) in the direction \(V \in \mathfrak{so}(n)\) is thus given by

\[
\gamma(t) = pe^{tV}.
\]

The symmetry is given by \(s_p(q) = pq^T p\). Indeed, the geodesic such that \(\gamma(0) = p\) and \(\gamma(1) = q\) is given by \(\gamma(t) = pe^{t \log(p^T q)}\), and thus \(\gamma(-1) = pq^T p\). The right and left actions are isometries, and the map \(q \mapsto q^T\) is also an isometry since its differential (seen as a map in the Lie algebra) is given by \(V \mapsto q(-V)q^T\), and so it preserves the inner product \(\langle V_1, V_2 \rangle = \frac{1}{2} \text{tr}(V_1^T V_2)\). Thus, \(q \mapsto pq^T p\) is a composition of isometries, and thus an isometry. \(SO(n)\) equipped with this bi-invariant metric is thus a Riemannian symmetric space.

The sphere \(S^n\) embedded in \(\mathbb{R}^{n+1}\)

The sphere can be seen as an homogeneous space: \(S^n = SO(n+1)/SO(n)\). So, we have \(G = SO(n+1)\) and \(H = SO(n)\). The involutive automorphism \(\sigma\) is given by \(g \mapsto \begin{pmatrix} -I_n & 0 \\ 0 & 1 \end{pmatrix} g \begin{pmatrix} -I_n & 0 \\ 0 & 1 \end{pmatrix}^{-1}\) and its set of fixed points is \(G_\sigma = \left\{ \begin{pmatrix} R & 0 \\ 0 & 1 \end{pmatrix} \big| R \in SO(n) \right\} \approx SO(n)\). Notice that another possibility is \(S^n = O(n+1)/O(n)\). In this case, we have \(G_\sigma = \left\{ \begin{pmatrix} R & 0 \\ 0 & r \end{pmatrix} \big| R \in O(n) \right\} \subset G_\sigma\) whose identity component is isomorphic to \(SO(n)\). Thus we have \(G_\sigma \subset H \subset G_\sigma\).

Its Riemannian geometry (with the induced Riemannian metric from the Euclidean space \(\mathbb{R}^3\)) is described in Section 4.4.1 of Chapter 4 for \(n = 2\). The extension to larger \(n\) is not difficult.

Symmetric positive definite matrices \(\mathcal{P}_n^+\)

It is described in Section 3.5 of Chapter 3.

The Grassmann manifold \(\text{Grass}(n, p)\)

The Grassmann manifold \(\text{Grass}(n, p)\) is the set of \(p\)-dimensional subspaces in \(\mathbb{R}^n\). It admits different homogeneous space representations. Indeed, we
can write $\text{Grass}(n, p) = GL(n)/GL(p)$, $\text{Grass}(n, p) = O(n)/(O(p) \times O(n-p))$ or $\text{Grass}(n, p) = SO(n)/SO(p) \times O(n-p))$, where $S(G)$ denotes the set of matrices of positive determinant of the matrix group $G$. It admits a Riemannian metric that makes it a Riemannian globally symmetric space. More details on the Riemannian geometry of the Grassmann manifold are given in Section 4.4.4.

**The Stiefel manifold $\text{St}(n, p)$**

It is the set of $p$-dimensional orthogonal frames in $\mathbb{R}^n$ with respect to the standard inner product. It is diffeomorphic to $SO(n)/SO(n-p)$. When it is endowed with the left invariant Riemannian metric induced by the inner product (2.6), it is a normal homogeneous space, see Section 5.1 of Chapter 5. Notice that it is not a symmetric space.

In this thesis, we stick to the real case but most of these manifolds have their complex counterpart, e.g. the complex Grassmann manifold $G_C(n, p) = U(n)/(U(p) \times U(n-p))$ where $U(n)$ is the unitary group.

### 2.8 Basics on optimization

Since all the algorithms presented in this thesis are regarded as optimization algorithms, we think that this subject deserves at least this small introduction. Let us assume that $f$ is a smooth function. We want to solve the following problem:

$$p^* = \arg \min_{p \in \mathcal{M}} f(p).$$

Even if, in the real world, we are often happy to be able to improve a situation, in our case to reduce the value of our objective function $f$, our main concern here will be about finding a stationary point $p^*$ of the function $f$, i.e. a point that satisfies

$$Df(p)[X] = 0 \quad \forall X \in T_p\mathcal{M},$$

or equivalently

$$\ker Df(p^*)[X] = T_p\mathcal{M}.$$

Many iterative optimisation schemes are based on the relaxation principle, i.e. they want to reduce the objective function $f$ at each iteration. Let us first see how we can do that. Let us assume that the current iteration is the point $p \in \mathcal{M}$. Our goal remains modest since we want to move to a $p^+$ such that $f(p^+) < f(p)$. To achieve this goal, one classical idea is to design an iterative method that makes a step of length $\alpha$ along some descent direction $d$. By descent direction we mean, a direction such that if $\alpha > 0$ is taken sufficiently small, we have $f(\gamma(\alpha)) \leq f(p)$, where $t \mapsto \gamma(t)$ is a curve in $\mathcal{M}$ such that $\gamma(0) = p$ and $\dot{\gamma}(0) = d$. A first question is then: **What are the descent directions?** Let us pick a chart $\phi$ around $p$ (i.e. we specify some local coordinates), and let us compute the differential of $f \circ \phi^{-1} : \mathbb{R}^n \to \mathbb{R}$. 

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If the differential is not degenerate, we are not at a stationary point, and its kernel defines a \( n - 1 \)-dimensional space of the tangent space at \( p \). So, this kernel induces a splitting of the tangent space \( T_p M \) at \( p \) into \( T_p^+ M \) and \( T_p^- M \). The former corresponding to the ascent directions and the latter to the descent directions. If we want to minimize \( f \), we are looking for a descent direction, in \( T_p^- \).

Let us pick an inner product on \( T_p M \), i.e. a symmetric positive definite form \( B \). Since \( B \) is non degenerate, there exists a unique \( \Delta \) such that

\[
Df(p)[\Delta] = B(\Delta, X) \quad \forall X \in T_p M,
\]

i.e. we have a vector space isomorphism \( \Delta \mapsto B(\Delta, X) \) between \( T_p M \) and its dual. Furthermore, since \( B \) is positive definite, \( \Delta \in T_p^+ \) since \( Df(p)[\Delta] = B(\Delta, \Delta) > 0 \) if \( \Delta \neq 0 \).

So, an inner product \( B \) on \( T_p M \) defines a unique direction \( \Delta \) in \( T_p^+ \), called a gradient direction. By linearity of \( Df(p) \), \( -\Delta \in T_p^- \). As \( B \), we can, of course, use the Riemannian metric of \( M \), if it is a Riemannian manifold. In that case, we say that \( \Delta \) is the Riemannian gradient. But note that we could choose any other metric.
Chapter 3

Karcher mean computation on $SO(3)$ and $\mathcal{P}_n^+$

In this chapter, Newton and gradient methods are studied to compute the Karcher mean of rotation matrices and symmetric positive definite matrices. We first introduce the Karcher means, and give some results about their uniqueness on some Riemannian ball. Then, we make a brief overview of the methods that have been proposed to compute the Karcher mean on $SO(3)$ and $\mathcal{P}_n^+$. Since $SO(3)$ and $\mathcal{P}_n^+$ are symmetric spaces, it is possible to get explicit expressions for the eigenpairs of the Jacobi operator, and thus for the Riemannian Hessian of the squared Riemannian distance function. These explicit expressions are derived on $SO(3)$ and $\mathcal{P}_n^+$, and are used to implement a Newton method to compute the Karcher mean. An adaptive step size selection rule that ensures the convergence of the Riemannian gradient method on $\mathcal{P}_n^+$ is also proposed. Finally, the case of structured covariance matrices is considered. It is shown that it is possible to take advantage of this specific structure in the computation of the Karcher mean.

Some of the ideas presented in this chapter have already been published in [45] which can be considered as a precursory work.

Main contributions:

- a Newton method to compute the Karcher mean on $SO(3)$ (faster than the gradient method in some cases),
- a step size selection rule ensuring the convergence of the Riemannian gradient method for the Karcher mean computation on $\mathcal{P}_n^+$,
- a comparison between Newton and gradient methods in terms of computational time for the Karcher mean computation on $\mathcal{P}_n^+$ (The Newton method is faster in some cases),
- a method to compute the Karcher mean of structured covariance matrices.
3.1 Karcher mean

One of the most classical data analysis techniques consists in computing an average to get a measure of locality or to reduce a measurement noise. Let \( \{q_1, \cdots, q_N\} \) be \( N \) points in the Euclidean space \( \mathbb{R}^n \), their mean (arithmetic) is defined by the well known formula:

\[
\mu = \frac{1}{N} \sum_{i=1}^{N} q_i. \tag{3.1}
\]

Another definition of the mean \( \mu \) is:

\[
\mu = \arg \min_{p \in \mathbb{R}^n} \frac{1}{2N} \sum_{i=1}^{N} \|p - q_i\|^2. \tag{3.2}
\]

Since this optimization problem is convex, \( \mu \) is uniquely defined. Observe that (3.1), cannot be generalized easily on spaces that have no vector space structure. But (3.2) can be generalized once we equipped our space \( \mathcal{M} \) with a notion of distance; i.e. when \( \mathcal{M} \) is a metric space. In the present work, one remains closer to the Euclidean case in the sense that we only consider Riemannian distance functions, i.e. the ones induced by a Riemannian metric. In fact, by replacing the Euclidean distance by the Riemannian distance in (3.2), one obtains a notion of mean on a Riemannian manifold. More precisely, let \( q_1, \ldots, q_N \in \mathcal{M} \) be \( N \) points in \( \mathcal{M} \), we can define:

\[
\mu = \arg \min_{p \in \mathcal{M}} F(p), \quad F : \mathcal{M} \rightarrow \mathbb{R}^+, \quad p \mapsto \frac{1}{2N} \sum_{i=1}^{N} d(p, q_i)^2. \tag{3.3}
\]

Notice that this is not the only possibility. We can also define extrinsic means. The main idea is to embed the manifold into some \( \mathbb{R}^n \), which is always possible (but might be not easy) by virtue of Theorem 2. Then, one can compute the mean of points in \( \mathbb{R}^n \) and project the result back to the manifold. Of course, this mean depends on the embedding and on the projection used but this approach can be computationally attractive if the projection is easy to compute, see [55] and [51] for an example of this approach on the Grassmann manifold and the special orthogonal group.

The mean \( \mu \) defined by (3.3) is called the Fréchet mean and it is intrinsic, it does not depend on a particular embedding. It is a (global) minimizer of \( F \). Not that since the distance function is continuous on any metric space, \( F \) is continuous. So, for compact Riemannian manifolds like the sphere, the special orthogonal group, the Grassmann manifold and the Stiefel manifold, a Fréchet mean always exists. The only non-compact Riemannian manifold that is considered in this thesis is \( P_n^+ \) but it is an Hadamard manifold, see below. Unfortunately, as opposed to \( \mathbb{R}^n \), there are often many \( \mu \) that are global minimizers of \( F \). As an example, we can take the sphere \( S^2 \) embedded
in $\mathbb{R}^3$ with the induced Riemannian metric. When there are two antipodal data points, say one at the north pole and the other at the south pole, all the points on the equator are global minimizers of $F$. Moreover, it could be that there exist many local minimizers. Since computing the global minimizer is a difficult task in general, and since many optimization schemes only ensure the convergence to a local minimizer, in this thesis, any local minimizer of $F$ is considered as a mean and is called a Karcher mean, see [29]. Notice that, in the literature, other denominations are used: centroid, barycenter, Riemannian center of mass.

On Hadamard manifolds, i.e. complete simply-connected Riemannian manifolds with non-positive sectional curvature, it has been shown that there is a unique global minimizer of $F$. This is due to the fact that the function $F$ is geodesically convex, i.e. $t \mapsto F(\gamma(t))$ is a convex function when $t \mapsto \gamma(t)$ is a geodesic curve, see [49, Proposition 4.3]. The set of symmetric positive definite matrices $\mathcal{P}_n^+$ equipped with the affine invariant metric is an Hadamard manifold, see Chapter 3.

However, on manifolds of positive curvature, like the sphere $S^2$ or the rotation group $SO(3)$, there are in general many Karcher means. In this case, many authors have proposed to assume that the data points belong to an open Riemannian ball $B(o,r)$ of radius $r$ centred at some point $o \in \mathcal{M}$. The question is then: "Give a radius $r$ such that there exists one and only one Fréchet mean and it is located in $B(o,r)$." To answer this question, let us introduce the following definition.

**Definition 31 (Convexity radius).** It is the maximal radius that ensures that $B(p,r_c)$ is a strongly convex ball, i.e. any geodesic fully contained in $B(o,r_c)$ is minimizing.

The value $r_c$ depends on the injectivity radius and on the curvature of the manifold. It is given by [3, Definition 2],

$$r_c = \frac{1}{2} \min \{ \frac{\pi}{\sqrt{\Delta}}, \text{inj}(\mathcal{M}) \},$$

where $\Delta$ is an upper bound on the sectional curvature $\kappa$ and by convention, $\frac{\pi}{\sqrt{\Delta}} = \infty$ if $\Delta \leq 0$. We have the following result.

**Theorem 20 ([3, Theorem 2]).** Let $\{q_i\}_{i=1}^N \subset B(o,r)$ with $r \leq r_c$, then the Fréchet mean $\mu$ is unique and it is inside $B(o,r)$. Moreover, it is the unique zero of the gradient vector field $\nabla F(p)$ in $\overline{B}(o,r)$ and $\mu$ is a non-degenerate critical point of $F$, i.e., the Hessian of $F$ at $p$ is positive definite.

Notice that, on $B(o,r_c)$, the function $F$ is not necessarily convex. It can be shown, see [3] and the references therein, that $F$ is convex on the ball $B(o, \frac{d}{2})$ if all the data points belong to that ball, since $p \mapsto \frac{1}{2}d(p,q)^2$ is convex if $d(p,q) \leq d_c$ where

$$d_c = \min \{ \text{inj}(\mathcal{M}), \frac{\pi}{2\sqrt{\Delta}} \}. \quad (3.4)$$
On the sphere $S^2$, we have $r_c = \frac{\pi}{2}$ and $d_c = \frac{\pi}{2}$. Thus, if all the data points belong to a ball $B(o, \frac{\pi}{2})$ (the open half of the sphere), then there exists a unique Karcher mean inside that ball. Moreover, if all the data points belong to $B(o, \frac{\pi}{4})$ then the function $F$ is convex on this ball. On $SO(n)$, the sectional curvature is bounded by $\Delta = \frac{1}{2}$ and $\text{inj}(SO(n)) = \pi$, and thus $r_c = \frac{\pi}{2}$ and $d_c = \frac{\sqrt{2}}{\pi}$. On the Grassmann manifold, the sectional curvature is bounded by $2$, see [63], and its injectivity radius is $\pi/2$. Thus $r_c = \pi/4$ and $d_c = \frac{\sqrt{2}}{\pi}$. On $SO(3)$, the sectional curvature $\kappa = \frac{1}{4}$, and the injectivity radius $\text{inj}(SO(3)) = \pi$, thus $r_c = \pi/2$ and $d_c = \pi$. So, in this case, $F$ is convex on the ball where the Karcher mean is ensured to be unique. On $\mathcal{P}^+_n$, the sectional curvature is negative and the Karcher mean is unique if no data point lies on the boundary of the cone. These results are due to Kendall, see [30].

This has an impact on the choice of a numerical scheme to compute the Karcher mean. More precisely, the Hessian could be singular or indefinite and the Newton iteration could leave the ball $B(o, r_c)$ as remarked in [3]. But this does not necessarily mean that the Newton method is useless in practice. Indeed, a Newton method could still be used after a few gradient iterations. The idea would be to iterate until the basin of quadratic convergence of the Newton method is reached. This strategy is followed in the scheme [41, Chapter 4, p. 173] defined for self-concordant functions. In fact, in that case, it is possible to ensure that the Newton method converges quadratically once the norm of the gradient with respect to the Hessian metric is lower than some computable threshold.

### 3.2 Computation of the Karcher mean

Many algorithms have already been proposed to compute the Karcher mean. In [33], a proof of convergence of a gradient method is given under some conditions on the curvature of the manifold and the step size, but no specific step size selection rule is given to ensure that these conditions are satisfied. Most of the gradient methods that have been introduced in the literature are Riemannian gradient methods, what differs is the step size selection rule. We will first describe the Riemannian gradient algorithm and recall the common step size selection rules proposed in the literature.

The gradient of the function $F$ in (3.3), see [29], is

$$
\text{grad} F(x) = \frac{1}{N} \sum_{i=1}^{N} \exp_x^{-1}(y_i),
$$

where $\exp_x^{-1}(y)$ stands for the Riemannian log-mapping that returns a tangent vector $v$ at $x$ such that the geodesic curve $t \mapsto \gamma(t)$ with $\gamma(0) = x$ and $\gamma(0) = v$ satisfies $\gamma(1) = y$. The Riemannian gradient method is presented in algorithm 1.

There are different strategies to chose $h_k$ in step (5) of algorithm 1. It is possible to choose $h_k \in \mathbb{R}^+_0$ such that the function $h_k \mapsto \exp_{p_k}(-h_k \text{grad} F(p_k))$
Algorithm 1 Riemannian gradient method

1: Given a set of \( N \) points \( q_i \in \mathcal{M} \) for \( 1 \leq i \leq n \) and an initial guess for the Karcher mean \( \mu_0 \);
2: Set \( \mu_k = \mu_0 \) and \( k = 1 \);
3: until \( g_{\mu_k}(\nabla F(\mu_k), \nabla F(\mu_k)) < \epsilon \) do
4: Compute the gradient of \( F \) at \( \mu_k \) using (3.5);
5: Move along the geodesic curve starting at \( \mu_k \): \( \mu_{k+1} = \exp_{\mu_k}(-h_k \nabla F(\mu_k)) \);
6: Set \( k = k + 1 \);
7: end until
8: return \( \mu_k \) (the estimation of the Karcher mean)

is minimized, or to use a line search technique to find a step size that satisfies the Armijo condition, see [41]. But these step size selection rules require the evaluation of the cost function \( F \) and rely on some parameters that must also be tuned. Another possibility is to fix the step size in advance. For instance, we can fix \( h_k = 1 \). This strategy is followed in [39] to compute the Karcher mean on compact Lie groups. The same strategy is used in [43] to compute the Karcher mean on \( \mathcal{P}_n^+ \). But to the best of our knowledge, there is no convergence proof for \( \mathcal{P}_n^+ \).

In [3], the behaviour of constant step size gradient algorithms is studied, under the assumption that we know beforehand the radius of a ball where all the data points belong. In particular, the authors have introduced the following conjecture.

Conjecture ([3, Conjecture 2.15 p.10]) Let us assume that the data points \( \{q_i\}_{i=1}^N \subset B(o,r) \) where \( r < r_c \), then no matter where we start inside \( B(o,r) \), the Riemannian gradient method, see algorithm 1, will converge to the unique Karcher mean inside \( B(o,r) \), if we choose a constant step size:

\[ h \in (0, 1/L) \]

where \( L \) is an upper bound on the Hessian \(^1\) of the squared Riemannian distance function on the ball \( B(o,r) \), i.e. \( L = \sqrt{3}2r \coth(\sqrt{3}2r) \) if \( \delta < 0 \) and \( L = 1 \) if \( \delta \geq 0 \), where \( \delta \) is a lower bound on the sectional curvature.

In [3], the conjecture is proven for manifolds of constant non-negative curvature.

On \( SO(3) \), the sectional curvature is \( k = 1/4 \) (constant curvature). So, the conjecture is proven in this case, and it suggests to choose \( h = 1 \). The unit step size gradient method will then converge to the unique Karcher mean inside a ball \( B(o,\pi/2) \) if all the data points belong to that ball.

On \( \mathcal{P}_n^+ \), the sectional curvature is non-positive. So the lower bound on the Hessian of \( F \) is 1, see section 3.3, and thus the function \( F \) is strongly geodesically convex. But, there is no global upper bound \( L \) on the Hessian.

---

\(^1\)By upper bound \( L \) and lower bound \( l \) on the Hessian, we mean \( l\|\Delta\|^2 \leq \text{Hess}_p(\Delta, \Delta) \leq L\|\Delta\|^2 \).
of $F$. We can only bound the Hessian on some ball of finite radius. On $\mathcal{P}_n^+$, $r_c = \infty$ and $\delta = -1/2$, see section 3.5.2. Thus, if all the data points belong to the ball $B(p_0, r)$ where $p_0$ is the starting point, $L = \sqrt{2r \coth(\sqrt{2r})}$, and if the conjecture is true, $1/L$ is a step size that ensures the convergence.

For strongly convex function, $h = \frac{2}{\mu + L}$ is the optimal step size selection rule if we know a lower bound $\mu$ and an upper bound $L$ on the Hessian of $F$, see [41, Theorem 2.1.14 p.66]. This step size is used in [7] to compute the Karcher mean on $\mathcal{P}_n^+$. The authors have considered a linearisation of the exponential map in (3.30), i.e. the exponential map is replaced by its linear approximation: $\text{Expm}(X) \approx I + X$. The authors prove the local convergence (if the algorithm starts close to the Karcher mean) of this linear approximation using this step size and deduce that it is also asymptotically optimal for the iteration (3.30), since the two iterations are equivalent up to first order. In this thesis, we propose a variable step gradient method. The main idea consists in choosing the step size $h_k = \frac{2}{\mu + L_k}$ at iteration $k$ based on the largest value $L_k$ of the Hessian of $F$ on a ball $B(p_k, r)$ centred at the current iteration $p_k$ such that the next iterate still belongs to that ball.

The recent paper [28], compares different algorithms (gradient, trust region, conjugate gradient,...) to compute the Karcher mean on $\mathcal{P}_n^+$. The comparison is done in terms of computational time, and it seems that the best method is, in most cases (depending on the data distribution and the size of the problem), the gradient method.

In this thesis, the potential interest of using a Newton method to compute the Karcher mean on $\mathcal{P}_n^+$ and $SO(3)$ is discussed. Such a technique has an asymptotic quadratic rate of convergence. So, in practice, a Newton method requires less iterations than first order techniques to reach a sufficiently high accuracy. But the cost per iteration is significantly higher since the Hessian of the objective function must be computed and the symmetric linear system of Newton equations must be solved at each iteration. Consequently, a gain in terms of computational time is not guaranteed. Here, explicit expressions for the eigenpairs of the Jacobi operator are derived and, from this, an implementation of the Newton method presented in [15] is proposed. Using this implementation, it is shown that the Newton method is faster than the gradient method in some cases (this depends on the data distribution) when a high accuracy is required.

### 3.3 Hessian of the squared Riemannian distance function

In this section, we derive an explicit expression for the Hessian of the Riemannian squared distance function and show how the eigenvalues of the Hessian can be bounded in function of the sectional curvature and the Riemannian distance.
Let $q \in \mathcal{M}$, $p \in \mathcal{M}/C(q)$, $\Delta p \in T_p\mathcal{M}$, and $s \mapsto c(s)$, a smooth curve in $\mathcal{M}$ such that $c(0) = p$ and $\dot{c}(0) = \Delta p$, see Figure 3.1; the Hessian of the Riemannian squared distance function

$$f_q(p) = \frac{1}{2}d(p,q)^2$$

is given by

$$\text{Hess} f_q(p)[\Delta p, \Delta p] \triangleq \frac{d}{ds} f_q(c(s))|_{s=0}, \quad (3.6)$$

where $\dot{J}(1) = D_tJ(t)|_{t=1}$ is the covariant derivative of the Jacobi field $J(t)$ along the unique (since $p \in \mathcal{M}/C(q)$) distance minimizing geodesic curve $t \mapsto \gamma(t)$ joining $q$ and $p$ such that $\gamma(0) = q$ and $\gamma(1) = p$, that satisfies

$$D_t^2 J(t) + R(J(t), \dot{\gamma}(t)) \dot{\gamma}(t) = 0, \quad (3.8)$$

$$J(0) = 0 \in T_q\mathcal{M},$$

$$J(1) = \Delta p \in T_p\mathcal{M},$$

see [29] or [44] for a proof.

From this expression of the Hessian of the squared Riemannian distance function $f_q$ using Jacobi fields, it is possible to obtain bounds [49] on the Hessian of $f_q$ valid on any Riemannian manifold with a lower, and an upper bound on its sectional curvature: $\delta \leq \kappa \leq \Delta$. Under the assumption that $d(p,q) < \min\{\text{inj}(p), \frac{\pi}{\sqrt{\kappa}}\}$, we have:

$$b_\Delta(d(p,q)) \leq \text{Hess} f_q(p) \leq c_\delta(d(p,q)) \quad (3.9)$$

where

$$b_\Delta(d) = \begin{cases} \sqrt{\Delta}d\cot(\sqrt{\Delta}d) & \text{if } \Delta \geq 0, \\ 1 & \text{if } \Delta < 0, \end{cases}$$

$$c_\delta(d) = \begin{cases} 1 & \text{if } \delta \geq 0, \\ \sqrt{\delta}d\coth(\sqrt{\delta}d) & \text{if } \delta < 0. \end{cases}$$

Note that $F(x) = \frac{1}{N} \sum_{i=1}^N f_{q_i}(x)$ with $f_{q_i}(x) = \frac{1}{2}d(x, q_i)^2$, so the bounds on the Hessian of $f$ are also valid for $F$. These bounds used in section 3.6 to choose a step size that guarantees the convergence of a Riemannian gradient method.
On symmetric spaces, the Hessian \( \text{Hess}_q(f)(\Delta p, \Delta p) \) can be computed explicitly. Indeed, since the curvature endomorphism \( R \) is parallel on symmetric spaces, this implies that (3.8) is a constant coefficient differential equation and it can be solved explicitly, see section 2.4 or [10, 13, 15] for more details. Let the \( \lambda_k \)'s be the eigenvalues of the Jacobi operator

\[
J \mapsto R(J, \dot{\gamma}(0)) \dot{\gamma}(0),
\]

and the \( E_k \)'s are its corresponding eigenvectors. Since the Jacobi operator (3.10) is a symmetric linear map, it admits an orthonormal basis of eigenvectors. Let us assume that \( E_1, ..., E_m \) form an orthonormal basis at \( q = \gamma(0) \) that can be extended to a frame \( E_1(t), ..., E_m(t) \) by parallel transport along the curve \( t \mapsto \gamma(t) \). Note that \( E_1(t), ..., E_m(t) \) is orthogonal for each \( t \) since the parallel transport is an isometry. Notice that \( \dot{\gamma}(0) = \exp_q^{-1}(p) \) and \( \|\dot{\gamma}(0)\| = d(p, q) \).

In general, the basis \( E_1(t), ..., E_m(t) \) is not a basis of eigenvectors of the Jacobi operator at \( \gamma(t) \) except at \( q = \gamma(0) \). But on symmetric spaces, the curvature endomorphism is parallel and thus we have

\[
R_{\gamma(t)}(E_i(t), \dot{\gamma}(t)) \dot{\gamma}(t) = \lambda_i E_i(t).
\]

That is why we obtain a constant coefficients differential equation for the Jacobi fields on symmetric spaces. Consequently we can compute the basis \( E_1(1), ..., E_m(1) \) that diagonalizes the Jacobi operator at \( p \) and then parallel translate this basis along \( \gamma \). We have,

\[
\text{Hess}_q(f)(p)(\Delta p, \Delta p) = g_p \left( \sum_{k=1}^{m} g_p(\Delta p, E_k(1))w_k(1) E_k(1), \Delta p) \right),
\]

\[
= m \sum_{k=1}^{m} g_p(\Delta p, E_k(1))^2 w_k(1),
\]

with

\[
w_k(t) = \begin{cases} 
\sqrt{\lambda_k} \cot(t\sqrt{\lambda_k}) & \text{if } \lambda_k > 0, \\
1/t & \text{if } \lambda_k = 0, \\
\sqrt{-\lambda_k} \coth(t\sqrt{-\lambda_k}) & \text{if } \lambda_k < 0.
\end{cases}
\]

If we know explicit expressions for the eigenpairs of the Jacobi operator on symmetric spaces, it is also possible to derive bounds (and maybe better bounds) on the Hessian of \( f_q \). Indeed, from (3.12), we have:

\[
\min_k w_k(1) ||\Delta p||^2 \leq \text{Hess}_q(f)(p)(\Delta p, \Delta p) \leq \max_k w_k(1) ||\Delta p||^2.
\]

The term \( w_k(1) \) is shown in Figure 3.2 as a function of \( \lambda_k \).
Observe that, on Riemannian manifolds of non-positive sectional curvature, like $\mathbb{P}^n_+$, all the $\lambda_k$’s are non-positive. Indeed, let $X, Y \in T_p\mathcal{M}$ be non-colinear (they define a section of $T_p\mathcal{M}$), the sectional curvature at $p$ is given by

$$
\kappa(X, Y) = \frac{g(R(X, Y)Y, X)}{g(X, X)g(Y, Y) - g(X, Y)^2} = \frac{\sum_{i=1}^n x_k^2 \lambda_k}{g(X, X)g(Y, Y) - g(X, Y)^2},
$$

where the $(\lambda_k, E_k)$’s are the eigenpairs of the Jacobi operator $J \mapsto R(J, Y)Y$ and $X = \sum_{i=1}^n x_k E_k$. Since $\kappa(X, Y) \leq 0$ for every $X, Y$, we have $\lambda_k \geq 0 \ \forall k$. So, $w_k(1)$ is greater or equal to 1 and the Hessian of the squared Riemannian distance function is positive definite and lower bounded by 1. This explains why the squared Riemannian distance function is strongly geodesically convex. Similarly, on Riemannian manifolds of non-negative sectional curvature, like $SO(3)$, all the $\lambda_k$’s are non-negative, and $w_k(1)$ is upper bounded by 1 and is positive if $\sqrt{\lambda_k} < \pi/2$.

The diagonalisation of the Jacobi operator on $SO(3)$ is done in the next section, and see also the Chapter 4 for other symmetric spaces.

### 3.4 Newton method on $SO(3)$

In this section, a Newton method to compute the Karcher mean on $SO(3)$ is proposed. Note however that the case of $SO(n)$ could be also interesting, and a Newton method that computes the Karcher mean on $SO(n)$ could be implemented using the results of Appendix A. We first recall the formulas to compute the geodesics and the log-mappings on $SO(3)$, then we give an explicit
expression of the eigenpairs of the Jacobi operator, which are useful to compute the Hessian of the squared Riemannian distance function.

Given \( p \in SO(3) \), a tangent vector at \( p \) can be represented by a matrix of the form \( pv \) where \( v \) is skew-symmetric, see the definition of the tangent space. But it is also possible to represent only \( v \in T_I SO(3) \) without forgetting that this tangent vector at the identity or in the Lie algebra is related to the point \( p \). This approach is computationally more efficient since it does not require to compute and store the matrix \( pv \). Furthermore, to represent an element of the Lie algebra, a vector \( \tilde{v} \in \mathbb{R}^3 \) is used, see Table 2.1. Using this representation and the Rodrigues formulas, we have

\[
\begin{align*}
\exp_p(v) & : so(3) \to SO(3), \\
\exp_p(v) &= p \exp(v) = p(I + \frac{\sin \|v\|}{\|v\|} v + \frac{(1-\cos(\|v\|))}{\|v\|^2} v^2), \\
\exp_p^{-1}(q) & : SO(3) \to so(3), \\
\exp_p^{-1}(q) &= \frac{\theta}{2 \sin \theta} \begin{bmatrix}
-R(1,2) + R(2,1) \\
R(1,3) - R(3,1) \\
-R(2,3) + R(3,2)
\end{bmatrix}, \\
\text{where } R &= p^\top q \text{ and } \theta = \arccos \frac{\text{trace}(R)^{-1}}{2},
\end{align*}
\]

where \( \exp \) stands for the matrix exponential.

On \( SO(3) \), an element of the Lie algebra can be represented by a \( 3 \times 3 \) skew-symmetric matrix. Using this representation, the curvature endomorphism is given by (see [42])

\[
R(X,Y)Z = \frac{1}{4}[Z,[X,Y]],
\]

(3.14)

where \( X,Y,Z \in so(3) \) are skew symmetric matrices. But, using the vector representation of the Lie algebra, see Table 2.1 we can write

\[
R(X,A)A = \frac{1}{4} A \times (X \times A),
\]

where \( A \in \mathbb{R}^3 \) represents \( \dot{\gamma}(0) \) and \( X \in \mathbb{R}^3 \) represents the Jacobi field \( J \). Consequently, the eigenpairs of the Jacobi operator (3.10) with the vector representation of the Lie algebra are described by

- \( \lambda = 0, \ E_1 \);
- \( \lambda = \frac{\|A\|^2}{4}, \ E_2, \ E_3 \);

where \( E_1 = \frac{A}{\|A\|} \) and \([E_1, E_2, E_3]\) is a positively oriented orthonormal basis of \( \mathbb{R}^3 \). The eigenpairs of the Jacobi operator are also given in section 4.4.3 with another representation of the Lie algebra.

Table 3.1 gives upper and lower bounds on the eigenvalue of the Hessian of \( f_q \) at \( p \) in function of the Riemannian distance \( d(p,q) \) on \( SO(3) \). Observe that
the squared Riemannian distance function is convex if $d < \pi$ on $SO(3)$. So, the Karcher mean is unique on a ball of radius $\pi/2$ as shown in [39]. And, if the data belongs to a ball of radius $\pi/2 \leq r \leq \pi$ centred at $p$, then there is a unique Karcher mean inside the ball of radius $\pi - r$. In fact, by the triangle inequality, the distance between any point inside this ball and the data points cannot exceed $\pi$, see [22].

To implement the Newton method, a basis of the Lie algebra is needed. On $SO(3)$ one can choose the canonical basis of $\mathbb{R}^3$. Then, using (3.12), one obtains a representation of the Hessian matrix in the chosen basis. Notice also that, since the current estimation of the mean is mapped back to $I$ at each iteration, the diagonalisation of the Jacobi operator is only required at the identity. Once a matrix representation of the Hessian is obtained in the chosen basis, the Newton equations consist of a $3 \times 3$ linear system of equations that can be solved using, e.g. a Cholesky factorization.

A set of $n$ points was generated around the identity, w.l.o.g. since $SO(3)$ is Riemannian homogeneous. The points are distributed uniformly (radially and in each direction) on a ball of radius $r$. The time required to execute the gradient and Newton algorithms to reach a given accuracy was computed using the \textit{tic; ... toc;} function of Matlab and averaged over 100 runs. To be independent of the computer power, we only report the time reduction $(1 - T_{\text{Newton}}/T_{\text{gradient}})100$ (in \%). This set of points was generated 100 times for different values of the radius $r$. The mean and the standard deviation of the time reduction is presented in Table 3.2.

On $SO(3)$, the accuracy was set to $\|\text{grad} F(\mu_k)\| < 10^{-15}$. The unit step size gradient technique was used since it guarantees the convergence. Notice that in the case $r = 3\pi/4$, the starting point was picked randomly inside the ball of radius $\pi/4$ since the Karcher mean is unique inside of this ball. For $r = \pi/4$, the Newton method does not perform better than the gradient method but for $r = \pi/2$ and $r = 3\pi/4$, one observes a significant improvement with the Newton method.

The Newton method is thus useful in some cases. Of course, it would be nice to be able to characterize the basin of attraction of the Newton method. But this goes beyond this thesis.
Table 3.2: Mean (first entry) and standard deviation (second entry) of the time reduction in % in function of the number of data points $n$ and the radius of the ball $r$ on $SO(3)$

<table>
<thead>
<tr>
<th>$r$ vs $n$</th>
<th>4</th>
<th>10</th>
<th>100</th>
<th>1000</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\pi/4$</td>
<td>(4,10)</td>
<td>(5,11)</td>
<td>(3,11)</td>
<td>(5,10)</td>
</tr>
<tr>
<td>$\pi/2$</td>
<td>(24,12)</td>
<td>(29,7)</td>
<td>(29,4)</td>
<td>(28,5)</td>
</tr>
<tr>
<td>$3\pi/4$</td>
<td>(34,14)</td>
<td>(45,7)</td>
<td>(46,3)</td>
<td>(43,3)</td>
</tr>
</tbody>
</table>

3.5 Geometry of $\mathcal{P}_n^+$

Let $\mathcal{P}_n^+$ be the set of symmetric positive definite $n$-by-$n$ matrices:

$$\mathcal{P}_n^+ = \{ p \in \mathbb{R}^{n \times n} | p = p^\top, p \succ 0 \}. \tag{3.15}$$

It is also the set of ellipsoids in $\mathbb{R}^n$, and for $n = 3$, it is often called the set of diffusions tensors. $\mathcal{P}_n^+$ endowed with the so called affine invariant Riemannian metric has been studied in [18, 43, 54]. In this section, we recall the Riemannian symmetric space structure of $\mathcal{P}_n^+$ and detail the derivation of the formulas for the geodesics, the log-mappings and the curvature endomorphism using its Riemannian symmetric space structure. Good references about Riemannian symmetric spaces include [23, 31, 42, 61].

The connected component containing the identity of the general linear group $GL^+(n)$

$$GL^+(n) = \{ g \in \mathbb{R}^{n \times n} | \det(g) > 0 \},$$

which is a Lie group\(^3\), acts on $\mathcal{P}_n^+$ by congruence:

$$\lambda : GL(n) \times \mathcal{P}_n^+ \to \mathcal{P}_n^+ \ (g, p) \mapsto gp^{\top}.$$  

This action is transitive since any element $p \in \mathcal{P}_n^+$ can be written as $p = gg^{\top}$, i.e. for all $p \in \mathcal{P}_n^+$, there exists a $g \in GL(n)$ that maps the identity to $p$ by congruence. Equivalently, $\mathcal{P}_n^+$ is the orbit in $\mathbb{R}^{n \times n}$ of the identity $I$ by the action $\lambda$. The isotropy group at the identity, i.e. the subgroup of $GL^+(n)$ that lets the identity tensor $I$ invariant, is given by the orthogonal group $SO(n)$ since $\lambda(U, I) = UIU^\top = I$ admits $SO(n)$ as solution set, included in $GL^+(n)$. And the isotropy group at any $p = gg^{\top}$ is given by:

$$\mathcal{H}_p = \{ gUg^{-1} | U \in SO(n) \}$$

since

$$\lambda(\mathcal{H}, p) = gUg^{-1}pg^{-\top}U^\top g^{\top} = p.$$  

This turns $\mathcal{P}_n^+$ into a homogeneous space and yields another representation of $\mathcal{P}_n^+$ as the set of left cosets or fibers denoted by $GL^+(n)/\mathcal{H}$, see Figure 3.3.

\(^3\) It is the inverse image of an open set, and so it is a submanifold of $\mathbb{R}^{n \times n}$.

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This kind of construction is often useful to get other representations of the element of $P_n^+$. In fact, by choosing one element in each fiber (specifying a section), we have a representation (a bijection) of the elements of $P_n^+$. One possible choice is the principal square root denoted by $p^{1/2}$. It is given in Matlab by $\text{sqrtm}(p)$, and it can be computed using an eigenvalue decomposition: if $p = UDU^\top$, then $p^{1/2} = UD^{1/2}U^\top$.

Using Theorem 14, since the action $\lambda$ is a smooth map, $P_n^+$ is a smooth submanifold of $\mathbb{R}^{n \times n}$ such that the map $\pi : GL^+(n) \to P_n^+$, $g \mapsto \lambda(g, I) = gg^\top$ is a smooth submersion.

The Lie Algebra of $GL(n)$ denoted by $\mathfrak{gl}_n$ is the set of $n \times n$ matrices. The subspace $\mathfrak{h}$ of $\mathfrak{gl}_n$ that corresponds to the isotropy group $H$ (which is a closed Lie subgroup of $GL^+(n)$) is the set of skew-symmetric matrices:

$$\mathfrak{h} = \text{skew}(n) = \{S \in \mathbb{R}^{n \times n} | S = -S^\top\}.$$

The submersion $\pi$ yields a representation of the tangent space at a point $p \in P_n^+$. In fact, the tangent space at $p$, seen as the vector space of derivations of smooth functions, can be identified with a sub-vector space of the Lie algebra $\mathfrak{gl}_n$ of $GL^+(n)$. In fact, we have the vector space isomorphism:

$$\mathfrak{gl}_n / \mathfrak{h} \to T_p \mathcal{M}, \ V \mapsto X_p(f) = \frac{d}{dt}f(\lambda(\exp(tV), p))|_{t=0}.$$

Notice that when $V \in \text{skew}(n)$, we have $\lambda(\exp(tV), p) = p$.

So to represent the tangent vectors, we can thus pick a sub-vector space $\mathfrak{m}$ of $\mathfrak{gl}_n$ that is also a section. There are particular choices of such a $\mathfrak{m}$ such that $\mathfrak{gl}_n = \mathfrak{h} \oplus \mathfrak{m}$, that satisfies the following properties

$$Ad_H(\mathfrak{m}) \subset \mathfrak{m} \ [\mathfrak{m}, \mathfrak{m}] \subset \mathfrak{h}. \quad (3.16)$$
The first one is called the reductive property, and it mainly ensures the existence of a $GL(n)$-invariant connection, see [31]. The last condition implies the existence of an involutive automorphism $\sigma$ of the Lie group $GL^+(n)$. In fact, we can choose $m = \text{sym}(n)$ where $\text{sym}(n)$ is the set of symmetric matrices. Since the adjoint representation on $GL^+(n)$ is given by $\text{Ad}_H(m) = h mh^{-1}$ for $h \in H = SO(n)$, the reductive condition is clearly satisfied, and we have also $[\text{sym}(n), \text{sym}(n)] \subseteq \text{skew}(n)$.

To turn $\mathcal{P}_n^+$ into a Riemannian symmetric space, we can introduce the following Riemannian metric called the affine invariant Riemannian metric:

$$g_p(X,Y) = \text{tr}(Xp^{-1}Yp^{-1}).$$

This metric is simply the image of the following symmetric positive define form at the tangent space at the identity:

$$g_I(X,Y) = \text{tr}(XY).$$

In fact, we have $\lambda(p^{1/2}, I) = p$ and its differential with respect to the second argument at the identity $I$ is the map: $X \mapsto p^{1/2}Xp^{1/2}$.

Consequently this metric is invariant with respect to the action of the group, or equivalently, the group $GL(n)$ acts by isometries, which makes $\mathcal{P}_n^+$ a Riemannian homogeneous space. Notice that the metric (3.17) corresponds to positive definite Euclidean Hessian of the barrier function: $x \mapsto -\log(\det(x))$ defined on $\mathcal{P}_n^+$.

$\mathcal{P}_n^+$ has actually more than an homogeneous space structure, it is also a Riemannian symmetric space. There exists a symmetry $s_p$ at each point $p \in \mathcal{P}_n^+$, i.e., an involutive isometry that has only $p$ as a local fixed point. At the identity, the symmetry is given by:

$$s_I(q) : \mathcal{P}_n^+ \to \mathcal{P}_n^+, q \mapsto q^{-1}. \quad (3.18)$$

This symmetry is globally defined on $\mathcal{P}_n^+$ (for all $q$) and it is an isometry since $Ds_I(q)[V] = -q^{-1}Vq^{-1}$ preserves the Riemannian metric:

$$g_q(V,V) = g_{s_I(q)}(Ds_I(q)[V], Ds_I(q)[V]).$$

It has only $I$ as a fixed point since the only solution $q \in \mathcal{P}_n^+$ of $q = q^{-1} \Leftrightarrow q^2 = I$ is the identity.

To obtain the symmetry of $q$ at another point $p$, it suffices to compose the action $\lambda(p^{-1/2},.)$ that maps $p$ to the identity and $q$ to $p^{-1/2}qp^{-1/2}$, with the isometry at the identity, and then to apply the inverse action $\lambda(p^{1/2},.)$. This gives:

$$s_p(q) = \lambda(p^{1/2}, s_I(\lambda(p^{-1/2}, q))) = pq^{-1}p.$$  

As a composition of isometries, it is an isometry and it is easy to verify that it is a symmetry.

Using Theorem 18, we have:
• the Riemannian curvature endomorphism is parallel, i.e., \( \nabla R = 0 \),

• the geodesics starting at \( I \) are given by \( \gamma(t) = \lambda(\exp(tS), I) = \exp(2tS) \) with \( S \in m \),

• the curvature endomorphism at the identity is given by \( R_I(X, Y)Z = -[[X, Y], Z] \) for \( X, Y, Z \in m \).

For more convenience, we will pose \( V = 2S \in \text{sym}(n) \) to represent a tangent vector. Notice that, with this convention, the curvature endomorphism becomes:

\[
R_I(X, Y)Z = -\frac{1}{4}[[X, Y], Z].
\]  

(3.19)

The geodesic \( t \to \gamma(t) \) such that \( \gamma(0) = p \) is obtained using the action by isometries:

\[
\gamma(t) = \lambda(p^{1/2}, \gamma(t)) = p^{1/2} \exp(tV)p^{1/2}.
\]  

(3.20)

In this formula, \( V \) must be interpreted as an element of \( m \) or \( T_I \mathcal{P}^+_n \). To obtain a formula for the geodesic that satisfies \( \dot{\gamma}(0) = X \), where \( X \in T_p \mathcal{P}^+_n \), we can use the differential of the isometry \( q \to \lambda(p^{-1/2}, q) = p^{-1/2} qp^{-1/2} \) given by \( X \to p^{-1/2}Xp^{-1/2} \) that maps a tangent vector \( X \in T_p \mathcal{P}^+_n \) to a tangent vector at the identity. This yields the following expression for the geodesic starting at \( p \) in the direction \( X \in T_p \mathcal{P}^+_n \):

\[
\gamma(t) = p^{1/2} \exp(tp^{-1/2}Xp^{-1/2})p^{1/2}.
\]  

(3.21)

With this formula, we can define the Riemannian exponential map and its inverse called the Riemannian log-mapping.

\[
\exp_p : T_p \mathcal{P}^+_n \to \mathcal{P}^+_n, \ v \mapsto p^{1/2} \exp(p^{-1/2}vp^{-1/2})p^{1/2},
\]

\[
\exp_p^{-1} : \mathcal{P}^+_n \to T_p \mathcal{P}^+_n, \ q \mapsto p^{1/2} \log(p^{-1/2} qp^{-1/2})p^{1/2}.
\]

where \( \exp \) and \( \log \) stands for the exponential and matrix logarithm.

We can now turn \( \mathcal{P}^+_n \) into a metric space by defining the Riemannian distance between any two points \( p \) and \( q \). This distance is the length of the shortest geodesic joining \( p \) and \( q \). On \( \mathcal{P}^+_n \); there is only one geodesic that links two points, i.e the cut locus of any point is empty. We have thus

\[
d(p, q) = \sqrt{q_p(\exp_p^{-1}, \exp_p^{-1})} = \sqrt{\text{tr}((\log(p^{-1/2}qp^{-1/2}))^2)}.
\]  

(3.22)

Let us assume that \( p = I \) and \( q = Ud(1, d_2, d_3)U^+ \) (eigenvalue decomposition), then

\[
d(I, q) = \sqrt{\sum_{i=1}^n \log(d_i)^2}.
\]  

(3.23)

Consequently, an ellipsoid on the border of the cone, i.e. a rank deficient ellipsoid, is at an infinite distance to the identity. Notice that the geodesics are defined for all \( t \), which implies by Hopf-Rinow that \( \mathcal{P}^+_n \) is complete as a metric space with this distance function.
3.5.1 Sectional curvature on $\mathbb{P}^n_+$

In this section, we provide a lower bound on the sectional curvature that will be useful further on to derive a bound on the Hessian of the Riemannian squared distance function. Since the curvature tensor is invariant by isometries, and since the group $GL^+(n)$ acts transitively by isometries on $\mathbb{P}^n_+$, we only compute the sectional curvature at the identity. Let us first describe how the Jacobi operator:

$$X \mapsto R(X,Y)Y = -\frac{1}{4}[[X,Y],Y],$$

can be diagonalized. Since the Jacobi operator is a symmetric linear map, it admits an orthonormal basis of eigenvectors. Since $Y$ is a symmetric matrix, let us consider its eigenvalue decomposition:

$$Y = U \begin{pmatrix} \sigma_1 & & \\ & \sigma_2 & \\ & & \ddots \\ & & & \sigma_n \end{pmatrix} U^\top. \quad (3.24)$$

Using this, the eigenvalues $\lambda_i$ and the corresponding eigenvectors $E_i$ of the Jacobi operator on $\mathbb{P}^n_+$ are given by

$$\lambda = 0, \quad E = U e_i e_i^\top U^\top \text{ for } 1 \leq i \leq n; \quad (3.25)$$

$$\lambda = -\frac{1}{4}(\sigma_i - \sigma_j)^2, \quad E = U \frac{1}{\sqrt{2}}(e_i e_j^\top + e_j e_i^\top)U^\top \text{ for } 1 \leq i < j \leq n; \quad (3.26)$$

where $e_i$ stands for the $i$-th identity vector.

The sectional curvature is defined in function of the Riemannian curvature endomorphism by

$$\kappa(X,Y) = \frac{g(R(X,Y)Y,X)}{g(X,X)g(Y,Y) - g(X,Y)^2}.$$ 

It can be shown [34] that it depends only on the section span $(X,Y)$, i.e. the subspace spanned by $X$ and $Y$. If $X$ and $Y$ are two orthogonal tangent vectors of unit norm, the denominator, which corresponds to the area of the parallelogram defined by $X$ and $Y$, equals 1.

**Theorem 21.** A lower bound on the sectional curvature $\kappa$ of $\mathbb{P}^n_+$ equipped with the affine invariant metric (3.17) is $-1/2$. This bound is tight.

**Proof.** Let us decompose $Y$ in (3.24) in the basis of eigenvectors of the Jacobi operator given by (3.25), and $X$ in the basis of eigenvectors of the Jacobi operator $\{E_k\}_{1 \leq k \leq N = \frac{n(n+1)}{2}}$ given by (3.25) and (3.26) such that

$$X = \sum_{i=1}^{N} \alpha_i E_i, \quad Y = \sum_{i=1}^{n} \sigma_i E_i.$$
If \( \|X\| = 1 \) and \( \|Y\| = 1 \), we have also: \( \sum_{i=1}^{N} \alpha_i^2 = 1 \) and \( \sum_{i=1}^{n} \sigma_i^2 = 1 \). The subspace span \((E_1, \ldots, E_n)\) is related to the eigenvalue \( \lambda = 0 \). So the component of \( X \) in this subspace makes no contribution to the sectional curvature. We can thus assume w.l.o.g., that \( X \) is in the orthogonal complement of span \((E_1, \ldots, E_n)\) and thus \( X \perp Y \) since \( Y \in \text{span} (E_1, \ldots, E_n) \). The sectional curvature then becomes:

\[
\kappa(X,Y) = g(R(X,Y)Y, X) = g\left( \sum_{i=n+1}^{N} \alpha_i \lambda_i E_i, \sum_{j=n+1}^{N} \sigma_j E_j \right) = \sum_{i=n+1}^{N} \sigma_i^2 \lambda_i,
\]

and we have the following tight bound:

\[
\min_{n+1 \leq i \leq N} \lambda_i \leq \kappa(X,Y) \tag{3.27}
\]

since we have a convex combination of the \( \lambda_i \)'s. It remains to find a bound on the eigenvalue

\[
\lambda = -\frac{(\sigma_1 - \sigma_2)^2}{4} \quad \text{s.t.} \quad \sigma_1^2 + \sigma_2^2 = 1.
\]

Let us go to polar coordinate:

\[
\sigma_1 = r \cos(\theta), \quad \sigma_2 = r \sin(\theta),
\]

with \( r = 1 \) to parametrize the constraint \( \sigma_1^2 + \sigma_2^2 = 1 \), we obtain

\[
\lambda = \frac{(\sigma_1 - \sigma_2)^2}{4} = \frac{(\sigma_1^2 + \sigma_2^2 - 2\sigma_1 \sigma_2)}{4} = \frac{(1 - \sin(2\theta))}{4}.
\]

\[a(1-\sin(2x))\text{, for } x \in [-\pi, \pi].\]
which is minimal, see 3.4 when $\theta = -\pi/4$ and $3\pi/4$, i.e. $\sigma_1 = \frac{\sqrt{2}}{2}$, $\sigma_2 = -\frac{\sqrt{2}}{2}$ or $\sigma_1 = -\frac{\sqrt{2}}{2}$, $\sigma_2 = \frac{\sqrt{2}}{2}$, and so a lower bound on the sectional curvature $\kappa(\text{span}\{X,Y\})$ is given by $-1/2$ and this bound is tight since (3.27) is tight.

3.5.2  Bound on the Hessian of $F$ on a ball for $P_n^+$

Since, on $P_n^+$, we have $-\frac{1}{2} \leq \kappa \leq 0$, using the results of section 3.3, the Hessian of the squared Riemannian distance function $f_q$ at $p$ is lower bounded by $1$ and upper bounded by

$$L(p) = \sqrt{-\kappa d(p,q) \coth(\sqrt{-\kappa d(p,q)})} = \frac{\sqrt{2}}{2} d(p,q) \coth(\frac{\sqrt{2}}{2} d(p,q)).$$

(3.28)

The same bounds are also valid for $F$. Notice that $x \coth(x)$ goes to $1$ when $x \to 0$, and is strictly increasing and bounded by $1 + x$ on $]0, \infty[$. It has also an oblique asymptote $y = x$. Thus, we have also

$$L(p) = 1 + \frac{\sqrt{2}}{2} \max_i d(p,q_i).$$

This bound is interesting since it depends on the distance $d(p,q)$, and in the next section it is used to derive a step size that ensures the convergence.

Now, we derive the exact value on the largest eigenvalue of the Hessian of $f_q$ at $p$. To do that first note that $f_q$ is invariant by isometries, i.e. we have $f_q(p) = f_{p^{-1/2}q^{-1/2}}(I)$ and more generally $f_q(\gamma(s)) = f_{p^{-1/2}q^{-1/2}}(\gamma_I(s))$ where $s \rightarrow \gamma(s)$ is a geodesic curve passing through $p$ and $\gamma_I(s) = p^{-1/2}\gamma(s)p^{-1/2}$. Thus, we have:

$$\text{Hess}_q(p)[\Delta, \Delta] = \text{Hess}_{f_{p^{-1/2}q^{-1/2}}(I)}[p^{-1/2}\Delta p^{-1/2}, p^{-1/2}\Delta p^{-1/2}].$$

Consequently to find the Riemannian Hessian, we can thus assume w.l.o.g. (by posing $q \leftarrow p^{-1/2}q^{-1/2}$), that $p = I$. Using our explicit expressions of the Jacobi fields on $P_n^+$. Let

$$q = U\text{diag}(d_1, \ldots, d_n)U^\top,$$

be an eigenvalue decomposition of $q$ such that $d_1 \geq \cdots \geq d_n$ and let $c = \frac{d_1}{d_n}$ be its condition number with respect to the 2-norm. We have

$$\exp^{-1}(q) = U\text{diag}(\log(d_1), \ldots, \log(d_n))U^\top,$$
and using (3.13), we obtain
\[
L(I) \leq \frac{(d_1 - d_n)}{2} \coth\left(\frac{(d_1 - d_n)}{2}\right)\|\Delta p\|^2
\]
\[
\leq \frac{\log(d_1) - \log(d_n)}{2} \coth\left(\frac{\log(d_1) - \log(d_n)}{2}\right)\|\Delta p\|^2
\]
\[
= \frac{\log(c)}{2} \coth\left(\frac{\log(c)}{2}\right)\|\Delta p\|^2.
\] (3.29)

This bound tends to 1 when \(c\) is going to 1 and is strictly increasing for \(c > 1\). So if the condition number of the ellipsoids are close to 1, then the upper bound \(L\) will be a bit larger than 1 and the Hessian will be close to the identity.

To get an insight on the conditioning of our problem, let us consider the data points \(\{q_i\}_{i=1}^N\). A good starting point, if we have no particular knowledge about the localization of the Karcher mean, is simply one of the data points. If we choose \(q_1\) as an initial guess, and map it at the identity using the isometry \(q \mapsto q_1^{-1/2}qq_1^{-1/2}\), the data set becomes
\[
\{I, q_1^{-1/2}q_2q_1^{-1/2} \cdots q_1^{-1/2}q_Nq_1^{-1/2}\}.
\]
The Hessian at \(I\) depends on the relative conditioning of the data matrices, i.e. the condition number of the data matrices after a translation by isometries that maps one of the data points to the identity.

### 3.6 Step size selection rule for the gradient method on \(P_n^+\)

In this section, a step size selection rule that ensures the convergence of the gradient algorithm is provided. The gradient iteration is given by:
\[
p_{k+1} = \exp_{p_k}(h_k \grad F_k), \text{ where } \grad F_k = \frac{1}{N} \sum_{i=1}^N \exp_{p_k}^{-1}(q_i). \tag{3.30}
\]

The main idea consists in choosing a step size \(h_k\) such that our objective function \(F\) defined in (3.3) is reduced. To guarantee that, a quadratic upper bound on \(F\) restricted to a geodesic curve starting at \(p_k\) is derived using an upper bound \(L_k\) on the largest value of its Hessian on a ball centred at the current iteration \(p_k\) that contains all the data points. Of course, we need to take care of the fact that our step size does not lead \(p_{k+1}\) outside of this ball, since in this situation our bound \(L_k\) will no longer be valid.

Notice that, in our case, \(L_k \geq 1\) and so
\[
\frac{1}{L_k} \leq \frac{2}{1 + L_k} \leq \min\left(\frac{2}{L_k}, 1\right).
\]
The following theorem provides a convergence proof for the two step size selection rules below.
Theorem 22. If the starting point is one of the data points, and if, in the iteration (3.30), the step size at iteration $k$, is chosen such that

$$h_k = \frac{1}{L_k} \quad \text{or} \quad h_k = \frac{2}{1 + L_k},$$

where

$$L_k = 1 + \frac{\sqrt{2}}{2} \left( \max_i d(p_k, q_i) + \|\text{grad} F_k\| \right),$$

(3.31)

then the gradient method Algorithm 2 converges to the unique Karcher mean.

Proof. The proof of convergence is based on the relaxation principle, i.e., the value of the cost function $F$ at each iteration must be strictly decreasing. So, the step size $h_k$ must be chosen to ensure this decrease. Let $r_k = \max_i d(p_k, q_i)$ and notice that by assumption $h_k \leq 1$ which ensures that $h_k \|\text{grad} F_k\| \leq \|\text{grad} F_k\| \leq r_k$ since:

$$\|\text{grad} F_k\| = \frac{1}{N} \sum_{i=1}^{N} \|\exp_{p_k}^{-1}(q_i)\| \leq r_k.$$

This ensures that $p_{k+1}$ will not leave the ball $B(p_k, r_k)$, see Figure 3.5. Furthermore, the bound on the Hessian $L_k$, see Section 3.5.2, is valid at every point of the geodesic segment $\{\exp_{p_k}(-th_k\text{grad} F_k) | t \in [0, 1]\}$. In fact, we have

$$d(q_i, \exp_{p_k}(-th_k\text{grad} F_k)) \leq r_k + \|\text{grad} F_k\| \quad \forall i \quad \forall t \in [0, 1].$$
We can now apply a classical 1-dimensional argument as in [41]. Let $h_k \mapsto \gamma(h_k) = \exp_{p_k}(-h_k \nabla F_k)$ be the geodesic curve such that $\gamma(0) = p_k$ and $\frac{d}{dh} \gamma|_{h=0} = - \nabla F_k$. Using a Taylor expansion we obtain

$$F(\gamma(h_k)) = F(\gamma(0)) - h_k g_{\gamma(0)}(\nabla F(\gamma(0)), \nabla F(\gamma(0))) + \frac{h_k^2}{2} \text{Hess}(\gamma(h_k))[\gamma^*(h_k^*), \gamma(h_k^*)],$$

with $h_k^* \in ]0, h_k[. \text{ With } L_k \text{ as in (3.31), we have}$

$$\text{Hess}(\gamma(h_k^*))[\gamma^*(h_k^*), \gamma(h_k^*)] \leq L_k \|\gamma(h_k^*)\|^2 \leq L_k \|\gamma(0)\|^2 = L_k \|\nabla F(\gamma(0))\|^2,$$

and thus

$$F(\gamma(h_k)) - F(\gamma(0)) \leq (-h_k + \frac{1}{2} h_k^2 L_k) \|\nabla F(\gamma(0))\|^2.$$ (3.32)

To guarantee the decrease of the objective function, the upper bound on the right-hand side must be strictly negative. This is true if $0 < h_k < \min(2/L_k, 1)$, and $h = 1/L_k$ minimizes the bound. By taking the sum from 1 to $k$ on the left-hand side and on the right-hand side, one obtains

$$\sum_{i=1}^{k} \|\nabla F(\mu_i)\|^2 \leq \sum_{i=1}^{k} \frac{(F(\mu_{i+1}) - F(\mu_i))}{(-h_i + \frac{1}{2} h_i^2 L_i)},$$

$$\leq \frac{1}{\min_{1 \leq i \leq k}(|-h_i + \frac{1}{2} h_i^2 L_i|)} \sum_{i=1}^{k} (F(\mu_{i+1}) - F(\mu_i)).$$

This implies $\|\nabla F(\mu_k)\| \to 0$ when $k \to \infty$ since the right-hand side is bounded. Indeed,

$$\sum_{i=1}^{k} (F(\mu_{i+1}) - F(\mu_i)) = (F(\mu_{k+1}) - F(\mu_1)),$$

is bounded since $F$ is bounded from below by 0 and $\exists \epsilon$ such that

$$\min_i (|-h_i + \frac{1}{2} h_i^2 L_i|) > \epsilon > 0.$$

Indeed, the function $F$ is coercive (strongly convex), thus there exists a ball $B(I, r_{\max})$ centred at the identity that contains all the data points and the starting points $p_k$ such that $F(p_k) \leq F(B) = \min_{p \in \partial B} F(p)$. Using (3.32), the iterations cannot escape this ball. So the maximal distance between the current iterate and the data points remains bounded by $2r_{\max}$, and using (3.31), $L_i \leq \frac{\sqrt{2}}{1}(1 + 4r_{\max})$, which implies the existence of $\epsilon$ since we can choose $\epsilon = \frac{\sqrt{2}}{2}(1 + 4r_{\max})$, $h_i = 1/L_i$, and $\epsilon = \frac{\sqrt{2}}{2}(1 + 4r_{\max}) L_i r_i$ when $h_i = \frac{1}{2} L_i r_i$.\]
This theorem proves the global convergence of our step size selection rules but does not say anything about the convergence rate. The convergence rate will be illustrated numerically on some examples in section 3.8.

3.7 Implementation

In this section, we provide a concrete algorithm, see Algorithm 2, that maps the current iteration \( \mu_k \) at the identity using the isometry \( x \mapsto \mu_k^{-1/2} x \mu_k^{-1/2} \) at each iteration and choose the step size using the rule derived in Theorem 22. The composition of all these isometries are stored in the matrix \( Y \) and its inverse is applied to the estimated Karcher mean at step 21. Mapping the current iteration at the identity at each iteration, and also the data points \( q_i \), could lead to numerical error accumulation if many iterations are performed. In fact, after a few iterations, it is like if we are solving the Karcher mean problem with a modified version of the data points \( q_i \). But the method could still be restarted with the original data if this problem occurs.

**Algorithm 2** Gradient method on \( \mathcal{P}_n^+ \)

**Require:** \( N \) data points \( q_1, \ldots, q_N \in \mathcal{P}_n^+ \), a required precision \( \epsilon \), and an initial iterate \( p_0 \in \mathcal{P}_n^+ \) (typically one of the data points);

**Ensure:** \( \mu \) is their Karcher mean

1: set \( k = 0 \), set \( \mu = p_0 \);
2: set \( Y = I \) to keep track of all the isometries;
3: until \( g(\text{grad} F(p_k), \text{grad} F(p_k)) < \epsilon \) do
4: compute \( \mu^{-1/2} \) (eigenvalue decomposition);
5: compute \( Y = \mu^{-1/2} Y \) the matrix representing all the isometries;
6: for \( i = 1 \rightarrow N \) do
7: \( q_i \leftarrow \mu^{-1/2} q_i \mu^{-1/2} \);
8: compute \( q_i = U D U^\top \) (diagonalisation) and set \( d = \text{diag}(D) \);
9: compute the condition number \( c_i = \max d / \min d \);
10: compute the distance \( l_i = \| \log d \| \);
11: compute \( K_i = U (\log(d)) U^\top \);
12: end for
13: compute \( \Delta = \frac{1}{N} \sum_{i=1}^{N} K_i \);
14: normalization \( \Delta = (\Delta + \Delta^\top)/2 \) (to reduce numerical errors);
15: bound on the Hessian valid on a ball \( L_{\text{ball}} = 1 + \frac{\sqrt{2}}{2} (\max_i l_i + \| \Delta \|) \);
16: compute the bound on the Hessian at \( I \): \( L = \log(\max(c_i)) \coth(\log(\max(c_i))) \approx 1 + \frac{\log(\max(c_i))}{\log(\max(c_i))} \approx 1 + \frac{1}{1 + \frac{\pi^2}{2} L_{\text{ball}}} \);
17: choose a step \( h = \frac{2}{1 + L} \) or \( h = \frac{2}{1 + L_{\text{ball}}} \);
18: compute \( h\Delta = U D U^\top \) and set \( \mu = U e^{\Delta} U^\top \);
19: \( k \leftarrow k + 1 \);
20: end until
21: return \( Y^{-1} \mu Y^{-1} \);
At step 17, we need to choose a step size $h$ using our bound on the Hessian $L$ valid only at the identity and our bound on the Hessian $L_{\text{ball}}$ valid on a ball containing all the data points. We can choose $h = \frac{2}{1+L_{\text{ball}}}$ or $h = \frac{1}{L_{\text{ball}}}$ to ensure the convergence see, Theorem 22, or choose $h = \frac{2}{1+L}$, even if the convergence is not guaranteed in that case.

3.8 Numerical experiments

In this section, we compare different step size strategies. Since the problem is invariant by isometries, the data points can be generated, w.l.o.g. around the identity $I$. We generated 5 data points of dimension $n = 10$ on a radial strip of interior radius $r_1 = 6$ and exterior radius $r_2 = 7$ centred around the identity. The results are shown on Figure 3.6. The unit step size gradient method (magenta) seems to converge but very slowly. It was stopped after 200 iterations. The step size selection rule $h = \frac{2}{1+L_{\text{ball}}}$ (red) is much better than $h = \frac{1}{L_{\text{ball}}}$ (blue). Notice that these two step size selection rules guarantee the converge, see Theorem 22. The green curve, corresponding to $h = \frac{2}{1+L}$ where $L$ is chosen as in step 16 algorithm 2, gives a better convergence rate but there is no proof of global convergence for this step size rule. This suggests to use the step size rule $h = \frac{2}{1+L_{\text{ball}}}$ at the beginning and then switch to $h = \frac{2}{1+L}$ to take advantage of its better convergence rate. When this switch must be done, is still an open question.

The value of $L_{\text{ball}}$ and $L$ are presented on Figure 3.7. We can observe a monotone decrease of the two bounds at the beginning and after a few iterations, the bounds remain constant, and so the related step sizes remain the same, and we have reached the asymptotic rate of convergence. The asymptotic gap between these two curves gives an idea of the level of conservatism we have introduced using the bound $L_{\text{ball}}$ on the Hessian. By Theorem 22, $L_{\text{ball}}$ cannot increase during the iterations since $L_{\text{ball}}$ at iteration $k$ is valid on $B(p_k, r_k)$ and the next iterate $p_{k+1}$ belongs to that ball. On the contrary, $L$ can increase as the next simulation demonstrates, see Figure 3.8. In that simulation, the data points are distributed around a geodesic curve.

3.9 Computation of the Newton step

To compute the Newton step, we need to solve the system of Newton’s equations:

$$H_{op}(\Delta) = -\text{grad}f,$$

where $H_{op} : T_pM \rightarrow T_pM$ is defined by

$$\text{Hess}(I)[\Delta, \Delta] = g_I(H_{op}(\Delta), \Delta).$$

A first approach is to build the Hessian matrix $H$ from the Hessian form
Figure 3.6: Norm of the gradient $\|\text{grad}F\|$ at the current iteration $k$ for different step size selection rules.

(3.12):

$$\text{Hess} f(I)[\Delta, \Delta] = \sum_{k=1}^{m} g_I(\Delta, E_k(1))^2 w_k(1),$$

by choosing a specific basis of $T_I\mathcal{M}$. Notice that we only need $\text{Hess} f[\Delta, \Delta]$ since the Hessian is a symmetric form, we have the following identity:

$$\text{Hess} f[\Delta_1, \Delta_2] = \frac{\text{Hess} f[\Delta_1 + \Delta_2, \Delta_1 + \Delta_2] - \text{Hess} f[\Delta_1, \Delta_1] - \text{Hess} f[\Delta_2, \Delta_2]}{2}.$$

But this Hessian matrix $H$ would be a $\frac{n^2-n}{2} \times \frac{n^2-n}{2}$ matrix. So, forming the Hessian matrix and storing it in memory will rapidly become an issue when $n$ increases.

To avoid computing the Hessian matrix $H$, the main idea consists in solving the Newton’s equations using an iterative method like the conjugate gradient method. Note that this method requires at most $\frac{n^2-n}{2}$ evaluations of the function $\Delta \mapsto H_{op}(\Delta)$. From the expression of the Hessian given in section 3.3, and the explicit expression of the eigenpairs of the Jacobi operator (3.25), one obtains
Figure 3.7: Value of $L_{\text{ball}}$ (triangle) and $L$ (dot) at each iteration $k$ for the step size rule $h = \frac{2}{1 + L_{\text{ball}}}$ (red curve) and $h = \frac{2}{1 + L}$ (green curve). The data points are distributed on a radial strip.

$$H_{op}(\Delta) = \sum_{k=1}^{m} g_1(\Delta_1, E_k(1)) w_k(1) E_k(1),$$

$$= \sum_{1 \leq i \leq j \leq n} \text{trace}(U^\top \Delta U E_{ij}) w_{ij} U E_{ij} U^\top,$$

where $E_{ij}$ is the symmetric matrix:

$$E_{ij} = \frac{1}{\sqrt{2}} (e_i e_j^\top + e_j e_i^\top),$$

and $w_{ij} \in \mathbb{R}$ is defined by:

$$w_{ij} = \frac{|\sigma_i - \sigma_j|}{2} \coth \left( \frac{|\sigma_i - \sigma_j|}{2} \right).$$

To implement this, let $B = U^\top \Delta U$ which is a symmetric matrix, we have

$$\text{trace}(U^\top \Delta U E_{ij}) = \frac{1}{\sqrt{2}} \left( \text{trace}(e_j^\top B e_i) + \text{trace}(e_i^\top B e_j) \right),$$

$$= \frac{1}{\sqrt{2}} (B(j,i) + B(i,j)),$$

$$= \frac{2}{\sqrt{2}} B(i,j) = \sqrt{2} B(i,j),$$

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Figure 3.8: Value of $L_{\text{ball}}$ (triangle) and $L$ (dot) at each iteration $k$ for the step size rule $h = \frac{2}{1 + L_{\text{ball}}}$ (red curve) and $h = \frac{2}{1 + T}$ (green curve). The data points are distributed around a geodesic curve.

where $B(i,j)$ is the entry $(i,j)$ of the matrix $B$.

Thus one obtains,

$$H_{\text{op}}(\Delta) = U \left( \sum_{1 \leq i \leq j \leq n} \sqrt{2}B(i,j)w_{ij}E_{ij} \right)U^T,$$

$$= U \left( \sum_{1 \leq i \leq j \leq n} B(i,j)w_{ij}(e_i e_j^T + e_j e_i^T) \right)U^T.$$

This last expression can be computed using the Hadamard product, $B \circ W$ with $W(i,j) = w_{ij}$, which is efficient in Matlab in terms of computational time. The computational complexity of evaluating $H_{\text{op}}(\Delta)$ is in $O(n^3)$ flops. The conjugate gradient method needs to evaluate $H_{\text{op}}(\Delta)$ for a few $\Delta$’s. To do that, observe that $W$ must be computed only once and the $U$ is known since we have already computed the gradient, see step 8 of Algorithm 2.

3.9.1 Numerical experiments

In this section, the Newton method, where the Newton equations are solved by means of a conjugate gradient scheme, is compared with the gradient method. A set of 5 data points was generated on a radial strip around the identity $I$.
using:
\[ q_r = \exp_1 ((r + u) \frac{V}{\|V\|}), \]

where \( u \) is uniformly distributed on \([0, 1]\) and \( V \) is a symmetric matrix whose entries are Gaussian and identically distributed. The interior radius of the radial strip is \( r \) and the exterior radius is \( r + 1 \). In Table 3.3 and in Table 3.4, the mean and the standard deviation of the computational time required by different methods to reach \( \|\text{grad} F\| \leq 1e^{-10} \) are presented for different values of \( r \). The average was taken over 40 runs with different data points distributed on the radial strip. The conjugate gradient method is stopped when the norm of the residues reaches \( 1e^{-12} \). Another approach would be to reduce this threshold at least for the first Newton iterations, but we have sometimes observed a degradation of convergence rate.

For \( n = 10 \), see figure 3.9, we observe that the gradient method with the step size \( h = \frac{2}{1 + L} \) is faster than for \( h = \frac{2}{1 + \text{Nest}} \) for all values of \( r \). This is due to the fact that the former needs less iterations to converge than the latter, see Table 3.3. The Newton method is comparable to the gradient method with \( h = \frac{2}{1 + L} \) when \( r \) is small. However, when \( r \) increases, the Newton method gets better. So, even if it has not been proved to be globally convergent, for \( n = 10 \), the gradient method with \( h = \frac{2}{1 + L} \) seems to be the best choice for small values of \( r \), and when \( r \) increases, the Newton method becomes competitive.

For \( n = 100 \), see figure 3.10, the Newton method is faster than the gradient method except for small values of \( r \). Notice that for small values of \( r \) the Hessian of \( F \) is close to the identity, and thus the gradient step and the Newton step are similar. Notice that the computational time of the Newton method does not depend a lot on \( r \). Consequently, the Newton method seems to be more robust to the way the data points are distributed. Observe also that the number of Newton steps remains almost constant when \( n \) increases as opposed to the number of CG iteration, see Table 3.4. This is due to the fact that the number of CG iterations is affected by the conditioning number of the Hessian which is upper bounded by \( L \) since the lower bound on the Hessian is 1.

The number of CG iterations is much lower than \( \frac{n^2 + n}{2} \), i.e. the dimension of the problem. This is one of the key computational facts, thanks to the choice of the opposite of the gradient as a starting point. A random initialization often lead to much more CG iterations.

When \( n \) increases, it seems that the difference in terms of computational time between the gradient method and the Newton method increases as well. This could be due to the fact that the computation of the diagonalisation of the data points at step 8 becomes the dominant component of the cost when \( n \) is large. Observe that the Matlab built-in function \( \text{eig} \) is used to compute the eigenvalue decomposition at step 8 of algorithm 2.

For all methods, we also observe an increase of the computational time when \( r \) is increasing. This is due to the fact that more steps are needed for the gradient method, and for the Newton method, more Newton steps but also more conjugate gradient iterations.
Figure 3.9: $n = 10$ The circle is the mean of the samples. The upper and lower side of the rectangle box are the upper quartile, i.e. 25% of the data are greater than this value, and lower quartile, respectively. The grey points are the outliers, i.e. lower or greater than $1.5$ times the lower or upper quartiles, respectively. The upper and lower bar are the maximum and minimum, respectively (excluding the outliers). The black bar in the middle of the box is the median.
Figure 3.10: \( n = 100 \) The circle is the mean of the samples. The upper and lower side of the rectangle box are the upper quartile, i.e. 25% of the data are greater than this value, and lower quartile, respectively. The grey points are the outliers, i.e. lower or greater than 1.5 times the lower or upper quartiles, respectively. The upper and lower bar are the maximum and minimum, respectively(excluding the outliers). The black bar in the middle of the box is the median.

<table>
<thead>
<tr>
<th>( r = 2 )</th>
<th>( r = 5 )</th>
<th>( r = 10 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>gradient with ( h = \frac{2}{1 + L_{ball}} )</td>
<td>(35, 1)</td>
<td>(59, 2)</td>
</tr>
<tr>
<td>gradient with ( h = \frac{2}{1 + L} )</td>
<td>(17, 1)</td>
<td>(35, 2)</td>
</tr>
<tr>
<td>CG iterations</td>
<td>(24, 1)</td>
<td>(46, 2)</td>
</tr>
<tr>
<td>Newton iterations</td>
<td>(5, 0)</td>
<td>(6, 0)</td>
</tr>
</tbody>
</table>

Table 3.3: \( n = 10 \) Number of iterations required to reach an accuracy of \( 1e-10 \) for the gradient method with \( h = \frac{2}{1 + L_{ball}} \) and \( h = \frac{2}{1 + L} \). The number of CG iterations is the sum of the CG iterations over all Newton iterations. The first entry is the mean and the second entry is the standard deviation (rounded).
gradient with $h = \frac{2}{1+L_{\text{ball}}}$ & (61, 2) & (101, 2) & (176, 2) & (212, 5) \\
gradient step $h = \frac{2}{1+L}$ & (15, 0) & (24, 0) & (43, 1) & (54, 1) \\
CG iteration & (21, 1) & (34, 1) & (63, 1) & (75, 2) \\
Newton iterations & (5, 0) & (5, 0) & (6, 0) & (6, 0) \\

Table 3.4: $n = 100$ Number of iterations required to reach an accuracy of $1e-10$ for the gradient method with $h = \frac{2}{1+L_{\text{ball}}}$ and $h = \frac{2}{1+L}$. The number of CG iterations is the sum of the CG iterations over all Newton iterations. The first entry is the mean and the second entry is the standard deviation (rounded).

3.10 Karcher mean of approximated covariance matrices

In this section, we consider that the data matrices are symmetric positive definite matrices that are a scaling of the identity plus a low rank matrix:

$$q_i = \alpha_i I + X_i X_i^\top$$

for $1 \leq i \leq m$, where the $X_i \in \mathbb{R}^{n \times p}$ with $n \gg mp$. This kind of $q_i$’s can be interpreted as an estimation of a covariance matrix using $p$ data vectors in $\mathbb{R}^n$, which are the columns of the matrix $X$. Notice that we are not considering low rank matrices, i.e. flat ellipsoids but simply ellipsoids that are isotropic on some subspace. Observe that these matrices are cheap to diagonalize. Indeed, let $X = QR$ (thin QR-factorization), we have $q = \alpha I + QRR^\top Q^\top$, and let $RR^\top = UDU^\top$, then the matrix $[QU | Q^\perp]$ where $Q^\perp$ is an orthogonal completion of $Q$, diagonalizes the matrix $q$. The eigenvalues related to $QU$ are the $\alpha + d_i$’s, and the eigenvalues related to $Q^\perp$ equal $\alpha$.

Note also that, under the assumption that $n \gg mp$, all the $q_i$’s have a common eigenspace related to the eigenvalue $\alpha_i$. Indeed, let $[X_1, \cdots, X_m] = QR$ and let $U_c$ be an orthogonal completion of $Q$, the column space of $U_c$ is a basis for this common eigenspace. So we can assume that all the data points can be diagonalized by

$$ q_i = \begin{bmatrix} U_i & U_c \end{bmatrix} \begin{bmatrix} D_i & 0 \\ 0 & \alpha_i I \end{bmatrix} \begin{bmatrix} U_i^\top \\ U_c^\top \end{bmatrix} = U_i D_i U_i^\top + \alpha_i U_c U_c^\top, $$

where $U_i \in \mathbb{R}^{n \times mp}$ with $U_c \in \mathbb{R}^{n \times (n-mp)}$. We may wonder how to compute the Karcher mean of such kind of data. Let us consider a subset $\tilde{M}$ of $\mathcal{P}_n^+$ that consists of symmetric matrices that have a common eigenspace. Let us fix $U_c$, an orthogonal basis of this common eigenspace we can define

$$ \tilde{M} = \{ U DU^\top + U_c \Lambda U_c^\top | U \in St(n, mp) \perp U_c, \ \Lambda \text{ is diagonal} \}. $$

The identity $I$ belongs to $\tilde{M}$ and the theorem below implies that $\tilde{M}$ is a geodesically complete submanifold of $\mathcal{P}_n^+$. 

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Theorem 23. [31, Theorem 4.3, chap XI, vol II] Let \((G, H, \sigma)\) be a symmetric space and let \(\mathfrak{g} = \mathfrak{m} + \mathfrak{h}\) be the canonical decomposition. Then there is a natural one-to-one correspondence (bijection) between the set of linear subspaces \(\mathfrak{m}\) of \(\mathfrak{m}\) such that: \([\tilde{\mathfrak{m}}, \mathfrak{m}] \subset \mathfrak{m}\) and the set of complete totally geodesic submanifolds \(\mathcal{M}\) through the origin \(o\) of the symmetric space \(\mathcal{M} = G/H\).

Let \(q \in \mathcal{M}\), its log-mapping at the identity is given by the matrix logarithm of \(q\), which yields a tangent vector:

\[
v = \log(q) = U \log(D) U^T + U_c \log(A) U_c^T.
\]

Let us define the subset \(\tilde{\mathfrak{m}} \subset \mathfrak{m}\) as the image of \(\tilde{\mathcal{M}}\) by the log-mapping at the identity. This subset \(\tilde{\mathfrak{m}}\) is a subvector space of \(\mathfrak{m}\). Let

\[
v_1 = U_1 L_1 U_1^T + U_c K_1 U_c^T,
\]

\[
v_2 = U_2 L_2 U_2^T + U_c K_2 U_c^T,
\]

\[
v_3 = U_3 L_3 U_3^T + U_c K_3 U_c^T,
\]

where the \(L_i\)'s and \(K_i\)'s are diagonal matrices. We have \(v_1 v_2 = U_1 L_1 U_1^T U_2 L_2 U_2^T + U_c K_1 K_2 U_c^T\), and thus

\[
[v_1, v_2] = U_1 L_1 U_1^T U_2 L_2 U_2^T - U_2 L_2 U_2^T U_1 L_1 U_1^T + U_c (K_1 K_2 - K_2 K_1) U_c^T \in \mathfrak{h},
\]

is a low rank matrix and

\[
[[v_1, v_2], v_3] = U_1 L_1 U_1^T U_2 L_2 U_2^T U_3 L_3 U_3^T - U_2 L_2 U_2^T U_1 L_1 U_1^T U_3 L_3 U_3^T
\]

\[
- U_3 L_3 U_3^T U_1 L_1 U_1^T U_2 L_2 U_2^T + U_3 L_3 U_3^T U_2 L_2 U_2^T U_1 L_1 U_1^T \subset \tilde{\mathfrak{m}},
\]

which is a low rank matrix. Since it belongs to \(\tilde{\mathfrak{m}}\), Theorem 23 implies that \(\tilde{\mathcal{M}}\) is a geodesically complete submanifold of \(\mathcal{P}_+^m\). This means that any geodesic curve between any two points \(q_1\) and \(q_2\) that belong to \(\tilde{\mathcal{M}}\) is entirely contained in \(\tilde{\mathcal{M}}\). This implies in particular that the Karcher mean of points in \(\tilde{\mathcal{M}}\) will be in \(\tilde{\mathcal{M}}\). Consequently, we expect the existence of an algorithm to compute the Karcher mean that do not compute \(U_c\).

Let \(\mu\) be the Karcher mean, which is the unique solution of:

\[
\sum_{i=1}^{m} \exp_{\mu}^{-1}(q_i) = \sum_{i=1}^{m} \mu^{1/2} \log(\mu^{-1/2} q_i \mu^{-1/2}) \mu^{1/2} = 0. \tag{3.33}
\]

Thus, if all the \(q_i\)'s are of the form

\[
q_i = U_i D_i U_i^T + U_c A_i U_c^T,
\]

the solution of (3.33) is of the form:

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\[ \mu = U_m D_m U_m^\top + U_c \Lambda_m U_c^\top. \]

Indeed, by replacing \( \mu \) in (3.33), one obtains

\[
\sum_{i=1}^{m} \log(\mu^{-1/2} q_i \mu^{-1/2}) = \sum_{i=1}^{m} [U_m \ U_c] \log \left( \begin{bmatrix} D_{m}^{-1/2} U_m^\top D_i U_i^\top U_m D_m^{-1/2} & 0 \\ \Lambda_m^{-1/2} \Lambda_i \Lambda_m^{-1/2} \end{bmatrix} \right) [U_m \ U_c]^\top = 0,
\]

which implies

\[
\sum_{i=1}^{m} \log(D_{m}^{-1/2} U_m^\top D_i U_i^\top U_m D_m^{-1/2}) = 0, \quad (3.34)
\]

\[
\sum_{i=1}^{m} \log(\Lambda_m^{-1/2} \Lambda_i \Lambda_m^{-1/2}) = 0. \quad (3.35)
\]

Since the \( \Lambda \)'s are diagonal matrices, (3.35) yields for each entry \( \lambda_i \) of \( \Lambda_i \) and \( \lambda_m \) of \( \Lambda_m \):

\[
\sum_{i=1}^{m} \log(\frac{\lambda_i}{\lambda_m}) = \sum_{i=1}^{m} \log(\lambda_i) - m \log(\lambda_m) = 0,
\]

which implies

\[ \lambda_m = \left( \prod_{i=1}^{m} \lambda_i \right)^{1/m}, \]

i.e. \( \lambda_m \) is the geometric mean of the \( \lambda_i \)'s.

Let us fix \( E \) such that \([E \ U_c]\) is an \( n \times n \) orthonormal matrix. We can choose \( E = U_1 \) for instance. Let us express the \( U_i \)'s in the basis formed by the columns of \( E \):

\[ u_i \in SO(mp) \] such that \( U_i = E u_i \) and \( U_m = E u_m \). We have \( U_m^\top U_i = u_m^\top E^\top U_i = u_m^\top u_i \) and (3.34) yields

\[
\sum_{i=1}^{m} u_m^\top \log(u_m D_m^{-1/2} u_m^\top u_i D_i u_i^\top u_m D_m^{-1/2} u_m^\top) u_m = 0,
\]

thus \( \tilde{\mu} = u_m D_m u_m^\top \) is the Karcher mean of the data points \( \tilde{q}_i = u_i D_i u_i^\top \in P^+_{mp} \) which can be computed using our gradient method. The solution of (3.33) is then given by:

\[ \mu = E \tilde{\mu} E^\top + U_c \Lambda_m U_c^\top. \]

\[ ^4 \text{This is possible since } U_i^\top U_c = 0 \forall i. \]
In terms of computational cost, this approach is interesting. Since computing the Riemannian exponential map and the log-mapping require an eigenvalue decomposition of a symmetric positive definite matrix of size $n \times n$. If we assume that we have only $m$ data matrices $q_i$ that are a scaling of the identity plus a matrix of rank at most $p$, we just have to compute a Karcher mean on $P^m_\text{mp}$. Consequently, if $mp$ is small with respect to $n$, the reduction in terms of computational cost will be significant.
Chapter 4

Geodesic data fitting

In this chapter, a method to compute the best geodesic approximation of a set of points that belong to a Riemannian manifold is proposed. This method is based on a gradient descent technique on the tangent bundle of the manifold. An expression for the gradient is derived using the theory of Jacobi fields and an efficient numerical technique is proposed to compute these Jacobi fields. The presented approach is valid on any Riemannian locally symmetric space like the sphere $S^2$, the set of symmetric positive definite matrices $P^+_n$, the special orthogonal group $SO(3)$, and the Grassmann manifold Grass$(n, p)$. This chapter has been published in [46].

Main contributions: formulas for the gradient for

- the sphere $S^2$,
- the special orthogonal group $SO(n)$,
- the set of symmetric positive definite matrices $P^+_n$,
- the Grassmann manifold Grass$(n, p)$.

4.1 Introduction

In many areas of signal and image processing, we have to deal with data that belong to nonlinear spaces or manifolds, see [16, 48] and the references therein. To extract some information out of these data, many authors have proposed different optimization schemes to compute the Karcher mean, i.e., a generalized notion of mean that is defined using the Riemannian distance, see [29]. Moreover, the problem of finding a smooth curve that interpolates a set of time labeled data points is discussed in [11], and a variational approach to find a smooth curve that approximates a set of time labeled data points is presented in [36]. In this chapter, we propose a method to compute the generalization of the best linear regression model. More precisely, we want to find the best geodesic,
\[ \gamma(0) = p \gamma(1) q_2 q_1 q_3 M \gamma(t_1) \gamma(t_2) \gamma(t_3) v \]

Figure 4.1: Problem illustration. The dashed line is the geodesic curve we want to find and the continuous lines are geodesics whose length equals \( d(q_i, \gamma(t_i)) \).

i.e., a generalization of a parameterized straight line that approximates a given set of data on the manifold.

This problem can be formulated as an optimization problem. Indeed, let \( \{ (q_i, t_i) | q_i \in \mathcal{M}, 0 \leq t_i \leq 1 \}_{i=1}^m \) be some time labeled data points on a Riemannian manifold \((\mathcal{M}, g)\). The goal is then to find a geodesic curve \( t \mapsto \gamma^*(t) \) that minimizes the sum of the squared Riemannian distances \( d \) between the data points \( q_i \)'s and their corresponding points on the geodesic curve \( \gamma(t_i) \), see Fig. 4.1. This yields the following optimization problem:

\[
\gamma^* = \arg\min_{\gamma \text{ is a geodesic in } \mathcal{M}} \frac{1}{2} \sum_{i=1}^m d(q_i, \gamma(t_i))^2.
\]

Such a best geodesic approximation can, e.g., be used to identify the parameters of constant velocity dynamical models. In fact, many methods have been proposed to deal with data that possess a dynamic behavior. For instance, this happens in the subspace tracking problem, see [47] and the references therein, and in filtering problems on the special orthogonal group \( SO(3) \), see [38]. In these situations a constant velocity model or geodesic model is often assumed (at least on some time window) to represent the dynamic behavior of the data on the manifold, and the \( t_i \)'s are the sampling instants. Our geodesic data fitting technique can be useful to assess the validity of such a model or to identify the parameters of a noise model as in [47].

A geodesic is a curve of zero acceleration, i.e., \( \nabla \dot{\gamma} \dot{\gamma} = 0 \), where \( \nabla \) stands for the Riemannian connection. So, a geodesic is the solution of a second order differential equation. This equation has a unique solution on some time window, if \( p = \gamma(0) \in \mathcal{M} \) and \( v = \dot{\gamma}(0) \in T_p \mathcal{M} \) are specified. Thus, a geodesic can be uniquely represented by a point \( (p, v) \) in the tangent bundle \( T\mathcal{M} = \{(p, v) \mid p \in \mathcal{M}, \ v \in T_p \mathcal{M} \} \). Notice that \( T\mathcal{M} \) is a manifold of dimension \( 2 \dim(\mathcal{M}) \). The problem (4.1) with this parameterization of the geodesics in \( \mathcal{M} \) is described in [36], where the authors give a first order necessary condition of optimality on the sphere \( S^2 \) and on the special orthogonal group \( SO(n) \). This necessary condition is a nonlinear system in \( p \) and \( v \) and no algorithm is given to solve this system.

In this chapter, a gradient descent technique on \( T\mathcal{M} \) is proposed to find
a stationary point of the objective function in (4.1). This gradient descent method is introduced in section 4.2. Our geometric approach to derive the gradient is described in section 4.3. Section 4.4 explains how to efficiently diagonalize the Jacobi operator, which is one of the key computational steps in the computation of the gradient. Section 4.5 presents some numerical experiments.

4.2 Steepest descent on the tangent bundle

In this section, some notations and concepts about the tangent bundle of $\mathcal{M}$ are introduced and our gradient descent technique on $\mathcal{T}\mathcal{M}$ is described. The tangent space of $\mathcal{T}\mathcal{M}$ at $(p,v)$ denoted by $T_{(p,v)}\mathcal{T}\mathcal{M}$ is a vector space of dimension $2 \dim(\mathcal{M})$. This tangent space can be expressed as the direct sum of two sub-vector spaces of dimension $\dim(\mathcal{M})$ called the vertical space and the horizontal space. A tangent vector $V \in T_{(p,v)}\mathcal{T}\mathcal{M}$ is vertical if it corresponds to a variation of $v$ only, $p$ remaining fixed. Equivalently, a tangent vector $V$ is horizontal if it corresponds to a variation of $p$ only, $v$ remaining constant, i.e., parallel. Notice that the horizontal space depends on the definition of a connection on $\mathcal{M}$, the Riemannian connection in our case. This splitting of $T_{(p,v)}\mathcal{T}\mathcal{M}$ makes it possible to represent a tangent vector $V \in T_{(p,v)}\mathcal{T}\mathcal{M}$ by two tangent vectors $\Delta p, \Delta v \in T_p\mathcal{M}$: $\Delta p$ representing a variation of $p$ and $\Delta v$ a variation of $v$. That is why, a tangent vector $V \in T_{(p,v)}\mathcal{T}\mathcal{M}$ is denoted by a couple $(\Delta p, \Delta v)$. To turn $\mathcal{T}\mathcal{M}$ into a Riemannian manifold, the Sasaki metric $G((\Delta p_1, \Delta v_1), (\Delta p_2, \Delta v_2))_{(p,v)} = g_p(\Delta p_1, \Delta p_2) + g_p(\Delta v_1, \Delta v_2)$ is chosen. This metric makes horizontal tangent vectors $(\Delta p, 0)$ orthogonal to vertical tangent vectors $(0, \Delta v)$, see [52] for more details. Using this metric, we can define the gradient of the a function $f : \mathcal{T}\mathcal{M} \to \mathbb{R}$, which is a tangent vector $\text{grad}_f(p,v) = (\text{grad}_p, \text{grad}_v) \in T_{(p,v)}\mathcal{T}\mathcal{M}$ such that

$$Df((p,v))[[(\Delta p, \Delta v))] \triangleq \left. \frac{d}{dt} f(c(t)) \right|_{t=0},$$

$$= G((\text{grad}_p, \text{grad}_v), (\Delta p, \Delta v))_{(p,v)},$$

where $c(t)$ is a curve in $\mathcal{T}\mathcal{M}$ such that $\left. \frac{d}{dt} c(t) \right|_{t=0} = (\Delta p, \Delta v)$.

To find the gradient of $f$, we need to compute the differential of $f$. The expressions for the differential of the objective function in (4.1) and the gradient are derived in section 4.3. Using this gradient, it is possible to implement a first order optimization algorithm as in [2]. Algorithm 3 presents a simple version of such a technique.

In step 8, we use a curve $t \mapsto \beta(t)$ in $\mathcal{T}\mathcal{M}$, i.e., a curve in $\mathcal{M}$ and a vector field along this curve, such that $\beta(0) = (p,v)$ and $\dot{\beta}(0) = (-\alpha \text{grad}_p, -\alpha \text{grad}_v)$. The following curve in $\mathcal{T}\mathcal{M}$ has been chosen:

$$\beta(t) = (\exp_p(-t \alpha \text{grad}_p), \Gamma_p \exp_p(-t \alpha \text{grad}_p)(v - t \alpha \text{grad}_v)), \quad (4.3)$$
Algorithm 3 Gradient descent

1: Given a required precision $\epsilon$ and an initial iterate $(p_0, v_0) \in TM$;
2: set $k = 0$, $\alpha = 0.5$ and set $(p_k, v_k) = (p_0, v_0)$;
3: until $G(\nabla f((p_k, v_k)), \nabla f((p_k, v_k))) < \epsilon$ do
4: compute $\nabla f((p_k, v_k))$, the gradient of $f$ with respect to the Sasaki metric;
5: set $\alpha = 2\alpha$ and $(p_{new}, v_{new}) = \beta(1)$, where $t \mapsto \beta(t)$ is a curve in $TM$ such that $\beta(0) = (p_k, v_k)$ and $\dot{\beta}(0) = (\alpha \nabla f(p_k, v_k))$;
6: until $f((p_{new}, v_{new})) < f((p_k, v_k))$ do
7: set $\alpha = \frac{\alpha}{2}$;
8: set $(p_{new}, v_{new}) = \beta(1)$ where $t \mapsto \beta(t)$ is a curve in $TM$ such that $\beta(0) = (p_k, v_k)$ and $\dot{\beta}(0) = (\alpha \nabla f(p_k, v_k))$;
9: end until
10: set $k = k + 1$;
11: set $(p_k, v_k) = (p_{new}, v_{new})$;
12: end until
13: return $(p_k, v_k)$

where $exp_p : T_pM \to M$ is the exponential map and $\Gamma_{p \to q} : T_pM \to T_qM$ is the parallel transport along the geodesic joining $p$ to $q$. This means that we move along the geodesic curve (in $M$) starting at $p$ in the direction $-\alpha \nabla p$ and parallel translate the vector $v - \alpha \nabla v$ along this geodesic curve.

4.3 Computation of the Gradient

In this section, the gradient of the $i$-th term of the objective function (4.1) is computed. More precisely, let us consider the following function:

$$f : TM \to \mathbb{R}, \,(p, v) \mapsto \frac{1}{2}d(q_i, \gamma(p, v, t_i))^2, \quad (4.4)$$

where $\gamma(p, v, t)$ is a geodesic curve such that $\gamma(p, v, 0) = p$ and $\dot{\gamma}(p, v, 0) = v$. In order to compute the differential of $f$, let us write $f = g \circ h$ where $g$ and $f$ are defined by:

$$g : M \to \mathbb{R}, \, c \mapsto \frac{1}{2}d(q_i, c)^2, \quad (4.5)$$

$$h : TM \to M, \,(p, v) \mapsto \gamma(p, v, t_i). \quad (4.6)$$

The following two theorems give the differential of $h$ and $g$.

**Theorem 24.** The differential of $g$ at $c \in M$, $Dg : T_cM \to TR \cong \mathbb{R}$ is given by

$$Dg(c)[\Delta c] = g_c(\Delta c, \dot{\beta}(1)),$$

where $\beta(t)$ is the minimizing geodesic curve such that $\beta(0) = q_i$ and $\beta(1) = c$. 

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For a proof, see [29].

The next theorem is a known fact, see [10].

Theorem 25. The differential of \( h \), \( Dh : T_{(p,v)}\mathcal{T}M \to T_{\gamma(p,v,t_i)}\mathcal{M} \) is given by

\[
Dh((p,v))[(\Delta p, \Delta v)] = J(t_i),
\]

where \( J(t_i) \) is the Jacobi field along the geodesic curve \( t \mapsto \gamma(p,v,t) \) such that

\[
\begin{align*}
D^2_t J(t) + R(J(t), \dot{\gamma}(p,v,t), \dot{\gamma}(p,v,t)) &= 0, & (4.7) \\
J(0) &= \Delta p, \\
\dot{J}(0) &= \Delta v,
\end{align*}
\]

where \( D_t J(t) \) is the covariant derivative of the vector field \( J(t) \) along \( \gamma(p,v,t) \) and \( R \) stands for the curvature endomorphism defined by:

\[
R(X,Y)Z = \nabla_X \nabla_Y Z - \nabla_Y \nabla_X Z - \nabla_{[X,Y]} Z.
\]

Proof. Let \( s \to c(s) \) be a curve in \( \mathcal{M} \) such that \( c(0) = p \) and \( \dot{c}(0) = \Delta p \). Thus, \( \alpha(s) = (c(s), \Gamma_{c(0) \to c(s)}(v + s\Delta v)) \) is a curve in \( \mathcal{T}\mathcal{M} \) such that \( \dot{\alpha}(s) = (\Delta p, \Delta v) \) since

\[
D_s \Gamma_{c(0) \to c(s)}(v + s\Delta v) = \lim_{s \to 0} \frac{\Gamma_{c(s) \to c(0)}(\Gamma_{c(0) \to c(s)}(v + s\Delta v)) - v}{s} = \Delta v.
\]

By definition we have:

\[
\begin{align*}
Dh(p,v)[(\Delta p, \Delta v)] &= \frac{d}{ds} h(\alpha(s))|_{s=0}, \\
&= \frac{d}{ds} \exp_{c(s)}(t_i \Gamma_{c(0) \to c(s)}(v + s\Delta v))|_{s=0}.
\end{align*}
\]

Observe that \( \Omega : [-\epsilon, \epsilon] \times [0, t_i] \to \mathcal{M} \), \( (s,t) \mapsto \exp_{c(s)}(t \Omega_{c(0) \to c(s)}(v + s\Delta v)) \) is a variation through geodesics. Thus, see section 2.4,

\[
\partial_s \Omega(s,t)|_{(s,t)=(0,t_i)} = J(t_i),
\]

where \( J(t_i) \) stands for the Jacobi field along the geodesic curve \( t \mapsto \exp_p(tv) \) at \( t_i \).

Using these two theorems, the differential of \( f \) at \( (p,v) \in \mathcal{T}\mathcal{M} \) in the direction \((\Delta p, \Delta v)\) is then given by

\[
Df((p,v))[(\Delta p, \Delta v)] = g_{\gamma(p,v,t_i)}(J(t_i), \dot{\beta}(1))
\]

\[
= g_p(\Gamma_{\gamma(p,v,t_i) \to p}(J(t_i)), \Gamma_{\gamma(p,v,t_i) \to p}(\dot{\beta}(1)))
\]

since the parallel transport is an isometry. Notice that \( \dot{\beta}(1) = -\exp^{-1}_{\gamma(p,v,t_i)}(q_i) \) where \( \exp^{-1}_p(q) : \mathcal{M} \to T_p\mathcal{M} \) stands for the log-mapping, i.e., the inverse of
the exponential map. This mapping can be computed efficiently on the spaces we have considered, see Section 4.4. Consequently, to compute the gradient, it remains to solve the Cauchy problem (4.7). Since the curvature is a linear operator, (4.7) is a second order time-varying linear differential equation in $J(t)$. But if we assume that $\mathcal{M}$ is a symmetric Riemannian manifold, which implies $\nabla R = 0$, i.e., the curvature tensor is parallel along $\gamma(p, v, t)$, then (4.7) becomes a second order constant coefficients linear differential equation that is easy to solve, see [10]. Let us define the Jacobi operator

$$L_{\gamma}(J) : J \mapsto R(J, \dot{\gamma}(p, v, 0)) \dot{\gamma}(p, v, 0),$$

(4.9)

that acts on tangent vectors $J$ at $p$. Since this operator is symmetric, it admits an orthogonal basis of eigenvectors and real eigenvalues. Let $E_1 = \frac{\dot{\gamma}}{\|\dot{\gamma}\|}, \ldots, E_{\dim(\mathcal{M})}$ be a basis of eigenvectors and $\lambda_1 = \ldots, \lambda_{\dim(\mathcal{M})}$, the corresponding eigenvalues, i.e.,

$$L_{\gamma}(E_k) = \lambda_k E_k \text{ for } k = 1, \ldots, \dim(\mathcal{M}).$$

Then, the Jacobi equation (4.7) can be expressed in this basis of eigenvectors. Let $J(t) = \sum_{k=1}^{\dim(\mathcal{M})} u_k(t) E_k(t)$ where $E_k(t)$ is the extension of $E_k = E_k(0)$ along the curve $\gamma$ by parallel transport. By replacing $J(t)$ in (4.7), one obtains

$$\sum_{k=1}^{\dim(\mathcal{M})} (\ddot{u}_k(t) + u_k(t) \lambda_k) E_k(t) = 0,$$

since $D_t E_k(t) = 0$. So, we end up with $\dim(\mathcal{M})$ decoupled second order time-invariant linear ode’s whose solutions are of the form

$$u_k(t) = c_k(t) \Delta p_k + s_k(t) \Delta v_k,$$

where

- $c_k(t) = 1$ and $s_k(t) = t$ if $\lambda_k = 0$,
- $c_k(t) = \cos(\sqrt{\lambda_k} t)$ and $s_k(t) = \frac{\sin(\sqrt{\lambda_k} t)}{\sqrt{\lambda_k}}$ if $\lambda_k > 0$,
- $c_k(t) = \cosh(\sqrt{-\lambda_k} t)$ and $s_k(t) = \frac{\sinh(\sqrt{-\lambda_k} t)}{\sqrt{-\lambda_k}}$ if $\lambda_k < 0$,

where $\Delta p_k = g_p(\Delta p, E_k)$ and $\Delta v_k = g_v(\Delta v, E_k)$. With this notation, we can write

$$J(t_i) = \sum_{k=1}^{\dim(\mathcal{M})} (c_k(t_i) \Delta p_k + s_k(t_i) \Delta v_k) E_k(t_i).$$

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and the differential (4.8) becomes
\[
g_p\left( \sum_{k=1}^{\dim(M)} (c_k(t_i)\Delta p_k + s_k(t_i)\Delta v_k)E_k(0), \Gamma_{\gamma(p,v,t_i)}(\dot{\beta}(1)) \right)
\]
\[
= g_p(\Delta p, \sum_{k=1}^{\dim(M)} c_k(t_i)g_p(\Gamma_{\gamma(p,v,t_i)}(\dot{\beta}(1)), E_k)E_k)
\]
\[
+ g_p(\Delta v, \sum_{k=1}^{\dim(M)} s_k(t_i)g_p(\Gamma_{\gamma(p,v,t_i)}(\dot{\beta}(1)), E_k)E_k).
\]

Consequently, the gradient \((\text{grad}_p, \text{grad}_v)\) in the Sasaki metric is given by
\[
(\text{grad}_p, \text{grad}_v) = \left( \sum_{k=1}^{\dim(M)} c_k(t_i)g_p(T, E_k)E_k, \sum_{k=1}^{\dim(M)} s_k(t_i)g_p(T, E_k)E_k \right),
\]
(4.10)

where \(T = \Gamma_{\gamma(p,v,t_i)}(\dot{\beta}(1))\). The procedure to compute the gradient of \(f\) defined in (4.4) is then the following:

1. computation of \(\dot{\beta}(1)\) using the log-mapping,
2. computation of \(\Gamma_{\gamma(p,v,t_i)}(\dot{\beta}(1))\), the parallel transport of \(\beta(1)\) at \(T_{pM}\) along the geodesic curve \(t \mapsto \gamma(p, v, t)\),
3. diagonalization of the operator \(L_{\dot{\gamma}}\),
4. computation of \((\text{grad}_p, \text{grad}_v) \in T_{(p,v)}T\mathcal{M}\) using (4.10).

To compute the gradient using this procedure and so, to implement Algorithm 3, it remains to find an efficient way to diagonalize \(L_{\dot{\gamma}}\) and to compute \((\text{grad}_p, \text{grad}_v)\) in (4.10). This is the subject of the next section.

### 4.4 Diagonalization of the curvature

The goal of this section is to describe an efficient way to diagonalize the Jacobi operator \(L_{\dot{\gamma}}\) in (4.9). This is done here by exploiting the specific structure of the algebraic representation of the curvature endomorphism \(R\) on symmetric spaces, see [31]. Indeed, it is possible to find an explicit solution for the eigenvalues and eigenvectors of the Jacobi operator \(L_{\dot{\gamma}}\) in terms of some factorization of a matrix \(A\) representing the tangent vector \(\dot{\gamma}(p, v, 0)\). A way to represent points and formulas for the geodesics, the parallel transports and the log-mappings are first recalled for the sphere \(S^2\), the set of symmetric positive definite matrices \(P_+^n\), the special orthogonal group \(SO(3)\), and the Grassmann manifold \(\text{Grass}(n, p)\). Then, explicit expressions for the eigenpairs of the Jacobi operator are given.
4.4.1 The sphere $S^2$

Let $S^2 = \{ p \in \mathbb{R}^3 | p^\top p = 1 \}$ be the unit sphere in $\mathbb{R}^3$ endowed with the ambient metric: $g_p(X, Y) = X^\top Y$. The tangent space at a point $p \in S^2$ is

$$T_pS^2 = \{ v \in \mathbb{R}^3 | p^\top v = 0 \}.$$ 

Using these representations of points and tangent vectors, one has the following formulas:

$$\exp_p(v) = p \cos(\|v\|) + \frac{v}{\|v\|} \sin(\|v\|),$$

$$\exp_p^{-1}(q) = \frac{(I_3 - pp^\top)q}{\sqrt{1 - (p^\top q)^2}} \cos(p^\top q),$$

$$\Gamma_{p\to q}(w) = \left(-p \sin(\|v\|) + \frac{v}{\|v\|} \cos(\|v\|)\right) v^\top w + \left(I_3 - \frac{vv^\top}{\|v\|^2}\right) w \text{ where } v = \exp_p^{-1}(q).$$

The curvature endomorphism is given by, see [10],

$$R(X, Y)Z = (Y^\top Z)X - (X^\top Z)Y.$$ 

Thus, the Jacobi operator (4.9) on the sphere $S^2$ becomes: $L_A(X) = R(X, A)A = A^\top AX - AA^\top X = \|A\|^2 \left(I - \frac{AA^\top}{\|A\|^2}\right) X$. So, the eigenpairs $(\lambda, X)$ of $L_A$ are $(0, \frac{A}{\|A\|})$, and $(\|A\|^2, V)$, where $V$ is a unit tangent vector orthogonal to $A$.

4.4.2 The set of symmetric positive definite matrices $P_n^+$

Let $P_n^+$ be the set of symmetric positive definite matrices endowed with the affine invariant metric

$$g_p(X, Y) = \text{trace}(Xp^{-1}Yp^{-1}), \quad (4.11)$$

defined on the tangent space at $p$:

$$T_pP_n^+ = \{ v \in \mathbb{R}^{n\times n} | v = v^\top \}.$$ 

The exponential map, the parallel transport and the log-mapping are given by, see [16, 18],

$$\exp_p(v) = p^{1/2}e^{(p^{-1/2}vp^{-1/2})p^{1/2}},$$

$$\exp_p^{-1}(q) = p^{1/2} \log(p^{-1/2}qp^{-1/2})p^{1/2},$$

$$\Gamma_{p\to q}(w) = p^{1/2}rp^{-1/2}wp^{-1/2}rp^{1/2}$$

where $r = e^{(p^{-1/2}vp^{-1/2})}$ and $v = \exp_p^{-1}(q)$. 76
Notice that the action \( x \mapsto p^{-1/2}xp^{-1/2} \) maps \( p \) to the identity \( I \) and it is an isometry. So, one can "translate" the problem to the identity using this isometry at each iteration. Thus, we can assume that \( p = I \) and the diagonalization of the Jacobi operator (4.9) will be only required at the identity. The curvature endomorphism at the identity \( I \) is given by, see [31],

\[
R_I(X_I,Y_I)Z_I = \frac{1}{4}[Z_I,[X_I,Y_I]].
\]

where \([A,B] = AB - BA\) stands for the matrix Lie bracket and \(X_I,Y_I,Z_I\) are tangent vectors at the identity, i.e., symmetric matrices. So, one obtains the following expression for the Jacobi operator (4.9) on \( \mathbb{P}^n_+ \):

\[
L_{A_I}(X_I) = \frac{1}{4}(-A_I^2X_I + 2A_I X_I A_I - X_I A_I^2).
\]

Since \( A_I \) is symmetric, it can be diagonalized by an orthogonal transformation denoted by \( A_I = UDU^\top \) where \( D = \text{diag}(d_1, \ldots, d_n) \). Using this, it can be shown that the eigenvalues \( \lambda \) and the corresponding eigenvectors \( X \) of the Jacobi operator on \( \mathbb{P}^n_+ \) are

- \( \lambda = 0 \), \( X = Ue_i e_i^\top U^\top \) for \( 1 \leq i \leq n \);
- \( \lambda = -\frac{1}{4}(d_i - d_j)^2 \), \( X = U \frac{1}{\sqrt{2}}(e_i e_j^\top + e_j e_i^\top)U^\top \) for \( 1 \leq i < j \leq n \);

where \( e_i \) stands for the \( i \)-th identity vector.

### 4.4.3 The special orthogonal group \( \text{SO}(3) \)

Let \( \text{SO}(3) = \{ p \in \mathbb{R}^{3 \times 3} | p^\top p = I_3 \, \text{det}(p) = 1 \} \) be the set of rotation matrices with the bi-invariant metric

\[
g(X,Y) = \frac{1}{2}\text{trace}(X^\top Y). \tag{4.12}
\]

The Lie algebra or the tangent space at the identity is given by

\[
\text{so}(3) = \{ v \in \mathbb{R}^{3 \times 3} | v^\top = -v \}.
\]

Notice that a tangent vector at any point can be represented by an element of the Lie algebra, see [10]. Using this representation, we have the following formulas:

\[
\exp_p(v) = pe^{(v)},
\]

\[
\exp_p^{-1}(q) = \log(p^\top q),
\]

\[
\Gamma_{p \to q}(v) = q^\top pe^{(v/2)}we^{(v/2)} \text{ where } v = \exp_p^{-1}(q).
\]

The curvature endomorphism on a Lie group with a bi-invariant metric is expressed by (see [42])

\[
R(X,Y)Z = \frac{1}{4}[Z,[X,Y]].
\]
Thus, the Jacobi operator in (4.9) is $L_A(X) = \frac{1}{4} (-A^2 X + 2AXA - XA^2)$. Since $A \in \text{so}(3)$ is skew-symmetric, we can consider its Schur decomposition $A = U\beta(e_3 e_2^\top - e_2 e_3^\top)U^\top$ and the eigenpairs of the Jacobi operator are described by

- $\lambda = 0, U(e_3 e_2^\top - e_2 e_3^\top)U^\top$;
- $\lambda = \frac{\beta^2}{4}, U(e_2 e_1^\top - e_1 e_2^\top)U^\top$.

Notice that all these eigenvectors are orthogonal and of unit norm with respect to the bi-invariant metric $g(X,Y)$ in (4.12).

4.4.4 The Grassmann manifold Grass($n,p$)

A point on the Grassmann manifold, i.e., a subspace, can be represented by the column space of an $n \times p$ orthogonal matrix $P$ and a tangent vector at $P$ by an $n \times p$ matrix $V$ such that $V^\top P = 0$, see [14]. Notice that the dimension of the tangent space, i.e., the dimension of the manifold, is $p(n - p)$. The following Riemannian metric:

$$g_P(X,Y) = \text{trace}(X^\top Y),$$

turns Grass($n,p$) into a symmetric space, see [31]. Using these representations for the subspaces and for the tangent vectors, we have the following formulas (see [14, 47]):

$$\exp_P (V) = (PW \cos(\Sigma) + U \sin(\Sigma))W^\top$$
where $V = U\Sigma W^\top$ (compact SVD),

$$\exp_P^{-1}(Q) = W_2 \Sigma W_1^\top$$
with

$$\left[ \begin{array}{c} X^\top Q \\ (I_n - XX^\top)Q \end{array} \right] = \left[ \begin{array}{c} W_1 \cos(\Sigma) Z^\top \\ W_2 \sin(\Sigma) Z^\top \end{array} \right]$$
(CS decomposition),

$$\Gamma_{P \to Q}(T) = (-XW\sin(\Sigma) + U \cos(\Sigma))U^\top T + (I_n - UU^\top)T$$
where $\exp_P^{-1}(Q) = U\Sigma W^\top$ (compact SVD).

Let $X,Y$ and $Z$ be $n \times p$ matrices representing tangent vectors at $P \in \text{Grass}(n,p)$. According to [63], the curvature endomorphism is given by

$$R(X,Y)Z = (XY^\top - YX^\top)Z + Z(Y^\top X - X^\top Y),$$
and thus, the Jacobi operator is

$$L_A(X) = XA^\top A - 2AX^\top A + AA^\top X,$$
where $A$ is an $n \times p$ matrix representing $\dot{\gamma}(p,v,0)$. Let $A = U\Sigma W^\top$ where $\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_p)$ be the compact SVD of $A$ and define $U_\perp \in \mathbb{R}^{n \times (n - 2p)}$ such that $[P|U|U_\perp]$ is an $n \times n$ orthogonal matrix. It can be shown that the eigenpairs $(\lambda, X)$ of the Jacobi operator (4.9) are given by

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• \( \lambda = 0 , X = UD_{i}W^{T} \) with \( D_{i} = e_i e_{i}^{T} \) for \( 1 \leq i \leq p \);

• \( \lambda = (\sigma_i - \sigma_j)^2 , X = US_{ij}W^{T} \) with \( S_{ij} = \frac{1}{\sqrt{2}}(e_i e_{j}^{T} + e_j e_{i}^{T}) \) for \( 1 \leq i < j \leq p \);

• \( \lambda = (\sigma_i + \sigma_j)^2 , X = UR_{ij}W^{T} \) with \( R_{ij} = \frac{1}{\sqrt{2}}(e_i e_{j}^{T} - e_j e_{i}^{T}) \) for \( 1 \leq i < j \leq p \);

• \( \lambda = \sigma_i^2 , X = U \tilde{e}_j e_{i}^{T}W^{T} \) for \( 1 \leq i \leq p \) and \( 1 \leq j \leq (n - 2p) \);

where \( e_i \) is the \( i \)-th identity vector in \( \mathbb{R}^p \) and \( \tilde{e}_j \), the \( j \)-th identity vector in \( \mathbb{R}^{n-2p} \). When \( n \gg p \), it is interesting to avoid computing and storing the orthogonal completion \( U_{\perp} \). This can be done, since only an orthogonal projection on \( U_{\perp} \) is required to compute (4.10). In fact, for \( \lambda = \sigma_i^2 \), the vectorized form of \( X = U \tilde{e}_j e_{i}^{T}W^{T} \) is \((W \otimes U_{\perp}) \text{vec}(\tilde{e}_j e_{i}^{T})\), and the components of the gradient in (4.10), in col\((U_{\perp})\), are of the form:

\[
(W \otimes U_{\perp}) \left( \begin{array}{c}
\begin{bmatrix}
c_i^2 & \ldots & c_i^2 \\
\vdots & \ddots & \vdots \\
c_p^2 & \ldots & c_p^2 \\
\end{bmatrix}
\end{array}
\right) \otimes I_{(n-2p)} (W \otimes U_{\perp})^{\top} \text{vec}(T),
\]

(4.13)

where \( T = \Gamma_{\gamma p,v,t_{\perp}}^{\beta 1}(\tilde{\beta}(1)) \). Using \((A \otimes B)(C \otimes D) = (AC \otimes BD)\) and \((W \otimes U_{\perp})^{\top} = (W^{\top} \otimes U_{\perp}^{\top})\), (4.13) becomes

\[
(WCW^{\top} \otimes U_{\perp} U_{\perp}^{\top}) \text{vec}(T) = (WCW^{\top} \otimes (I_n - [P|U][P|U]^{\top})) \text{vec}(T),
\]

whose matrix form is

\[
(I_n - [P|U][P|U]^{\top}) T(WCW^{\top}).
\]

This last formula has a computational complexity of \( O(np^2) \).

### 4.5 Numerical examples

To illustrate the method, we have first picked 3 points on the sphere \( S^2 \). The best geodesic approximation of these 3 points is presented in Fig. 4.2. In \( \mathbb{R}^n \), the best geodesic approximation passes through the two following points:

\[
\tilde{t} = \frac{1}{m} \sum_{i=1}^{m} t_i , \quad \gamma(\tilde{t}) = \frac{1}{m} \sum_{i=1}^{m} q_i,
\]

(4.14)

\[
\tilde{t} = \frac{1}{\sum_{i=1}^{m} t_i} \sum_{i=1}^{m} t_i^2 , \quad \gamma(\tilde{t}) = \frac{1}{\sum_{i=1}^{m} t_i} \sum_{i=1}^{m} t_i q_i,
\]

(4.15)
Figure 4.2: The data points $q_i$, $1 \leq i \leq 3$ are in red. The best geodesic $\gamma^*(t)$ is the blue curve and the black arrow represents $\dot{\gamma}^*(0)$. The points $\gamma^*(t_i)$ for $t_1 = 0.1, t_2 = 0.5, t_3 = 0.9$, are in magenta. The Karcher mean of the $q_i$’s is $\kappa_1$, and $\kappa_2$ is the weighted Karcher mean.

Notice that $\gamma(\bar{t})$ is the center of mass of the data points, and $\gamma(\bar{\bar{t}})$ is a weighted mean where the $t_i$’s can be seen as the mass attached to each $q_i$. This mean (4.14) and this weighted mean (4.15) defined in $\mathbb{R}^n$ can be generalized to our setting using the Karcher mean. In [36], the authors have proved that the best geodesic passes through the Karcher mean $\kappa_1$ of the data points if the data belong to an abelian subgroup of $SO(n)$ and they believe that this property does not hold in general. As shown in Fig. 4.2, the best geodesic does neither pass through the Karcher mean $\kappa_1$ nor to the weighted Karcher mean $\kappa_2$ defined as the global minimizer of the function $p \mapsto \frac{1}{\sum_{i=1}^m t_i} \sum_{i=1}^m t_i d(p,q_i)^2$. But this is still interesting because the geodesic passing through these two points $\kappa_1$ and $\kappa_2$ can be a good initial condition for our gradient descent technique. In fact, our numerical experiments on the sphere $S^2$ have shown that the Karcher mean is close to the best geodesic if the data points are not located too far apart.

Our best geodesic fitting method was also tested on the Grassmann manifold with 10 data points. Table 4.1 shows that the number of gradient iterations required to reach an accuracy of $\epsilon = 10^{-6}$, does not depend on the dimension of the Grassmann manifold.

To illustrate the filtering capability of the proposed method, 5 data points $p_1, ..., p_5$ on $P_2^+$, i.e., the set of ellipsoids in $\mathbb{R}^2$, were generated on a geodesic curve according to the model:

$$p_k = \exp_p(t_kv)$$ for $t_k = k \cdot 0.1$,

where $v$ is a tangent vector at $p \in P_2^+$. To perturb these points, for each point $p_k$, a Gaussian random vector of mean 0 was generated on $T_p P_2^+$. Then, this
random vector was parallel translated along the geodesic curve $t \mapsto \exp_p(tv)$ to $T_{p_k} P_2^+$ and a perturbed version of $p_k$ was computed by moving in the direction of this tangent vector along a geodesic curve. This ensures that all the points $p_k$ are perturbed with the same probability distribution with respect to the Riemannian metric (4.11) since the parallel transport is an isometry.

To reduce the noise, our geodesic fitting method was applied to these perturbed data. The points $p_1, \ldots, p_5$ are drawn in blue in Fig.4.3. Since the filtered data points are close to the true data points $p_k$, the true geodesic is almost recovered.
Figure 4.3: (upper) The ellipsoids $p_1, \ldots, p_5$ are in blue. The ellipsoids in red represent the perturbed data and the ellipsoids in green are the filtered data. (lower) Riemannian distance between the $p_k$’s and their perturbed version (in red) and their corresponding filtered version (in green).
Chapter 5

Log-mapping on the Stiefel manifold

Recently, many algorithms have been proposed to deal with data that belong to the Stiefel manifold $\text{St}(n, p)$, the set of $p$-dimensional orthogonal frames in $\mathbb{R}^n$. This situation appears in optimization [2, 14], in signal processing [57], and image analysis [21, 56, 58]. Two of the classical computational tasks that these algorithms have to perform are the computation of Riemannian exponential maps and the computation of Riemannian log maps. Let $t \mapsto \gamma(t)$ be a geodesic curve, i.e., the generalization of a straight line on a Riemannian manifold. The exponential map returns $\gamma(1)$ given $\gamma(0)$ and its time derivative at $t = 0$ denoted by $\dot{\gamma}(0)$. The Riemannian log map returns $\dot{\gamma}(0)$ given $\gamma(0)$ and $\gamma(1)$. This last problem is also called the endpoint geodesic problem.

In [14], the Stiefel manifold is equipped with two different Riemannian metrics: the Euclidean metric, and the canonical metric. The first one is the inherited metric when the Stiefel manifold is seen as a submanifold of $\mathbb{R}^{n \times p}$, and the second one comes from the Riemannian homogeneous space structure of $\text{St}(n, p)$. Notice that these two Riemannian metrics are different, and yield different geodesic curves. Formulas to compute the exponential maps relative to the Euclidean metric and relative to the canonical metric are provided in [14]. These formulas have a numerical complexity of $O(np^2)$. Since the computation of the log map is much harder to perform, some authors have proposed some approximations, see for instance [2]. In [56], a shooting method is proposed to compute the Riemannian log map related to the Euclidean metric, but to the best of our knowledge, no algorithm has been proposed to handle the case with the canonical metric.

In this chapter, we propose an iterative method to compute the Riemannian log mapping related to the canonical metric. Our approach consists in seeking for the closest point to $\gamma(0)$ in the fiber containing $\gamma(1)$ using a gradient method. Our numerical experiments show that this algorithm exhibits a linear rate of convergence, and that only a few iterations are required to reach the machine
precision if $\gamma(0)$ is not too far from $\gamma(1)$. The computation of the gradient only requires a log map on the special orthogonal group $SO(n)$, i.e., the set of orthonormal matrices of determinant $+1$, which can be computed efficiently using an eigenvalue decomposition. If $p < n/2$, the problem is first reduced to $St(2p, p)$ as in [56]. Thus, in this case, the total numerical complexity of our algorithm is in $O(np^2)$, which is particularly interesting when $n$ is much larger than $p$.

The simplest application of the log map consists in computing the Riemannian distance between two points on the Stiefel manifold. Our algorithm computes a geodesic curve between two points but this geodesic is not necessarily minimizing. A condition under which the minimizing geodesic curve is computed is given. In particular, we provide a lower bound on the injectivity radius of the Stiefel manifold.

Another related application is the computation of the Karcher mean [29]. In fact, the Riemannian log map can be used to compute the gradient of the squared Riemannian distance function, and thus to compute the Karcher mean of a set of points on the Stiefel manifold. This is illustrated in Section 5.4.

Main contributions:

- We propose an iterative scheme to compute the Riemannian log-mapping on the Stiefel manifold $St(n, p)$.
- We give a lower bound on the injectivity radius $\text{inj}(St(n, p))$.

5.1 Geometry of the Stiefel manifold

In this section, the Stiefel manifold is described as a normal homogeneous space. This important geometric structure yields nice formulas for the geodesics and for the sectional curvature.

The Stiefel manifold $St(n, p)$ is the set of orthonormal $p$-frames in $\mathbb{R}^n$. We can represent an element of $St(n, p)$ using an $n$-by-$p$ orthogonal matrix. This yields the following definition:

$$St(n, p) = \{X \in \mathbb{R}^{n \times p} \mid X^\top X = I_p\}.$$  

It defines $St(n, p)$ as an embedded submanifold of $\mathbb{R}^{n \times p}$. Indeed, this is a consequence of Theorem 1 since $St(n, p) = F^{-1}(0)$ with the constant rank smooth map $F: \mathbb{R}^{n \times p} \to \mathbb{R}^{p \times p}$ $X \mapsto X^\top X - I_p$.

Let us look at some particular cases.

- $St(1, 1) \equiv \{1, -1\}$;
- $St(2, 1)$ is the unit sphere $S^1$ and $St(2, 2)$ is the orthogonal group $O(2)$;
- $St(n, 1) \equiv S^{n-1}$ is the $n - 1$ dimensional sphere embedded in $\mathbb{R}^n$;
- $St(n, n) \equiv O(n)$;
\[ St(n, n - 1) \equiv O(n)/\{1, -1\} \equiv SO(n) \] since once an \( n - 1 \) orthonormal basis of \( \mathbb{R}^n \) is chosen, it remains only one orthogonal completion that makes it a basis with a positive orientation;

\[ St(4, 2) \] the first non trivial case.

The orthogonal group \( O(n) \) (the set of rotations and reflections) acts smoothly on \( St(n, p) \) by multiplication on the left as follows

\[ \lambda : O(n) \times St(n, p) \to St(n, p), \quad (Q, X) \mapsto QX. \]

This action is transitive \(^1\), i.e., it is possible, starting from any \( X_1 \in St(n, p) \), to reach any \( X_2 \in St(n, p) \) using this action. In fact, we can choose \( Q = [X_2 \quad X_2^\perp] [X_1 \quad X_1^\perp]^\top \in O(n) \). Actually, it is only necessary to show that you can reach any element from one specific element called the origin \( o \). Indeed, if we have \( X_1 = \lambda(Q_1, o) \) and \( X_2 = \lambda(Q_2, o) \), we have also \( X_2 = \lambda(Q_2, \lambda(Q_2^\perp, X_1) = \lambda(Q_2Q_1^{-1}, X_1) \). Here, we can choose \( o = \begin{bmatrix} I_p \\ 0 \end{bmatrix} \), i.e. the identity frame, and we have, for any \( X \in St(n, p) \):

\[ X = \underbrace{[XX^\perp]}_{Q} \begin{bmatrix} I_p \\ 0 \end{bmatrix}. \tag{5.1} \]

Notice that, when \( p < n \), the special orthogonal group \( SO(n) \), acts also transitively on \( St(n, p) \). If \( p < n \), we always have the freedom to find an orthonormal completion \( X^\perp \) in (5.1) such that \( Q \in SO(n) \). However, for \( p = n \), this is not the case since \( St(n, n) = O(n) \). Observe that computing the geodesic on \( O(n) \) is not difficult. In fact, \( SO(n) \) is composed of two connected components, the orthogonal matrices of determinant \(+1\) and the ones of determinant \(-1\). Each component being isometric to \( SO(n) \), a geodesic curve between two points belonging to the same connected component is a geodesic in \( SO(n) \), which is easy to compute. So, in the remaining part of this chapter, we will consider the action of \( SO(n) \) only and assume, \( p < n \).

One can define the isotropy group at the origin \( o \) denoted by \( H \), i.e., a subgroup of \( G = SO(n) \) that leaves the origin invariant. All the \( Q \)’s that satisfy:

\[ o = \begin{bmatrix} I_p \\ 0 \end{bmatrix} = Q \begin{bmatrix} I_p \\ 0 \end{bmatrix}, \]

must be of the form \( Q = [o \quad o^\perp] \). Thus, the only degrees of freedom we have are in the choice of the orthogonal basis \( o^\perp \). So, the isotropy group at the origin is given by:

\(^1\)This yields another way to show that \( St(n, p) \) is a submanifold of \( \mathbb{R}^{n \times p} \). Indeed, \( St(n, p) \) is the orbit of the identity frame \( \begin{bmatrix} I_p \\ 0 \end{bmatrix} \) by the smooth action (multiplication on the left) of the orthogonal group \( O(n) \) on \( \mathbb{R}^{n \times p} \). By Theorem 14, \( St(n, p) \) is a submanifold of \( \mathbb{R}^{n \times p} \) by Theorem 14.
\[ H = \text{Iso}(o) = \{ \begin{bmatrix} I_p & 0 \\ 0 & O_{n-p} \end{bmatrix} \mid O_{n-p} \in \text{SO}(n-p) \}. \]

Notice that the isotropy groups are conjugate, i.e. \( \text{Iso}(X) = QHQ^{-1} \) where \( X = Qo \). Consequently \( \text{St}(n,p) \) is in one to one correspondence (bijection) with the set of left cosets \( G/H = \text{SO}(n)/\text{SO}(n-p) = \{ QH \mid Q \in \text{SO}(n) \} \). An element of \( \text{SO}(n)/\text{SO}(n-p) \), i.e., an equivalence class, is denoted by \([Q]\) where \( Q \in \text{SO}(n) \), and we can also write \([Q] \in \text{St}(n,p)\). By Theorem 14, we know that \( H \) is a closed subgroup of \( G \), and by requiring that the canonical projection \( \pi : \text{SO}(n) \rightarrow \text{SO}(n)/\text{SO}(n-p), Q \mapsto [Q] \) (or \( Q \mapsto Qo \)) is a smooth submersion, \( G/H \) inherits a unique smooth structure, see Theorem 15 and Fig 5.1.

\[
\begin{pmatrix}
\text{SO}(n) \\
\pi \\
\text{SO}(n)/\text{SO}(n-p) \\
\phi \text{ (diffeomorphism)} \\
\text{St}(n,p)
\end{pmatrix}
\]

\( \lambda(.,o) \) group action with fixed origin

Figure 5.1: Illustration of the homogeneous space construction on the Stiefel manifold

Let \( \text{so}_n \) be the Lie algebra of \( \text{SO}(n) \) or the tangent space at the identity element \( I \in \text{SO}(n) \). It has been shown in the first chapter that the Lie algebra consists of skew-symmetric matrices:

\[ \text{so}_n = \text{skew}(n) = \{ V \in \mathbb{R}^{n \times n} \mid V^\top = -V \}. \]

When this Lie algebra is endowed with the bi-invariant inner product:

\[ \langle X, Y \rangle = \frac{1}{2} \text{trace}(X^\top Y), \]

the corresponding Riemannian metric on \( \text{SO}(n) \) is defined by

\[ q_p(X_p, Y_p) = \langle p^{-1}X_p, p^{-1}Y_p \rangle, \]

and makes \( \text{SO}(n) \) a Riemannian manifold where the left and right actions of \( \text{SO}(n) \) (on itself) are isometries.

The Lie algebra corresponding to the subgroup \( H \) is given by

\[ \mathfrak{h} = \{ \begin{bmatrix} 0 & 0 \\ 0 & C \end{bmatrix} \mid C \in \text{skew}(n-p) \}. \]
and thus the tangent space at any point \( p \in St(n, p) \) can be identified with \( so_n/h \) via

\[
V_p f = \frac{d}{dt} f(\lambda(\exp(tV), p))|_{t=0} \quad \text{with} \quad V \in so_n/h,
\]

where \( \exp \) stands for the \( SO(n) \) Lie group exponential map. Roughly speaking, the elements of \( so_n/h \) represent infinitesimal rotations that make a variation of \( p \), and the elements of \( h \) represent infinitesimal rotations that let \( p \) invariant.

A priori, any particular section in \( so_n \) that represents the element in \( so_n/h \) can be chosen to represent tangent vectors. A simple possibility would be to choose a subvector space \( m \subset so_n \) complementary to \( h \), i.e. such that \( so_n = m \oplus h \) (direct sum of vector spaces). But, sometimes there are particular choices of \( m \). The particular choice here, corresponds to the normal Riemannian homogeneous space structure. The philosophy here, is to make the Riemannian structure of \( St(n, p) \) compatible with the Riemannian structure of \( SO(n) \) in the hope of getting simpler formulas for the geodesics and the curvature.

**Definition 32.** A homogeneous space \( M = G/H \) is a normal homogeneous space, see [23] or [10], if the Riemannian metric \( g \) on \( M \) is the induced metric from a bi-invariant Riemannian metric \( q \) on \( G \), and \( m = h^\perp \) with respect to \( q \).

In our case, we have \( St(n, p) = SO(n)/SO(n-p) \) where \( SO(n) \) is endowed with the Riemannian metric (5.2), and thus

\[
m = h^\perp = \{ \begin{bmatrix} X_1 & -X_2^\top \\ X_2 & 0 \end{bmatrix} \mid X_1 \in \text{skew}(p), \, X_2 \in \mathbb{R}^{(n-p) \times p} \}.
\]

Observe also that the structure of normal homogeneous space is more specific than the structure of naturally reductive homogeneous spaces or reductive spaces, see the theorem below.

**Theorem 26.** [31, Theorem 3.5] Let \( G/H \) be an homogeneous space. Assume that the Lie algebra \( \mathfrak{g} \) of \( G \) admits an \( \text{Ad}_G \)-invariant non-degenerate symmetric bilinear form \( B \) such that its restriction \( B_h \) to \( h \) is non-degenerate (in our case, \( B \) will be an inner product). Then

- The decomposition \( \mathfrak{g} = m \oplus h \) defined by

\[
m = \{ X \in \mathfrak{g} \mid B(X, Y) = 0 \quad \forall Y \in h \},
\]

is \( \text{Ad}_H \)-invariant, i.e. it is a reductive decomposition.

- \( G/H \) is naturally reductive with respect to the decomposition \( \mathfrak{g} = m \oplus h \) defined above and the \( G \)-invariant metric \( g \) defined by \( B_m \), i.e.

\[
B(X, [Z, Y]_m) + B([Z, X]_m, Y) = 0.
\]

- The sectional curvature is given by:

\[
\kappa(X, Y) = ||[X, Y]_h||^2 + \frac{1}{4} ||[X, Y]_m||^2,
\]

and it is thus non-negative.
In our case, so\(_{n} = h \oplus m\) is a reductive decomposition:

\[
Ad_{H}(m) \subset m \quad \forall h \in H \quad \forall m \in m,
\]

since

\[
Ad_{H}(m) = hmh^{-1} = \begin{bmatrix} I_{p} & 0 \\ 0 & O_{n-p} \end{bmatrix} \begin{bmatrix} X_{1} & -X_{2} \\ X_{2} & 0 \end{bmatrix} \begin{bmatrix} I_{p} & 0 \\ 0 & O_{n-p}^{-1} \end{bmatrix}
= \begin{bmatrix} X_{1} & -X_{2} \top O \top \\ OX_{2} & 0 \end{bmatrix} \subset m.
\]

Furthermore, the restriction of the inner product (5.2) to \(m\) is then given by:

\[
g(X,Y) = \frac{1}{2} \text{trace}(X \top Y) = \frac{1}{2} \text{trace}(X_{1} \top Y_{1}) + \text{trace}(X_{2} \top Y_{2}),
\]

with \(X = \begin{bmatrix} X_{1} & -X_{2} \top \\ X_{2} & 0 \end{bmatrix} \in m\) and \(Y = \begin{bmatrix} Y_{1} & -Y_{2} \top \\ Y_{2} & 0 \end{bmatrix} \in m\), and we have also

\[
g([X,Z],Y) = -g(Z,[X,Y]) \quad \forall X, Y, Z \in m.
\]

For a fixed \(X\), this means that the linear operator \(Y \mapsto [X,Y]\) is skew-symmetric or skew-adjoint with respect to the metric \(g\). Consequently, with this Riemannian metric, \((St(n,p),g)\) is a naturally reductive homogeneous space, see [42]. Observe that it is not a symmetric space since the last condition in (2.5) is not satisfied.

The geodesics starting at \(o\) in \((St(n,p),g)\) are then given by the following theorem:

**Theorem 27.** [42, Proposition 25] If \(M = G/H\) is naturally reductive, its geodesics starting at \(o\) are given by \(\gamma(t) = \lambda(e^{tV}, o) = \pi(e^{tV})\) where \(V \in m\).

So, since SO\((n)\) acts on \((St(n,p), g)\) by isometries, the geodesic in \((St(n,p), g)\) starting at \([Q]\) in the direction represented by \(V \in m\) is given by:

\[
t \mapsto \gamma(t) = Qe^{tV} \begin{bmatrix} I_{p} \\ 0 \end{bmatrix},
\]

where \(X \mapsto e^{X} = \sum_{k=0}^{\infty} \frac{X^{k}}{k!}\) stands for the matrix exponential. Letting \(Q = [Y_{0}Y_{0}^{\perp}]\) and \(X = \begin{bmatrix} A & -R \top \\ R & 0 \end{bmatrix} \in \text{skew}(n)\), with \(A \in \text{Skew}(p)\) and \(R \in \mathbb{R}^{(n-p) \times p}\); the Riemannian exponential map \(X \mapsto \gamma(1)\), is then given by:

\[
Y_{1} = \gamma(1) = [Y_{0}Y_{0}^{\perp}]e^{ \begin{bmatrix} A & -R \top \\ R & 0 \end{bmatrix} } \begin{bmatrix} I_{p} \\ 0 \end{bmatrix}.
\]

Since \(X\) is a real skew-symmetric matrix, it can be computed using a real Schur decomposition \(X = USU\top\) with \(S = -S\top\).
The geodesics in $G$ starting at $Q$ of the form $t \mapsto \gamma(t) = Qe^{tV}$ with $V \in \mathfrak{m}$ are called horizontal geodesics (denoted by $\hat{\gamma}(t) = \gamma(t)V$ with $V \in \mathfrak{m}$) and the length of geodesics in $G/H$ are the length of their corresponding horizontal geodesics in $G$, i.e. the length of the geodesic segment in $G/H$ from $\gamma(0)$ to $\gamma(1)$ is $\|V\|$. This follows from the fact that $\pi$ is a Riemannian submersion, i.e. $D\pi|_{m}$ preserves the metric, see [10] for more details. Note that a similar result, i.e. the one to one correspondence between the geodesic curves in $G/H$ starting at $p$ (with respect to the Riemannian connection) and the one parameter subgroups $t \mapsto e^{tV}$ with $V \in \mathfrak{m}$ is also obtained in [31], see chapter 10 corollary 2.5, Theorem 2.10 and Theorem 3.3.

However there are many non-horizontal geodesics in $G$ that are mapped to the same geodesic in $G/H$. Indeed, let $V \in \mathfrak{m}$ and $H \in \mathfrak{h}$, in our case, we have: $e^{t(V+H)}p = e^{tV}p$, or equivalently, $e^{-t(V+H)}e^{tV}p = p$, which is equivalent to $e^{-tH}p = p$ when $[V,H] = 0$. This means that all the geodesics $t \mapsto \gamma(t)$ in $SO(n)$ such that $\dot{\gamma}(0) = V + H$ with $[H,V] = 0$ are mapped to the same geodesic in $St(n, p)$. All these geodesics can be chosen as a representation of this geodesic in $St(n, p)$. But the length of these geodesics equals $\sqrt{\|V\|^2 + \|H\|^2}$ since $\mathfrak{h} \perp \mathfrak{m}$, and the one of smaller length is the horizontal one ($H = 0$).

### 5.2 Computation of the Riemannian log-mapping

Let us assume that we know $Y_{0}, Y_{1} \in St(n, p)$, we want to find a geodesic curve that links them, and if possible a geodesic of shortest length. Since the geodesics in $St(n, p)$ are the image by $\pi$ of horizontal geodesics in $SO(n)$, the main idea here is to start from a geodesic in $SO(n)$ that links the two fibers $Y_{0}H$ \(^2\) and $Y_{1}H$, and update it until it gets horizontal. Notice that there exists infinitely many horizontal geodesics in $SO(n)$ whose image by $\pi$ is the same geodesic in $St(n, p)$. To ensure that a geodesic in $St(n, p)$ is the image of only one horizontal geodesic in $SO(n)$ (a lifted geodesic), we have to fix a point on the first fiber $Y_{0}H$, i.e. to fix an orthogonal completion $Y_{0}^{\perp}$.

Then, notice that $SO(n)$ acts on $St(n, p)$ by isometries, which map geodesics to geodesics, thus one can assume, w.l.o.g. that $[Y_{0} \; Y_{0}^{\perp}] = I$. It suffices to set $Y_{1} \leftarrow [Y_{0} \; Y_{0}^{\perp}]^\top Y_{1}$, and to apply the reverse transformation afterwards.

We are then looking for $V = \begin{bmatrix} A & -R^\top \\ R & 0 \end{bmatrix} \in \mathfrak{m}$ such that

$$Y_{1} = \pi(e^{V}) = e^{Vo}.$$  

Or equivalently, we are seeking for a point $Q^*$, see Fig. 5.2, on the left coset $Y_{1}H$ such that the geodesic $t \mapsto \gamma(t)$ in $SO(n)$ linking the identity $I$ to $Q \in Y_{1}H$ is horizontal. Since we are also looking for a minimizing geodesic, the main idea

---

\(^2\) $Y_{0}H = \pi^{-1}(Y_{0})$ stands for the left coset corresponding to $Y_{0}$. 

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Figure 5.2: Illustration: log-mapping computation. This picture makes sense if $SO(n)$ is seen as $\mathbb{R}^3$ and $St(n,p)$ as a plane in $\mathbb{R}^3$. The geodesics are then straight lines.

is to solve the following optimization problem:

$$Q^* = \arg \min_{Q \in Y_1 H} f_I(Q)$$

where $d(I, Q)$ stands for the Riemannian distance function in $SO(n)$. Observe that, $f_I : Y_1 H \to \mathbb{R}_+$ is continuous but not differentiable everywhere, see Section 5.2.1 for more details. But at any stationary point (the function is then differentiable by assumption) of this function, it corresponds an horizontal geodesic. This is due to the fact that $m \perp h$, thanks to the normal Riemannian homogeneous space structure. As shown later on, it could be that there exist many geodesics that link two points on the Stiefel manifold and they are not necessarily minimizing. Note that the problem (5.5) is equivalent to finding an orthogonal completion $Y_1^\perp$ that yields a zero in the lower right part of $V$ in the equation $[Y_1 ~ Y_1^\perp] = eV$.

To solve the optimization problem (5.5), a simple gradient algorithm is proposed. The gradient is readily available using the Riemannian log-mapping on $SO(n)$: $\exp_{Q_I}(Q_2) = Q_1 \log(Q_1^\top Q_2)$. In fact, since $SO(n)$ acts on $St(n,p)$ by isometries, the Riemannian gradient (with respect to the induced metric on the fiber $Y_1 H$) of the function in (5.5) is given by:

$$\nabla f_I(Q) = -Q P_h Q^{-1} \exp_{Q_I}^{-1}(I) = -Q P_h \log(Q^\top),$$

where $P_h$ and $P_m$ stand for the orthogonal projection on $h$ and on $m$, respectively. Since $m \perp h$, $P_m A$ is simply the $m$ component of $A$. This yields algorithm 4.

Remarks:

• To initialize the algorithm, we need to choose $Y_1^\perp$. It can be generated randomly but it is, of course, better to choose it such that $[Y_1 ~ Y_1^\perp]$ is
Algorithm 4 log-mapping on $St(n, p)$

1: Let $Q = [Y_1 \ Y_1^\perp] \in SO(n - p)$ be an orthogonal completion of $Y_1$;
2: until $\|\Delta\|_F^2 < \epsilon$ do
3: Compute the Schur Decomposition of $Q = USU^\top$ where the elements on the diagonal of $S$ are either a $1$, or a 2-by-2 block of the form
   \[
   \begin{bmatrix}
   \cos(\theta) & \sin(\theta) \\
   -\sin(\theta) & \cos(\theta)
   \end{bmatrix};
   \]
4: Form the log-mapping in $SO(n)$:
   \[
   \exp^{-1}(Q) = U \log(S) U^\top \in \text{skew}(n)
   \]
   using:
   \[
   \log\left(\begin{bmatrix}
   \cos(\theta) & \sin(\theta) \\
   -\sin(\theta) & \cos(\theta)
   \end{bmatrix}\right) = \begin{bmatrix} 0 & \theta \\ -\theta & 0 \end{bmatrix}, \quad \log(1) = 0;
   \]
5: Compute $f_I(Q) = \frac{1}{2} d(I, Q)^2 = \frac{1}{2} \|\exp^{-1}(Q)\|_F^2$;
6: Set: $\Delta = [0_{(n-p)\times p} \ I_{n-p}] \exp^{-1}(Q) \begin{bmatrix} 0_{p\times(n-p)} \\ I_{n-p} \end{bmatrix}$;
7: Choose a step size $\alpha > 0$ such that the function (5.5) is decreased (backtracking method using $f_I(Q)$ computed at step 5), and set: $Q \rightarrow [Y_1 \ Y_1^\perp e^{(-\alpha\Delta)}]$;
8: end until
9: return $v = P_m(\exp^{-1}(Q))$

close to $Q^*$. One possibility is to choose the element of the coset $Y_1H$ that is the closest to the identity $I$ in Frobenius distance. Let $Y_1^+$ such that $[Y_1 \ Y_1^+] \in so(n)$, this yields the following optimization problem:

$$R^* = \arg\min_{R \in SO(n-p)} \frac{1}{2} \|I - [Y_1 \ Y_1^+ R]\|_F^2, \quad (5.6)$$

whose solution is given by

$$R = W \begin{bmatrix} I_{n-p-1} & 0 \\ 0 & \det W U^\top \end{bmatrix} U^\top,$$

with $[0 \ 0 \ I_{n-p}] Y_1^+ = U\Sigma W^\top$ (singular value decomposition). When the singular values are distinct, the solution is unique.

This initialization is justified when $Q^*$ is close to the identity. In fact, the objective function in (5.6) is

$$\frac{1}{2} d(I, Q)^2 = \frac{1}{2} \|\log(Q)\|_F^2 \approx \frac{1}{2} \|I - Q\|_F^2.$$

- Let us consider the case where $Y_1$ spans the same $p$-dimensional subspace as $o$, i.e. $Y_1 = \begin{bmatrix} R_1 \\ 0 \end{bmatrix}$ where $R_1 \in SO(p)$. In this case, the algorithm
converges in one iteration if $\alpha = 1$, no matter how it is initialized. In fact, if we take the initial condition $\begin{bmatrix} R_1 & 0 \\ 0 & R_2 \end{bmatrix}$ with $R_2 \in SO(n-p)$, in step 6, we have $\Delta = \log(R_2)$, and thus the update in step 7 is $Q \begin{bmatrix} R_1 & 0 \\ 0 & R_2 R_2^{-1} \end{bmatrix}$.

- Let $Y_0, Y_1 \in St(n, p)$ such that the two frames $Y_0$ and $Y_1$ have $p - 1$ vectors in common. Let us denote by $t \mapsto e(t)$ the trajectory of the vector that changes ($e(0)$ and $e(1)$ belong to the frame $Y_0$ and $Y_1$, respectively). Then, a geodesic between these two frames is simply a rotation in the plane span$(e(0), e(1))$ and it is thus easy to compute.

- At step 3, one could also compute an approximation of the matrix logarithm $\log(Q)$, see for example [27]. Moreover, note that we do not necessarily need to compute a Schur decomposition to compute $\Delta = \begin{bmatrix} 0_{(n-\rho) \times \rho} & I_{n-p} \end{bmatrix} \exp^{-1}(Q) \begin{bmatrix} 0_{\rho \times (n-p)} \\ I_{n-p} \end{bmatrix}$; only the lower right part of $\exp^{-1}(Q)$ is important. Designing an algorithm that uses this specific structure is still an open problem.

- Note that $\exp_I(P_m \exp^{-1}(Q))$ does not belong to the coset $Y_1 H$.

- The Schur decomposition of different points inside a coset seems to be unstructured, i.e., the 2-dimensional invariant subspaces change. It could be possible to update it using the decomposition in the direct sum of 2-dimensional vector spaces.

### 5.2.1 Selection of the step size $\alpha$

To choose the step size $\alpha$ in step 7 different heuristics can be chosen, but the main idea is often the same: choose a step size; and if it does not yield a reduction of the cost function, reduce it until it does. Of course, it is very difficult to say something about the number of step sizes that will have to be chosen before finding one that works.

To tune the step size it is insightful to look at the Hessian of the objective function (5.5). Since any two points in $Y_1 H$ can be linked by a geodesic curve entirely contained in $Y_1 H$ (all the one parameter subgroups are geodesics), $Y_1 H$ is a totally geodesic submanifold of $SO(n)$. Thus, the Riemannian Hessian of the squared Riemannian distance function $q \mapsto \frac{1}{2}d(I, q)^2$ in $SO(n)$ and the Riemannian Hessian of the same function restricted to $Y_1 H$, i.e. $f_I$, coincide. Since $SO(n)$ is a manifold of positive curvature, an upper bound on the Riemannian Hessian of the squared Riemannian distance function is given by $L = 1$, see Section 3.3 for more details. Thus the Riemannian Hessian of $f_I$ in (5.5) is bounded by $L = 1$. Then, under the assumption that $Q \mapsto f_I(Q)$ is $C^2$, using a Taylor expansion of $f_I$ along a geodesic curve $t \mapsto \gamma(t) \subset Y_1 H$ such that
\[ \gamma(0) = Q \quad \text{and} \quad \dot{\gamma}(t) = \text{grad} f_I(Q), \]

one obtains:

\[ f_I(\gamma(h)) \leq f_I(Q) - \|\text{grad} f_I(Q)\|^2 h + \frac{L}{2} h^2 \|\text{grad} f_I(Q)\|^2. \tag{5.7} \]

So, if we choose \( h \in [0, \frac{2}{L}] \), a decrease of \( f_I \) is ensured. Since \( f_I \) is continuous, on the compact \( Y_1 H \), it is bounded from below. Then, by a classical argument, it is possible to show that the sequence \( \{f_I\}_k \) corresponding to our gradient method converges, and from that, to show that the sequence of gradient \( \{\|\text{grad} f_I\|\}_k \to 0 \) when \( k \to \infty \), see Theorem 22 for more details. The algorithm converges to a stationary point, and thus a geodesic in \( St(n, p) \). Note that, in our case \( L = 1 \), and \( h = 1 \) maximizes the potential (according to the bound (5.7)) decrease of the cost function. So \( h = 1 \) is probably a good step size.

Unfortunately, \( f_I \) is continuous but not differentiable everywhere. To describe this, we need the concept of conjectivity radius and injectivity radius, see [10] for more details or Section 2.4. The points on the coset \( Y_1 H \), where \( f_I \) is not differentiable are intersections of \( Y_1 H \) with the cut locus of the identity \( C(I) \). In fact, only at these points the squared Riemannian distance function in \( SO(n) \) fails to be smooth. Unfortunately, the cut locus of the identity is difficult to describe in general. However, our numerical experiments on \( St(4, 2) \) (note that in that case, the points on the Stiefel manifold are seen as left cosets isomorphic to \( S^1 \) inside \( SO(4) \)) seem to show that there is only 1 intersection.

Nonetheless, the nature of \( C(I) \cap Y_1 H \) is unknown to the author. However, let \( Q^* \) be a stationary points of \( f_I \), and let us assume that \( d(I, Q^*) < \pi - \epsilon \) with \( 0 < \epsilon < \pi \). Then on the ball \( B(Q^*, \epsilon) \subset Y_1 H \), there is no cut point, since by the triangle inequality we have \( \forall Q \in B(Q^*, \epsilon), \quad d(I, Q) \leq d(I, Q^*) + d(Q, Q^*) < \pi = \text{inj}(SO(n)) \).

As we have shown, all the geodesics (in \( St(n, p) \)) linking \( o \) to \( Y_1 \) are stationary points of the function \( f_I \) in (5.5) since they are horizontal. We may wonder when there is only one stationary point. In that case, there is only one minimizing geodesic between \( o \) and \( Y_1 \). It is the case when \( d(o, Y_1) < \text{inj}(St(n, p)) \). Thus, it would be nice to have a lower bound on the injectivity radius of \( St(n, p) \).

We have the following estimate.

**Theorem 28** ([10] Lemma 5.6). Let \( \mathcal{M} \) be a compact (and thus complete) Riemannian manifold, its injectivity radius

\[ \text{inj}(\mathcal{M}) = \min\{\text{conj}(\mathcal{M}), \frac{l}{2}\}, \]

where \( l \) is the length of the shortest periodic (or closed) geodesic and \( \text{conj}(\mathcal{M}) \) is the conjugate radius of \( \mathcal{M} \). Furthermore, the conjugate radius of \( \mathcal{M} \) satisfies

\[ \text{conj}(\mathcal{M}) \geq \frac{\pi}{\sqrt{\Delta}}, \]

where \( \Delta \) is an upper bound on the sectional curvature of \( \mathcal{M} \).
Let us first look at the length of the shortest periodic geodesics in $SO(n)$, w.l.o.g. we can assume that these geodesics start and end at the identity $I$. Thus, we want to find the $V$'s of smallest norm such that $I = Ie^V$. Since $V \in \text{skew}(n)$, we can consider its Schur decomposition $V = USU^\top$. Then, the constraint $I = e^S$ implies that $\theta_i = k_i 2\pi k_i \in \mathbb{Z}$. Thus, the shortest non trivial minimizing geodesic in $SO(n)$ is of length $2\pi$.

Let us now look at the shortest periodic geodesics in $St(n,p)$, which w.l.o.g., start at the identity since the space is Riemannian homogeneous. These geodesics are the images of horizontal geodesics in $SO(n)$ that start in the fiber containing the identity, and end in this fiber. But they are not necessarily periodic in $SO(n)$. We are thus looking for the $V$'s $\in m$ of smallest norm such that

$$\begin{bmatrix} I_p & 0 \\ 0 & R \end{bmatrix} = e^V \text{ with } R \in SO(n-p).$$

Let $e_1, \ldots, e_p$ be the first $p$ identity vectors, i.e. $[e_1 \ldots e_p] = o = \begin{bmatrix} I_p \\ 0 \end{bmatrix}$ and let $t \mapsto \gamma(t)$ be a geodesic curve such that $\gamma(0) = o = \gamma(1)$. If this geodesic is not a trivial geodesic ($\gamma(t) = o \forall t$), at least one of these identity vectors must move. Let us assume, w.l.o.g., that it is $e_1$. The rotation $Q = e^V \in SO(n)$ that realizes this movement satisfies $Qe_1 = e_1$. Let $Q$ be defined by the set of orthogonal subspaces $S_1, S_2, \ldots$ and corresponding rotations $r_1, r_2, \ldots$ (Schur decomposition). The vector $e_1$ has at least a component in one of these subspaces that depends on $t$, let say $S_i$. To have $Qe_1 = e_1$, this component must make one rotation of $2\pi$ in the subspace $S_i$, and thus $\|V\| \geq 2\pi$.

The sectional curvature on the Stiefel manifold is given by

$$\kappa(X,Y) = \|[X,Y]_h\|^2 + \frac{1}{4}\|[X,Y]_m\|^2.$$

The following theorem is helpful to bound the curvature.

**Theorem 29.** [6, Theorem 1] For general complex matrices $X$ and $Y$, and for the Frobenius norm $\|\cdot\|_F$, we have

$$\|X,Y\|_F \leq \sqrt{2}\|X\|_F\|Y\|_F.$$

The inequality is sharp.

In fact,

$$\|[X,Y]_h\|^2 = \frac{1}{2}\|[X,Y]_h\|_F^2$$

$$\leq \frac{1}{2}\|[X,Y]_m\|_F^2$$

$$= \frac{1}{2}2\|X\|_F^2\|Y\|_F^2 \text{ using Theorem 29}$$

$$= 1.$$
The same argument yields $\|[X, Y]_m\| \leq 1$. So an upper bound on the sectional curvature is given by:

$$\Delta = \max \kappa(X, Y) = \frac{5}{4} = 1.25.$$  

This bound is achieved if one considers the section spanned by the two following vectors:

$$X = \frac{\sqrt{2}}{2} \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, \quad Y = \frac{\sqrt{2}}{2} \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}.$$  

Then, using Theorem 28, the injectivity radius is lower bounded by

$$\text{inj}(St(n, p)) \geq \frac{\pi}{\sqrt{\Delta}} = 0.89\pi.$$  \hspace{1cm} (5.13)

We will see, in our numerical experiments, that this bound seems to be tight. Furthermore, using the bound in (A.2), see Appendix A, it is possible to guarantee that, when

$$d(I, Q^*) < d_c = \frac{\sqrt{2}}{2} \pi \approx 0.71\pi \leq \text{inj}(St(n, p)),$$  \hspace{1cm} (5.14)

there exists a ball contained in $Y_1 H$, and centred at $Q^*$, such that the objective function (5.5) is convex inside of that ball. When the objective function $f_I$ is strictly convex on a sufficiently large ball around $Q^*$, it could be valuable to use a Newton method to take advantage of its asymptotic quadratic rate of convergence. Notice that the bound (5.14) is very restrictive since the Hessian of the squared Riemannian distance function can be positive definite when it is restricted to the directions tangential to the fiber $Y_1 H$, and so $f_I$ could still be positive definite.

5.2.2 Numerical examples with $p = 2$

To gain some insight into the minimization problem (5.5), let us consider the case where $p = 2$ and $n = 4$. It should be considered as the simplest non trivial case but it is particularly important in shape space analysis, see [56] and [65].

Let

$$A = \begin{bmatrix} 0 & -1 & -1 & 0 \\ 1 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix},$$

and let $t \mapsto \gamma(t) = \exp_I(t\frac{A}{|A|})$ be a unit speed geodesic (parametrized by arc length), starting at the identity $I \in SO(n)$. Since $A \in m$, $t \mapsto \gamma(t)o$ is a
geodesic in \( St(n, p) \). Since \( H \equiv S^1 \) when \( p = 2 \), it is possible to make a graphic of the cost function (5.5) in function of an angle \( \theta \) defined by

\[
H = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & \cos(\theta) & \sin(\theta) \\
0 & 0 & -\sin(\theta) & \cos(\theta)
\end{pmatrix} \quad | \quad \theta \in [-\pi, \pi].
\]

The result is presented on Fig. 5.3. Just below our lower bound (5.13) on the injectivity radius, i.e. \(0.89\pi\), there is only one minimizer (green curve). Once \( t \) is larger than the injectivity radius, it is possible to have many stationary points, and so many geodesics (not necessarily minimizing) are linking \( o \) and \( Y_1 \) (blue curve).

Choosing the point on the fiber \( Y_1 H \) that is the closest to the identity in Frobenius norm, which only requires a singular value decomposition, yields an initial guess quite close to the minimizer when \( t \) is small, see Fig. 5.4. The number of iterations required to reach a given accuracy \( \epsilon \), increases with the distance \( d(I, Q^*) \). Another important point to notice is that, in these examples there is only one point where the cost function (5.5) is not differentiable (one angular point), and it is often a maximum.

5.3 Computation of the log-mapping when \( n \gg p \)

In this section, the method proposed in [14] to compute the geodesic (5.3) when \( n \gg p \) is described in more details. Then, it is shown how the same method can be used to compute the log-mapping in that case. The key idea is to remark that the geodesic curve \( t \mapsto \gamma(t) \) remains inside a \( 2p \)-dimensional subspace.

In fact, let \( R = [QQ^\perp]_r = QR \) be the QR-decomposition of \( R \), we have

\[
\begin{bmatrix}
A & -R^T \\
R & 0
\end{bmatrix} =
\begin{bmatrix}
I_p & 0 \\
0 & [QQ^\perp]
\end{bmatrix}
\begin{bmatrix}
A & -r^T \\
r & 0
\end{bmatrix}
\begin{bmatrix}
I_p & 0 \\
0 & [QQ^\perp]^T
\end{bmatrix}.
\]

By replacing (5.15) into (5.4), one obtains

\[
Y_1 = [Y_0 Y_0^\perp]
\begin{bmatrix}
I_p & 0_p \\
0_p & Q_p^\perp
\end{bmatrix}
\begin{bmatrix}
\exp\left( A \begin{bmatrix} 0 & -r^T \\ r & 0 \end{bmatrix} \right) \\
0_p & 0_p
\end{bmatrix}
\begin{bmatrix}
I_p \\
0_p
\end{bmatrix},
\]

\[
= [Y_0 Y_0^\perp Q \ Y_0^\perp Q^\perp]
\begin{bmatrix}
\exp\left( A \begin{bmatrix} 0 & -r^T \\ r & 0 \end{bmatrix} \right) \\
0_p & 0_p
\end{bmatrix}
\begin{bmatrix}
I_p \\
0_p
\end{bmatrix},
\]

\[
= [Y_0 Y_0^\perp Q \ Y_0^\perp Q^\perp] \exp\left( A \begin{bmatrix} 0 & -r^T \\ r & 0 \end{bmatrix} \right) \begin{bmatrix}
I_p \\
0_p
\end{bmatrix}.
\]

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Figure 5.3: Objective function $f_I(Q)$ where $Q \in Y_1 H$ parametrized by $\theta$ for different values of $t$

Let us define

$$H = \dot{\gamma}(0) = [Y_0 \quad Y_0^\perp] \begin{bmatrix} A & -R^T \\ R & 0 \end{bmatrix} \begin{bmatrix} I_p \\ 0 \end{bmatrix} = Y_0 A + Y_0^\perp R = Y_0 A + Y_0^\perp Q r. \quad (5.17)$$

Notice that $H$ is the tangent vector to the curve

$$t \mapsto [Y_0 \quad Y_0^\perp] e \left( t \begin{bmatrix} A & -R^T \\ R & 0 \end{bmatrix} \right) \begin{bmatrix} I_p \\ 0 \end{bmatrix},$$

in $\mathbb{R}^{n \times p}$ at the origin $t = 0$.

Observe also that this last formula requires $O(np^2)$ flops to compute the geodesic in (5.4). In fact, it suffices to compute $A = Y_0^\top H$ and $(I - Y_0 Y_0^\top) H = Y_0^\top R = Y_0^\top Q r$ where $U$ and $r$ are computed using a QR-decomposition to find $A$, a $r$ and a $U$. Then replacing $Y_0^\perp Q$ in (5.16) by $U$, we can compute $Y_1$ using:

$$Y_1 = [Y_0 \quad U] \exp \left( t \begin{bmatrix} A & -r^\top \\ r & 0 \end{bmatrix} \right) \begin{bmatrix} I_p \\ 0 \end{bmatrix}. \quad (5.18)$$
Figure 5.4: Objective function $f_I(Q)$ parametrized by $\theta$ for different values of $t$. The red triangle is the starting point. It is chosen here as the closest element of the fiber $Y_1^t H$ to the identity with respect to the Frobenius norm. $N$ is the number of iterations required to reach an accuracy of $\epsilon = 10^{-14}$. When $t$ is small $f_I(Q)$ is very close to a (wrapped) parabola whose Hessian is 1.
This does not tell you how to compute the exponential in (5.16) but the problem involves only the computation of the exponential of a $2p \times 2p$ matrix, and $Y_1$ can be computed in $O(np^2)$ flops. This is thus an interesting approach when $n \gg p$.

The same tricks can be used to compute the Riemannian log-mapping. In fact, let us assume that we know $Y_0$ and $Y_1$, the aim is to compute $A$ and $R$, or equivalently $H$ such that (5.4) is satisfied. First, note that $Y_1$ in (5.16) can be decomposed on the basis $[Y_0 \ Y_0^\perp Q]$:

$$Y_1 = Y_0 M + Y_0^\perp Q N,$$

with

$$\begin{bmatrix}
M \\
N 
\end{bmatrix} = \exp \left( \begin{bmatrix}
A & -r \top \\
r & 0
\end{bmatrix} \right) \begin{bmatrix}
I_p \\
0_p
\end{bmatrix},$$

where $M$ and $N$ are the components of $Y_1$ in this basis. These components can be computed from $Y_1$ and $Y_0$

$$M = Y_0 \top Y_1, \quad (5.19)$$

$$N = R \text{ where } (I - Y_0 Y_0 \top) Y_1 = U R. \quad (5.20)$$

Note that $[M \ N]$ is an orthogonal matrix by construction. Consequently, we end up to the following baby problem: Finding $A$ and $r$ such that

$$\begin{bmatrix}
M \\
N 
\end{bmatrix} = \exp \left( \begin{bmatrix}
A & -r \top \\
r & 0
\end{bmatrix} \right) \begin{bmatrix}
I_p \\
0_p
\end{bmatrix}. \quad (5.21)$$

Note that the decomposition in (5.20) is not unique but $H = Y_0 A + U r$ in (5.17) will be unique. This problem is a log-mapping problem on a $St(2p, p)$ and computing the baby problem requires $O(np^2)$ flops. Thus, the total cost of computing a log-mapping on $St(n, p)$, when $n \gg p$ is in $O(np^2) + O(kp^3)$ where $k$ is the number of iterations required in our gradient method. The baby problem is not simpler, it is just smaller.

### 5.4 Related applications

Once we have an algorithm to compute the Riemannian log-mapping on the Stiefel manifold, we can implement a gradient method to compute the Karcher mean of a set of points, see Chapter 3. Since the Stiefel manifold has positive curvature, there exist many Karcher means, and our gradient method converges to one of them. To guarantee the uniqueness of the Karcher mean, we have to assume that the data points all belong to a ball of some radius, and inside that ball the Karcher mean will be unique. In particular, if all the data points belong to an open Riemannian ball of radius $r = r_c$, there is a unique Karcher mean inside that ball. On the Stiefel manifold, $r_c = \frac{\Delta}{2 \sqrt{3/4}} \approx 0.45 \pi$ since $\Delta = \frac{\pi}{4}$. 

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Figure 5.5: Karcher mean computation on $St(10, 2)$. (upper left): norm of the gradient at step $k$; (lower left) mean over each data point of the number of Schur decompositions required to reach an accuracy of $\epsilon = 10^{-14}$ in Algorithm 4 when the log-mapping is computed; (right) same experiment except that the required accuracy $\epsilon$ in the log-mapping computation using Algorithm 4 depends now on the gradient of the Karcher mean cost function $F$ at the current iteration: $\epsilon = \|\text{grad} F_k\|10^{-2}$.

A unit step size gradient method was implemented to compute the Karcher mean of a set of 5 data points located on a radial strip of inner radius $0.4\pi$ and outer radius $0.44\pi$ around the identity frame $o$. The starting point is one of the data points. The result is presented in Fig. 5.5.

Notice that the Karcher mean could be used to compute an approximation of a partial joint diagonaliser of a set of symmetric matrices following the approach given in [40], or be used as an initial condition for another joint diagonalisation algorithm.

Another related application is in data fitting on $SO(n)$ using cosets, see [32]. We will only give the main idea here. Let us assume that we want to approximate a set of points $\{q_1, \cdots, q_N\}$ on $SO(n)$ by a coset $pH$ where $p \in SO(n)$ and $H = \{ \begin{bmatrix} I_p & 0 \\ 0 & R_{n-p} \end{bmatrix} \mid R_{n-p} \in SO(n) \}$, i.e. the isotropy group at the identity on $St(n,p)$. In other words, we want to find a rotation $p$ such that the $p^Tq_i$’s are rotations close to $H$. To do that, we can consider the following optimization problem:

$$p^* = \arg \min_{p \in SO(n)} \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2} d(q_i, pH)^2,$$

(5.22)

where $d$ stands for the classical bi-invariant Riemannian distance on $SO(n)$, and the distance between a point and a coset is defined by

$$d(q_i, pH) = \min_{h \in H} d(q_i, ph).$$

Using $p \in SO(n)$ to parametrize the set of cosets $pH$ is a big over parametriza-
tion. But it is possible to work on the coset space \( SO(n)/H = St(n,p) \), which is here the Stiefel manifold. In fact, \( d \) is bi-invariant, thus we have \( d(q_i, pH) = d(q_iH, pH) \). This optimization problem is thus equivalent to a Karcher mean problem on the Stiefel manifold where the \( q_iH \)'s are the data points.
Chapter 6

Log-mapping on $GL_n$

In this chapter, a shooting method is proposed to solve the endpoint geodesic problem on the general linear group equipped with a left invariant metric. Let $g_1$ be in the identity component of $GL(n)$. This problem consists in finding $V \in \mathbb{R}^{n \times n}$ (the solution is not necessarily unique) such that:

$$g_1 = e^{V^T} e^V - V^T,$$

where $e^X$ stands for the matrix exponential function. We first review the geometry of $GL(n)$ equipped with a left invariant metric. Then, a shooting method is proposed to estimate $V$. The particular case of symplectic matrices which has recently deserved some interest in the recent literature [17] is also discussed. Some potential applications are the computation of the Riemannian distance between invertible matrices or the computation of the Karcher mean.

Main contributions:

- We propose a gradient method to compute the Riemannian log-mapping on the general linear group equipped with a left invariant metric.
- We apply our approach to averaging problems on the symplectic group and compare it to other approaches.

6.1 Generalities on the general linear group

The general linear group $GL(n, \mathbb{R})$ is the set of invertible linear maps from $\mathbb{R}^n$ to $\mathbb{R}^n$. These maps can be represented by matrices whose determinant is non-zero once a basis has been chosen. In this chapter, we will only consider the real general linear group, and use the shorthand notation $GL(n)$ for $GL(n, \mathbb{R})$. As a topological space $GL(n)$ has two connected components: the matrices of positive determinant denoted by $GL^+(n)$ (it is also called the identity component since it contains the identity); and the ones of negative determinant.
denoted by $GL^{-}(n)$. The Lie group exponential map is simply given by the matrix exponential $e^{tV} = \sum_{k=0}^{\infty} \frac{(tV)^{k}}{k!}$.

6.1.1 Riemannian geometry of the general linear group $GL(n)$.

In this section, the Riemannian geometry of the general linear group equipped with a left invariant metric is described. For more information about this geometry, see [4, 5]. A formula for the Riemannian connection on $GL^{+}(n)$ has already been derived in [4, 60]. A formula for the geodesics related to a right invariant metric was derived in [60] using Lax pairs. In [4], see also the references therein, the geodesics are described as the extrema of a length functional. More precisely, let $t \mapsto g(t)$ be a smooth curve in $GL^{+}(n)$, its length with respect to the $p$-norm $\|X\|_{p} = (\text{tr}(X^{T}X)^{1/p})$ is given by

$$L_{p}(g) = \int_{0}^{1} \|g(t)^{-1} \dot{g}(t)\|_{p} dt.$$ 

In [4], the case where $p$ is even is studied. Here, we will only consider the case $p = 2$. The distance is then induced by a Riemannian metric, and the infima of $L_{2}$ such that $g(0) = g_{0}$ and $g(1) = g_{1}$ are distance minimizing geodesics.

At each inner product $g_{I}(.,.)$ on $gl_{n} \cong T_{I} GL^{+}(n)$, it corresponds a left invariant Riemannian metric defined by:

$$g_{P}(X_{P},Y_{P}) = g_{I}(P^{-1}X_{P},P^{-1}Y_{P}).$$ (6.1)

This metric is in fact left invariant since the differential of the left action is $X \mapsto PX$. So $X_{P} = PX_{I}$, and

$$g_{P}(X_{P},Y_{P}) = g_{I}(X_{I},Y_{I}).$$

or equivalently, the left action or left translation (group action on itself), is an isometry. In this work, only the following inner product is considered:

$$\langle X,Y \rangle = \text{tr}(X^{T}Y).$$ (6.2)

The Lie group structure and the Riemannian metric are made compatible in the hope of getting simpler formulas to compute the geodesics. Indeed, let us assume that we want to compute the geodesics on the Riemannian manifold $(GL^{+}(n), g)$. Since the left action is an isometry, we only have to compute the geodesics that start at the identity $\gamma(0) = I$ and such that $\dot{\gamma}(0) = X_{I}$. In fact, the geodesic that starts at $P$ in the direction $X_{P} = PX_{I}$ is given by $P\gamma(t)$.

Let $t \mapsto \gamma(t)$ be a geodesic and $t \mapsto (\gamma(t), \dot{\gamma}(t))$ its tangent vector field, we have

$$\nabla_{\dot{\gamma}(t)} \dot{\gamma}(t) = 0,$$
where $\nabla$ stands for the Riemannian connection. Let us define the curve in the Lie algebra $\mathfrak{gl}_n$ that corresponds to $t \mapsto \gamma(t)$ by

$$x(t) = \gamma(t)^{-1} \dot{\gamma}(t).$$

If $x(t)$ was constant, $(\gamma(t), \dot{\gamma}(t))$ would be a left invariant vector field whose integral curve is given by the Lie group exponential map. Unfortunately, $x(t)$ is not always constant, and the Riemannian exponential map and the Lie group exponential map are different in general.

Since $GL^+(n)$ is a linear Lie group, the adjoint representation is $Ad : GL^+(n) \to GL(g), \ g \mapsto g \ast g^{-1}$ and $ad = DAd(e), \ g \mapsto GL(g), \ V \mapsto [V, \ast]$. Its adjoint with respect to the inner product (6.2) is

$$ad^*_g \gamma = [x^T, \gamma].$$

Let us consider two vector fields $X = (g, gx(g))$ and $Y = (g, gy(g))$ on $GL^+(n)$. If we know a formula for the Riemannian connection of left invariant vector fields, see [10], it is possible to derive a formula for any vector field. Indeed, using the locality of the connection, we have

$$\nabla_X Y|_p = \nabla_{gx(g)}gy(g)|_p = \nabla_{px(p)}gy(g)|_p.$$

Let $(E_1, \cdots, E_n)$ be a basis of $\mathfrak{gl}_n$, we have $y(g) = \sum_{i=1}^n y^i(g) E_i$, where $g \mapsto y^i(g)$ are smooth functions from $GL^+(n)$ to $\mathbb{R}$ that represent the coordinates of $y(g)$ in the basis $(E_1, \cdots, E_n)$. Note that if $Y$ is left invariant, then the $y^i(g)$’s are constant functions. Using the Leibniz rule: $\nabla_X fY = (\nabla_X f)Y + f\nabla_X Y$, we have

$$\nabla_{px(p)}y^i(g)\sum_{i=1}^n \nabla_{px(p)}y^i(g)\sum_{i=1}^n (gE_i)|_p + \sum_{i=1}^n y^i(g)|_p \nabla_{px(p)}gE_i|_p.$$  \hfill (6.3)

We have also $\nabla_{px(p)}y^i(g)|_p = (px(p))_p y^i(g) = \frac{d}{ds} y^i(\beta(s))|_{s=0}$ where $s \mapsto \beta(s)$ is a curve in $GL^+(n)$ such that $\beta(0) = p$ and $\beta(0) = px(p)$. Thus, the first term in the right-hand side of (6.3) becomes $pDy(g)[px(p)]|_p$, and the second one is

$$\sum_{i=1}^n y^i(p)\nabla_{px(p)}gE_i|_p = \nabla_{px(p)}g\sum_{i=1}^n y^i(p)E_i|_{y(p)}.$$ 

since the $y^i(p)$’s are constant. Eventually, one obtains:

$$\nabla_X Y|_p = pDy(g)[px(p)]|_p + p\nabla_X y(g)|_p,$$

where the second term is the covariant derivative of left invariant vector fields. This equation can be interpreted as follows. The first term represents the derivative of the components of $Y$, and the second term represents the covariant derivative of the basis elements.
The Riemannian connection for left invariant vector fields \( x, y \) on Lie groups equipped with a left invariant Riemannian metric can be derived from the Koszul defining equation of the Riemannian connection and is well known, see e.g., [10, Proposition 3.18]:

- \( \nabla_x y = \frac{1}{2}([x, y] - ad_x^*(y) - ad_y^*(x)) \);
- one-parameter subgroups are geodesics if and only if \( ad_x^*(X) = 0 \) for all \( X \).

Thus the Riemannian connection with respect to the metric \( g \) is given by

\[
\nabla_{X(g)}Y(g) = g(Dy(g)[gx(g)] + \nabla_{x(g)}y(g))
\]

\[
= g(Dy(g)[gx(g)] + \frac{1}{2}([x(g), y(g)] - ad_{x(g)}^*(y(g)) - ad_y^*(g)(x(g))))
\]

\[
= g(Dy(g)[gx(g)] + \frac{1}{2}([x(g), y(g)] - [x(g)^\top, y(g)] - [y(g)^\top, x(g)])).
\]

(6.4)

### 6.1.2 Geodesics

Let \( g(t) \) be a geodesic curve in \( GL^+(n) \), and define \( x(t) = g(t)^{-1}g(t) \), we have

\[
\dot{x} + \nabla_x x = 0.
\]

Using (6.4), this yields

\[
\dot{x} - [x^\top, x] = \dot{x} - x^\top x + xx^\top = 0.
\]

The solution of this differential equation in the Lie algebra \( \mathfrak{gl}_n \) is given by, see Appendix C for more details,

\[
x(t) = e^{-t(x_0 - x_0^\top)}x_0e^{t(x_0 - x_0^\top)}.
\]

To find a formula for the geodesics, we then need to integrate the vector field \( (g(t), g(t)x(t)) \), i.e. to find the solution \( t \mapsto g(t) \) of

\[
\dot{g}(t) = g(t)x(t) = g(t)e^{-t(x_0 - x_0^\top)}x_0e^{t(x_0 - x_0^\top)}.
\]

To do this, we can proceed as in [60]. Let \( b(t) = g(t)e^{-t(x_0 - x_0^\top)} \), we have

\[
\dot{b}(t) = g(t)e^{-t(x_0 - x_0^\top)}x_0 - g(t)e^{-t(x_0 - x_0^\top)}(x_0 - x_0^\top),
\]

\[
= g(t)e^{-t(x_0 - x_0^\top)}(x_0 - (x_0 - x_0^\top)),
\]

\[
= b(t)x_0^\top.
\]

Thus \( b(t) = b(0)e^{tx_0^\top} \) and this yields

\[
\gamma(t) = g_0e^{tx_0}e^{t(x_0 - x_0^\top)},
\]

(6.5)

which is the geodesic curve that starts at \( g_0 \) and such that \( \dot{\gamma}(0) = g_0x_0 \). Notice that when \( ad_{x_0}^*(x_0) = [x_0^\top, x_0] = 0 \), i.e., \( x_0 \) is normal, the Riemannian exponential map corresponds to the Lie group exponential map since \( x(t) = x_0 \).
6.1.3 The 2-by-2 case

When \( p = 2 \), it is possible to derive explicit expressions for the geodesics:

\[
g(t) = e^{tV^\top} e^{t(V - V^\top)}
\]

where \( V \in \mathfrak{gl}_2 \). We can assume, w.l.o.g., that \( V \) is upper triangular. Indeed, let us consider the real Schur canonical decomposition in the Euclidean space \((\mathfrak{gl}_2, \langle \cdot, \cdot \rangle)\), we have

\[
V = USU^\top,
\]

where \( U \) is orthogonal and \( S \) can have the following two forms:

1. When the eigenvalues of \( V \) are real:

\[
S_1 = \begin{bmatrix}
\lambda_1 & \sigma \\
0 & \lambda_2
\end{bmatrix},
\]

\( S \) is normal when \( \sigma = 0 \).

2. When the eigenvalues of \( V \) are complex conjugate:

\[
S_2 = \begin{bmatrix}
\alpha & \beta_1 \\
\beta_2 & \alpha
\end{bmatrix},
\]

where \( \beta_1 \) and \( \beta_2 \) are of opposite sign. \( S \) is normal when \( \beta_1 = -\beta_2 \).

Using this decomposition we have:

\[
\tilde{g}(t) = U^\top g(t) U = e^{tS^\top} e^{t(S - S^\top)}.
\]

Then, using the definition of the matrix exponential, one obtains

\[
e^{tS} = \begin{bmatrix}
e^{t\lambda_1} & 0 \\
\sigma e^{t\lambda_1 - \lambda_2 t} & e^{t\lambda_2}
\end{bmatrix}.
\]

Thus in case (1), we have

\[
\tilde{g}(t) = \begin{bmatrix}
e^{t\lambda_1} & 0 \\
\sigma e^{t\lambda_1 - \lambda_2 t} & e^{t\lambda_2}
\end{bmatrix} \begin{bmatrix}
\cos(t\sigma) & \sin(t\sigma) \\
-\sin(t\sigma) & \cos(t\sigma)
\end{bmatrix}.
\]

In the case (2), we have

\[
e^{S_2} = e^{\alpha t} \begin{bmatrix}
0 & \beta_1 \\
\beta_2 & 0
\end{bmatrix},
\]

\[
e^{S_2} = e^{\alpha t} \begin{bmatrix}
\cos(\sqrt{d}) & -\sin(\sqrt{d}) \frac{\sqrt{d}}{\beta_2} \\
-\sin(\sqrt{d}) \frac{\sqrt{d}}{\beta_1} & \cos(\sqrt{d})
\end{bmatrix},
\]

where \( d = |\beta_1\beta_2| \). Notice that \( e^{S_2} \) is skew-symmetric when \( \beta_1 = -\beta_2 \) and in that case \( S_2 \) is normal. Eventually, one obtains:

\[
\tilde{g}(t) = e^{\alpha t} \begin{bmatrix}
\cos(t\sqrt{d}) & -\sin(t\sqrt{d}) \frac{\sqrt{d}}{\beta_1} \\
-\sin(t\sqrt{d}) \frac{\sqrt{d}}{\beta_2} & \cos(t\sqrt{d})
\end{bmatrix} \begin{bmatrix}
\cos(t(\beta_1 - \beta_2)) & \sin(t(\beta_1 - \beta_2)) \\
-\sin(t(\beta_1 - \beta_2)) & \cos(t(\beta_1 - \beta_2))
\end{bmatrix}.
\]
6.2 Shooting method

The main idea of our approach is to use a shooting method to compute the Riemannian log-mapping, i.e., given $\gamma(1) = g_1$ and $\gamma(0) = g_0$ in (6.5), we want to find $x_0$. Since the left translation is an isometry, the geodesic that starts at $g_0$ is simply the image of a geodesic $t \mapsto \gamma(t)$ that starts at the identity by the left translation, i.e. $g_0 \gamma(t)$. Let $g = g_0^{-1} g_1$, our problem then becomes: finding $V \in \mathfrak{gl}_n$ such that:

$$g = e^{V^\top e(V - V^\top)}.$$

Note that this problem does not necessarily admit a unique solution. Indeed, if $g = I_2$, we can choose $V = 0_2$ or $V = \begin{bmatrix} 0 & 2\pi \\ -2\pi & 0 \end{bmatrix}$. When there are many solutions, we are looking for the ones of smaller norm $\|V\|$.

To tackle this problem, we propose a shooting strategy. The main principle is the following. Starting from an initial guess $V_i$, one computes $g_i = e^{V_i^\top e(V_i - V_i^\top)}$. Then, using a measure of discrepancy, given by a function $f_g(g)$ that measures a kind of distance between $g$ and $g_i$, we try to adapt our initial guess $V_i$. More precisely, the problem can be seen as the following optimization problem on the Lie algebra $\mathfrak{gl}_n$:

$$V^* = \arg\min_{V \in \mathfrak{gl}_n} G(V), \quad G(V) = f_g(e^{V^\top e(V - V^\top)}).$$

(6.6)

Since this problem is defined on the vector space $\mathfrak{gl}_n$, implementing a gradient method or a more elaborate optimization scheme is not an issue once one can compute the differential of $G$. This will be the subject of the next section. A more important problem is to choose a function $f_g$. This function should be sufficiently smooth, easy to differentiate and must at least have an isolated global minimizer at $g$. Actually, it would be nice to tune $f_g$ such that $G$ is a smooth well conditioned convex function but this is not an easy task and even not always possible since in some cases, $V$ is not unique.

If the function $G$ in (6.6) has many local minimizers, a simple optimization scheme, like the gradient method, will only find one of them. Moreover, the $V$ corresponding to a local minimizer is not necessarily the $V$ of smaller norm, i.e. the $V$ that corresponds to the shortest geodesic between $g_0$ and $g_1$. But when it is the case, the norm of $V$ is the Riemannian distance between $g_0$ and $g_1$.

Here are different choices of functions $f_g(p)$ which are listed next along with their gradient $\Delta$ with respect to the Riemannian metric (6.1).

- Using the embedding of $GL^+(n)$ in $\mathbb{R}^{n \times n}$, we can use the squared (to be differentiable everywhere) of the Euclidean distance:

$$f_g(p) = \frac{1}{2} \| g - p \|^2,$$

(6.7)

whose differential is given by $Df_g(p)[Z] = \tr((p - g)^\top Z)$ where $Z$ is a tangent vector at $p$. Its gradient $\Delta$ with respect to the metric (6.1) is...
given by
\[ \Delta = pp^\top (p - g). \]

- Another possibility is given by the squared norm of the logarithm:
\[ f_g(p) = \frac{1}{2} \| \log(g^{-1}p) \|_F^2. \quad (6.8) \]

This function, as opposed to the previous one, has the nice property to be left invariant. Indeed, if we replace \( g \) by \( qg \) and \( p \) by \( qp \), for some \( q \in GL^+(n) \), the value of the function does not change. This property respects probably more the geometry of the problem. Its differential is given by
\[ Df_g(p)[Z] = \text{tr}(\log(g^{-1}p)^\top D\log(g^{-1}p)(p)[Z]), \]

where the differential of the logarithm is given by the following integral:
\[ D\log(g^{-1}p)(p)[Z]) = \int_0^1 (\alpha((g^{-1}p) - I)) + I)^{-1} g^{-1} Z(\alpha((g^{-1}p) - I)) + I)^{-1} d\alpha, \quad (6.9) \]

which can be computed numerically using the approach proposed in [25] and implemented in [24]. Notice that when \( g \) is close to \( p \), in the sense that \( g^{-1}p \) is close to the identity, the differential of the logarithm is close to the identity map and thus \( Df_g(p)[Z] \cong \text{tr}(\log(g^{-1}p)^\top g^{-1} Z) = \text{tr}((g^{-T} \log(g^{-1}p))^\top Z). \) So the gradient will be close to
\[ \Delta \cong pp^\top g^{-T} \log(g^{-1}p). \quad (6.10) \]

Using (6.9), it is easy to compute the adjoint of the differential of the logarithm with respect to the inner product (6.2):
\[ \langle D\log(X)[Z], W \rangle = \langle Z, (D\log(X)[W^\top])^\top \rangle. \]

The differential is then given by:
\[ Df_g(p)[Z] = \langle \log(g^{-1}p), D\log(g^{-1}p)(p)[Z] \rangle, \]
\[ = \langle (D\log(g^{-1}p)(p)[\log(g^{-1}p)^\top])^\top, Z \rangle, \]

and thus, the actual gradient of (6.8) is given by:
\[ \Delta = pp^\top D\log(g^{-1}p)(p)[\log(g^{-1}p)^\top]^\top. \]

So to compute the differential, one needs to compute the logarithm of a matrix and its differential, which is computationally more demanding than a simple difference \( g - p \), which was required to compute the differential of the previous function. Another potential issue with this cost function is the non-existence of the real matrix logarithm, see Appendix D for more details.
Let $G$ be the gradient of $f$ with respect to the metric $G$. In order to minimize the function $G$ in (6.6) related to one of the functions $f_g$ presented above, we will now compute its gradient with respect to the metric (6.1). Let us first compute the differential of the map: $Df_g(p)[Z] \triangleq \frac{d}{ds} \left( \| I - g^{-1}(p + sZ) \|^2_F \right)_{s=0},$

$$= \frac{d}{ds} \left( \| I - (p^\top + sZ^\top)g - (I - g^{-1}(p + sZ)) \|_F \right)_{s=0},$$

$$= \frac{d}{ds} \left( \| I - (p^\top + sZ^\top)g - (I - g^{-1}(p + sZ)) \|_F \right)_{s=0},$$

and thus the gradient is given by

$$\Delta = pp^\top(g^{-1}p - g^{-\top}) = pp^\top(g^{-1}p - I).$$

Notice that this expression is close to (6.10), when $g^{-1}p \cong I$ since, in that case, $\log(g^{-1}p) \cong (g^{-1}p - I)$. In order to minimize the function $G$ in (6.6) related to one of the functions $f_g$ presented above, we will now compute its gradient with respect to the metric (6.1). Let us first compute the differential of the map:

$$G : TGL^+(n) \cong GL^+(n), \quad V \mapsto f_g(e^{V}e^{-V^\top}).$$

Let $G = f_g \circ F$ with $F(V) = e^{V^\top}e^{-V^\top}$, and thus by the chain rule:

$$DG(V)[Z] = (Df_g(F(V)) \circ DF(V))[Z].$$

Let also $\Delta$ be the gradient of $f_g$ with respect to $g(F(V))$, i.e.

$$Df_g(F(V))[Z] = g_{F(V)}(\Delta, Z).$$

One obtains

$$DG(V)[Z] \triangleq \frac{d}{ds} G(V + sZ)_{s=0},$$

$$= Df_g(F(V)) \circ DF(V)[Z],$$

$$= g_{F(V)}(\Delta, DF(V)[Z]),$$

$$= g_I(F(V)^{-1}\Delta, F(V)^{-1}DF(V)[Z]) \quad (p \mapsto F(V)^{-1}p \text{ is an isometry}),$$

$$= g_I((F(V)^{-1}DF(V))^*F(V)^{-1}\Delta, Z),$$
where the $*$ stands for the adjoint with respect to the metric $g_I$. It is computed in the next section. Then, the gradient of $G$ with respect to the Riemannian metric $g_I$ (6.1) is given by

$$\text{grad} G(V) = (F(V)^{-1}DF(V))^*F(V)^{-1}\Delta.$$ 

### 6.3 Computation of the differential of $F$

The derivative of the Lie group exponential map is given by [62]:

$$\frac{d}{ds} e^{X(s)} = \int_0^1 e^{\alpha X(s)} \dot{X}(s) e^{(1-\alpha)X(s)} d\alpha,$$

$$= \int_0^1 e^{\alpha X(s)} \dot{X}(s) e^{-\alpha X(s)} d\alpha e^{X(s)},$$

$$= \int_0^1 e^{(1-u)X(s)} \dot{X}(s) e^{uX(s)} du. \quad (6.12)$$

where the last equality is obtained using the change of variable $\alpha = 1 - u$.

Using this, it is easy to compute the differential of the function

$$F : T_I GL^+(n) \rightarrow GL^+(n), V \mapsto F(V) = e^V e^{V^T}.$$ 

Indeed, we have:

$$DF(V)[Z] \triangleq \frac{d}{ds} F(V + sZ)|_{s=0}$$

$$= \frac{d}{ds} e^{(V+sz)}|_{s=0} e^{(V^T)} + e^V \frac{d}{ds} e^{(V^T + s(Z-Z^T))}|_{s=0},$$

and using (6.12), one obtains:

$$\int_0^1 e^{\alpha V^T} Z^T e^{-\alpha V^T} d\alpha e^{V^T} e^{V^T}$$

$$+ e^V \int_0^1 e^{\alpha(V^T-Z^T)} (Z - Z^T) e^{-\alpha(V^T)} d\alpha e^{V^T} \in T_{F(V)} GL(n).$$

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Thus
\[ F(V)^{-1} DF(V)[Z] = e^{V^T - V} e^{-V^T} DF(V)[Z] \]
\[ = e^{V^T - V} e^{-V^T} \int_0^1 e^{\alpha V^T} Z^T e^{-\alpha V^T} d\alpha e^{V^T} e^{-V^T} \]
\[ + e^{V^T - V} \int_0^1 e^{\alpha(V^T - V)} (Z - Z^T) e^{\alpha(V^T - V)} d\alpha e^{V^T} e^{-V^T} \]
\[ = T_A(Z) + T_B(Z) = T(Z). \]

Let us now determine the adjoint operator with respect to the inner product \( g \), i.e.
\[ g(T(Z), W) = g(Z, T^*(W)). \]

Since by linearity of the transposition and of the trace, we have
\[ \left( \int_0^1 A(t) dt \right)^T = \int_0^1 A^T(t) dt \quad \text{tr} \left( \int_0^1 A(t) dt \right) = \int_0^1 \text{tr} A(t) dt, \]
and using \( \text{tr}(A) = \text{tr}(A^T) \) and \( \text{tr}(AB) = \text{tr}(BA) \), one obtains
\[ g_I(T_A(Z), W) = \text{tr}(T_A(Z)^T W) \]
\[ = \int_0^1 \text{tr}(F(V)^T e^{-\alpha V} Z e^{\alpha V^T} F(V)^{-1} W) d\alpha \]
\[ = g_I \left( \int_0^1 e^{-\alpha V^T} F(V)^T F(V)^{-1} e^{\alpha V^T} d\alpha, Z \right), \quad (6.14) \]

and
\[ g_I(T_B(Z), W) = \text{tr}(T_B(Z)^T W) \]
\[ = \int_0^1 \text{tr}(e^{V^T - V} e^{-\alpha(V^T - V)} (Z - Z^T) e^{\alpha(V^T - V)} e^{V^T - V} W) d\alpha \]
\[ = g_I \left( \int_0^1 e^{-\alpha(V^T - V)} e^{V^T - V} (W - W^T) e^{\alpha(V^T - V)} d\alpha, Z \right). \quad (6.15) \]

The differential of the matrix exponential at \( A \) in the direction \( E \) is given by
\[ L(A, E) = e^A \int_0^1 e^{-\alpha A} E e^{\alpha A} d\alpha. \]
Using the numerical method presented in [25] and implemented in [24], it is possible to approximate the differential of the matrix exponential. From this, it is easy to compute the integral in (6.14) and (6.15), and so the adjoint $T^*$ of $T$, and thus the gradient of $G$.

A simple gradient scheme to compute the Riemannian log-mapping $\exp^{-1}(q_2)$ on $GL^+(n)$ is then the following:

1. compute $g = q_1^{-1}q_2$;
2. find an initial guess $V \in \mathfrak{gl}_n$ using, for instance, the Lie group log-mapping given by the matrix logarithm $\log(g)$ (when it exists, see Appendix D);
3. compute $p = e^{V^T} e^{(V - V^T)}$;
4. compute the gradient $\Delta$ at $p$ of one of the cost functions $f_g(p)$ and compute the gradient $\Delta V$ of $G$;
5. find a step size $\alpha > 0$ that ensures the decrease of the cost function $f_g(e^{V^T} e^{(V - V^T)})$ (backtracking for instance) and set $V = V - \alpha \Delta V$;
6. if $\|\Delta V\| \geq \epsilon$ goto step 3.; otherwise return $V$.

Note that other optimization schemes are also possible, like quasi Newton schemes.

6.4 The symplectic group

In this section, the geometry of a nice subgroup of the general linear group, the symplectic group $SP(2n)$ is described. The interest in averaging problems on the symplectic group, and a review of its geometry are provided in [17].

The real symplectic group is

$$SP(2n) = \{ P \in \mathbb{R}^{2n \times 2n} \mid P^T Q P = Q \},$$

(6.16)

where

$$Q = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \in \mathbb{R}^{2n \times 2n},$$

whose determinant is 1.

To show that $SP(2n)$ is a subgroup of $GL^+(2n)$, it is necessary and sufficient to show that it is a non-empty subset of $GL^+(2n)$, and that it is closed under the group operation and inversion, i.e. $\forall P_1, P_2 \in SP(2n), \ P_1 P_2 \in SP(2n)$ and $P_1^{-1} \in SP(2n)$. This is easy to show using the definition (6.16). To prove that $SP(2n)$ is a Lie subgroup, it remains to show that $SP(2n)$ is a submanifold of $GL^+(2n)$. To do this, we can use the definition (6.16). Indeed, $SP(2n) = F^{-1}(0)$ where $F : GL^+(2n) \subset \mathbb{R}^{2n \times 2n} \rightarrow \mathbb{R}^{2n \times 2n}, \ P \mapsto P^T Q P - Q$ is a smooth map, and its differential is

$$DF(P)[Z] = P^T Q Z + Z^T Q P.$$
Since $P \in SP(2n)$ implies $P$ is invertible, we have
\[ \ker DF(P)[Z] = \{YP \mid Y \in \mathfrak{sp}_{2n}\}, \]
where $\mathfrak{sp}_{2n}$ is the set of Hamiltonian matrices:
\[ \mathfrak{sp}_{2n} = \{X|X^TQ + QX = 0\}. \] (6.17)

If $X = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$, this is equivalent to $C = C^T$, $B = B^T$ and $A + D^T = 0$. So the dimension of the vector space of Hamiltonian matrices is $2(\frac{n^2+n}{2}) + n^2 = 2n^2 + n$.

Using Theorem 1, $SP(2n)$ is thus a submanifold of $GL^+(2n)$ of dimensions $2n^2 + n$.

Another way to show that $SP(2n)$ is a Lie subgroup is to remark that the Hamiltonian matrices form a sub-vector space of $\mathbb{R}^{2n \times 2n}$ but also a Lie sub-algebra of $\mathfrak{gl}_{2n}$ since we have:
\[ [\mathfrak{sp}_{2n}, \mathfrak{sp}_{2n}] \subset \mathfrak{sp}_{2n}. \]

Indeed, let $V_1, V_2 \in \mathfrak{sp}_{2n}$, i.e.
\[ V_1^TQ + QV_1 = 0, \quad V_2^TQ + QV_2 = 0, \]
we have:
\[ [V_1, V_2]^TQ + Q[V_1, V_2] = V_2^TV_1^TQ - V_1^TV_2^TQ + QV_1V_2 - QV_2V_1 = 0, \]
thus $[V_1, V_2] \subset \mathfrak{sp}_{2n}$. Using the Theorem 2 in [9], there exists one and only one Lie subgroup of $GL^+(2n)$ corresponding to $\mathfrak{sp}_{2n}$. This subgroup is $SP(2n)$. Notice that we have also $\text{tr}(V) = 0$, and thus $\mathfrak{sp}_{2n}$ is actually a Lie sub-algebra of $\mathfrak{sl}_n$, the Lie algebra of the special linear group. Consequently, $SP(2n)$ can be also regarded as a Lie subgroup of the special linear group. Observe that for $n = 1$, the symplectic matrices are the matrices of determinant 1, so $SP(2) = SL(2)$.

One can equip $SP(2n)$ with a left invariant Riemannian metric using the inner product (6.2) restricted to $\mathfrak{sp}_{2n}$. The derivation of the Riemannian connection and the formula for the geodesics in Section 6.1.1 are exactly the same, and the geodesics starting at the identity are of the form:
\[ g(t) = e^{tV^T}e^{t(V-V^T)}, \]
with $V \in \mathfrak{sp}_{2n}$. Notice that $g(t)$ is symplectic since it is the product of two symplectic matrices. Indeed, $V \in \mathfrak{sp}_{2n}$ implies that $V^T \in \mathfrak{sp}_{2n}$, and thus $V - V^T \in \mathfrak{sp}_{2n}$. To show this, just multiply the equation in (6.17) by $Q$ on the left and on the right to obtain the equivalent condition $XQ + QX^T = 0$. This condition is also equivalent to (6.17), when $X$ is replaced by $X^T$, so $X^T \in \mathfrak{sp}_{2n}$. Furthermore $V - V^T \in \mathfrak{sp}_{2n}$ since $\mathfrak{sp}_{2n}$ is a vector space.
6.5 Application to Karcher mean computation

The Riemannian log-mapping enables us to implement a gradient method to compute a Karcher mean on $GL(n)$ if the data points all belong to $GL^+(n)$ or $GL^-(n)$. Since the Riemannian distance function is left invariant, this mean is also left invariant. In [17], the authors proposed an extrinsic mean of symplectic matrices. Their approach is first described and compared to the Karcher mean. Then, some numerical experiments are carried out to illustrate our approach.

The following extrinsic mean is proposed in [17],

$$
\mu_e(q_1, \cdots, q_N) = \arg\min_{p \in SP(2n)} \frac{1}{2N} \sum_{i=1}^{N} \|p - q_i\|_F^2,
$$

$$
= \arg\min_{p \in SP(2n)} \frac{1}{2} \left\| p - \frac{1}{N} \sum_{i=1}^{N} q_i \right\|_F^2.
$$

(6.18)

It is an extrinsic mean since it consists in computing the mean of the data points $q_i$ in $\mathbb{R}^{n \times n}$, and then projecting the result on the symplectic manifold (seen as a submanifold of $\mathbb{R}^{n \times n}$). By projection, here one means: finding the closest point of $C$ in $SP(2n)$ with respect to the Euclidean metric, i.e. the Frobenius metric. This approach is attractive, mainly for its simplicity and potentially low computational cost. But $\mu_e$ is not invariant with respect to the group action on the left, i.e.

$$
\mu_e(pq_1, \cdots, pq_N) \neq p\mu_e(q_1, \cdots, q_N).
$$

To circumvent this, but still keeping the same approach, one could use another projection. A simple idea could be, for instance, to replace $\|p - C\|_F^2$ by $\|I - p^{-1}C\|_F^2$.

On the general linear group, this approach is difficult to extend since $GL^+(n)$ is dense in $\mathbb{R}^{n \times n}$. Indeed, with the Frobenius norm, the projection will be $p = C$ if $C \in GL^+(n)$, and if $C \notin GL^+(n)$, there are many $p$’s in $GL^+(n)$ that can approximate $C$ with a desired accuracy. The same problem appears with $\|I - p^{-1}C\|_F^2$. However, if we generate some random matrices, the probability that one of them does not belong to $GL^+(n)$ is zero; since if $p \notin GL(n)$, the entries of $p$ satisfy the polynomial equation $\det(p) = 0$, whose solution set is of measure zero. Notice that the same holds for $C$, since $\det(C) = 0$ is also a polynomial in the the entries of the matrices $q_i$’s. So $C$, will be invertible almost all the time. But $C$ could be not invertible even if the $q_i$’s belong to $GL(n)$, and are well conditioned as in the following example.

Example 8. Let

$$
q_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad q_2 = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix},
$$

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then $C = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$, which does not belong to $GL(n)$.

Consequently, this extrinsic mean, based on the embedding of $GL(n)$ in $\mathbb{R}^{n \times n}$ is probably not the best strategy. Even though, it could be that it makes sense in some applications.

Let us now look at some Karcher means of the data in Example 8. Since $q_2 \in SO(2)$ corresponds to a rotation of $\pi + k\pi \ k \in \mathbb{Z}$, a Karcher mean, which is the mid-point of the geodesic linking $q_1$ to $q_2$ is given by $\mu_1 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$.

It corresponds to a rotation of $\pi/2$ and is not unique since $\mu_2 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$, a rotation of $-\pi/2$, will be also a Karcher mean. There is thus two Karcher means in $SO(2)$.

Observe that $SO(n)$ is a totally geodesic submanifold of $GL^+(n)$ since any geodesic in $SO(n)$ is also a geodesic in $GL^+(n)$. But all the geodesics in $GL^+(n)$ that start and end in $SO(n)$ are not fully contained in $SO(n)$, see Appendix B. However, for $n = 2$, the geodesics that start and end in $SO(2)$ without being fully contained in $SO(2)$ are of length at least $\pi$, see Appendix B. This ensures that $\mu_1$ and $\mu_2$ are also Karcher means in $GL^+(2)$ since

$$\|\exp_{\mu_1}^{-1}(q_1)\|_{SO(2)} = \|\exp_{\mu_2}^{-1}(q_2)\|_{SO(2)}$$

$$= \|\exp_{\mu_1}^{-1}(q_1)\|_{SO(2)} = \|\exp_{\mu_2}^{-1}(q_2)\|_{SO(2)} = \frac{\pi}{2} \leq \pi.$$

It is unknown if there exist other Karcher means in $GL^+(2)$.

Observe also that, due to the metric in (6.1), non invertible matrices are at an infinite distance of any matrix in $GL^+(n)$. For instance, the geodesic starting at the identity at $t = 0$ given by

$$V = e^{t \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix}}$$

is going to the matrix $C$ in the example when $t$ is going to the infinity. This geodesic is thus of infinite length and the zero matrix is thus at an infinite distance of the identity. Thus, the Riemannian distance is probably more suitable to compare invertible matrices than the Frobenius distance.

To illustrate our approach, we generated a set of 10 matrices of size 2-by-2 at a distance $r = 1$ of the identity. A unit step size gradient method was then used to find a Karcher mean. The result is presented on Fig. 6.1. Note that, when $r$ is small, the Lie group log-mapping is ensured to exist, and it is chosen as an initial guess.

The main issue with our method to compute the Riemannian log-mapping is that it cannot guarantee that the returned $V$ is the one of minimal norm if $V$ is not unique. Thus $V$ is not necessarily the opposite of the gradient of
the squared Riemannian distance function. Consequently, we cannot guarantee that the point returned by our algorithm is a Karcher mean. Finding conditions under which it is possible to guarantee the uniqueness of $V$ or under which $V$ is of minimal norm are open problems in $GL^+(n)$ and in $SP(2n)$. This could be done by estimating the injectivity radius of $GL^+(n)$.

![Figure 6.1](image)

Figure 6.1: (left) Riemannian distance between the initial point, here the first data point, and the other data points. (middle) Norm of the gradient (3.5) at each iteration. (right) Riemannian distance between the Karcher mean and the data points.

Our method to approximate the Karcher mean on $GL^+(n)$ can be used to compute Karcher means on $SP(2n)$, endowed with the induced Riemannian metric from $GL^+(2n)$, see Section 6.4. Observe that for $n = 2$, $SO(2) \subset SP(2) = \{P \mid \det(P) = 1\}$ but this is no longer true for $n > 2$. The two matrices in the Example 8 are thus symplectic. These two matrices have two Karcher means in $SO(2)$ (rotation of $+\pi/2$ or $-\pi/2$), and these two Karcher means are also Karcher means in $SP(2)$. Indeed, as in the case of $GL^+(n)$, there is no geodesic in $SP(2)$ that ends and starts in $SO(2)$ of length smaller than $\pi$ that is not fully contained in $SO(2)$, see Appendix B. Note that it could be that there exist other Karcher means.

One could also compute the extrinsic mean as in [17]. Since $C = 0$, computing the projection on $SP(2n)$ is equivalent to find $\mu_c \in SP(2n)$ such that
$\frac{1}{2}\|\mu_e\|_F^2$ is minimized. This problem admits all the points on the submanifold $SO(2)$ as non isolated global minimizers. To show this, let us apply a Schur decomposition $\mu_e = USU^\top$ where $S$ is of the form

$$S_1 = \begin{bmatrix} \lambda & \sigma \\ 0 & \frac{1}{\lambda} \end{bmatrix} \quad S_2 = \begin{bmatrix} \alpha & \beta_1 \\ \beta_2 & \alpha \end{bmatrix} \text{ with } \alpha^2 - \beta_1\beta_2 = 1. $$

In the first case, we have $\|\mu_e\|_F^2 = \|S_1\| = \lambda^2 + \frac{1}{\lambda^2} + \sigma^2$ which is minimum when $\sigma = 0$ and $\lambda = \pm 1$. In the second case, one obtains $\|S_2\| = 2\alpha^2 + \beta_1^2 + \beta_2^2$. By replacing $\alpha^2$ by $1 + \beta_1\beta_2$, $\|S_2\|$ becomes $2 + (\beta_1 + \beta_2)^2$ which is minimal when $\beta_1 = -\beta_2 = \beta$. This corresponds to

$$S_2 = \begin{bmatrix} \pm \sqrt{(1 - \beta^2)} & \beta \\ -\beta & \pm \sqrt{(1 - \beta^2)} \end{bmatrix},$$

with the existence condition $-1 \leq \beta \leq 1$, so $S_2 \in SO(2)$. It is proven in [64], that once $C \in SP(2n)$, the extrinsic mean defined by (6.18) is unique. But, nothing can ensure that $C$ is in $SP(2n)$ as the Example 8 suggests. A set of 10-by-10 symplectic matrices located at a distance 1 of the identity was generated. A Karcher mean was then computed using a unit step size gradient method. The result is presented on Fig.6.2.
Figure 6.2: (left) Riemannian distance between the initial point, here the first data point, and the other data points. (middle) Norm of the gradient (3.5) at each iteration. (right) Riemannian distance between the Karcher mean and the data points.
Conclusion and perspectives

In this thesis, some algorithms to compute the Riemannian distance, the Karcher mean(s) and to solve geodesic fitting problems on some common Riemannian homogeneous spaces have been proposed and studied. This thesis is at the border between Riemannian geometry, optimization and signal processing. In fact, most of the related applications come from the signal processing community. We can think of subspace tracking, shape analysis, diffusion tensor imaging, to just cite a few. The algorithms are always presented as optimization algorithms derived from the variational description of our problems. And, of course, to understand the structure of these problems, differential geometry, and more precisely Riemannian geometry plays a key role. We will briefly review our main contributions and give some perspectives and put the emphasis on some interesting open questions.

In the first chapter, some concepts of Riemannian geometry were first presented. Since our end goal was to design algorithms, explicit formulas to compute the basic objects used in Riemannian geometry like the geodesics, the parallel transports and the sectional curvature were in need. In general, on a Riemannian manifold, this is almost impossible to obtain. In particular, the geodesic equation in a coordinate system is a second order non-linear differential equation that is extremely difficult to solve. So, one has to be more modest and add some extra structures. That is why, a brief introduction to Lie group theory, homogeneous spaces and symmetric spaces was provided. From the point of view of the author, these are the spaces for which algorithms can be designed. In particular, all the Lie subgroups and homogeneous spaces related to the general linear group $GL(n)$ possess a natural matrix representation that is commonly used in numerical programming language. Fortunately, almost all manifolds appearing in practical applications have such kind of structure.

In Chapter 3, we compared gradient and Newton methods to compute the Karcher mean on the cone of symmetric positive definite matrices equipped with the so-called affine invariant Riemannian metric. Since this is a Hadamard manifold, the Karcher mean is unique and the problem is geodesically convex. A convergence proof for a gradient method with an adaptive step size selection rule was provided. And, it was shown that a Newton method can be faster than a gradient method. A similar result has been also obtained for $SO(3)$. Our Newton algorithm and our analysis was mainly based on explicit expres-
tions for the eigenpairs of the Jacobi operator on $\mathbb{P}^n_+$. Observe that, with the material presented in Chapter 4, it is possible to implement Newton methods on other symmetric spaces like $SO(n)$ or the Grassmann manifold. Even if, the advantage of a Newton method in the positive curvature case is probably more limited.

In Chapter 4, we studied the generalization of linear regression of time labeled data points to Riemannian manifolds. We investigated the problem on some Riemannian symmetric spaces where the Jacobi fields can be computed explicitly. In particular, we derived explicit expressions for the eigenvalues and eigenvectors of the Jacobi operator on the sphere, the special orthogonal group, the set of symmetric positive definite matrices and the Grassmann manifold. Based on this, a simple gradient method on the tangent bundle is proposed. The study of a second order method for geodesic data fitting, and the uniqueness of the solution of (4.1) in function of the data distribution is still an open problem and could be considered as a nice perspective of future research.

In Chapter 5, we proposed a simple gradient method to compute the endpoint geodesic problem, or the Riemannian log-mapping, on the Stiefel manifold equipped with the induced Riemannian metric of the special orthogonal group $SO(n)$. In this case, the Stiefel manifold is a normal homogeneous space, and the geodesics in $St(n,p)$ are "projected versions" of some geodesics in $SO(n)$. The uniqueness of the Riemannian logarithm was also discussed, and, in particular, the injectivity radius of the Stiefel manifold was estimated. As an application, the computation of the Karcher mean was considered as well as a related application to coset fitting. Furthermore, the log-mapping is also useful in shape space analysis or in filtering problems, see [57]. Characterizing the nature of the intersection of a coset with the cut locus of the identity is a nice, but probably very hard, open problem. The computation of the Jacobi fields on the Stiefel manifold is also an open problem that could be of interest.

In Chapter 6, a shooting technique was proposed to compute the Riemannian log-mapping on the general linear group equipped with a left invariant Riemannian metric. Once again, our algorithm was applied to compute the Karcher mean on the general linear group. The symplectic group, which is one of its Lie subgroup is also considered. The sectional curvature is unknown to the present author and estimating it, even in simple cases, could be a nice subject of research. Another interesting question would be to study the effect of the curvature on the uniqueness of the Karcher mean on $GL(n)$. 

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Appendix A

Hessian of the squared Riemannian distance function on $SO(n)$

Let $SO(n)$ be endowed with the metric

$$g(A, B) = \frac{1}{2} \text{tr}(A^\top B), \quad (A.1)$$

where $A$ and $B$ belong to the Lie algebra of $SO(n)$, which is the set of skew-symmetric matrices. Let $k = \frac{n}{2}$ if $n$ is even and $k = \frac{n-1}{2}$ when $n$ is odd, and let us consider the Schur decomposition of $A = USU^\top$ with

$$S = \begin{bmatrix} 0 & -\alpha_1 \\ \alpha_1 & 0 \\ & \ddots \\ & & 0 & -\alpha_p \\ & & \alpha_p & 0 \end{bmatrix},$$

which consists of $k$ $2 \times 2$-blocks on its diagonal. For odd dimensions, a 0 must be also added on the diagonal of $S$. One can then write

$$g(A, A) = \frac{1}{2} \text{tr}(A^\top A) = \alpha_1^2 + \alpha_2^2 + \cdots + \alpha_p^2.$$

Let $p$ and $q$ be two points on $SO(n)$, and let $A = \exp_{p^{-1}}^1(q) = p \log (p^\top q)$. Observe that the $\alpha_i$’s represent the angles of rotation in the 2-dimensional planes of rotation, and thus $0 \leq \alpha_i \leq \pi$. Actually, we have $-\pi \leq \alpha_i \leq \pi$, but a rotation of negative angle can be represented by multiplying one of the two corresponding columns in the $U$ matrix by $-1$. Consequently,

$$d(p, q) \leq \sqrt{g(A, A)} = \sqrt{k/2\pi}.$$
and the injectivity radius of $SO(n)$ is $\pi$ and its diameter is $k\pi$.

Since $SO(n)$ is a Lie group, when it is equipped with the bi-invariant metric (A.1), its curvature tensor at the identity is given by [31]:

$$R_I(X,Y)Z = \frac{1}{4} [Z, [X,Y]].$$

The eigenvalues $\lambda$ and corresponding eigenvectors $E$ of the Jacobi operator $X \mapsto R(X,A)$ are then given by the following expressions. Let $E = (X)_{ij}$ be a $2k \times 2k$ skew-symmetric matrix with a $2 \times 2$ block $X$ in position $(2i-1 : 2i, 2j-1 : 2j)$, and when $i \neq j$ the block $-X^\top$ in position $(2j-1 : 2j, 2i-1 : 2i)$.

When $n$ is even, we have:

- $\lambda = 0$, $E = (B_1)_{ii}$ for $1 \leq i \leq k$;
- $\lambda = \frac{1}{4}(\alpha_i - \alpha_j)^2$, $E = (B_2)_{ij}$, and $E = (B_3)_{ij}$ for $1 \leq j < i \leq k$;
- $\lambda = \frac{1}{4}(\alpha_i + \alpha_j)^2$, $E = (B_3)_{ij}$, and $E = (B_4)_{ij}$ for $1 \leq j < i \leq k$;

where

$$B_1 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad B_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad B_3 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix},$$
$$B_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad B_4 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Notice that there are $k$ eigenpairs of the first kind, $k^2 - k$ of the second kind, and $\frac{k^2}{2} - k$ of the third kind. This makes a total of $2k^2 - k = \frac{n^2 - n}{2}$ eigenpairs, which is equivalent to the dimension of $SO(n)$. So, fortunately, no eigenpairs has been lost in the battle !!! When $n$ is odd, we have the same eigenpairs as in $SO(n-1)$ plus the following ones:

$$\lambda = \frac{\alpha_i^2}{4}, \quad E = e_n e_i^\top - e_i e_n^\top$$
and for $1 \leq i \leq k = \frac{n-1}{2}$.

The eigenvalues of the Hessian of the squared Riemannian distance function $q \mapsto \frac{1}{2}d(I,q)^2$ at the identity are given by $\sqrt{\lambda} \cot \sqrt{\lambda}$, see (3.3). This function is upper bounded by 1, and strictly decreasing and positive if $\sqrt{\lambda} < \pi/2$. This last condition implies that

$$|\alpha_i - \alpha_j| < \pi \quad \text{and} \quad |\alpha_i + \alpha_j| < \pi \quad \forall i, j.$$

An illustration is provided on Figure A.1.
A sufficient condition for this to hold is

\[ D(p, q) = \|A\| < d_c = \frac{\sqrt{2}}{2} \pi, \quad (A.2) \]

where \( \|\cdot\| \) stands for the norm related to the metric (A.1). Notice that this condition is quite restrictive when \( n \) is large since the diameter increases with \( n \).

So, when \( d(p, q) \leq \frac{\sqrt{2}}{2} \pi \), the squared Riemannian distance function is positive definite at \( p \). This radius should not be confused with the so called convexity radius defined by

\[ r_c = \frac{1}{2} \min\left\{ \frac{\pi}{\sqrt{\Delta}}, \text{inj}(\mathcal{M}) \right\}, \]

which is the maximal radius that ensures that \( B(p, r_c) \) is a strongly convex ball.
Appendix B

Geodesics in $GL^+(2)$ that start and end in $SO(2)$

In this section, we look at the geodesics $t \mapsto \gamma(t)$ in $GL^+(2)$ that end and start in $SO(2)$. We can assume, w.l.o.g., that $\gamma(0) = I$, and $\gamma(1) \in SO(2)$. Using the explicit expressions for the geodesic curves derived in Section 6.1.3, it is possible to find all the $V$’s that satisfy:

$$g = e^{V^T} e^{V} \text{ with } g^T g = I_2.$$  

Indeed, in case 1 (see Section 6.1.3), $V = \begin{bmatrix} \lambda_1 & \sigma \\ 0 & \lambda_2 \end{bmatrix}$, and the condition $g^T g = I$ implies:

$$e^{2\lambda_1} + \sigma^2 \left( \frac{e^{\lambda_1} - e^{\lambda_2}}{\lambda_1 - \lambda_2} \right)^2 = 1,$$

$$e^{2\lambda_2} = 1.$$  

The last equation implies $\lambda_2 = 0$, the second equation implies $\sigma = 0$ and so, using the first equation, $\lambda_1 = 0$. Thus the only solution is $V = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$.

In case 2, $V = \begin{bmatrix} \alpha & \beta_1 \\ \beta_2 & \alpha \end{bmatrix}$ and

$$g = U e^{\alpha} \begin{bmatrix} \cos(t\sqrt{d}) & -\sin(t\sqrt{d}) \frac{\sqrt{d}}{\beta_1} \\ -\sin(t\sqrt{d}) \frac{\sqrt{d}}{\beta_2} & \cos(t\sqrt{d}) \end{bmatrix} \begin{bmatrix} \cos(t(\beta_1 - \beta_2)) & \sin(t(\beta_1 - \beta_2)) \\ -\sin(t(\beta_1 - \beta_2)) & \cos(t(\beta_1 - \beta_2)) \end{bmatrix} U^T,$$  

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where \( d = \sqrt{|\beta_1 \beta_2|} \). The condition \( g^\top g = I_2 \) implies
\[
e^{2\alpha} \left( \cos(\sqrt{d})^2 + \sin(\sqrt{d})^2 \frac{d}{\beta_1^2} \right) = 1, \\
- e^{2\alpha} \cos(\sqrt{d}) \sin(\sqrt{d}) \sqrt{d} \left( \frac{1}{\beta_2} + \frac{1}{\beta_1} \right) = 0, \\
e^{2\alpha} \left( \sin(\sqrt{d})^2 \frac{d}{\beta_2^2} + \cos(\sqrt{d})^2 \right) = 1.
\]

Let us look at the second equation, either

- \( \sqrt{d} = 0 \), which implies \( \beta_1 = \beta_2 = 0 \) since \( \beta_1 \) and \( \beta_2 \) must be of opposite sign. In this case, the first equation implies \( \alpha = 0 \) and so \( V = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \).

- \( \beta_2 = -\beta_1 = \beta \), in this case the first equation implies that \( \alpha_0 \) and thus \( V = \begin{bmatrix} 0 & -\beta \\ \beta & 0 \end{bmatrix} \) is skew-symmetric. The geodesics corresponding to skew-symmetric \( V \)'s are fully contained in \( SO(2) \).

- \( \cos(\sqrt{d}) = 0 \) this implies that \( \sqrt{d} = \frac{\pi}{2} + k\pi > 0 \) \((k = 0, 1, 2, ...)\) and \( \sin(\sqrt{d}) = \pm 1 \). The first and last equations then imply that \( |\beta_1| = |\beta_2| \) and \( \alpha = 0 \). Thus \( V = \begin{bmatrix} 0 & -\beta \\ \beta & 0 \end{bmatrix} \) is skew-symmetric.

- \( \sin(\sqrt{d}) = 0 \) which implies \( \cos(\sqrt{d}) = \pm 1 \) and \( \sqrt{d} = k\pi > 0 \) for \( k = 1, 2, ... \) \((k = 0 \text{ corresponds to } \beta_1 = \beta_2 = 0)\). The first equation implies that \( \alpha = 0 \) and the corresponding \( V \)'s are of the form
\[
V = \begin{bmatrix} 0 & -\frac{k\pi}{2} \\ \beta & 0 \end{bmatrix}.
\]

Observe that, some of the \( V \)'s are not skew-symmetric and their corresponding geodesics leave the orthogonal group \( SO(2) \). Let us look at the \( V \) of this kind that is of minimal norm. Let \( f(\beta) = \|V\|^2 = \beta^2 + \frac{\pi^2 \beta^2}{4} \), we have \( \frac{df}{d\beta} = 2\beta(1 - \frac{\pi^2}{4\beta^2}) \) and \( \frac{d^2 f}{d\beta^2} = \frac{6\pi^2 \beta^2}{\beta^4} + 2 > 0 \). Thus, the local minimizers of \( f \) are of the form \( \beta = k\pi \). Observe that \( V \) is skew-symmetric if \( \beta = k\pi \), and thus the corresponding geodesics are fully contained in \( SO(2) \). The global minimizer of \( f \) is \( \beta = \pi \) \((k = 1)\), and thus the shortest geodesic that links the identity to another element of \( SO(2) \) without staying in \( SO(2) \) is of length at least \( \|V\| = \sqrt{f(\beta)} = \sqrt{2}\pi \). Note that the standard metric \((A.1)\) in \( SO(n) \) can be seen as the induced metric from \( GL^+(n) \) defined by \((6.2)\) but divided by 2. So, the corresponding distance on \( SO(2) \) is \( \|V\|_{SO(2)} = \pi \).
Consequently, if \( p, q \in SO(2) \) and \( d_{SO(2)}(p, q) < \pi \) (where \( d_{SO(2)} \) is the Riemannian distance induced by (A.1)), then the minimizing geodesic in \( GL^+(2) \) between them is fully contained in \( SO(2) \).
Appendix C

More about Lax pairs

Let us consider the following differential equation:

\[ \dot{x}(t) = [p(t), x(t)] \text{ with } x(0) = x_0. \]

(C.1)

Its solution is of the form \( x(t) = U(t)x(0)U(t)^{-1} \), where \( t \mapsto U(t) \) is the solution of

\[
\dot{U}(t) = P(t)U(t), \quad U(0) = I.
\]

(C.2)

This means that the spectra of \( x \) is independent of \( t \). It is also called an isospectral flow. In our case, we have \( p(t) = x(t)^\top \). Thus (C.2) becomes

\[
\dot{U}(t) = U(t)^{-T}x(0)^\top U(t)^{-1}U(t),
\]

\[
U(0) = I,
\]

whose solution is given by:

\[
U(t) = e^{-t(x_0-x_0^\top)}e^{-tx_0},
\]

and so

\[
x(t) = e^{-t(x_0-x_0^\top)}e^{-tx_0}x_0^\top e^{tx_0}e^{t(x_0-x_0^\top)},
\]

\[
\quad = e^{-t(x_0-x_0^\top)}x_0e^{t(x_0-x_0^\top)},
\]

since \( e^{-tx_0}x_0 = x_0e^{-tx_0} \).
Appendix D

Properties of the Lie group exponential map

Let \( p \in GL(n) \), the exponential map is given by the matrix exponential

\[
\exp : \mathfrak{gl}_n(\mathbb{R}) \to GL(n, \mathbb{R}) \quad p \mapsto \exp(p).
\]

This map is not a global diffeomorphism. So, it is not always possible to define its inverse the Lie group log-mapping:

\[
\exp^{-1} : GL(n, \mathbb{R}) \to \mathfrak{gl}_n(\mathbb{R}).
\]

For instance, \( \log(-1) \) does not exist in \( \mathfrak{gl}_1(\mathbb{R}) \cong \mathbb{R} \). The following two theorems describe the surjectivity and bijectivity of the real Lie group exponential map.

**Theorem 30** (Surjectivity of the Lie group exponential map, see [12]). Let \( C \) be a real square matrix. Then there exists (at least) a real solution \( X \) of the equation \( e^X = C \) if and only if \( C \) is non-singular and each Jordan block of \( C \) belonging to a negative eigenvalue occurs an even number of times.

**Theorem 31** (Bijectivity of the Lie group exponential map, see [12]). Let \( C \) be a real square matrix. Then the equation \( e^X = C \) has a unique real solution \( X \) if and only if all the eigenvalues of \( C \) are positive real and no Jordan block of \( C \) belonging to any eigenvalue appears more than once.

In the complex case, i.e. when we consider

\[
\exp : \mathfrak{gl}_n(\mathbb{C}) \to GL(n, \mathbb{C}),
\]

the situation is actually simpler. This map is always surjective (any element of \( GL(n, \mathbb{C}) \), i.e. invertible matrices, can be reached by the Lie group exponential map) but not necessarily injective. For example, we have \( \log(-1) = i\pi + 2k\pi \) with \( k \in \mathbb{Z} \). So, the Lie group exponential map is not injective. To make it
injective in the complex plane ($n = 1$), we have at least to make a restriction to a strip of height $2\pi$.

The log function of Matlab, see [25], returns the principal logarithm, which is the unique logarithm for which every eigenvalue has an imaginary part lying strictly between $-\pi$ and $\pi$. This principal logarithm exists when $X$ has no eigenvalue with strictly negative real part.

Let us take the following example:

$$
\begin{bmatrix}
-1 & 0 \\
0 & -1
\end{bmatrix},
$$

it has a logarithm but it is not unique. Indeed, we have

$$
\exp\left(\begin{bmatrix}
0 & -\pi - 2k\pi \\
\pi + 2k\pi & 0
\end{bmatrix}\right) = \begin{bmatrix}
-1 & 0 \\
0 & -1
\end{bmatrix} \quad \forall k \in \mathbb{Z}.
$$

Notice that it also has a complex logarithm given by $\begin{bmatrix} \pi i & 0 \\ 0 & \pi i \end{bmatrix}$: This is the logarithm returned by the log function of Matlab.

To compute the Riemannian log-mapping, the Lie group log-mapping is used to compute the gradient and to initialize the method. The main issue with this strategy is that the Lie group exponential map is not surjective, i.e. there exist some $P \in GL^+(n, \mathbb{R})$ such that there is no curve of the form $\gamma(t) = e^{tV}$ for some $V \in \mathfrak{gl}_n(\mathbb{R})$ such that $\gamma(1) = P$. How to handle this issue is an open question. Theorem 30 gives a condition on $P$ such that it is possible. On the contrary, the Riemannian geodesic $\gamma(t) = e^{tV} e^{t(V - V^\top)}$ is defined on the whole $\mathfrak{gl}_n(\mathbb{R})$, and so, by virtue of the Hopf-Rinow Theorem 8, any two points of $GL(n)$ that belong to the same connected component can be joined by a geodesic. Here is an example.

**Example 9.** Let us consider

$$g = \begin{bmatrix}
-1 & 0 \\
0 & -2
\end{bmatrix}.
$$

This matrix does not admit a real logarithm. But it admits a Riemannian log-mapping given approximatively by

$$
\begin{bmatrix}
1.2707 & 3.6678 \\
-1.8339 & -0.5776
\end{bmatrix}.
$$

This is not a normal matrix. It has complex conjugate eigenvalues: $0.3466 + 2.4233i$ and $0.3466 - 2.4233i$.

Finally, in this work, we have only considered the case of real matrices, the complex case could be also interesting to study. But the author does not know any applications related to that case. In the complex case, the metric will be given by taking the real part of the trace in (6.1) and by replacing the transposition by a conjugation. Furthermore, the complex Lie group exponential map is surjective, i.e. the Lie group logarithm always exists.
Bibliography


List of Notations

\( \Gamma_{\gamma(0)\rightarrow\gamma(1)} \) Parallel transport along the curve \( t \mapsto \gamma(t) \) .................. 15
\( \exp_p \) Riemannian exponential map at \( p \in \mathcal{M} \) ......................... 15
\( \exp_p^{-1} \) Riemannian log-mapping at \( p \) .................................................. 15
\( \mathfrak{sp}_{2n} \) Lie algebra of \( SP(2n) \) .................................................. 114
\( \text{Grass}(n,p) \) The Grassmann manifold .................................. 31
\( \kappa(X,Y) \) Sectional curvature of the section spanned by \( X \) and \( Y \) ........... 17
\( \lambda(g,p) = g \cdot p \) Left action of \( g \) at \( p \in \mathcal{M} \) .................. 24
\( \mathcal{M} \) A manifold .......................................................... 7
\( \mathfrak{gl}(n) \) Lie algebra of the general linear group ....................... 22
\( \mathfrak{o}(n) \) Lie algebra of the orthogonal group .......................... 22
\( \mathfrak{sl}(n) \) Lie algebra of the special linear group ..................... 22
\( \nabla \) Affine connection .......................................................... 13
\( \mathcal{P}_n^+ \) The set of symmetric positive definite matrices ............. 31
\( \text{skew}(n) \) Set of \( n \times n \) skew-symmetric matrices ....................... 47
\( SP(2n) \) The real symplectic group ........................................ 113
\( \text{sym}(n) \) Set of \( n \times n \) symmetric matrices ............................. 48
\( \text{inj}(\mathcal{M}) \) Injectivity radius of \( \mathcal{M} \) ........................................ 16
\( \text{inj}(p) \) Injectivity radius of \( \mathcal{M} \) at \( p \) ........................... 16
\( C(p) \) Cut locus at \( p \) ......................................................... 16
\( D\phi \) or \( \phi^* \) The differential of the map \( \phi \) .......................... 8
\( d(p,q) \) Riemannian distance between \( p \) and \( q \) ................. 16
$D_t X$ Covariant derivative of $X$ along a curve $t \mapsto \gamma(t)$ .......................... 14
$e^V$ Matrix exponential ................................................................. 23
$G/H$ The set of left cosets $gH$ ...................................................... 26
$GL(n)$ The general linear group ...................................................... 20
$GL^+(n)$ The identity component of the general linear group .............. 20
$O(n)$ The orthogonal group ............................................................ 21
$R(X,Y)Z$ Curvature endomorphism .................................................. 14
$S^n$ The sphere embedded in $\mathbb{R}^{n+1}$ ........................................ 31
$s_p$ Symmetry at $p$ ........................................................................ 29
$SL(n)$ The special linear group .......................................................... 21
$SO(n)$ The special orthogonal group .................................................. 21
$St(n,p)$ The Stiefel manifold ............................................................. 32
$T\mathcal{M}$ Tangent bundle of $\mathcal{M}$ ............................................... 10
$T_p \mathcal{M}$ Tangent space at $p \in \mathcal{M}$ ............................................. 7
$X_p$ Tangent vector at $p \in \mathcal{M}$ ..................................................... 7