The Log-composition of Stationary Velocity Fields in Diffeomorphic Image Registration

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Abstract

Medical imaging employs techniques and tools belonging to several branches of mathematics and physics that, when applied to morphometric and statistical study of biological shape variability, are collected under the name of *computational anatomy*. One of its critical tool, image registration, is widely used in both academical studies and applications, and continuously challenges researchers to enhance accuracy, improve reliability and reduce the time of the computations. The use of diffeomorphisms in image registration and the concomitant introduction of the log-euclidean framework to compute statistics, provide an interesting options to model the organs' deformations and to quantify the variations of anatomies. One of the challenges of this setting is the numerical computation of the Lie exponential of stationary velocity fields (SVF), the Lie logarithm of the corresponding transformation and their combinations as they appear in the BCH formula: concept at the core of the underpinning theory of the *log-demons* algorithm.

The necessity of finding fast numerical computation techniques of the BCH formula gave birth to the concept of log-composition presented in this thesis, with some strategies for its computation.

Contents

Chapter 1

Introduction to Diffeomorphic Image Registration

> *The series is divergent, therefore we may be able*
> *to do something with it.*
> - Oliver Heaviside

1.1 Toward an ill-posed Problem

The process of determining correspondences between two or more images acquired from patients scans is a challenging task that has seen the application of a growing number of mathematical theories contributing to its solution.

The challenge and the concomitant difficulties in approaching the problem is a consequence of the fact that dealing with image registration problem means dealing with an ill-posed problem. Transformations between anatomies are not unique, and the impossibility to recover spatial or temporal evolution of an anatomical transformation from temporally isolated images, makes any validation a difficult, if not an impossible task. In addition each situation inevitably brings some prior knowledge within the initial data, that may imply some modifications in the problems' setting and affect the choice some constraints. This, of course, impact dramatically the range of possibilities and possible outcomes.

It is often the practical situation that provides the hint in choosing the optimal constraints, but it almost never provides enough information to reduce the large amount of options involved. A wide range of variants in methodologies and approaches to solve the registration problem has been thus proposed in the last decades: a quick glance to Google scholar reveals about 1200000 papers in *medical image registration* (55% of the whole *image registration* resources). See [SDP13], [ZF03] for surveys in medical image registration.

1.1.1 Examples of applications

One of the main application of image registration is in the domain of brain imaging: this tool can be used to examine differences between subjects and distinguish their biological features (cross-sectional studies) or to compare different acquisition of the same subject, before and after a surgery or after a fixed period of time (longitudinal studies). In both cases an accurate comparison between images and the parameters of the transformation involved may result in a quantification of anatomical variability and in a better understanding of the patients' features. For example, brain atrophy is considered a biomarker to diagnose the Alzheimer

disease and to analyze its evolution; most of the algorithms and techniques involved in the atrophy measurement requires longitudinal or cross-sectional scans to be aligned, and so are directly affected by the solution of the registration algorithm (See [FF97], [GWRNJ12], [PCL+15] for studies on brain atrophy involving registration).

Also when dealing with motion correction, if the sequence of images is affected by the motion of cardiac pulses or respiratory cycles, registration algorithms are often used for the realignment. For example, in lungs radiotherapy, lungs' motion is directly computed using a registration algorithm, and it is related with the respiratory surrogate signal. The correspondence model is then used to direct the X-ray or electrons beam on the cancerous tissue, minimizing the unaffected cells' damages (See for example [MHSK], [MHM+11]).

Another application is to compose together several images to obtain a bigger picture -also called *mosaicing*. In this case image registration is used to align images in the overlapping regions (See [VPM+06], [Sze94] as examples of image registration applied to mosaicing processes).

1.1.2 Diffeomorphisms in medical imaging: State of the Art

In the attempt to classify image registration algorithms, one of the most relevant feature that distinguish them is the choice of the family to whom the transformation belongs and its parametrization. Since anatomies are in a continuous process of modification over time, in general without any variation in the topological features, the use of diffeomorphisms to model transformations of organs appears as one of the most natural. Not accidentally diffeomorphisms are as well an important class of solutions of partial and ordinary differential equation aimed to model the dynamics of fluids.

In the development of diffeomorphic image registration, we can broadly identify some steps that led to the concept of log-composition presented in this research:

1981-1996 ▷ The use of diffeomorphisms in medical image registration starts from the research of a solution to partial differential equations: deformations are modeled as the consequent effect of two balancing forces applied to an elastic body [Bro81] or to conserve the energy momentum [CRM96]. In this early stage, diffeomorphisms are the domain of the solution to differential equation, and are not considered with their Lie group structure.

1998-2004 ▷ Based on the concept of attraction, the Demons algorithm [Thi98], [PCA99] propose the computation of the transformation between images in an iterative framework, where the update of the transformation at each step is parametrized with a vector field that is optimized at each step. This vector field is defined as the set of vectors (demons) that moves one image into the other.
Here diffeomorphisms are not directly involved and the vectors at each voxel are considered as independent elements. In the same year of [Thi98], the set of diffeomorphism was taken into account in image matching and computational anatomy, not only as the set of solutions of some family of differential equations, but with its tangent space [DGM98, Tro98, GM98].

2005-2006 ▷ The almost concomitant appearance of the Large Deformation Diffeomorphic Metric Mapping (LDDMM) [BMTY05] and the further investigation on the tangent space to the Lie group of diffeomorphisms as the space where to perform statistics (the so called log-Euclidean framework) [ACPA06b, AFPA06] keep the valuable approach in using diffeomorphisms as Lie group and to consider them with their Lie algebra, to model the little deformation in the tangent space as well as to rely on this normed space in computing the distance between transformations.

2007-2013 ▷ The LDDMM revealed all the opportunities provided by differential geometry in considering tangent vectors to the space of transformation in a framework for the computation of image registration. In this setting, the tangent vector field comes from the solution of the ODE that models the transformations and it consists of the set of the non-stationary vector field (also time varying vector field or TVVF). After the log-Euclidean framework [ACPA06b] aimed at the computation of statistics of diffeomorphisms, the set of tangent vector field is restricted to the time-independent vector field (also stationary velocity field or SFV); the same restriction was subsequently considered in some further improvements of LDDMM (DARTEL, Stationary LDDMM [Ash07], [HBO07]). Log-Euclidean framework brought new life also to the Demons algorithm, that become, in 2007, the diffeomorphic demons [VPPA07]. Subsequent approaches that involves the symmetrization of the energy function and a different norm (local correlation coefficient instead of L^2) are proposed in symmetric log-demons [VPPA08] and LCC-demons [LAF$^+$13] respectively.

1.1.3 Using Diffeomorphisms: Utility and Liability

If the algorithm is meant to model transformations that only preserves distances, orientations and angles, then the set of transformations involved can bonded to the rigid body transformations group $SE(3)$. The consequent registration algorithm will be suitable for example to compensate the motion in a rapid sequence of scans, or if some little differences has happened, to compare them in longitudinal and cross sectional scans.

If the algorithm is meant to model transformations that only preserves topology, as often happen for medical images, then the set of transformations can be bonded to the set of diffeomorphism *Diff*. This is, on one hand, particularly appealing for its algebraic group structure (see, for example [Art11]) and for its analytical properties. On the other side, due to its infinite-dimensional nature, a mathematical formalization of *Diff* as Lie group (so as differentiable manifold within a group structure, see [War13]) not of immediate understanding, and it is still an open field of research.

Attempt to provide some handles to this object for easy manipulation was done for the first time in 1966 by Vladimir Arnold [Arn66] (see also [Arn98], more readable for non-French speakers): to solve differential equation in hydrodynamic, the set *Diff* is considered as a Lie group possessing a Lie algebra. This assumption is not formally prosecuted in accordance to the problem-oriented nature of this paper. Subsequent steps in the exploration of the set of diffeomorphisms as a Lie group can be found in [MA70, EM70, Omo70, Les83]. A survey on early development of infinite dimensional Lie group can be found in [Mil84a], while more recent results and applications on diffeomorphisms has been published in [OKC92, BHM10, Sch10, BBHM11].

Considering *Diff* as a differentiable manifold involves the idea of having it locally in correspondence with some generalized "infinite-dimensional Euclidean" space. Attempt to set this correspondence showed that for some infinite-dimensional group the transition functions are smooth over Banach spaces [KW08]. This led to the idea of Banach Manifolds. Unfortunately the group of diffeomorphisms do not belongs to the category of Banach manifold but requires a more generals space on which the transition maps are smooth: the Frechet spaces. Here, important theorems from analysis, as the inverse function theorem, or the main results from the Lie group theory in a finite dimensional settings, as Lie correspondence theorems, do not holds anymore. These difficulties led some researchers in approaching the set of diffeomorphisms from other perspectives: for example, instead of treating *Diff* as a group equipped with differential structures, it is seen, in [Woj94], as a quotient of other

well behaved group. In other cases, in [MA70] first and in [Mil84b] later, Banach spaces are substituted with more general locally convex spaces to underpin the definition of smooth manifolds.

Without denying the importance of fundamentals and underestimating the doors research in this domain may open, we will approach the matter in as similar way of what has been done in set theory: we will use a *naive approach* to infinite dimensional Lie group, where the fundamental definition of infinite dimensional Lie group is a generalization of the finite dimensional case left more to the intuition than to a robust formalization.

For the practical purposes of medical imaging, it is enough to consider vector fields that vanishes outside a compact subset of $\mathbb{R}^d$, whose corresponding diffeomorphisms are the identity outside the corresponding compact set Ω (domain of an image) - see [Mil84a] pag. 1017. In addition, in this research, every findings is tested before in the finite dimensional settings (in this case $SE(2)$), where important theorems and close forms are available. Afterwards we will extend methods and results in the infinite dimensional case of diffeomorphisms with proper precautions.

It is important as well to remember that there is another limitation in the use of diffeomorphisms that do not comes down to the theoretical difficulties of handling them as formal structures. It is a consequence of the practical necessity of dealing with discrete images and softwares. Two subset of some topological space have the same topology if exists an homeomorphism between them: this analytical property do not holds if the objects involved are considered in a discretized space. Separated subset remains separated until their distance is less than the size of a voxel for a significant region; if this happen, even with a homeomorphic underpinning model, the discretization process do not preserve the topology.

1.2 Image Registration Framework

A *d-dimensional image* is a continuous function from a subset Ω of the coordinate space $\mathbb{R}^d$ (having in mind particular cases $d = 2, 3$) to the set of real numbers $\mathbb{R}$. Given two of them, $F : \Omega_F \to \mathbb{R}$ and $M : \Omega_M \to \mathbb{R}$, called respectively *fixed image* and *moving image*, the *image registration problem* consists in the investigation of features and parameters of the transformation function

$$\varphi : \mathbb{R}^d \supseteq \Omega_F \longrightarrow \Omega_M \subseteq \mathbb{R}^d$$
$$\mathbf{x} \longmapsto \varphi(\mathbf{x})$$

such that for each point $\mathbf{x} \in \Omega_F$ the element $M(\varphi(\mathbf{x}))$ and $F(\mathbf{x})$ are as closed as possible according to a chosen measure of similarity. The function defined as the composition of the moving image after the transformation, $M \circ \varphi$, is called *warped image*.

The underpinning idea can be represented by the following diagram, where φ is the solution that makes f the identity function:

$$\begin{array}{ccc} \Omega_F & \xrightarrow{\quad \varphi \quad} & \Omega_M \\ \Big\downarrow{\scriptstyle F} & & \Big\downarrow{\scriptstyle M} \\ \mathbb{R} & \dashrightarrow{\quad f \quad} & \mathbb{R} \end{array}$$

If $\Omega_F \neq \Omega_M$, it is always possible to apply an homeomorphism to transform them into a common domain Ω, called *background space*, on which both of the images are defined.

The definition of image registration problem proposed here, leaves two key degrees of freedom in searching for a solution: the transformation's domain (also called *deformation model*), and the metric to measure the similarity between images.
Once these are chosen, they can be used as constituent of an *image registration framework*: we define it as an iterative process that, at each step provides a new function φ that approaches f to the identity. Each iteration involves the optimization of a function that measure the similarity between the fixed image and the warped image computed at the previous step. To refine the energy function, the metric can be considered with an additive regularization term, that introduces a constraint based on prior knowledge about the searched solution:

$$\mathcal{E}(F, M, \varphi) = \text{Sim}(F, M, \varphi) + \text{Reg}(\varphi) \tag{1.1}$$

where Sim is a function that measure the similarity, while Reg is a regularization term. The optimization algorithm on which the framework is based and the resampling strategy - process of resize the image from one dimension to another - provide additional degrees of freedom in defining a framework for an algorithm aimed to solve image registration problem.

1.2.1 Iterative Registration Algorithm

The definition of registration problem and the iterative framework described above, raise several issues. For example there are no reasons to believe that such a correspondence is unique and that there is at least one of them whose behaviour corresponds to a reasonable biological transformation between anatomies. One way to deal with this problem is to add some constraints on the transformation φ, such that it models realistic changes that can occur in biological tissues. The kind and quality of the constraints are one of the features that distinguish one registration algorithm from the other.
The image registration framework here presented can be see as a electronic device with 5 knobs, each with its range:

$$\{\varphi\} \in \{\text{Transformations}\}$$
$$\text{Sim} \in \{\text{Similarity measures}\}$$
$$\text{Reg} \in \{\text{Regularization Terms}\}$$
$$\text{Opt} \in \{\text{Optimization techniques}\}$$
$$\text{Res} \in \{\text{Resampling techniques}\}$$

Under the hood of this ideal device we may see an engine that can be schematically represented as in figure 1.1.
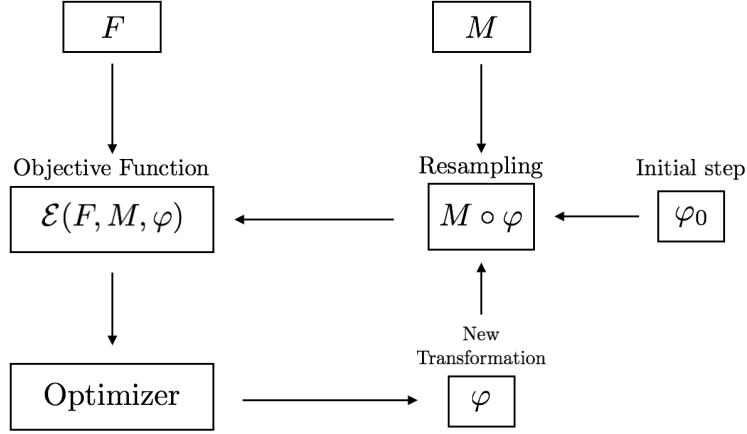
Figure 1.1: Image registration framework scheme.

Modulating on the value of each knob, changing for example the set of transformation or the resampling technique, we change between the possible registration algorithms that generally falls in this framework.

Far from being a complete overview of all of the possible frameworks, it does not take into account the fact that each version or implementation inevitably involves different needs and consequent challenges. Solutions found for each case may fall outside this simplification scheme: for example the parametrization of the transformations (or the deformation field's update) at each iterative step do not appear in this picture, even though is a fundamental feature.

In the following subsections we will going from the generalized framework to some specific algorithms. We are interested in particular in the parametrization of the *diffeomorphisms* (bijective differentiable maps with differentiable inverse, for example [Lee12]) of the latest important algorithms: the LDDMM and the diffeomorphic Demons.

1.2.2   LDDMM: Classic, Shooting and Stationary

As previously done in the elastic registration [Bro81], the LDDMM framework [BMTY05] originates by considering motion between images as the motion of a fluid, and utilizes ODE from fluid dynamics to compute the deformation between fixed and moving. A *time varying vector field* (TVVF) is the continuously differentiable map defined as

$$
\begin{aligned}
V : [0,1] &\longrightarrow \mathcal{V}(\Omega) \\
t &\longmapsto V_{(t)} : \Omega \longrightarrow \mathbb{R}^d \\
&\qquad \mathbf{x} \longmapsto V_{(t,\mathbf{x})}
\end{aligned}
$$

Once initial conditions are given, at each TVVF, corresponds a unique time varying (or non-stationary) homomorphisms defined by the following ODE

$$
\frac{d\phi_t(\mathbf{x})}{dt} = V_{(t,\phi_t(\mathbf{x}))} \tag{1.2}
$$

6

where the function ϕ is a path on the set of homeomorphisms (continuous function from the background space Ω to itself with continuous inverse), indicated with $\mathrm{Hom}(\Omega)$:

$$\phi : [0,1] \longrightarrow \mathrm{Hom}(\Omega)$$
$$t \longmapsto \phi_t : \Omega \longrightarrow \Omega$$
$$\mathbf{x} \longmapsto \phi_t(\mathbf{x})$$

The sought transformation φ between fixed and moving images (such that it satisfies $F \circ \varphi^{-1} \simeq M$), is modeled in the LDDMM as the solution of the equation 1.2 at time 1. Using the fundamental theorem of calculus we obtain:

$$\varphi := \phi_1 = \phi_0 + \int_0^1 V_{(t,\phi_t(\mathbf{x}))} dt$$

The set of homeomorphisms is taken into account since it can define a partition of the set of images into equivalence classes, as orbits of the action on the set of images from the background space $\mathcal{I}_\Omega$ (see for example [Art11]). In other words, given a subgroup of homeomorphisms $\mathbb{G} \subseteq \mathrm{Hom}(\Omega)$ and an image F, the orbit of the action of $\mathbb{G}$ over F, given by

$$\mathcal{O}_{\mathbb{G}}(F) = \{ F \circ \varphi^{-1} \mid \varphi \in \mathbb{G} \}$$

consists in the set of the images having the same topology of F.

The LDDMM framework put a first constraint $\mathbb{G}$ to the set of diffeomorphisms, and a second constraint considering ϕ_t as the shortest path between the identity function on $\mathbb{G}$ and φ. In this way the resulting vector field $V_{(t,\phi_t(\mathbf{x}))}$ is the one that minimize the distance l between transformations:

$$\hat{l} = \inf_{V_{(t,\phi_t(\mathbf{x}))} \, : \, \dot{\phi}_t(\mathbf{x}) = V_{(t,\phi_t(\mathbf{x}))}} \int_0^1 ||V_{(t,\phi_t(\mathbf{x}))}||_{L^2}^2 dt$$

For the similarity term the LDDMM uses the L^2 norm (see for example [SS09], chapter 4) between the moving image and the fixed image in the same orbit:

$$\mathrm{Sim}(F,M,\varphi) = \frac{1}{\sigma^2} ||F(\varphi^{-1}) - M||_{L^2}^2$$

while the regularization term is defined on the norm of the velocity vector field tangent to the transformation: the optimization function is given by

$$\mathcal{E}(F,M,\varphi) = \frac{1}{\sigma^2} ||F(\varphi^{-1}) - M||_{L^2}^2 + \int_0^1 ||LV_{(t,\phi_t(\mathbf{x}))}||_{L^2}^2 dt$$

In the LDDMM implementation, the data structure utilized to store deformation fields are 5-dimensional matrices

$$M = M(x_i, y_j, z_k, t, d) \qquad (i,j,k) \in L, \quad t \in T \quad d = 1,2,3 \qquad (1.3)$$

where (x_i, y_j, z_k) are discrete position of a lattice L in the domain of the images, t is the time parameter in a discretized domain T and d is index of the coordinate axis. So, the discretized *tangent vector* $\mathbf{v}_\tau(x_i, y_j, z_k)$ at time t, has coordinates defined by

$$\mathbf{v}_t(x_i, y_j, z_k) = (M(x_i, y_j, z_k, t, 1), M(x_i, y_j, z_k, t, 2), M(x_i, y_j, z_k, t, 3))$$

Therefore at the k-th step, the algorithm provides the 5-dim matrix $\mathbf{v}_k$ that is the approximation of the discretized time varying velocity fields $V_{(t,\phi_t(\mathbf{x}))}$. The update at each step is computed as

$$\mathbf{v}_{k+1} = \mathbf{v}_k - \epsilon\vec{\nabla}(\Delta\mathcal{E})$$

where $\Delta\mathcal{E}$ is the discretized version of the energy function and ϵ is the gradient descent step size.

A direct upgrade of the classical LDDMM performs the optimization on the geodesic flows, defined by a set of Hamiltonian equation (Shooting LDDMM [VRRC12]).
In this algorithm the iterative evolution of the deformation field, solution of the optimization algorithm, is regularized with the constraint imposed by an additional scalar field called *initial momentum*. As proved by the authors, the evaluation of this constraint at each step provides geodesics flows of homeomorphisms, but it is computationally expensive. Using the log-Euclidean framework presented in [AFPA06], the algorithm proposed in [Ash07] uses a constraint based on the stationarity of the involved velocity field. Instead of considering time varying velocity fields constrained by a set of Hamiltonian equations, the domain of vector field is reduced to the stationary, which is an -almost- equivalent constraint, that considerably reduces the computational complexity. Resulting algorithm, the DARTEL (Diffeomorphic Anatomical Registration using Exponentiated Lie Algebra), was published in contemporary with [HBO07] based on the same concept of the parametrization of geodesics path of diffeomorphisms with stationary velocity fields, and with [VPPA07] that uses SVF in the Demons framework. Aim of the next section is to present this algorithm.

1.2.3 Demonology: Classic, Additive, Diffeomorphic, Log and Symmetric

The first demons-based algorithm in image registration was proposed by [Thi98], in analogy with the Maxwell's demon in thermodynamics. This early version - often called *classic demons* - do not involves diffeomorphisms. The floating image is deformed with a vector field resulting from the computation of the optical flow regularized by a gaussian filter at each step. The optical flow is based on the idea that a voxel in the moving image is attracted by some force to all the points in the fixed with similar intensity.
Let $\mathbf{x}$ be a point in the background space Ω, the unknown vector field $V : \Omega \to \mathbb{R}^d$ is the function that at each voxel satisfies:

$$V(\mathbf{x}) \cdot \vec{\nabla}F(\mathbf{x}) = M(\mathbf{x}) - F(\mathbf{x}) \tag{1.4}$$

whose solution provides the update of the deformation field at each step.

The final deformation, solution to the registration problem is obtained composing at each step the previous transformation with an update: let $\{T_k\}_{k=1}^N$ be the sequence of deformation and let δT_k be the update at the step k. Then they can be expressed as the identity plus the displacement field:

$$T_k(\mathbf{x}) = \mathbf{x} + V_k(\mathbf{x})$$
$$\delta T_k(\mathbf{x}) = \mathbf{x} + \delta V_k(\mathbf{x})$$

And the k-th deformation is computed by composition as:

$$T_{k+1}(\mathbf{x}) := (\delta T_k \circ T_k)(\mathbf{x})$$
$$= \mathbf{x} + \delta V_k(\mathbf{x}) + V_k(\mathbf{x} + \delta V_k(\mathbf{x}))$$

Since the third addend is close to $V_k(\mathbf{x})$, some implementation - as for example ITK - consider only the sum between V_{k+1} and V_k in the computation of the update:

$$T_{k+1}(\mathbf{x}) := (\delta T_k + T_k)(\mathbf{x})$$
$$= \mathbf{x} + V_k(\mathbf{x}) + \delta V_k(\mathbf{x})$$

Demons algorithms with this implementation are often called *additive demons*.

In the paper that presents the PASHA demons [CBD$^+$03], authors underline the fact that the scalar product 1.4 underpinning the classic demon consists in the minimization of a local energy function, one per volxel. They reformulate the algorithm using a global energy function, aimed to make the method easier to be analyzed and compared with others. With some modifications, the Classic demons algorithm is accompanied back to the framework presented in the previous section, having a global energy function which optimization provides at each step the update of the transformation.
Again the PASHA algorithm does not involve any diffeomorphism. The solution is smoothed with the widespread stratagem of applying a Gaussian filter G at each of the global transformation T_k involved in the registration:

$$T_{k+1}(\mathbf{x}) := G_1(T_k(\mathbf{x}) + G_2(\delta T_k(\mathbf{x})))$$

If G_1 is omitted the model is sometime called *fluid*, while if G_2 is omitted is called *elastic*.

Diffeomorphisms were introduced within the demons algorithm (*diffeomorphic demons* [VPM$^+$06]) after the presentation of the log-Euclidean framework [AFPA06]. To each stationary velocity field $V \in \mathcal{V}(\Omega)$ is associated a diffeomorphisms φ by the ODE $d\varphi/dt = V_{(t,p)}$. Using Lie theory, SVF are elements of the *Lie algebra* - usually denoted with $\mathfrak{g}$ - while the set of diffeomorphisms are elements of the Lie group - denoted with $\mathbb{G}$ -.
Roughly speaking, the lie algebra $\mathfrak{g}$ is the tangent space (as local linear approximation of a manifold) to the Lie group $\mathbb{G}$, and these two spaces are in local correspondence thanks to two crossing-structure functions: the *Lie exponential* and the *Lie logarithm*. *Lie exponential* maps vector fields on the corresponding Lie group elements, while the *Lie logarithm* - inverse of the Lie exponential under some condition [Lee12]- maps each diffeomorphisms in the correspondent tangent vector field:

$$\varphi = \exp(V) \quad V = \log(\varphi) \qquad \varphi \in \mathbb{G} \quad V \in \mathfrak{g}$$

In this settings, the update can not be computed simply with a sum of vector fields, since it must reflect the composition of diffeomorphisms defined by the corresponding vector fields.

It has been presented several approaches to face the problem of the computation of the update: diffeomorphic demons compute each new diffeomorphisms as the composition between the diffeomorphism obtained at the previous step φ_k with the exponential of the SVF δV_k obtained by the optimization algorithm :

$$\varphi_{k+1} := \varphi_k \circ \exp(\delta V_k)$$

while in the subsequent log-demon [VPPA08] the composition is performed in the tangent space toward exponential and logarithm functions

$$V_{k+1} := \log(\exp(V_k) \circ \exp(\delta V_k)) \tag{1.5}$$

For this last computation, another treasure from the theory of Lie group has been stolen: the BCH formula. Defined as the solution for Z of the equation

$$\exp(Z) = \exp(X) \circ \exp(Y)$$

As we will see in this research, it involves an infinite series of nested Lie bracket, that do not makes its computation as straightforward as we wish. This thesis is devoted to the research of some numerical method for its computation and the last section of this chapter is aimed to introduce the definition of log-composition, whose numerical approximation will help in the computation of equation 1.5.

1.3 The Log-composition at the Service of Image Registration

Every non-rigid registration algorithm requires to be implemented and to work with discretized images. The nature of the computers' memory prevent from the possibility of storing the continuous fluid transformations that, for example, solves the differential equations of the LDDMM or any of the diffeomorphisms resulting from the demons. The only manipulation we are allowed to perform, unfortunately, are storing the discretized vector fields and resampling them with the images using one of the available techniques.
When relying on diffeomorphisms, we still have to consider discretized vector fields our objects, but we need the Lie group of diffeomorphisms as support to compute their composition in the equation 1.5. This operation of composition is baptized here under the name of *log-composition* and it is defined as

$$X \oplus Y := \log(\exp(X) \circ \exp(Y)) \qquad \forall \, X, Y \in \mathfrak{g}$$

The main aim of this document is to present a comparison between numerical methods to compute it.

It is worthed to notice that a fast log-composition is not useful only for the diffeomorphic demons. It may be used to solve some of the problems that rely on Lie groups and need to be implemented in a computer. In medical imaging it can be used for

1. Diffeomorphic demon, and symmetric diffeomorphic demon [VPM$^+$06, VPPA08].

2. Fast computation of the logarithm [BO08] (discussed in chapter 4).

3. Calculus on diffusion tensor [AFPA06].

4. Compute the discrete ladder for Parallel Transport in Transformation Groups [LP14a].

The next chapter is aimed to the formal definition of the log-composition, underpinned with the tools from differential geometry theory and to present two new numerical technique to compute it.

Chapter 2

Tools from Differential Geometry

> *People know or dimly perceive, that if thinking is not kept pure and keen, if spirit's contemplation do not holds, even mechanics of automobiles and ships will soon cease to run. Even engineer's slide rule, computations of banks and stock exchanges will wonder aimlessly for the lost of authority, and chaos will ensue.*
>
> -Hermann Hesse, *Magister Ludi*

2.1 A Lie Group Structure for the Set of Transformation

We consider every group $\mathbb{G}$ as a group of transformations acting on $\mathbb{R}^d$, having in mind the particular case $d = 2, 3$ for 2-dimensional or 3-dimensional images. We will focus out attention to transformations defined by matrices or diffeomorphism. Other than group they also have the structure of Lie group: they are considered with a maximal atlas that makes them differentiable manifold, in which the composition of two transformation and the inverse of each transformation are well defined differentiable maps:

$$\mathbb{G} \times \mathbb{G} \longrightarrow \mathbb{G}$$
$$(x, y) \longmapsto xy^{-1}$$

Differential geometry is in general a technique to use the well known calculus features and operators on spaces different from the usual $\mathbb{R}^n$. Adding the differentiable structure to a group of transformations gives us new handles to hold and manipulate them: in particular provides the opportunity to define a tangent space to each point of the group (and so a fiber bundle), a space of vector fields, a set of flows and one parameter subgroup as well as other features that enrich this structure. The abstract idea of vector field over a manifold will be concretized for image registration introducing the concepts of *displacement field, deformation field* and *velocity field (stationary or time varying)* that will be there presented. Due to space limitations we will refer to [DCDC76], [Lee12] for the definitions and concepts of differential geometry and [dCV92] for definition and concepts of Riemannian geometry.

2.2 Lie Exponential, Lie logarithm, Lie log-composition and the BCH formula

Let $\mathbf{v}$ be an element in the tangent space fo the Lie group $\mathbb{G}$ indicated with $\mathfrak{g}$. The *Lie exponential* is defined as

$$\exp : \mathfrak{g} \longrightarrow \mathbb{G}$$
$$\mathbf{v} \longmapsto \exp(\mathbf{v}) = \gamma(1)$$

where $\gamma : [0,1] \to \mathbb{G}$ is the unique one-parameter subgroup of $\mathbb{G}$ having $\mathbf{v}$ as its tangent vector at the identity ([dCV92], [EMP06], [AFPA06]). It satisfies the following properties:

1. $\exp(t\mathbf{v}) = \gamma(t)$.

2. $\exp(\mathbf{v}) = e$ if $\mathbf{v} = \mathbf{0}$.

3. $\exp(\mathbf{v}) \circ \exp(-\mathbf{v}) = e$

4. The exponential function satisfies the one parameter subgroup property:

$$\exp((t+s)\mathbf{v}) = \gamma(t+s) = \gamma(t) \circ \gamma(s) = \exp(t\mathbf{v})\exp(s\mathbf{v})$$

5. $\exp(\mathbf{v})$ is invertible and $(\exp(\mathbf{v}))^{-1} = \exp(-\mathbf{v})$.

6. $\exp$ is a diffeomorphism between a neighborhood of $\mathbf{0}$ in $\mathfrak{g}$ to a neighborhood of e in $\mathbb{G}$.

The neighborhoods of $\mathbb{G}$ and of $\mathfrak{g}$ such that the last property holds, are called *internal cut locus* of $\mathbb{G}$ and $\mathfrak{g}$ respectively. The *cut locus* is the boundary of the internal cut locus.

When we deal with a matrix Lie group of dimension n, we have the following remarkable properties:

1. for all $\mathbf{v}$ in a matrix Lie algebra $\mathfrak{g}$:

$$\exp(\mathbf{v}) = \sum_{k=0}^{\infty} \frac{\mathbf{v}^k}{k!}$$

2. If $\mathbf{u}$ and $\mathbf{v}$ are commutative then $\exp(\mathbf{u} + \mathbf{v}) = \exp(\mathbf{u})\exp(\mathbf{v})$.

3. If $\mathbf{c}$ is an invertible matrix then $\exp(\mathbf{c}\mathbf{v}\mathbf{c}^{-1}) = \mathbf{c}\exp(\mathbf{v})\mathbf{c}^{-1}$.

4. $\det(\exp(\mathbf{v})) = \exp(\operatorname{trace}(\mathbf{v}))$

5. For any norm, $||\exp(\mathbf{v})|| \leq \exp(||\mathbf{v}||)$.

6. $\exp(\mathbf{u} + \mathbf{v}) = \lim_{m \to \infty} (\exp(\frac{\mathbf{v}}{m})\exp(\frac{\mathbf{v}}{m}))^m$

7. If $\exp(\mathbf{w}) = \exp(\mathbf{u}) \circ \exp(\mathbf{v})$ then $\exp(-\mathbf{w}) = \exp(-\mathbf{v}) \circ \exp(-\mathbf{u})$.

The idea of defining an inverse of the Lie exponential leads to the idea of the Lie logarithm, defined

$$\log : \mathbb{G} \longrightarrow \mathfrak{g}$$
$$p \longmapsto \log(p) = \mathbf{v}$$

where $\mathbf{v}$ is the tangent vector having p as it exp.

If $\mathbb{G}$ is a matrix Lie group of dimension n, the following properties hold:

1. for all $\mathbf{v}$ in the matrix Lie algebra $\mathfrak{g}$:

$$\log(\mathbf{v}) = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{(\mathbf{v} - I)^k}{k!}$$

where I is the identity matrix.

2. For any norm, and for any $n \times n$ matrix $\mathbf{c}$, exists an α such that

$$||\log(I + \mathbf{c}) - \mathbf{c}|| \leq \alpha ||\mathbf{c}||^2$$

3. For any $n \times n$ matrix $\mathbf{c}$ and for any sequence of matrix $\{\mathbf{d}_j\}$ such that $||\mathbf{d}_j|| \leq \alpha/j^2$ it follows:

$$\lim_{k \to \infty} \left(I + \frac{\mathbf{c}}{k} + \mathbf{d}_k\right)^k = \exp(\mathbf{c})$$

Here we may see the beginning of the problem we have to deal with for the rest of the research, when passing from the finite dimensional case to the infinite dimensional case.
The domain of the logarithm is the matrix Lie group in which only the composition is defined. Nevertheless it is possible to compute $I + \mathbf{c}$, and this still make sense (and satisfy remarkable properties) when applied to the log. In addition the domain of the exponential is the matrix Lie algebra, but the exponential can be nevertheless applied to any matrix.
This can be done thanks to the fact that for matrices, $\mathfrak{g}$ and $\mathbb{G}$ are subset of a bigger algebra, the algebra of invertible matrix. In this structure the operation of sum is still defined over the group that admits only compositions, and infinite series are doors to pass from the structure of group to the algebra and vice versa. When presenting the rigid body transformation in chapter 3 we will see another couple of access doors based on numerical approximations.

When dealing with diffeomorphism in practical application we have to deal with a theoretical and a practical issues: on one side the the operations in Lie algebra are not compatible with the composition in the Lie group: expression as $e + \mathbf{v}$ contains a sum that is undefined (and therefore meaningless) in the Lie group structure. On the other side the (extremely) continuous nature of diffeomorphisms is not compatible with the (extremely) discrete nature of computers. It is not possible to implement something that maintains any of the property of diffeomorphism in a computer. The only options we have for practical implementations are the vector fields discretized on a d dimensional grid. In the paper of Arsigny [ACPA06a], scaling and squaring and inverse scaling and squaring are proposed for the computation of exponential and logarithm respectively; they transform a discretized vector field in another discretized vector field, while theoretical domain and codomain of these transformations are radically different. In addition, as shown in [HOP08] for some parameters of Stationary LDDMM and the diffeomorphic Demons the diffeomorphisms involved do not preserve the signs of the Jacobian determinant, and therefore are not diffeomorphisms anymore.
A different situation arises when dealing with classic Lie group: their matrix representation is not only ideal for implementation, but the Lie algebra $\mathfrak{g}$ of a classic Lie group $\mathbb{G}$ can be still represented with a set of matrices whose sum and products are compatible with the composition, since $\mathfrak{g}$ and $\mathbb{G}$ are both subset of a bigger algebra of the general linear group $GL(n)$ [KKK08]. case the exponential and logarithm have domain and codomain in the appropriate restriction of $GL(n)$.

The passage from finite dimensional case of matrices to infinite dimensional case of diffeomorphisms requires a way to represent diffeomorphisms having only discrete vector fields

to deal with, where operations within Lie algebra and Lie group are not anymore compatible. The strategy here proposed is to define an operation in the Lie algebra Lie algebra $\mathfrak{g} = \mathcal{V}(\Omega)$ that reflects the properties of the composition in the corresponding Lie group structure $\mathbb{G} = \mathrm{Diff}(\Omega)$.

The Lie log-composition (because based on the Lie log and exp maps) is defined here as the inner binary operation on the Lie algebra that reflects the composition on the lie group:

$$\oplus : \mathfrak{g} \times \mathfrak{g} \longrightarrow \mathfrak{g} \tag{2.1}$$
$$(\mathbf{v}_1, \mathbf{v}_2) \longmapsto \mathbf{v}_1 \oplus \mathbf{v}_2 = \log(\exp(\mathbf{v}_1) \circ \exp(\mathbf{v}_2)) \tag{2.2}$$
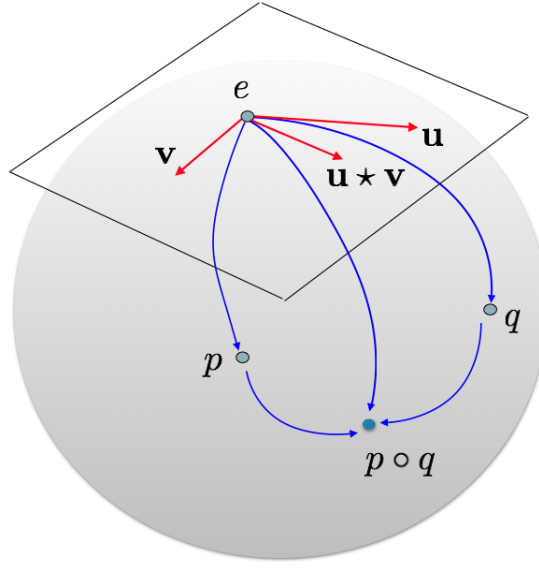
Figure 2.1: graphical visualization of the Lie log-composition.

Following properties holds for the Lie log-composition:

1. $\mathfrak{g}$ with the Lie log-composition $\oplus$ is a local topological non-commutative group (local group for short): if $C_{\mathfrak{g}}$ is the internal cut locus of $\mathfrak{g}$ then:

   (a) $(\mathbf{u}_1 \oplus \mathbf{u}_2) \oplus \mathbf{u}_3 = \mathbf{u}_1 \oplus (\mathbf{u}_2 \oplus \mathbf{u}_3)$ for all $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3$ in $C_{\mathfrak{g}}$.
   (b) $\mathbf{u} \oplus \mathbf{0} = \mathbf{0} \oplus \mathbf{u} = \mathbf{u}$ for all $\mathbf{u}$ in $C_{\mathfrak{g}}$.
   (c) $\mathbf{u} \oplus (-\mathbf{u}) = \mathbf{0}$ for all $\mathbf{u}$ in $C_{\mathfrak{g}}$.

2. For all t, s real, such that $(t + s)\mathbf{u}$ is in $C_{\mathfrak{g}}$,

$$(t\mathbf{u}) \oplus (s\mathbf{u}) = (t + s)\mathbf{u}$$

   And in particular, if the Lie algebra $\mathfrak{g}$ has dimension 1 the local group structure is compatible with the additive group of the vector space $\mathfrak{g}$.

We refer to $(\mathfrak{g}, \oplus)$ as the Lie Log-group. Additional observation of this algebraic structure in the particular case of diffeomorphisms, are contained in the next chapter.

To compute the log-composition there is a formula, the BCH (for Lie group [Hal15], general case [Woj94], applied to medical imaging [VPPA08]), that provides the exact solution to the Log-composition.

$$BCH(\mathbf{u}, \mathbf{v}) = \mathbf{u} + \mathbf{v} + \frac{1}{2}[\mathbf{u}, \mathbf{v}] + \frac{1}{12}([\mathbf{u}, [\mathbf{u}, \mathbf{v}]] + [\mathbf{v}, [\mathbf{v}, \mathbf{u}]]) - \frac{1}{24}[\mathbf{v}, [\mathbf{u}, [\mathbf{u}, \mathbf{v}]]] + ...$$

This expansion will provide the most immediate way to obtain a numerical computation of the log-composition.

2.3 Parallel Transport: Definition and Properties

In this section we introduce the concept of parallel transport for a generic Lie group $\mathbb{G}$. On this definition, again borrowed from differential geometry (for introduction and general definition: [MTW73], [Kne51], [KMN00]. For medical imaging applications [LAP11], [LP13] [LP14b], [PL$^+$11]), relies an important method for the computation of the Log-composition.

Definition 2.3.1. Let $\mathbb{G}$ be a finite dimensional connected Lie group defined with a connection ∇. Given $p, q \in \mathbb{G}$ and $\gamma : [0, 1] \rightarrow \mathbb{G}$ such that $\gamma(0) = p$ and $\gamma(1) = q$, then the vector $V_p \in T_p\mathbb{G}$, belonging to some vector field V is parallel transported along γ up to $T_q\mathbb{G}$ if V satisfies

$$\forall t \in [0, 1] \qquad \nabla_{\dot{\gamma}} V_{\gamma(t)} = 0$$

The parallel transport is the function that maps V_p from $T_p\mathbb{G}$ to $T_q\mathbb{G}$ along γ:

$$\Pi(\gamma)_p^q : T_p\mathbb{G} \longrightarrow T_q\mathbb{G}$$
$$V_p \longmapsto \Pi(\gamma)_p^q(V_p) = V_q$$

In the next properties we explore how did parallel transport and affine exponential behave when expressed as a composition and when there are changing in the signs.

Property 2.3.1 (Inversion)**.** $\mathbb{G}$ Lie group, ∇ connection, $p, q \in \mathbb{G}$. Given γ such that $\gamma(0) = p$, $\gamma(1) = q$ and $\mathbf{u} \in T_p\mathbb{G}$, we have:

1. $\Pi(\gamma)_p^q(-\mathbf{u}) = -\Pi(\gamma)_p^q(\mathbf{u}))$

2. $q = \exp_p(\mathbf{u}) \iff p = \exp_q(-\Pi(\gamma)_p^q(\mathbf{u}))$

Property 2.3.2 (change of signs of the composition for affine exponential)**.** $\mathbb{G}$ Lie group, ∇ connection, $p, q \in \mathbb{G}$, $\mathbf{u} \in T_p\mathbb{G}$, $\mathbf{v} \in T_q\mathbb{G}$ and $q = \exp_p(\mathbf{u})$. Let β be the tangent curve to $\mathbf{u}$ at p such that $\beta(1) = q$ and $r = \exp_b(\mathbf{v})$. Given $\mathbf{w} \in T_p\mathbb{G}$ such that

$$\exp_p(\mathbf{w}) = \exp_q(\mathbf{v}) \circ \exp_p(\mathbf{u})$$

Then

$$\exp_p(-\mathbf{w}) = \exp_{\beta(-1)}(-\Pi(\beta)_q^{\beta(-1)}(\mathbf{v})) \circ \exp_p(-\mathbf{u})$$

Lemma 2.3.1. Let $\mathbb{G}$ be a finite dimensional connected Lie group defined with a Cartan connection ∇ and $\mathbf{u}$ tangent vector in $T_e\mathbb{G}$. Let γ be a geodesic defined on $\mathbb{G}$ such that $\gamma(0) = e$, $\dot{\gamma}(0) = \mathbf{u}$ and $p = \gamma(1)$, point in the Lie group. Let β be the curve over $\mathbb{G}$ defined as $\beta(t) = p \circ \gamma(t)$, then the two following conditions hold:
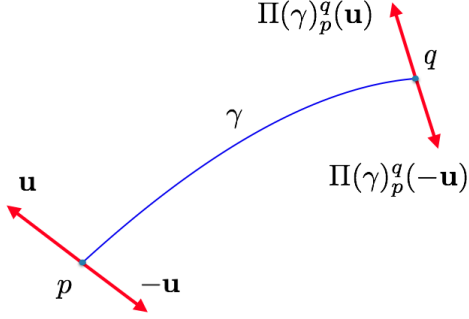
Figure 2.2: First inversion property.
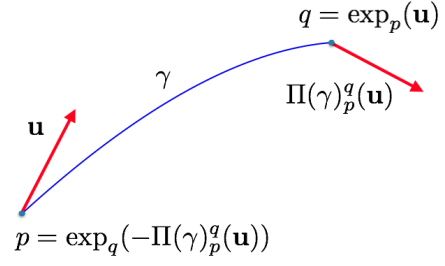
Figure 2.3: Second inversion property.
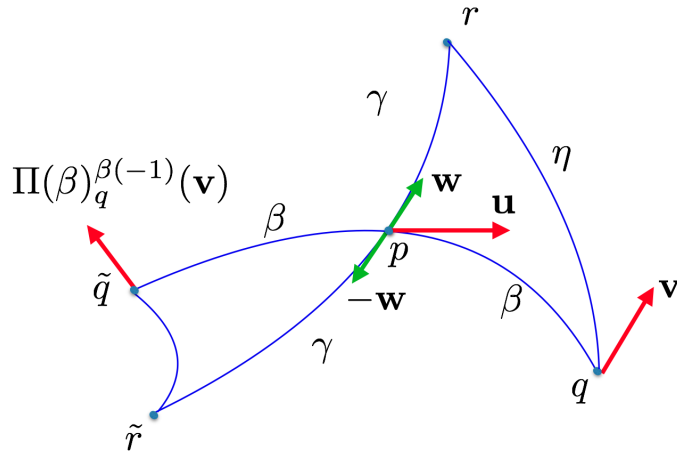
Figure 2.4: Change of sign property.

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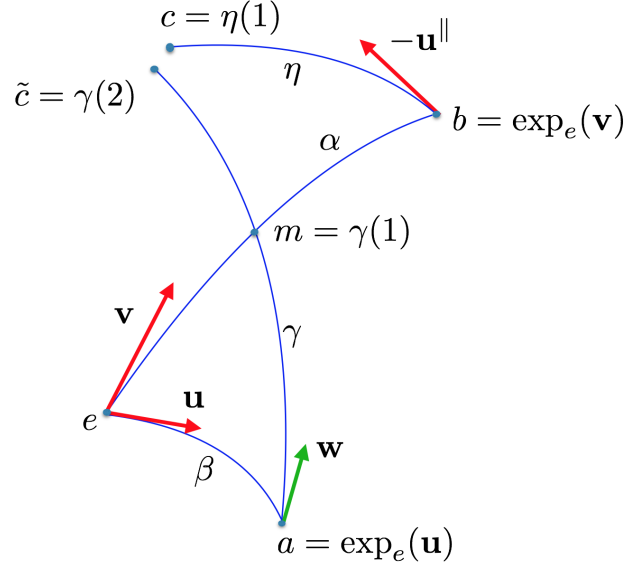
Figure 2.5: Pole ladder applied to parallel transport.

1. If ∇ is a Cartan connection then β is a geodesic.

2. For $\mathbf{u}_p := D(L_p)_e(\mathbf{u}) \in T_p\mathbb{G}$, push forward of the left-translation:

$$\exp_p(t\mathbf{u}_p) = p \circ \exp_e(tD(L_{p^{-1}})_p(\mathbf{u}_p)) = p \circ \exp_e(t\mathbf{u}) \tag{2.3}$$

The following theorem is an application of the pole ladder [LAP11] for the computation of the exponential that will underpin one of the numerical methods for the computation of the log-composition.

Theorem 2.3.1. Let $\mathbb{G}$ be a finite dimensional connected Lie group defined with a Cartan connection ∇. If, for each couple of linearly independent vectors $\mathbf{u}, \mathbf{v} \in T_e\mathbb{G}$, we consider the following elements:

$$a = \exp_e(\mathbf{u}) \qquad b = \exp_e(\mathbf{v})$$
$$\mathbf{v}_a^{\|} = \Pi(\gamma)_e^a(\mathbf{v})$$
$$\gamma : [0, 1] \to \mathbb{G} \quad \gamma(0) = e \quad \dot{\gamma}(0) = \mathbf{u}$$

$$\mathbf{v}^{\|} := D(L_{a^{-1}})_e(-\Pi(\alpha)_a^e(\mathbf{v}_a^{\|}))$$

Then it follows that if $\mathbf{u}$ is in the open ball $B(\mathbf{0}, \epsilon)$, then exists a $\tilde{\epsilon} > 0$ such that $\mathbf{u}_e^{\|}$ belongs to $B(\mathbf{0}, \tilde{\epsilon})$, and exists a $\delta(\epsilon + \tilde{\epsilon}) > 0$ such that the inequality

$$\|\log(\exp_e(\mathbf{v}^{\|})) - \log(\exp_e\left(\frac{\mathbf{u}}{2}\right) \circ \exp_e(\mathbf{v}) \circ \exp_e\left(-\frac{\mathbf{u}}{2}\right))\| < \delta(\epsilon + \tilde{\epsilon})$$

holds.

The last statement can be rewritten as the approximation:

$$\exp_e(\mathbf{v}^{\|}) \simeq \exp_e\left(\frac{\mathbf{u}}{2}\right) \circ \exp_e(\mathbf{v}) \circ \exp_e\left(-\frac{\mathbf{u}}{2}\right) \tag{2.4}$$

that will turn out to be the main tool for the computation of the log-composition using parallel transport.

When considering the equation 2.3, we use implicitly the formula for the change of base for affine exponential and logarithm [APA06]. It is in fact possible, using the derivative of the left-translation L_p, to bring back the exp and the log functions based at the point p of the manifold to the exp and the log evaluated at the identity using the following formulas:

$$\log_p(q) = DL_p(e)\log_e(q) \tag{2.5}$$

$$\exp_p(\mathbf{u}) = p \circ \exp_e(DL_p(e)^{-1}\mathbf{u}) \tag{2.6}$$

Further theoretical developments are beyond the aim of this research, but the reader can refer to the bibliography.

2.4 Numerical Computations of the Log-composition

In this section we provide explicit formulas for the computation of the log composition:

$$\mathbf{v}_1 \oplus \mathbf{v}_2 = \log(\exp(\mathbf{v}_1) \circ \exp(\mathbf{v}_2))$$

using the tools introduced in the previous sections.

2.4.1 Truncated BCH formula for the Log-composition

To compute the Lie log-composition, literature provides the BCH formula (for matrices [Hal15], general case: [KO89] , [Ser09]), defined as the solution of the equation $exp(\mathbf{w}) = \exp(\mathbf{u}) \circ \exp(\mathbf{v})$, for $\mathbf{u}$ and $\mathbf{v}$ in the Lie algebra $\mathfrak{g}$:

$$BCH(\mathbf{u}, \mathbf{v}) = \mathbf{u} + \mathbf{v} + \frac{1}{2}[\mathbf{u}, \mathbf{v}] + \frac{1}{12}([\mathbf{u}, [\mathbf{u}, \mathbf{v}]] + [\mathbf{v}, [\mathbf{v}, \mathbf{u}]]) - \frac{1}{24}[\mathbf{v}, [\mathbf{u}, [\mathbf{u}, \mathbf{v}]]] + ...$$

It consists of an infinite series of Lie bracket whose asymptotic behaviour cannot be predicted only from the coefficient of each nested Lie bracket term. In practical applications it can be computed using its *approximation of degree k*, defined as the sum of the BCH terms having no more than k nested Lie bracket. For example:

$$BCH^0(\mathbf{u}, \mathbf{v}) = \mathbf{u} + \mathbf{v}$$

$$BCH^1(\mathbf{u}, \mathbf{v}) = \mathbf{u} + \mathbf{v} + \frac{1}{2}[\mathbf{u}, \mathbf{v}]$$

$$BCH^2(\mathbf{u}, \mathbf{v}) = \mathbf{u} + \mathbf{v} + \frac{1}{2}[\mathbf{u}, \mathbf{v}] + \frac{1}{12}([\mathbf{u}, [\mathbf{u}, \mathbf{v}]] + [\mathbf{v}, [\mathbf{v}, \mathbf{u}]])$$

These numerical approximations of the log-composition $\mathbf{u} \oplus \mathbf{v}$ can be considered as a first step but are not satisfactory since they do not provide any condition to consider the error carried by each term.

2.4.2 Taylor Expansion Method for the Log-composition

A more sophisticated numerical method for the computation of the log-composition that relies on the Taylor expansion, that holds only for matrix Lie groups.

As shown in the appendix of [KO89] the terms of the BCH can be recollected using the Hausdorff method: each of the therm containing the n-th power of the vector $\mathbf{v}$ are collected together in the formal series V^n. Therefore

$$BCH(\mathbf{u}, \mathbf{v}) = \mathbf{u} + V^1\mathbf{v} + V^2\mathbf{v} + V^3\mathbf{v} + \cdots$$

Given the adjoint map:

$$ad_{\mathbf{u}} : \mathfrak{g} \longrightarrow \mathfrak{g}$$
$$\mathbf{v} \longmapsto ad_{\mathbf{u}}\mathbf{v} := [\mathbf{u}, \mathbf{v}]$$

and the multiple adjoint maps, defined as:

$$\mathrm{ad}_{\mathbf{u}}^n\mathbf{v} := [\underbrace{\mathbf{u}, [\mathbf{u}, ...[\mathbf{u}}_{\text{n-times}}, \mathbf{v}]...]]$$

$$\mathrm{ad}_{\mathbf{u}}^{-n}\mathbf{v} := [[...[\mathbf{v}, \underbrace{\mathbf{u}]...], \mathbf{u}}_{\text{n-times}}] = (-1)^n\mathrm{ad}_{\mathbf{u}}^n\mathbf{v}$$

it can be proved that the operator V_1 that when applied to $\mathbf{v}$ provides the linear part of $\mathbf{v}$ in the BCH results in

$$V_1 = \frac{\mathrm{ad}_{\mathbf{u}}^{-1}}{\exp{(\mathrm{ad}_{\mathbf{u}})} - 1} = \sum_{n=0}^{\infty} \frac{(-1)^n B_n}{n!}\mathrm{ad}_{\mathbf{u}}^{-n} = \sum_{n=0}^{\infty} \frac{B_n}{n!}\mathrm{ad}_{\mathbf{u}}^n$$

Where $\{B_n\}_{n=0}^{\infty}$ is the sequence of the second-kind Bernoulli number. If first-kind Bernoulli number are used, then each term of the summation must be multiplied for $(-1)^n$, as did for example in [KO89]. The denominator is defined within the structure of the formal power series ring [MT13].

In conclusion, the log-composition can expressed as:

$$\mathbf{u} \oplus \mathbf{v} = \mathbf{u} + \frac{\mathrm{ad}_{\mathbf{u}}^{-1}}{\exp{(\mathrm{ad}_{\mathbf{u}})} - 1}\mathbf{v} + \mathcal{O}(\mathbf{v}^2)$$

$$\mathbf{u} \oplus \mathbf{v} = \mathbf{u} + \sum_{n=0}^{\infty} \frac{B_n}{n!}\mathrm{ad}_{\mathbf{u}}^n\mathbf{v} + \mathcal{O}(\mathbf{v}^2) \tag{2.7}$$

that will turn out to be an important tool for the computation of the log-composition in the finite dimensional case.

2.4.3 Parallel Transport Method for the Log-composition

To obtain a numerical computation for the log-composition using parallel transport, three assumptions has to be made:

1. If $\mathbf{v}^{\|}$ is defined as in theorem 2.3.1, then exists an $\hat{\epsilon} > 0$ such that

$$\|\mathbf{u} \oplus \mathbf{v} - (\mathbf{u} + \mathbf{v}^{\|})\| < \hat{\epsilon}$$

2. If the vector $\mathbf{w} \in \mathfrak{g}$ is small enough, then:

$$\exp(\mathbf{u}) \simeq e + \mathbf{u}$$

The second condition is valid if the hypothesis of proposition 8.6 pag. 163 [You10] holds. A deepening in this direction is not in the scope of this research. For our purposes we will consider $\mathbf{w}$ small enough to make the approximation questioned here reasonable.

From these assumptions and from equation 2.4 it follows that

$$\mathbf{u} \oplus \mathbf{v} \simeq \mathbf{u} + \mathbf{v}^{\|}$$
$$e + \mathbf{v}^{\|} \simeq \exp_e \big(\frac{\mathbf{u}}{2} \big) \circ \exp_e(\mathbf{v}) \circ \exp_e \big(-\frac{\mathbf{u}}{2} \big)$$

Therefore

$$\mathbf{u} \oplus \mathbf{v} \simeq \mathbf{u} + \exp_e \big(\frac{\mathbf{u}}{2} \big) \circ \exp_e(\mathbf{v}) \circ \exp_e \big(-\frac{\mathbf{u}}{2} \big) - e \tag{2.8}$$

This is the third numerical method for the computation of the log-composition explored in this thesis.
We have to notice that when we apply it on the infinite dimensional case, the approximation 2.8 holds under the following additional assumption:

3. Theorem 2.3.1 holds when the Lie group is infinite dimensional.

whose eventual confirmation is at the moment not known to the author. We assume it is true in coherence with what has been said in the introduction, section 1.1.3.

Chapter 3

Spatial Transformations for the Computations of the Log-composition: SE(2) and SVF

Every working mathematician knows that if one does not control oneself (best of all by examples), then after some ten pages half of all the signs in formulae will be wrong and twos will find their way from denominators into numerators.
-V.I. Arnold

In the previous chapter we have introduced some essential mathematical tools for the numerical computation of the log-composition. They can be applied for several groups of transformation. In this research we show how they behave on two selected groups:

$SE(2)$ - The group of rigid body transformation of the plane (any combination of bi-dimensional rotations and translations) is the optimal playground to test the numerical methods introduced so far. Here all the closed form can be derived analytically, and therefore a ground truth is always available for comparisons. A representation of this Lie group as a subgroup of the real linear group $GL(2)$, with corresponding Lie algebra will be provided, with all of the closed form of the numerical computations presented in this research.

SVF - The subgroup of the set of diffeomorphisms parametrized by SVF, is the second group used to test the numerical methods here presented for the computation of the log-composition. Each one can be applied for the composition of SVF in the diffeomorphic demons and for the log-demons. In this case we do not know any closed form, but if we consider an improper norm in the space of transformation we still have a method to compare SVF and assess the quality of the results.

Since each of the theoretical elements at the core of the Lie group theory, depends strongly on the transformations considered, in this chapter we will see how they can be applied for the cases of SE(2) and the Lie group of diffeomorphisms parametrized with stationary velocity fields.

3.1 The Lie Group of Rigid Body Transformations

Each element of the group of rigid body transformation (or euclidean group) $SE(2)$ can be computed as the consecutive application of a rotation and a translation applied to any point $(x, y)^T$ of the plane:

$$\begin{pmatrix} X \\ Y \end{pmatrix} = R(\theta) \begin{pmatrix} x \\ y \end{pmatrix} + t = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} t_x \\ t_y \end{pmatrix}$$

where the rotation matrix defined by θ belongs to the special orthogonal group $SO(2)$. We can represent the elements of $SE(2)$ in two different form: as ternary vector (restricted form)

$$SE(2)^v := \{(\theta, t_x, t_y) \mid \theta \in [0, 2\pi), t_x, t_y \in \mathbf{R}^2\}$$

or with matrices (matrix form)

$$SE(2) := \left\{ \begin{pmatrix} R(\theta) & t \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} \cos(\theta) & -\sin(\theta) & t_x \\ \sin(\theta) & \cos(\theta) & t_y \\ 0 & 0 & 1 \end{pmatrix} \mid \theta \in [0, 2\pi), (t_x, t_y) \in \mathbf{R}^2 \right\}$$

The group $SE(2)$ it is a manifold with a differentiable structure compatible with the operation of composition, whose Lie algebra is given in matrix form by (see [Hal15, Gal11] for an introduction).

$$\mathfrak{se}(2) := \left\{ \begin{pmatrix} dR(\theta) & dt \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -\theta & dt_x \\ \theta & 0 & dt_y \\ 0 & 0 & 0 \end{pmatrix} \mid \theta \in [0, 2\pi), (tx, ty) \in \mathbf{R}^2 \right\}$$

and it is indicated with $\mathfrak{se}(2)^v$ in its vector form.

Given r, element of $SE(2)$ with $\theta \neq 0$. Its image with the Lie group logarithm is

$$\log(r) = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{(r-I)^k}{k} = \begin{pmatrix} dR(\theta) & L(\theta)t \\ 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & -\theta & \frac{\theta}{2}\left(\frac{\sin(\theta)}{1-\cos(\theta)}t_x + t_y\right) \\ \theta & 0 & \frac{\theta}{2}\left(-t_x + \frac{\sin(\theta)}{1-\cos(\theta)}t_y\right) \\ 0 & 0 & 0 \end{pmatrix}$$

where therefore

$$dR(\theta) = \begin{pmatrix} 0 & -\theta \\ \theta & 0 \end{pmatrix} \qquad L(\theta) = \frac{\theta}{2} \begin{pmatrix} \frac{\sin(\theta)}{1-\cos(\theta)} & 1 \\ -1 & \frac{\sin(\theta)}{1-\cos(\theta)} \end{pmatrix}$$

On the way back, the exponential of $dr \in \mathfrak{se}(2)$ is given by:

$$\exp(dr) = \sum_{k=1}^{\infty} \frac{dr^k}{k!} = \begin{pmatrix} R(\theta) & L(\theta)^{-1}t \\ 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} \cos(\theta) & -\sin(\theta) & \frac{1}{\theta}(\sin(\theta)dt_x - (1-\cos(\theta))dt_y) \\ \sin(\theta) & \cos(\theta) & \frac{1}{\theta}(-(1-\cos(\theta))dt_x + \sin(\theta)dt_y) \\ 0 & 0 & 1 \end{pmatrix}$$

where

$$L(\theta)^{-1} = \frac{1}{\theta} \begin{pmatrix} \sin(\theta) & -(1 - \cos(\theta)) \\ (1 - \cos(\theta)) & \sin(\theta) \end{pmatrix}$$

When θ is zero, $R(\theta)$ and $dR(\theta)$ coincide with the identity, and the transformation results in a translation. For proof and further details see for example [Gal11] [Hal15].

At this point it is important to notice that:

1. The infinite series of matrices do not raises any theoretical issues, since the sum is defined in the group as subset of a bigger algebra that contains both the Lie group and the Lie algebra. The infinite series of matrices appears to be the natural way to back and forth from the group to the algebra. A second door to passing from one structure to the other, when **r** has a little rotation element appears to be provided by the following approximations:

$$\exp(r) \simeq I + r \qquad \log(dr) \simeq dr - I$$

In fact for little θ, $\sin(\theta) \simeq \theta$, $\cos(\theta) \simeq 0$ and $L(\theta)^{-1} \simeq I$.

2. The map exp is not well defined over its whole domain $\mathfrak{se}(2)$. Given two elements $(\theta_0, dr_{0x}, dr_{0y})$ and $(\theta_1, dr_{1x}, dr_{1y})$, they have the same image with exp function if the two following conditions are both satisfied:

   i) Exists an integer k such that $\theta_0 = \theta_1 + 2k\pi$.
   ii) the translation (dr_{0x}, dr_{0y}) coincides with (dr_{1x}, dr_{1y}) up to a factor $\frac{\theta_0 \mod 2\pi}{\theta_1}$.

   To have a bijective correspondence we have to restrict the domain of exp to a space where if $\exp(\theta_0, dr_{0x}, dt_0y) = \exp(\theta_1, dr_{1x}, dr_{1y})$ it implies $(\theta_0, dr_{0x}, dr_{0y}) = (\theta_1, dr_{1x}, dr_{1y})$. It can be easy to prove that the sought space is the quotient of $\mathfrak{se}(2)$ over the equivalence relation $\sim$, defined as

   $$(\theta_0, dr_{0x}, dr_{0y}) \sim (\theta_1, dr_{1x}, dr_{1y})$$
   $$\overset{\text{def}}{\Longleftrightarrow}$$
   $$\exists k \in \mathbb{Z} \mid \theta_0 = \theta_1 + 2k\pi \quad \text{and} \quad (dr_{0x}, dr_{0y}) = \frac{\theta_0 \mod 2\pi}{\theta_1}(dr_{1x}, dr_{1y})$$

   The new algebra defined by the set of equivalence classes of this relation is indicated - with the standard convention, see [Art11] - with $\mathfrak{se}(2)/\sim$. With this restriction of the domainexp is a bijection having log as its inverse. What said so far can be summarize in the following commutative diagram:
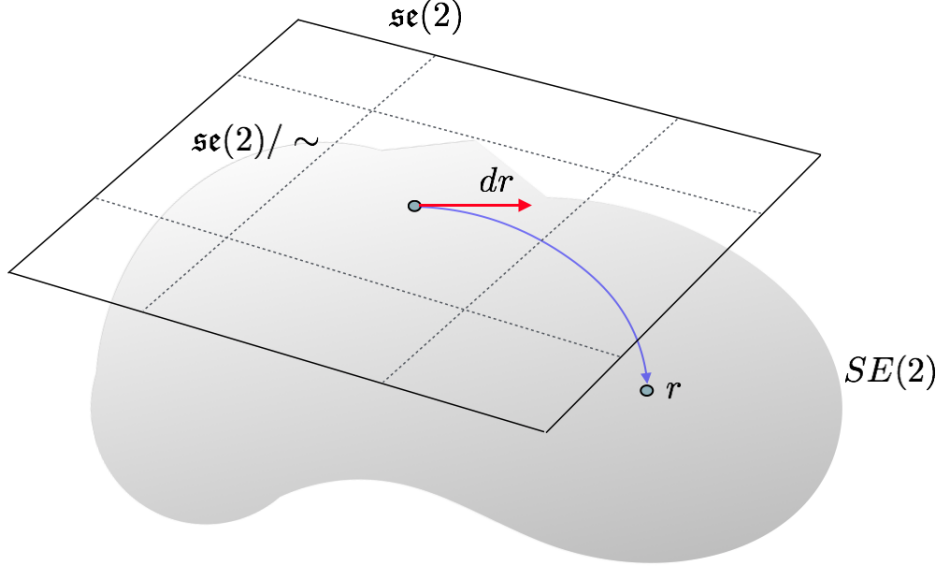

and with the schematic figure 3.1.

Figure 3.1: The Lie algebra $\mathfrak{se}(2)/\sim$ defined as the quotient of the Lie algebra $\mathfrak{se}(2)$ over the equivalence relation $\sim$ is in bijective correspondence with $SE(2)$.

3.1.1 Computations of Log-composition in $\mathfrak{se}(2)$

The log composition of two elements $dr_0 = (\theta_0, dr_{0x}, dr_{0y}), dr_1 = (\theta_1, dr_{1x}, dr_{1y})$ in $\mathfrak{se}(2)/\sim$ is provided as a direct applications of the definitions provided for this case. It results

$$dr_0 \oplus dr_1 = \log(\exp(dr_0) \circ \exp(dr_1)) \tag{3.1}$$

for the computation of the ground truth.
The approximations of the log-composition using truncated BCH formulas are straightforward:

$$dr_0 \oplus dr_1 \simeq BCH^0(dr_0, dr_1) = dr_0 + dr_1$$

$$dr_0 \oplus dr_1 \simeq BCH^1(dr_0, dr_1) = dr_0 + dr_1 + \frac{1}{2}[dr_0, dr_1]$$

$$dr_0 \oplus dr_1 \simeq BCH^2(\mathbf{u}, \mathbf{v}) = dr_0 + dr_1 + \frac{1}{2}[dr_0, dr_1] + \frac{1}{12}([dr_0, [dr_0, dr_1]] + [dr_1, [dr_1, dr_0]])$$

To compute the approximation with the Taylor method, and so to compute the equation 2.7, we observe that the vector form of the Lie bracket is given by

$$[dr_0, dr_1] = (0, dR(\theta_0)dt_1 - dR(\theta_1)dt_0)^T$$
$$= (0, -\theta_0 dr_{1y} + \theta_1 dr_{0y}, \theta_0 dr_{1x} - \theta_1 dr_{0x})^T$$

Therefore, the adjoint operator can be written in matrix form as a dual matrix of dr:

$$\mathrm{ad}_{dr} = \begin{pmatrix} 0 & 0 & 0 \\ dr_y & 0 & -\theta \\ -dr_x & \theta & 0 \end{pmatrix}$$

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In fact, when applied to dr_1 it results in the Lie bracket:

$$\mathrm{ad}_{dr_0}dr_1 = \begin{pmatrix} 0 & 0 & 0 \\ dr_{0y} & 0 & -\theta_0 \\ -dr_{0x} & \theta_0 & 0 \end{pmatrix} \begin{pmatrix} \theta_1 \\ dt_{1x} \\ dt_{1y} \end{pmatrix} = \begin{pmatrix} 0 \\ -\theta_0 dt_{1y} + \theta_1 dt_{0y} \\ \theta_0 dt_{1x} - \theta_1 dt_{0x} \end{pmatrix}$$

To compute the Taylor approximation proposed in equation 2.7 of the log composition, indicating $dt^\star = (dt_y, -dt_x)$ it can be proved easily by induction that

$$\mathrm{ad}_{dr}^n = \begin{pmatrix} 0 & 0 \\ dt^\star & dR(\theta) \end{pmatrix}^n = \begin{pmatrix} 0 & 0 \\ dR(\theta)^{n-1}dt^\star & dR(\theta)^n \end{pmatrix}$$

And so the series involved in the equation 2.7 become

$$\sum_{n=0}^{\infty} \frac{B_n}{n!}\mathrm{ad}_{dr}^n = \sum_{n=0}^{\infty} \frac{B_n}{n!} \begin{pmatrix} 0 & 0 \\ dR(\theta)^{n-1}dt^\star & dR(\theta)^n \end{pmatrix}$$

We can split it in two part, the rotational part and the translational part. The rotational part, using the nature of Bernoulli numbers and its generative equation, when $\theta \neq 0$ become

$$\sum_{n=0}^{\infty} \frac{B_n}{n!}dR(\theta)^n = I + \frac{1}{2}dR(\theta) + \sum_{n=1}^{\infty} \frac{B_{2n}}{2n!}dR(\theta)^{2n}$$

$$= I + \frac{1}{2}dR(\theta) + \left(\sum_{n=1}^{\infty} \frac{B_{2n}}{2n!}(i\theta)^{2n}\right)I$$

$$= \frac{1}{2}dR(\theta) + \left(\sum_{n=0}^{\infty} \frac{B_n}{n!}(i\theta)^n - \frac{1}{2}i\theta\right)I$$

$$= \frac{1}{2}dR(\theta) + \left(\sum_{n=0}^{\infty} \frac{i\theta e^{i\theta}}{e^{i\theta} - 1} - \frac{1}{2}i\theta\right)I$$

$$= \frac{1}{2}dR(\theta) + \frac{\theta/2}{\tan(\theta/2)}I$$

while for the translational part

$$\sum_{n=1}^{\infty} \frac{B_n}{n!}dR(\theta)^{n-1}dt^\star = dR(\theta)^{-1}\left(\sum_{n=1}^{\infty} \frac{B_n}{n!}dR(\theta)^n\right)dt^\star$$

$$= dR(\theta)^{-1}\left(\sum_{n=0}^{\infty} \frac{B_n}{n!}dR(\theta)^n - I\right)dt^\star$$

$$= dR(\theta)^{-1}\left(\sum_{n=0}^{\infty} \frac{1}{2}dR(\theta) + \frac{\theta/2}{\tan(\theta/2)}I - I\right)dt^\star$$

$$= dR(\theta)^{-1}\left(\sum_{n=0}^{\infty} \frac{1}{2}dR(\theta) + \frac{\theta/2}{\tan(\theta/2)}I - I\right)dt^\star$$

$$= \left(\frac{1}{2}I + \left(\frac{\theta/2}{\tan(\theta/2)} - 1\right)dR(\theta)^{-1}\right)dt^\star$$

Finally the closed form for the Taylor approximation of the log-composition is [Ver14]:

$$dr_0 \oplus dr_1 = dr_0 + \sum_{n=0}^{\infty} \frac{B_n}{n!}\mathrm{ad}_{dr_0}^n dr_1 + \mathcal{O}(dr_1^2) = dr_0 + \mathbf{J}(dr_0, dr_1)dr_1 + \mathcal{O}(dr_1^2) \qquad (3.2)$$

where

$$\mathbf{J}(dr_0, dr_1) = \begin{pmatrix} 1 & 0 & 0 \\ -\frac{\theta_0/2 - \tan(\theta_0/2)}{\theta_0 \tan(\theta_0/2)} dr_{0x} + \frac{1}{2} dr_{0y} & \frac{\theta_0/2}{\tan(\theta_0/2)} & -\theta_0/2 \\ -\frac{1}{2} dr_{0x} - \frac{\theta_0/2 - \tan(\theta_0/2)}{\theta_0 \tan(\theta_0/2)} dr_{0y} & \theta_0/2 & \frac{\theta_0/2}{\tan(\theta_0/2)} \end{pmatrix}$$

The approximation of the log-composition using parallel transport is a straightforward application of the equation 2.8:

$$dr_0 \oplus dr_1 \simeq dr_0 + \exp\left(\frac{dr_0}{2}\right) \exp(dr_1) \exp\left(-\frac{dr_0}{2}\right) - I \tag{3.3}$$

where the composition in the Lie group coincides with the product of matrix in the bigger algebra $GL(3)$ that contains both the Lie group $SE(2)$ and the Lie algebra $\mathfrak{se}(2)$.

3.2 One-parameter Subgroup Generated by Stationary Velocity Fields

As previously said, the passage from the finite to the infinite dimensional case is not free of deceptions. For the particular case of diffeomorphisms over the compact subset $\Omega \subset \mathbb{R}^d$, indicated with $Diff(\Omega)$, the exponential map is not a local bijection (see the counterexample in [LP13], pag. 6 or the definition of Koppel-diffeomorphisms [Gra88] pag. 115). We will consider only the subset G of $Diff(\Omega)$ that are in the image of the exponential function exp, or, in other world, the diffeomorphisms that belongs to the one-parameter subgroup.
If we indicate with G the one-parameter subgroup of $Diff(\Omega)$, each of the element of G are generated by a tangent vector field in $\mathcal{C}^\infty(\Omega)$ (see definitions in subsection 1.2.2) through an ordinary differential equation (see [Arn06]). These generating tangent vector field can be divided into two classes that split the ODE in two classes:

1. Stationary - or homogeneous

$$\frac{d\varphi(t)}{dt} = V_{\varphi(t)}$$

2. Non-stationary - or non-homogeneous

$$\frac{d\varphi(t)}{dt} = V_{(t,\varphi(t))}$$

For a fixed t both the stationary vector field (or SVF) $V_{\varphi(t)}$ and the time varying vector field (or TVVF) $V_{(t,\varphi(t))}$ belong to G. When varying t, the TVVFs behave as continuous paths over the tangent vector field, corresponding to the one-parameter subgroup G through the map exp.
Thanks to the Cauchy theorem that ensures the uniqueness of the solution of the ODE under the initial condition $\varphi(0) = e$, the local bijection between G and the Lie algebra of the tangent vector fields over Ω is ensured (see [Mil82], [KW08]):

$$\mathcal{V}(\Omega) \simeq G \subset \mathrm{Diff}(\Omega)$$

and, as consequence of the definition of exp and log it follows that

$$G = \exp(\mathcal{V}(\Omega))$$
$$\mathcal{V}(\Omega) = \log(G)$$

In the LDDMM framework (see section 1.2.2) only TVVFs are considered, while after subsequent paper of [ACPA06a] only SVF has been considered for practical applications.
For our purposes when talking about diffeomorphisms, we will take into account only the one-parameter subgroup G, or in other world the image of a SVF through the exp map.

3.2.1 Computations of Log-composition for SVF

A closed-form for the Taylor Expansion method 2.4.2 to compute the log-composition with SVF is not known. We will therefore compare the truncated BCH formula with the parallel transport method 2.3. Since there is closed form for the log-composition, we will exploit the parametrization of discretized SVF using matrices to have a ground truth to compare results. Norm will be computed in the group as the L_2 norm of matrices that represents the SVF.
Given $\mathbf{u}$ and $\mathbf{v}$ SVF, $\mathbf{w}_{\text{ground}} = \mathbf{u} \oplus \mathbf{v}$ solution of the log-composition and $\mathbf{w}_{\text{app}}$ its approximation using a numerical method, then their difference is computed in the group as:

$$\text{error} = ||\exp(\mathbf{w}_{\text{ground}}) - \exp(\mathbf{w}_{\text{app}})||_{L^2}$$

where $\exp(\mathbf{w}_{\text{ground}})$ is computed as the composition of the exponentials of $\mathbf{u}$ and $\mathbf{v}$:

$$\exp(\mathbf{w}_{\text{ground}}) = \exp(\mathbf{u}) \circ \exp(\mathbf{v})$$

As previously said, the norm L^2 is considered improperly in a group structure. It can be done only thanks to the fact that the discrete SVF are implemented with 5-dimensional matrices (see equation 1.3).

Further details about the methodology utilized to compare log-composition for SVF will be provided in chapter 5.

Chapter 4

Log-computation Algorithm using Log-composition

> I think you might do something better with the time
> than wasting it in asking riddles that have no answers.
> *-Alice in Wonderland.*

The *logarithm computation problem* can be stated as follows:

> *Given p in a Lie group $\mathbb{G}$,*
> *what is the element $\mathbf{u}$ in its Lie algebra $\mathfrak{g}$*
> *such that $\exp(\mathbf{u}) = p$?*

This chapter is devote to the numerical computation of the logarithm, based on an iterative algorithm called here *log-computation algorithm* [BO08]. Since the log-computation algorithm is based on the log-composition, each of the numerical methods presented in these pages can be applied to find a numerical method to solve the logarithm computation problem.

The first step toward this direction is to introduce the space of the approximations of a Lie algebra and a the Lie group.

4.1   Spaces of Approximations

As seen in section 3.1 of the previous chapter for the particular case of $SE(2)$, if the matrix dr is small enough we can approximate $\exp(dr)$ with $1 + dr$. Aim of this section is to generalize the same approximation for the SVF.

We define two approximating functions:

$$\mathrm{app} : \mathfrak{g} \longrightarrow \mathfrak{g}^{\sim}$$
$$\mathbf{u} \longmapsto \exp(\mathbf{u}) - 1$$

$$\mathrm{App} : \mathbb{G} \longrightarrow \mathbb{G}^{\sim}$$
$$\exp(\mathbf{u}) \longmapsto 1 + \mathbf{u}$$

Where $\mathfrak{g}^\sim$ is the space of approximations of elements of $\mathfrak{g}$, and $\mathbb{G}^\sim$ is the space of approximations of elements in $\mathbb{G}$, defined as

$$\mathfrak{g}^\sim := \{\exp(\mathbf{u}) - 1 \mid \mathbf{u} \in \mathfrak{g}\} \cup \mathfrak{g}$$
$$\mathbb{G}^\sim := \{1 + \mathbf{u} \mid \mathbf{u} \in \mathbb{G}\} \cup \mathbb{G}$$

In general $\mathfrak{g}^\sim \neq \mathfrak{g}$ and $\mathbb{G}^\sim \neq \mathbb{G}$, but in the considered cases of $\mathfrak{se}(2)$ and SVF, when $\mathbf{u}$ is *small enough* it follows that $\exp(\mathbf{u}) - 1 \in \mathfrak{g}$ and $1 + \mathbf{u} \in \mathbb{G}$. Therefore the elements of $\mathfrak{g}^\sim$ are compatible with all of the operations of Lie algebra $\mathfrak{g}$ and the elements of $\mathbb{G}^\sim$ are compatible with all of the operations of Lie group $\mathbb{G}$.

Lets examine what does *small enough* means in these two cases:

$\mathfrak{se}(2)$ - Since $\mathfrak{se}(2)$ and $SE(2)$ are subset of the bigger algebra $SE(2)$ then exp and log can be defined as infinite series. From

$$\exp(\mathbf{u}) = I + \mathbf{u} + O(\mathbf{u}^2)$$

It follows that $\text{app}(\mathbf{u}) - \mathbf{u} = O(\mathbf{u}^2)$. Thus for all $\mathbf{u}$ smaller than δ for any norm, exists $M(\delta)$ such that

$$||\text{app}(\mathbf{u}) - \mathbf{u}|| < M(\delta)||\mathbf{u}^2||$$

SVF - In case of SVF we do not have any Taylor series and big-O notation available but, according to the proposition 8.6 at page 163 of [You10], if $\mathbf{u}$ is, for any norm, smaller than $\epsilon < 1/C$, where C is the Lipschitz constant of the same norm, then $e + \mathbf{u}$ is a diffeomorphism. With this condition holds that $\text{SVF}^\sim = \text{SVF}$.

Therefore, for each small enough $\mathbf{u}$ in $\mathfrak{se}(2)$ or SVF, and considering the definition of the log-composition (equation 2.1) the following properties holds:

1. The approximations $\mathbf{u} \simeq \text{app}(\mathbf{u})$, $\exp(\mathbf{u}) \simeq \text{App}(\exp(\mathbf{u}))$ are meaningful.

2. $\mathbf{u} = \mathbf{v} \oplus (-\mathbf{v} \oplus \mathbf{u})$

3. $\text{app}(\mathbf{v} \oplus \mathbf{u}) = \exp(\mathbf{v})\exp(\mathbf{u}) - 1 \in \mathfrak{g}^\sim$

With this machinery, we can finally reformulate the algorithm presented in [BO08] for the numerical computation of the Lie logarithm map using the log-composition.

4.2 The Log-computation Algorithm using Log-composition

If the goal is to find $\mathbf{u}$ when its exponential is known, we can consider the sequence transformations $\{\mathbf{u}_j\}_{j=0}^\infty$ that approximate $\mathbf{u}$ as consequence of

$$\mathbf{u} = \mathbf{u}_j \oplus (-\mathbf{u}_j \oplus \mathbf{u}) \implies \mathbf{u} \simeq \mathbf{u}_j \oplus \text{app}(-\mathbf{u}_j \oplus \mathbf{u})$$

This suggest that a reasonable approximation for the $(j+1)$-th element of the series can be defined by

$$\mathbf{u}_{j+1} := \mathbf{u}_j \oplus \text{app}(-\mathbf{u}_j \oplus \mathbf{u})$$

If we chose the initial value $\mathbf{u}_0$ to be zero, then the algorithm presented in [BO08] become:

$$\begin{cases} \mathbf{u}_0 = 0 \\ \mathbf{u}_{j+1} = \mathbf{u}_j \oplus \text{app}(-\mathbf{u}_j \oplus \mathbf{u}) \end{cases} \tag{4.1}$$

Each strategy that we have examined to compute the Lie composition, become a numerical method for the computation of the logarithm.

4.2.1 Truncated BCH Strategy

At each step, we compute the approximation $\mathbf{v}_{j+1}$ with the k-th truncation of the BCH formula:

$$\begin{cases} \mathbf{u}_0 = 0 \\ \mathbf{u}_{j+1} = \mathrm{BCH}^k(\mathbf{u}_j, \mathrm{app}(-\mathbf{u}_j \oplus \mathbf{u})) \end{cases} \tag{4.2}$$

thus, for $k = 1$ results

$$\begin{aligned} \mathrm{BCH}^1(\mathbf{u}_j, \mathrm{app}(-\mathbf{u}_j \oplus \mathbf{u})) &= \mathbf{u}_j + \mathrm{app}(-\mathbf{u}_j \oplus \mathbf{u}) \\ &= \mathbf{u}_j + \exp(-\mathbf{u}_j)\exp(\mathbf{u}) - 1 \end{aligned}$$

And $k = 2$ it follows

$$\begin{aligned} \mathrm{BCH}^2(\mathbf{u}_j, \mathrm{app}(-\mathbf{u}_j \oplus \mathbf{u})) &= \mathbf{u}_j + \mathrm{app}(-\mathbf{u}_j \oplus \mathbf{u}) + \frac{1}{2}[\mathbf{u}_j, \mathrm{app}(-\mathbf{u}_j \oplus \mathbf{u})] \\ &= \mathbf{u}_j + \exp(-\mathbf{u}_j)\exp(\mathbf{u}) - 1 + \\ &\quad + \frac{1}{2}(\mathbf{u}_j(\exp(-\mathbf{u}_j)\exp(\mathbf{u}) - 1) - (\exp(-\mathbf{u}_j)\exp(\mathbf{u}) - 1)\mathbf{u}_j) \end{aligned}$$

The following theorem presented in [BO08], provides an error bound when $k = \infty$ so when the BCH formula is used, instead one of its truncation.

Theorem 4.2.1 (Bossa)**.** The iterative algorithm

$$\begin{cases} \mathbf{u}_0 = 0 \\ \mathbf{u}_{j+1} = \mathrm{BCH}(\mathbf{u}_j, \mathrm{app}(-\mathbf{u}_j \oplus \mathbf{u})) = \mathbf{u}_j \oplus \mathrm{app}(-\mathbf{u}_j \oplus \mathbf{u}) \end{cases} \tag{4.3}$$

converges to $\mathbf{v}$ with error $\delta_n \in \mathbb{G}$, where

$$\delta_n := \log(\exp(\mathbf{v}) \circ \exp(-\mathbf{v}_n)) \in O(||p - e||^{2^n})$$

We observe that this upper limit holds only when a closed-form for the log-composition is available, as for example $\mathfrak{se}(2)$.

4.2.2 Parallel Transport Strategy

If we apply the parallel transport method for the computation of the log-composition, we obtain another version of the log-computation algorithm:

$$\begin{cases} \mathbf{u}_0 = \mathbf{0} \\ \mathbf{u}_t = \mathbf{u}_{t-1} + \exp(\frac{\mathbf{u}_{t-1}}{2}) \circ \exp(\delta \mathbf{u}_{t-1}) \circ \exp(-\frac{\mathbf{u}_{t-1}}{2}) - e \end{cases} \tag{4.4}$$

We notice that mixing the operation of composition, sum and scalar product makes sense when the involved vectors are *small enough*, as stated in 4.1. Analytical computation of an upper bound error is not straightforward in this case. See section 5.3 for further details and other possible researches.

4.2.3 Symmetrization Strategy

The algorithm 4.1 could have been reformulated alternatively as $\mathbf{u}_{j+1} = \mathrm{app}(\mathbf{u} \oplus -\mathbf{u}_j) \oplus \mathbf{u}_j$. The log-composition is not symmetric therefore the two version in some cases may not return the same value. In an attempt to move toward the solution of this issue we consider

$$\begin{cases} \mathbf{u}_0 = 0 \\ \mathbf{u}_{j+1} = \mathbf{u}_j \oplus \frac{1}{2}\big(\mathrm{app}(-\mathbf{u}_j \oplus \mathbf{u}) + \mathrm{app}(\mathbf{u} \oplus -\mathbf{u}_j)\big) \end{cases} \tag{4.5}$$

Writing directly the approximations and using the BCH approximation of degree 1 it become:

$$\begin{cases} \mathbf{u}_0 = 0 \\ \mathbf{u}_{j+1} = \mathbf{u}_j + \frac{1}{2}\big(\exp(-\mathbf{u}_j)\exp(\mathbf{u}) - e + \exp(\mathbf{u})\exp(-\mathbf{u}_j) - e \big) \end{cases} \qquad (4.6)$$

Experimental results of the methods presented in this section are presented in the next chapter.

Chapter 5

Experimental Results

> *"A victory is twice itself when the achiever brings home full numbers."*
> Much ado about nothing, *Leonato, scene 1.*

In this chapter we show the present the application of the numerical methods presented in 4 to the transformations presented in 3.

5.1 Methods

5.1.1 Log-composition for $\mathfrak{se}(2)$

5.1.2 Log-composition for SVF

Using a python software, we created synthetic random matrices in $\mathfrak{se}(2)$. We considered the difference between the log composition computed with the closed form 3.1. A sample of 500 couples (dr_0, dr_1) of elements in $\mathfrak{se}(2)$ are created,

5.1.3 Log-computation Algorithm

5.2 Results

5.2.1 Log-composition for $\mathfrak{se}(2)$

5.2.2 Log-composition for SVF

5.2.3 Log-computation Algorithm

5.3 Conclusion and Further Research

Considering only the results, this one-year research can be considered much ado about nothing, but...

Computational time...!

Bibliography

[ACPA06a]   Vincent Arsigny, Olivier Commowick, Xavier Pennec, and Nicholas Ayache. A
            log-euclidean framework for statistics on diffeomorphisms. In *Medical Image
            Computing and Computer-Assisted Intervention–MICCAI 2006*, pages 924–
            931. Springer, 2006.

[ACPA06b]   Vincent Arsigny, Olivier Commowick, Xavier Pennec, and Nicholas Ayache.
            Statistics on diffeomorphisms in a log-euclidean framework. In *1st MICCAI
            Workshop on Mathematical Foundations of Computational Anatomy: Geomet-
            rical, Statistical and Registration Methods for Modeling Biological Shape Vari-
            ability*, pages 14–15, 2006.

[AFPA06]   Vincent Arsigny, Pierre Fillard, Xavier Pennec, and Nicholas Ayache. Log-
            Euclidean metrics for fast and simple calculus on diffusion tensors. *Magnetic
            Resonance in Medicine*, 56(2):411–421, August 2006.

[APA06]   Vincent Arsigny, Xavier Pennec, and Nicholas Ayache. Bi-invariant means in
            lie groups. application to left-invariant polyaffine transformations. 2006.

[Arn66]   Vladimir Arnold. Sur la géométrie différentielle des groupes de lie de dimension
            infinie et ses applications à l'hydrodynamique des fluides parfaits. In *Annales
            de l'institut Fourier*, volume 16, pages 319–361. Institut Fourier, 1966.

[Arn98]   Vladimir Igorevich Arnold. *Topological methods in hydrodynamics*, volume 125.
            Springer Science & Business Media, 1998.

[Arn06]   Vladimir I Arnold. Ordinary differential equations. translated from the russian
            by roger cooke. second printing of the 1992 edition. universitext, 2006.

[Art11]   Michael Artin. Algebra. 2nd, 2011.

[Ash07]   J. Ashburner. A fast diffeomorphic image registration algorithm. *NeuroImage*,
            38(1):95–113, 2007.

[BBHM11]   MARTIN BAUER, MARTINS BRUVERIS, PHILIPP HARMS, and PE-
            TER W MICHOR. Geodesic distance for right invariant sobolev metrics of
            fractional order on the diffeomorphism group. 2011.

[BHM10]   Martin Bauer, Philipp Harms, and Peter W Michor. Sobolev metrics on shape
            space of surfaces in n-space. *Arxiv preprint arXiv:1009.3616*, 2010.

[BMTY05]   M Faisal Beg, Michael I Miller, Alain Trouvé, and Laurent Younes. Comput-
            ing large deformation metric mappings via geodesic flows of diffeomorphisms.
            International journal of computer vision, 61(2):139–157, 2005.

[BO08]   Matias Bossa and Salvador Olmos. A New Algorithm for the Computation of the Group Logarithm of Diffeomorphisms. In Xavier Pennec and Sarang Joshi, editors, *Second International Workshop on Mathematical Foundations of Computational Anatomy - Geometrical and Statistical Methods for Modelling Biological Shape Variability*, New York, USA, 2008.

[Bro81]   Chaim Broit. *Optimal Registration of Deformed Images*. PhD thesis, Philadelphia, PA, USA, 1981. AAI8207933.

[CBD+03]   Pascal Cachier, Eric Bardinet, Didier Dormont, Xavier Pennec, and Nicholas Ayache. Iconic feature based nonrigid registration: the pasha algorithm. *Computer vision and image understanding*, 89(2):272–298, 2003.

[CRM96]   Gary E Christensen, Richard D Rabbitt, and Michael I Miller. Deformable templates using large deformation kinematics. *Image Processing, IEEE Transactions on*, 5(10):1435–1447, 1996.

[DCDC76]   Manfredo Perdigao Do Carmo and Manfredo Perdigao Do Carmo. *Differential geometry of curves and surfaces*, volume 2. Prentice-hall Englewood Cliffs, 1976.

[dCV92]   Manfredo Perdigao do Carmo Valero. *Riemannian geometry*. 1992.

[DGM98]   Paul Dupuis, Ulf Grenander, and Michael I. Miller. Variational problems on flows of diffeomorphisms for image matching, 1998.

[EM70]   David G Ebin and Jerrold Marsden. Groups of diffeomorphisms and the motion of an incompressible fluid. *Annals of Mathematics*, pages 102–163, 1970.

[EMP06]   DAVID G Ebin, GERARD Misiołek, and STEPHEN C Preston. Singularities of the exponential map on the volume-preserving diffeomorphism group. *Geometric and Functional Analysis*, 16(4):850–868, 2006.

[FF97]   Nick C Fox and Peter A Freeborough. Brain atrophy progression measured from registered serial mri: validation and application to alzheimer's disease. *Journal of Magnetic Resonance Imaging*, 7(6):1069–1075, 1997.

[Gal11]   Jean Gallier. *Geometric methods and applications: for computer science and engineering*, volume 38. Springer Science & Business Media, 2011.

[GM98]   Ulf Grenander and Michael I Miller. Computational anatomy: An emerging discipline. *Quarterly of applied mathematics*, 56(4):617–694, 1998.

[Gra88]   Janusz Grabowski. Free subgroups of diffeomorphism groups. *Fundamenta Mathematicae*, 2(131):103–121, 1988.

[GWRNJ12]   Serge Gauthier, Liyong Wu, Pedro Rosa-Neto, and Jianping Jia. Prevention strategies for alzheimer's disease. *Translational neurodegeneration*, 1(1):1–4, 2012.

[Hal15]   Brian Hall. *Lie groups, Lie algebras, and representations: an elementary introduction*, volume 222. Springer, 2015.

[HBO07]   Monica Hernandez, Matias N Bossa, and Salvador Olmos. Registration of anatomical images using geodesic paths of diffeomorphisms parameterized with stationary vector fields. In *Computer Vision, 2007. ICCV 2007. IEEE 11th International Conference on*, pages 1–8. IEEE, 2007.

[HOP08]   Monica Hernandez, Salvador Olmos, and Xavier Pennec. Comparing algorithms for diffeomorphic registration: Stationary lddmm and diffeomorphic demons. In *2nd MICCAI workshop on mathematical foundations of computational anatomy*, pages 24–35, 2008.

[KKK08]   Alexander A Kirillov, Aleksandr Aleksandrovič Kirillov, and Aleksandr Aleksandrovič Kirillov. *An introduction to Lie groups and Lie algebras*, volume 113. Cambridge University Press Cambridge, 2008.

[KMN00]   Arkady Kheyfets, Warner A Miller, and Gregory A Newton. Schild's ladder parallel transport procedure for an arbitrary connection. *International Journal of Theoretical Physics*, 39(12):2891–2898, 2000.

[Kne51]   MS Knebelman. Spaces of relative parallelism. *Annals of Mathematics*, pages 387–399, 1951.

[KO89]   S Klarsfeld and JA Oteo. The baker-campbell-hausdorff formula and the convergence of the magnus expansion. *Journal of physics A: mathematical and general*, 22(21):4565, 1989.

[KW08]   Boris Khesin and Robert Wendt. *The geometry of infinite-dimensional groups*, volume 51. Springer Science & Business Media, 2008.

[LAF+13]   Marco Lorenzi, Nicholas Ayache, Giovanni B Frisoni, Xavier Pennec, and Alzheimer's Disease Neuroimaging Initiative. LCC-Demons: a robust and accurate symmetric diffeomorphic registration algorithm. *NeuroImage*, 81:470–483, 2013.

[LAP11]   Marco Lorenzi, Nicholas Ayache, and Xavier Pennec. Schild's ladder for the parallel transport of deformations in time series of images. In *Information Processing in Medical Imaging*, pages 463–474. Springer, 2011.

[Lee12]   John Lee. *Introduction to smooth manifolds*, volume 218. Springer Science & Business Media, 2012.

[Les83]   JA Leslie. A lie group structure for the group of analytic diffeomorphisms. *Boll. Un. Mat. Ital. A (6)*, 2:29–37, 1983.

[LP13]   Marco Lorenzi and Xavier Pennec. Geodesics, parallel transport & one-parameter subgroups for diffeomorphic image registration. *International journal of computer vision*, 105(2):111–127, 2013.

[LP14a]   Marco Lorenzi and Xavier Pennec. Discrete Ladders for Parallel Transport in Transformation Groups with an Affine Connection Structure. In Frank Nielsen, editor, *Geometric Theory of Information*, Signals and Communication Technology, pages 243–271. Springer, 2014.

[LP14b]   Marco Lorenzi and Xavier Pennec. Efficient parallel transport of deformations in time series of images: from schild's to pole ladder. *Journal of Mathematical Imaging and Vision*, 50(1-2):5–17, 2014.

[MA70]   J Marsden and R Abraham. Hamiltonian mechanics on lie groups and hydrodynamics. *Global Analysis,(eds. SS Chern and S. Smale), Proc. Sympos. Pure Math*, 16:237–244, 1970.

[MHM+11]   JR McClelland, S Hughes, M Modat, A Qureshi, S Ahmad, DB Landau, S Ourselin, and DJ Hawkes. Inter-fraction variations in respiratory motion models. *Physics in medicine and biology*, 56(1):251, 2011.

[MHSK]   J. R. McClelland, D. J. Hawkes, T. Schaeffter, and A. P. King. Respiratory motion models: A review. *Medical Image Analysis*, 17(1):19–42, 2015/04/01.

[Mil82]   John Milnor. On infinite dimensional lie groups. *Preprint, Institute for Advanced Study, Princeton*, 1982.

[Mil84a]   J Milnor. Remarks on infinite-dimensional lie groups, in 'relativity, groups and topology, ii'(les houches, 1983), 1007–1057, 1984.

[Mil84b]   John Milnor. Remarks on infinite-dimensional lie groups. In *Relativity, groups and topology. 2.* 1984.

[MT13]   Carlo Mariconda and Alberto Tonolo. *Calcolo discreto: Metodi per contare.* Apogeo Editore, 2013.

[MTW73]   Charles W Misner, Kip S Thorne, and John Archibald Wheeler. *Gravitation.* Macmillan, 1973.

[OKC92]   V Yu Ovsienko, BA Khesin, and Yu V Chekanov. Integrals of the euler equations of multidimensional hydrodynamics and superconductivity. *Journal of Soviet Mathematics*, 59(5):1096–1101, 1992.

[Omo70]   Hideki Omori. On the group of diffeomorphisms on a compact manifold. In *Proc. Symp. Pure Appl. Math., XV, Amer. Math. Soc*, pages 167–183, 1970.

[PCA99]   Xavier Pennec, Pascal Cachier, and Nicholas Ayache. Understanding the "demon's algorithm": 3d non-rigid registration by gradient descent. In *Medical Image Computing and Computer-Assisted Intervention–MICCAI'99*, pages 597–605. Springer, 1999.

[PCL+15]   Ferran Prados, Manuel Jorge Cardoso, Kelvin K Leung, David M Cash, Marc Modat, Nick C Fox, Claudia AM Wheeler-Kingshott, Sebastien Ourselin, Alzheimer's Disease Neuroimaging Initiative, et al. Measuring brain atrophy with a generalized formulation of the boundary shift integral. *Neurobiology of aging*, 36:S81–S90, 2015.

[PL+11]   Xavier Pennec, Marco Lorenzi, et al. Which parallel transport for the statistical analysis of longitudinal deformations. In *Proc. Colloque GRETSI*. Citeseer, 2011.

[Sch10]   Rudolf Schmid. Infinite-dimensional lie groups and algebras in mathematical physics. *Advances in Mathematical Physics*, 2010, 2010.

[SDP13]   A. Sotiras, C. Davatzikos, and N. Paragios. Deformable medical image registration: A survey. *Medical Imaging, IEEE Transactions on*, 32(7):1153–1190, July 2013.

[Ser09]   Jean-Pierre Serre. *Lie algebras and Lie groups: 1964 lectures given at Harvard University.* Springer, 2009.

[SS09]   Elias M Stein and Rami Shakarchi. *Real analysis: measure theory, integration, and Hilbert spaces.* Princeton University Press, 2009.

[Sze94]   Richard Szeliski. Image mosaicing for tele-reality applications. In *Applications of Computer Vision, 1994., Proceedings of the Second IEEE Workshop on*, pages 44–53. IEEE, 1994.

[Thi98]   J-P Thirion. Image matching as a diffusion process: an analogy with maxwell's demons. *Medical image analysis*, 2(3):243–260, 1998.

[Tro98]   Alain Trouvé. Diffeomorphisms groups and pattern matching in image analysis. *International Journal of Computer Vision*, 28(3):213–221, 1998.

[Ver14]   Tom Vercauteren. Technical memo. Pre-print, 2014.

[VPM⁺06]   Tom Vercauteren, Aymeric Perchant, Grégoire Malandain, Xavier Pennec, and Nicholas Ayache. Robust mosaicing with correction of motion distortions and tissue deformations for in vivo fibered microscopy. *Medical image analysis*, 10(5):673–692, 2006.

[VPPA07]   Tom Vercauteren, Xavier Pennec, Aymeric Perchant, and Nicholas Ayache. Non-parametric diffeomorphic image registration with the demons algorithm. In *Medical Image Computing and Computer-Assisted Intervention–MICCAI 2007*, pages 319–326. Springer, 2007.

[VPPA08]   Tom Vercauteren, Xavier Pennec, Aymeric Perchant, and Nicholas Ayache. Symmetric log-domain diffeomorphic registration: A demons-based approach. In Dimitris N. Metaxas, Leon Axel, Gabor Fichtinger, and Gábor Székely, editors, *Medical Image Computing and Computer-Assisted Intervention - MICCAI 2008, 11th International Conference, New York, NY, USA, September 6-10, 2008, Proceedings, Part I*, volume 5241 of *Lecture Notes in Computer Science*, pages 754–761. Springer, 2008.

[VRRC12]   François-Xavier Vialard, Laurent Risser, Daniel Rueckert, and Colin J Cotter. Diffeomorphic 3d image registration via geodesic shooting using an efficient adjoint calculation. *International Journal of Computer Vision*, 97(2):229–241, 2012.

[War13]   Frank W Warner. *Foundations of differentiable manifolds and Lie groups*, volume 94. Springer Science & Business Media, 2013.

[Woj94]   Wojciech Wojtyński. One-parameter subgroups and the bch formula. *Studia Mathematica*, 111(2):163–185, 1994.

[You10]   Laurent Younes. Shapes and diffeomorphisms, volume 171 of applied mathematical sciences, 2010.

[ZF03]   Barbara Zitova and Jan Flusser. Image registration methods: a survey. *Image and vision computing*, 21(11):977–1000, 2003.