

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

Sebastiano Ferraris



Universtiy College London
Medical Physiscs and Biomedical Engineering

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Supervisor
Tom Vercauteren

Co-Supervisor
Marc Modat

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 these techniques, 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. Main challenges of this setting are the numerical computation of the Lie logarithm and Lie exponential, 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.

Thesis' Organization

- Chapter 1** The first chapter is devoted to the introduction of diffeomorphic image registration and the main recent advancements. Here are introduced advantages and disadvantages of using diffeomorphisms as well as some of the milestone frameworks that led to, or are directly affected by the log-composition.
- Chapter 2** The second one is the chapter of mathematical elements and tools; called from Lie group theory and hired to service image registration, techniques and tools are formally defined with a particular attention to flows, left translation, push forward, Lie logarithm, Lie exponential, connections and parallel transport. The concept of log-composition, around which the research gravitates, is defined as consequence of the need of generalize the BCH formula. Since its computation is impractical, other paths as Taylor expansion, parallel transport and accelerating convergence series are proposed as feasible alternatives.
- Chapter 3:** Each of the numerical methods for the computation of the log-composition are not computed and tested directly on the group of diffeomorphisms. Initially it they are applied to the finite dimensional group of rigid body transformation, where logarithms and exponentials possess a closed form. This chapter is aimed to present the customization of the tools defined in the previous chapter for the group of rigid body transformation and for the group of diffeomorphisms.
- Chapter 4:** Since the algorithm to compute the logarithm (here called *log-computation algorithm*) presented in [BHO07] relies on the BCH formula, the log-composition provides a range of methodologies for its computation. Each of the tools presented here for the log-composition become naturally available to challenge its performance.
- Chapter 5:** Here we are at the experimental results. The log-composition applied to rigid and diffeomorphic registration is applied to synthetic data and clinical images.

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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 leads to consider some prior knowledge within the initial data, that may affect the problems' parameters and chose some constraints, that, of course, impact dramatically the range of possible results.

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)¹.

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 biological features between subjects (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

¹Surveys in medical image registration can be found in [SDP13], [ZF03].

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 [FF97], [GWRNJ12], [PCL⁺15].

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 damage on the unaffected cells [MHSK], [MHM⁺11].

Another application is to compose together several images to obtain a bigger picture (mosaicing): in this case image registration is used to align images in the overlapping regions [VPM⁺06], [Sze94].

1.1.2 State of the Art

In the attempt to classify image registration algorithms, 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 minimize at each step an energy function. 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 solution of some family of differential equations, but with its Lie group structure [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 Lie group and Lie algebra embedded 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 (or log-demons) [VPPA07]². 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 diffeomorphic demons [VPPA08] and LCC-demons [LAF⁺13] respectively.

1.1.3 Using Diffeomorphisms: Utility and Liability

If the set of transformations is bonded to the rigid body transformations group $SE(3)$ (mostly utilized in robotics and classical mechanics), the registration algorithm will be adequate to align 3d images. In clinical practice, brain images are aligned using rigid registration to compensate the motion, or to compare differences in longitudinal and cross sectional scans. If we assume that the motion of internal anatomy is continuous, then the group $SE(3)$ is not versatile enough to transform images. The choice goes on the Lie group of diffeomorphism Diff, that appears particularly appealing in computational anatomy since their topology-preserving nature. Their mathematical formalization as Lie group, is on the other hand not of immediate understanding, and it is still an open field of research.

Attempt to provide this object some handles for easy manipulation was done for the first time in 1966 by Vladimir Arnold [Arn66]³: to solve differential equation in hydrodynamic, 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 [Mil84], 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 general space on which the transition map 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

²An accurate comparison between stationary LDDMM and Diffeomorphic Demons with emphasis in both theoretical and practical aspects can be found in [HOP08].

³And on a second time in the sequel [Arn98], more readable for non-French speakers.

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 as a quotient of other well behaved group [Woj94].

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. We work then mostly on finite dimensional settings, relying on important theorems and available close forms, and we will extend methods and results developed here in the infinite case -clearly - with proper precautions.

Another limitation that the reader should be aware of do not comes down to the theoretical difficulties of handling diffeomorphisms, but from the necessity of deal with discrete images and softwares. Two subset of some space have the same topology if exists an homeomorphism between them, but this analytical definition 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

1.2.1 Introductory Definitions

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, $F : \Omega_F \rightarrow \mathbb{R}$ and $M : \Omega_M \rightarrow \mathbb{R}$, called respectively *fixed image* and *moving image*, the *image registration problem* consists in the investigation of features and parameters of the transformation function

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

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:

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

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. In practice, this transformation between domains can be performed with a resampling technique, eventually with the well known artefacts related problem.

The definition of image registration here proposed, leaves two 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:

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

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 alternative options to define the registration algorithm based on this framework.

1.2.2 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:

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

Under the hood of this ideal device we may see an engine that can be schematically represented as in figure 1.1.

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

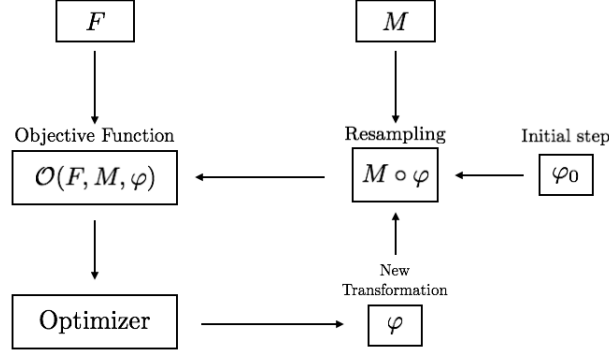


Figure 1.1: Image registration framework scheme.

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*⁴ of the latest important algorithms: the LDDMM and the diffeomorphic Demons.

1.2.3 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 reference and floating. Although, the discretized vector fields that can be stored in the computers' memory, are 5-dimensional matrix on a grid G over the background space Ω . The standard structure, used by most of the available software for image manipulation (Nibabel, py-NIfTI, niftilib, ...) is

$$M = M(x_i, y_j, z_k, t, d) \quad (i, j, k) \in G, \quad t \in T \quad d = 1, 2, 3 \quad (1.2)$$

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

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

Consider the set of homeomorphisms $\text{Hom}(\Omega)$ (continuous function from the background space Ω to itself with continuous inverse) that act⁵ on the set of images from the background

⁴bijjective differentiable maps with differentiable inverse; take the real valued $f(x) = x^3$: it is bijective differentiable but the inverse is not everywhere differentiable.

⁵In this action it is preferable to consider the composition with the inverse, because this same action in differential geometry, called pull-back play the role of the contravariant operator of the push-forward, widely used to make a vector field act on a domain different from the one has been originally defined. For definitions on group's action and orbits, we refer to [Art11]. For modern definitions of push-forward, pull-back and an introduction on Differential Geometry (in a non-Riemannian settings) [Lee12].

space \mathcal{I}_Ω :

$$\begin{aligned} \text{Hom}(\Omega) \times \mathcal{I}_\Omega &\longrightarrow \mathcal{I}_\Omega \\ (\varphi, F) &\longmapsto F \circ \varphi^{-1} \end{aligned}$$

its orbit, given an image F and a subgroup of the homeomorphisms $\mathbb{G} \subset \text{Hom}(\Omega)$, consists in the set of the images having the same topology of F :

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

The similarity term in the LDDMM is the L^2 norm⁶ between the moving image and the fixed image in the same orbit:

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

while the regularization term that provides the optimal φ at each step is defined on the norm of the velocity vector field tangent to the transformation. Limiting its length means impose a constrain on the speed of the transformation at each step.

Let $\text{Vect}(\Omega)$ be the set of all of the vector field over Ω . A generic time varying vector field (TVVF) is the continuously differentiable map defined as

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

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

$$\frac{d\phi_t(\mathbf{x})}{dt} = V^{(t)}(\mathbf{x}) \quad (1.3)$$

where

$$\begin{aligned} \phi : [0, 1] &\longrightarrow \text{Hom}(\Omega) \\ t &\longmapsto \phi_t : \Omega \longrightarrow \Omega \\ \mathbf{x} &\longmapsto \phi_t(\mathbf{x}) \end{aligned}$$

The transformation φ between fixed and moving images ($F \circ \varphi^{-1} = M$), can be defined by the couple $(V^{(t)}, \phi_t)$, such that, for $t = 0$, $\phi_t = Id$, identity of the group of homeomorphisms, and for $t = 1$, $\phi_t = \varphi$ is the sought homomorphism.

$$\varphi := \phi_1 = \phi_0 + \int_0^1 V^{(t)}(\phi) dt$$

To have an efficient algorithm and a meaningful constraint on the resulting transformation, it is reasonable to consider ϕ_t as the shortest path between the identity and φ , so to have $V^{(t)}$ as the one that minimize the distance between transformations⁷:

$$l = \inf_{V^{(t)} : \phi_t(\mathbf{x}) = V^{(t)}(\mathbf{x})} \int_0^1 \|V^{(t)}\|_{L^2}^2 dt$$

⁶For an introduction on the L^2 norm in the continuous we refer to chapter 4 of [SS09].

⁷This next equation can provide a metric on the manifold of the transformations, making it a Riemannian manifold. On the other side starting with a metric previously defined on the manifold (by a Levi-Civita connection so to be compatible with the shortest length of the integral curve), the consequent existence of geodesics may avoid the computation of the inf. In both cases this ‘‘Riemannian approach’’ makes unavoidable the passage toward a metric, and makes the LDDMM a metric based algorithm.

Ending points of path on the set of diffeomorphisms, whose tangent vector field (that varies over time), are used as regularization term:

$$\text{Reg}(F, M, \varphi) = \int_0^1 \|LV^{(t)}\|_{L^2}^2 dt \quad \dot{\phi}_t(\mathbf{x}) = V^{(t)}(\mathbf{x}) \quad \phi_0 = Id \quad \phi_1 = \varphi$$

Where L is a linear operator that can be dependent on some parameters that makes the approach even more general; it is defined as $L = (\alpha \vec{\nabla}^2 + \gamma)$ for α and γ real parameters and $\vec{\nabla}^2$ the Laplace operator. From the differential equation 1.3, and in consequence of the definition of φ the energy function 1.1 become

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

And so the optimization algorithm, at each step of the registration will look for

$$\hat{V} = \underset{V^{(t)} : \dot{\phi}_t(\mathbf{x})=V^{(t)}(\mathbf{x})}{\text{argmin}} \int_0^1 \|LV^{(t)}\|_{L^2}^2 dt + \frac{1}{\sigma^2} \|F(\varphi^{-1}) - M\|_{L^2}^2$$

Each transformation involved in the optimization algorithm are discretized time varying velocity fields; the update at each step is given by

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

where \mathbf{v}^k is the k -th step of the approximation of the velocity vector field V , $\Delta \mathcal{E}$ 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 on the Demons framework instead on the LDDMM.

1.2.4 Demonology: Classic, Pasha, Diffeomorphic, Symmetric and LCC

The first demons-based algorithm in image registration was proposed by [Thi98] in analogy with the Maxwell's demon in thermodynamics. This early version, called classic (or additive) demons, do not involves diffeomorphisms; the floating image is deformed with a vector field resulting from the computation of the optical flow⁸ regularized by a gaussian filter at each

⁸Previously introduced for small deformation of optical sequence of images [HS81].

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, therefore it works under the hypothesis that the intensity of a moving object is constant over time.

Let \mathbf{x} be a point in the background space Ω , the unknown vector field $V : \Omega \rightarrow \mathbb{R}^d$ is the function that at each point satisfies:

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

Thus it can be defined pointwise as

$$V(\mathbf{x}) = \frac{(M(\mathbf{x}) - F(\mathbf{x}))\vec{\nabla} F(\mathbf{x})}{\|\vec{\nabla} F(\mathbf{x})\|^2} \quad \forall \mathbf{x} \in \Omega \quad (1.5)$$

To reduce the instability for small values of $\|\vec{\nabla} F\|$ and to satisfy the condition $V \rightarrow \mathbf{0}$ for little $\vec{\nabla} F$, the equation 1.5 is multiplied by $\|\vec{\nabla} F(\mathbf{x})\|^2 / (\|\vec{\nabla} F(\mathbf{x})\|^2 + (M(\mathbf{x}) - F(\mathbf{x}))^2)$:

$$V(\mathbf{x}) = \frac{(M(\mathbf{x}) - F(\mathbf{x}))\vec{\nabla} F(\mathbf{x})}{\|\vec{\nabla} F(\mathbf{x})\|^2 + (M(\mathbf{x}) - F(\mathbf{x}))^2} \quad \forall \mathbf{x} \in \Omega \quad (1.6)$$

Therefore, the classical demons algorithm defines the update of the transformation field at each step with 1.6 or with $V(\mathbf{x}) = \mathbf{0}$ when

$$\|\vec{\nabla} F(\mathbf{x})\|^2 + (M(\mathbf{x}) - F(\mathbf{x}))^2 < \epsilon$$

for ϵ spacing of floating point number.

In the paper that presents the PAHSA demons [CBD⁺03], the 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 voxel. They reformulate the algorithm using a global energy function, aimed to makes the method easier to be analyzed and compared with others. With some modification, the Classic demons algorithm is accompanied back to the framework presented in the previous section, having as energy function

$$\mathcal{E}(F, M, \mathbf{c}, \mathbf{v}) = \frac{1}{\sigma_s^2} \text{Sim}(F, M, \mathbf{c}) + \frac{1}{\sigma_d^2} \text{dist}(\mathbf{c}, \mathbf{v}) + \frac{1}{\sigma_r^2} \text{Reg}(\mathbf{v}) \quad (1.7)$$

where C and V are both vector fields defined on the background space Ω and each σ accounts for the uncertainty of each of the involved measure.

It differs from the energy function 1.1 because of the additional *hidden variable* C , whose purpose is to use alternating minimization algorithm⁹ to optimize \mathcal{E} . Functions of involved in this new version of the energy function can be defined as

$$\begin{aligned} \text{Sim}(F, M, C) &= \|F - M \circ C\|^2 \\ \text{dist}(C, V) &= \|C - V\| \\ \text{Reg}(V) &= \|\vec{\nabla} V\|^2 \end{aligned}$$

⁹ The optimization algorithm is divided in two phase: at the step t , in the first phase the first two addend of the energy function are optimized to obtain the approximation of C , \mathbf{c}_t holding the variable V to \mathbf{v}_{t-1} , approximation obtained from the previous step. In the second phase, the last two addend of the energy function are optimized to obtain the approximation of V for C kept constant at \mathbf{c}_t obtained in the previous phase.

or with more advanced criteria proposed in [CBD⁺03]. In this context an equivalent version of the Classical demon, involving the global optimization function, can be reformulated from the previous equations, keeping $C = V$:

$$\begin{aligned}\text{Sim}(F, M, V) &= \|F - M \circ V\|^2 \\ \text{dist}(C, V) &= 0 \\ \text{Reg}(V) &= \|\vec{\nabla} V\|^2\end{aligned}$$

and applying a Gaussian smoother at each step to regularize the solution.

The update of the vector field obtained with the optimization of the energy function and the Gaussian smoother is summed at each step with the previously computed vector field¹⁰. Let $\{\mathbf{v}_j\}$ be the vector fields' sequence approximating V and $\delta\mathbf{v}$ the one computed at the iteration $j + 1$ by the optimization algorithm, then the *update* is computed with

$$\mathbf{v}_{j+1} := \mathbf{v}_j + \delta\mathbf{v} \quad (1.8)$$

Again the PASHA algorithm do not involves any diffeomorphism. This development was made in [VPM⁺06], with the diffeomorphic demons (or log-demon). Within the log-euclidean framework the involved vector fields are element in the tangent space of the group of diffeomorphisms. As in LDDMM, to each vector field $V \in \text{Vect}(\Omega)$ is associated a diffeomorphisms p by the ODE $dp/dt = V^{(t)}(p)$.

In this settings, the update can not be computed simply with a sum, since it must reflect the composition of diffeomorphisms that defines the corresponding vector fields. Intuitively if $dp/dt = V^{(t)}(p)$ and $dq/dt = W^{(t)}(q)$ do not implies $dp \circ q/dt = V^{(t)}(p) + W^{(t)}(q)$. To define the composition in the tangent space, we need to use two functions to transform vector fields into diffeomorphisms and vice-versa; they are already provided by Lie group theory. The *Lie algebra*, usually denoted with \mathfrak{g} , contains the set of the tangent vector fields, while the Lie group, denoted with \mathbb{G} , contains the set of transformations; the function *Lie exponential* maps vector fields on the corresponding Lie group elements while the *Lie logarithm*, its inverse under some condition defined in chapter 2, maps each diffeomorphisms in the correspondent tangent vector field:

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

The addition of tangent vector fields 1.8 that defines the update of the additive demons, becomes, in the diffeomorphic demon, the logarithm of the composition of the two diffeomorphisms that corresponds to the vector fields in the Lie group:

$$\mathbf{v}_{j+1} = \log(\exp(\mathbf{v}_j) \circ \exp(\delta\mathbf{v})) \quad (1.9)$$

And again the theory of Lie group provides a formula to compute this composition: the BCH formula. This involves an infinite series of nested Lie bracket, that do not makes its computation a straightforward task:

$$BCH(\mathbf{v}_j, \delta\mathbf{v}) := \mathbf{v}_j + \delta\mathbf{v} + \frac{1}{2}[\mathbf{v}_j, \delta\mathbf{v}] + \frac{1}{12}([\mathbf{v}_j, [\mathbf{v}_j, \delta\mathbf{v}]] + [\delta\mathbf{v}, [\delta\mathbf{v}, \mathbf{v}_j]]) + \dots$$

Remarkably, if we set to 0 all the lie brackets in the BCH formula (so we neglect the curvature of the space), the resulting composition of vector field in the log domain will coincide with 1.8:

$$BCH(\mathbf{v}_j, \delta\mathbf{v}) \simeq \mathbf{v}_j + \delta\mathbf{v}$$

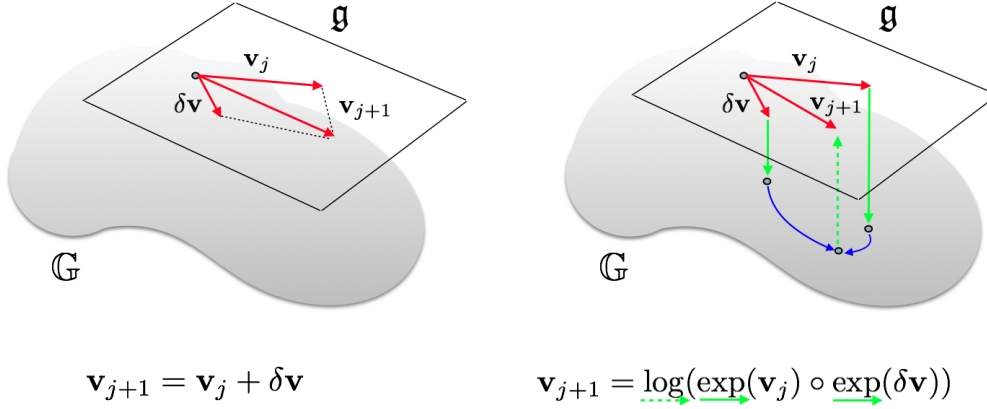


Figure 1.2: Each update computed in the additive demons algorithm is the sum of vector fields (left). In diffeomorphic demons algorithm vector fields are considered as elements of the lie algebra \mathfrak{g} , tangent space of the Lie group of diffeomorphisms. The update is compute as the composition of the correspondent transformations in the Lie group \mathbb{G} using the canonical transformations \exp and \log (right).

An extension of the diffeomorphic demons, that involves the optimization of the energy function $\mathcal{E}(F, M, V)$, exploits the existence of the inverse transformation and optimizes instead a symmetrised version of the energy function [VPPA07]. If $V = \log(p)$, then the *symmetric diffeomorphic demons algorithm* finds at each step

$$\tilde{V}_{t+1} = \operatorname{argmin}_{p \in \mathbb{G}} \mathcal{E}(F, M, \log(p)) + \mathcal{E}(F, M, \log(p^{-1}))$$

A further development of the diffeomorphic demons algorithm, presented in [LAF⁺13], preserve the structure of the symmetric version, but uses the LCC measure of similarity instead of L^2 to compute the energy function.

Last section of this chapter is devoted to introduce the intuition of this concept, while chapter 2 is devoted to the introduction the formal definitions and to its development.

1.3 The Composition of SVF in the Diffeomorphisms Group

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 solves the differential equations of the LDDMM and the diffeomorphic demons approach: the only thing that we can do, unfortunately, is to store 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 as input and output, but we need the Lie group of diffeomorphisms as support to compute the

¹⁰This is the reason why in demonology, the classical demons is sometime classified as additive demon.

composition 1.9 from the tangent space. This operation is baptized under the name of *log-composition* and it is defined as

$$U \oplus V := \log(\exp(U) \circ \exp(V)) \quad \forall U, V \in \mathfrak{g}$$

The main aim of this research is to find and compare numerical ways to compute it.

A fast log-composition is not useful only for the diffeomorphic demons. It can be used to solve every problem that uses 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].
3. Calculus on diffusion tensor [AFPA06].
4. Compute the discrete ladder for Parallel Transport in Transformation Groups [LP14a].

The next chapter is devoted to the formal definition of the log-composition, underpinned with the tools from differential geometry theory and to present the numerical technique developed so far 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:

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

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.

Some notes about these topics, tailored for image registration can be found on the github repository [?]

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

Let \mathbf{v} be an element in the tangent space \mathfrak{g} and $V \in \mathcal{V}(\mathbb{G})$ the unique vector field defined by \mathbf{v} over a local coordinate system around the origin. Let Φ_V be the flow associated with the vector field and $\gamma(t)$ the unique integral curve of V passing through the identity of the group. The *Lie exponential* is defined as ([dCV92], [EMP06])

$$\begin{aligned} \exp : \mathfrak{g} &\longrightarrow \mathbb{G} \\ \mathbf{v} &\longmapsto \exp(\mathbf{v}) = \gamma(1) \quad \dot{\gamma}(t) = V_{\gamma(t)}, \gamma(0) = e \end{aligned}$$

It satisfies the following properties:

1. $\exp(\mathbf{v}) = \Phi_V(e, 1)$.
2. $\exp(t\mathbf{v}) = \gamma(t) = \Phi_V(e, t)$.
3. $\exp(\mathbf{v}) = e$ if $\mathbf{v} = \mathbf{0}$.
4. $\exp(\mathbf{v}) \circ \exp(-\mathbf{v}) = e$
5. The exponential function satisfies the one parameter subgroup property:

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

6. $\exp(\mathbf{v})$ is invertible and $(\exp(\mathbf{v}))^{-1} = \exp(-\mathbf{v})$.
7. \exp is a diffeomorphism between a neighborhood of $\mathbf{0}$ in \mathfrak{g} to a neighborhood of Id 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 locus¹. 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. $\det(\exp(\mathbf{v})) = \exp(\text{trace}(\mathbf{v}))$
5. For any norm, $\|\exp(\mathbf{v})\| \leq \exp(\|\mathbf{v}\|)$.
6. $\exp(\mathbf{u} + \mathbf{v}) = \lim_{m \rightarrow \infty} (\exp(\frac{\mathbf{v}}{m}) \exp(\frac{\mathbf{u}}{m}))^m$
7. If $\exp(\mathbf{w}) = \exp(\mathbf{u}) \circ \exp(\mathbf{v})$ then $\exp(-\mathbf{w}) = \exp(-\mathbf{v}) \circ \exp(-\mathbf{u})$.

¹Here we define cut locus starting from the exp and log function, and in both domains. Traditionally it is defined only on Riemannian manifolds and using the geodesics (see [dCV92], p. 267). For Levi Civita connection we have that the definition are coincident.

8. For ad adjoint map in the Lie algebra we have $\exp(\text{Ad}_{\mathbf{u}}\mathbf{v}) = \text{Ad}_{\mathbf{u}}\exp(\mathbf{v})$

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

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

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:

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

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. On the other side the domain of the exponential is the matrix Lie algebra, but the exponential can be nevertheless applied to a generic 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 admit only compositions. The sum between element of a group can be performed on a Lie group, every time he and its Lie algebra are subset of a bigger algebra [KKK08]. In these cases infinite series are doors to pass from the structure of group and the algebra. When presenting the rigid body transformation in chapter 3 we will see another couple of access doors based on numerical approximations.

The (extremely) continuous nature of a diffeomorphism 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. As shown in [HOP08], for some parameters the Stationary LDDMM and the diffeomorphic Demons, the transformations involved in diffeomorphic framework may not preserve the signs of the Jacobian determinant. As previously said, 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 vector field in another vector field, and reasonably the domain and codomain of these transformations are radically different from the exp

2.2. LIE EXPONENTIAL, LIE LOGARITHM, LIE LOG-COMPOSITION AND THE BCH FORMULA

and log function defined for diffeomorphisms.

Matrices are much easier to handle, since the Lie group of a Lie algebra is still an algebraic structure defined by matrices, in which products are compatible with the composition. In this case the exponential and logarithm have domain and codomain in the appropriate restriction of the general linear group.

Passing from finite dimensional case of matrices to infinite dimensional case of diffeomorphisms requires a way to represent diffeomorphisms having only vector fields to deal with. The strategy here proposed is to embed the Lie group structure $\mathbb{G} = \text{Diff}(\Omega)$ in the Lie algebra $\mathfrak{g} = \mathcal{V}(\Omega)$, whose implementation better reflect the discretization of the diffeomorphisms. This is done toward the definition of an operation, defined on \mathfrak{g} , that utilizes the group structure of \mathbb{G} on its elements.

We define now the Lie Log-composition (Lie to distinguish it from the Affine Log-composition of the next section) as inner binary operation on the Lie algebra that reflects the composition on the lie group:

$$\begin{aligned} \oplus : \mathfrak{g} \times \mathfrak{g} &\longrightarrow \mathfrak{g} \\ (\mathbf{v}_1, \mathbf{v}_2) &\longmapsto \mathbf{v}_1 \oplus \mathbf{v}_2 = \log(\exp(\mathbf{v}_1) \circ \exp(\mathbf{v}_2)) \end{aligned}$$

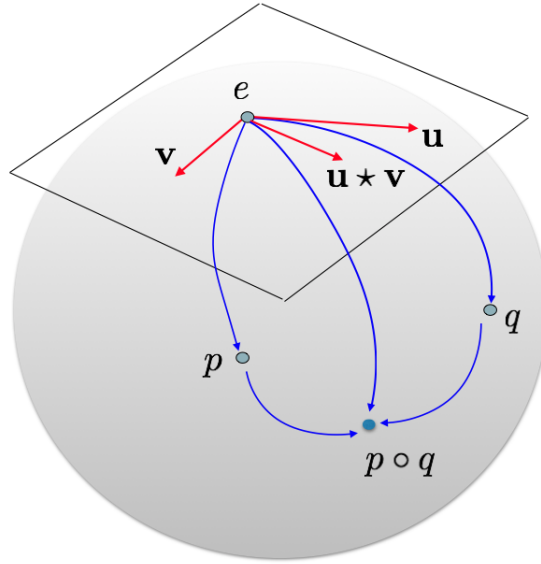


Figure 2.1: graphical visualization of the Lie log-composition.

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.

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

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 group composition leave the difficulty of managing the problem of the error carried by each term.

2.3 Affine Exponential, Affine logarithm and affine log-composition

Considering a Lie Group \mathbb{G} with a connection ∇ (that provides geodesics and curvature over manifold on which no Riemannian metric has been defined, see [dCV92]), the vector field $\nabla_U(V)$ associates at each point of the manifold the projection on the tangent plane of the covariant derivative of U in the direction of V .

First consequence of the definition of the connection is the possibility of define *geodesics* between points p and q of the manifold. A geodesic is a curve γ such that:

$$\gamma : [0, 1] \longrightarrow \mathbb{G} \quad \gamma(0) = p, \gamma(1) = q, \nabla_{\dot{\gamma}}\dot{\gamma} = 0$$

Note that in this case the concept of geodesic did not involves any metric defined on the surface of the manifold. If also a Riemannian metric is defined on \mathbb{G} , then geodesics defined by the metric coincides with the geodesics defined by the connection only for the particular Levi-Civita connection (see [dCV92]). A connection is said to be left invariant if it is closed for left invariant vector fields, i.e. if for any $V, W \in \text{Left}\mathcal{V}(\mathbb{G})$ their connection $\nabla_U V$ is still left invariant.

Second straight consequence of the definition of connection allows us to define a new kind of exponential from the Lie algebra to the Lie group that relies on the concept of geodesics.

2.3. AFFINE EXPONENTIAL, AFFINE LOGARITHM AND AFFINE LOG-COMPOSITION

This time the tangent plane that defines the Lie algebra is considered at the point p of the Lie group and $\mathbf{v} \in T_p\mathbb{G} \simeq \mathfrak{g}$ is a tangent vector at the point p :

$$\begin{aligned} \exp : \mathbb{G} \times \mathfrak{g} &\longrightarrow \mathbb{G} \\ (p, \mathbf{v}) &\longmapsto \exp_p(\mathbf{v}) = \gamma(1; p, \mathbf{v}) \end{aligned}$$

The curve $\gamma(t; p, \mathbf{v}) = \gamma(t)$ on \mathbb{G} is the unique one with the following features:

$$\gamma(0) = p \quad \dot{\gamma}(0) = \mathbf{v} \quad \nabla_{\dot{\gamma}} \dot{\gamma} = 0$$

This second kind of exponential is called affine exponential² The following properties hold:

1. If ∇ is a Cartan connection then \exp_e and \exp coincides.
2. For all p in \mathbb{G} , $\mathbf{v} \in T_p\mathbb{G}$ and t real

$$\exp_p(t\mathbf{v}) = \gamma(t; p, \mathbf{v})$$

3. Given $\mathbf{u} \in T_e\mathbb{G}$, $\mathbf{v} \in T_{\exp_e(\mathbf{u})}\mathbb{G}$, exists a $\mathbf{w} \in T_e\mathbb{G}$ such that

$$\exp_e(\mathbf{w}) = \exp_{\exp_e(\mathbf{u})}(\mathbf{v}) \circ \exp_e(\mathbf{u})$$

4. If V is a unitary left-invariant vector field, then for $V_e \in T_e\mathbb{G}$

$$\exp_e(2V_e) = \exp_{\exp_e(V_e)}(V_{\exp_e(V_e)}) \circ \exp_e(V_e)$$

Last two properties provides the intuitive idea that it is possible to move on the fiber bundle of the Lie group transporting in some sense a tangent vector defined at the identity on another tangent space. Certainly the Lie group possess a unique Lie algebra, as the tangent space at some point (the group's identity by convention), but two different tangent space (so two times the same Lie algebra structure) may not be oriented in the same way.

To approach the inverse of the affine exponential we consider the affine logarithm:

$$\begin{aligned} \log : \mathbb{G} \times \mathbb{G} &\longrightarrow T_p\mathbb{G} \simeq \mathfrak{g} \\ (p, q) &\longmapsto \log_p(q) = \mathbf{v} \end{aligned}$$

Where \mathbf{v} is the vector at the tangent plane defined at p such that the curve on \mathbb{G} with the following features

$$\gamma(0) = p \quad \gamma(1) = q \quad \nabla_{\dot{\gamma}} \dot{\gamma} = 0$$

has as its tangent in p the vector \mathbf{v} .

Any Lie group \mathbb{G} considered with a left-invariant connection ∇ can be equipped with a metric, based on the elements of its tangent space and on the log, for example:

$$\text{dist}(x, y) := ||\log_e(x^{-1} \circ y)|| \quad \forall x, y \in \mathbb{G}$$

² Note on the notation: to distinguish the affine exp and log from the Lie exp and log presented in the previous section, the affine will always have the subscript of the point of application even when it is the identity.

This metric is not necessarily coincident with the Riemannian one.

Is now time to extend the definition of Log-composition, with the definition of affine logarithm and affine exponential. The first step is to extend the definition of internal cut locus of the Lie algebra, even when not centered at the zero. If the tangent space is not considered at e of \mathbb{G} but at some general point p , we still have a diffeomorphism between a neighborhood of $\mathbf{0}$ in \mathfrak{g} to a neighborhood of p in \mathbb{G} . The internal cut locus of \mathfrak{g} this time is based on p and it is denoted with $C_{\mathfrak{g}}(p)$.

Given a point p_1 and a vector \mathbf{v}_1 on its tangent space $T_{p_1}\mathbb{G}$, the *affine Log-composition* is defined as the operation $\tilde{\oplus}$ over the fiber bundle of \mathbb{G} such that

$$\begin{aligned} \cdot \tilde{\oplus} \mathbf{v}_1 : T_{\exp_{p_1}(\mathbf{v}_1)}\mathbb{G} &\longrightarrow T_{p_1}\mathbb{G} \\ \mathbf{v}_2 &\longmapsto \mathbf{v}_2 \tilde{\oplus} \mathbf{v}_1 = \log_{p_1}(\exp_{\exp_{p_1}(\mathbf{v}_1)}(\mathbf{v}_2) \circ \exp_{p_1}(\mathbf{v}_1)) \end{aligned}$$

Note that not necessarily $\mathbf{v}_1 \tilde{\oplus} \mathbf{v}_2$ is a vector belonging to the internal cut locus based on the starting point p_1 .

2.4 Parallel Transport: Definition and Properties

In this section we present 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 2.4.1. 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 for all $t \in [0, 1]$ $\nabla_{\dot{\gamma}} V_{\gamma(t)} = 0$.

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

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

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

$$\Pi(\gamma)_p^q(-\mathbf{u}) = -\Pi(\gamma)_p^q(\mathbf{u}) \quad (2.1)$$

$$p = \exp_q(\mathbf{u}) \iff q = \exp_p(-\Pi(\gamma)_q^p(\mathbf{u})) \quad (2.2)$$

Property 2.4.2 (change of signs of the composition for affine exponential). \mathbb{G} Lie group, ∇ connection, $a, b \in \mathbb{G}$, $\mathbf{u} \in T_a\mathbb{G}$, $\mathbf{v} \in T_b\mathbb{G}$. Let β be the tangent curve to \mathbf{u} at a and $c = \exp_b(\mathbf{v})$. Given $\mathbf{w} \in T_c\mathbb{G}$ such that

$$\exp_a(\mathbf{w}) = \exp_b(\mathbf{v}) \circ \exp_a(\mathbf{u})$$

Then

$$\exp_a(-\mathbf{w}) = \exp_{\tilde{b}}(-\Pi(\beta)_{\tilde{b}}^{\tilde{b}}(\mathbf{v})) \circ \exp_a(-\mathbf{u})$$

where \tilde{b} is the affine exponential of $-\mathbf{u}$ or the element $\beta(-1)$.

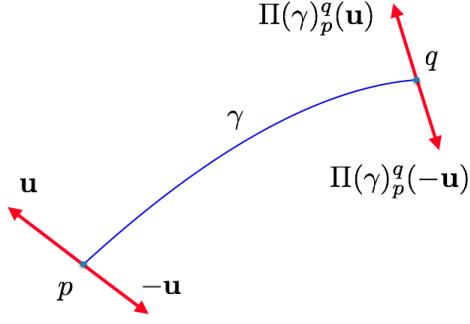


Figure 2.2: First inversion property.

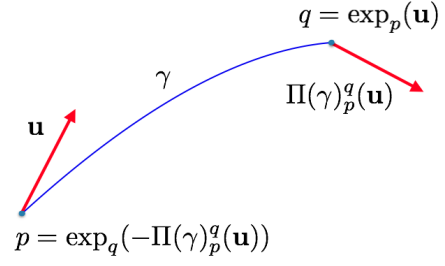


Figure 2.3: Second inversion property.

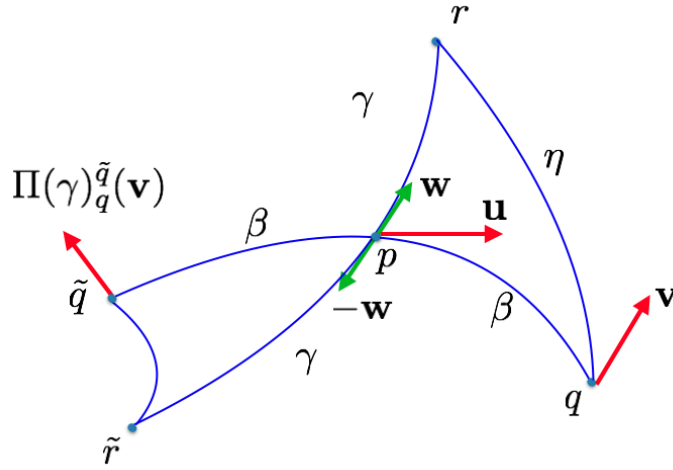


Figure 2.4: Change of sign property.

1. If ∇ is a Cartan connection then β is a geodesic.
2. For $\mathbf{u}_a := D(L_a)_e(\mathbf{u}) \in T_a\mathbb{G}$, push forward of the left-translation:

$$\exp_a(t\mathbf{u}_b) = b \circ \exp_e(tD(L_{a^{-1}})_a(\mathbf{u}_a)) = b \circ \exp_e(t\mathbf{u}) \quad (2.3)$$

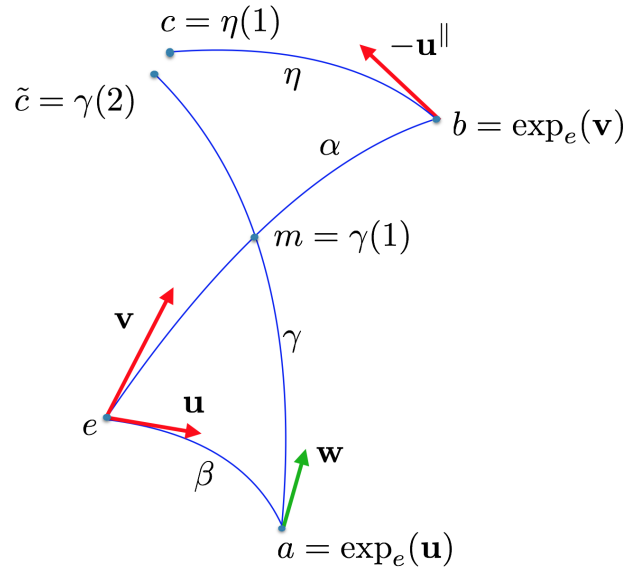


Figure 2.5: Pole ladder applied to parallel transport.

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 2.4.1. 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:

$$\begin{array}{l} a = \exp_e(\mathbf{u}) \quad b = \exp_e(\mathbf{v}) \\ \mathbf{u}^\parallel = \Pi(\alpha)_e^b(\mathbf{u}) \\ \gamma : [0, 1] \rightarrow \mathbb{G} \quad \gamma(0) = e \quad \dot{\gamma}(0) = \mathbf{v} \end{array}$$

Then, for $\mathbf{u}_e^\parallel := D(L_{b-1})_e(-\Pi(\alpha)_a^b(\mathbf{u}))$, the approximation

$$\exp_e(\mathbf{u}_e^\parallel) \simeq \exp_e\left(\frac{\mathbf{v}}{2}\right) \circ \exp_e(\mathbf{u}) \circ \exp_e\left(-\frac{\mathbf{v}}{2}\right)$$

holds.

Corollary 2.4.2. xxx attempt to measure the error in the formula... to be done in a more effective way! If, with previous notations, the condition (1) is an approximation

$$\exp_C\left(\frac{\mathbf{k}}{2}\right) = \exp(\xi) \circ \exp_M\left(\frac{\mathbf{k}}{2}\right)$$

for some ξ in \mathfrak{g} such that $\|\xi\| < \delta$ then the approximation has error

$$O(\|\delta\mathbf{u}\|^2) + O(\|\mathbf{u} + \delta\mathbf{u}\|^3) + \text{xxx something that must be investigated depending on } \delta$$

In considering the equation 2.3 we used implicitly the formula for the change of base for affine exponential and logarithm. 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:

$$\log_p(q) = DL_p(e) \log_e(q) \quad (2.4)$$

$$\exp_p(\mathbf{u}) = p \circ \exp_e(DL_p(e)^{-1}\mathbf{u}) \quad (2.5)$$

The interested reader can refer to the extended version on github [?], where proofs and examples are provided and relations between 2.4 and parallel transport are investigated.

2.5 Four Strategies for the Computation of Log-composition

In this section we provide explicit formulas for the computation of the log composition, using the tools introduced in the previous sections.

2.5.1 Truncated BCH formula

To compute the Lie Log composition, literature provides the BCH formula, 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} :

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

xxx derivation of the bch formula, constraints on the Lie algebra elements involved in its computation.

2.5.2 Taylor Expansion

Once *adjoint action* of \mathbf{u} on the Lie algebra is defined, nested Lie bracket can be reformulated as multiple composition of this operator:

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

So

$$\underbrace{[\mathbf{u}, [\mathbf{u}, \dots [\mathbf{u}, \mathbf{v}] \dots]]}_{\text{n-times}} = ad_{\mathbf{u}}^n(\mathbf{v})$$

In the appendix of xxx Klarsfeld xxx adjoint action are used to provide an expansion of the BCH formula. This can be rewritten as

$$\mathbf{u} \oplus \mathbf{v} = \mathbf{u} + \frac{ad_{\mathbf{u}} \exp(ad_{\mathbf{u}})}{\exp(ad_{\mathbf{u}}) - 1} \mathbf{v} + O(\mathbf{v}^2)$$

xxx intermediate passages to be written from zachos, blane!

The functional applied to \mathbf{v} can be rewritten as

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

Where $\{B_n\}$ is the sequence of the second-kind Bernoulli number³.

2.5.3 Parallel Transport

2.5.4 Numerical Computations of the Log-composition for SE(n)

Taylor Approximation to compute the Log-composition

We can apply the Taylor expansion formula for the computation of the affine log-composition to matrices in $SE(2)$. From previous subsection we have:

$$\mathbf{u} \star \mathbf{v} = \mathbf{u} + \frac{ad_{\mathbf{u}} \exp(ad_{\mathbf{u}})}{\exp(ad_{\mathbf{u}}) - 1} \mathbf{v} + O(\mathbf{v}^2) \quad \frac{ad_{\mathbf{u}} \exp(ad_{\mathbf{u}})}{\exp(ad_{\mathbf{u}}) - 1} = \sum_{n=0}^{\infty} \frac{B_n}{n!} ad_{\mathbf{u}}^n$$

Where $\{B_n\}$ is the sequence of the second-kind Bernoulli number⁴.

Parallel Transport to compute the Log-composition

Log and Exp Approximations for Small Rotations

Computations of logarithm and exponential obtained so far are a consequence of these formula:

$$\exp(\mathbf{r}) = \sum_{k=0}^{\infty} \frac{\mathbf{v}^k}{k!} \quad \log(\mathbf{r}) = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{(\mathbf{v} - I)^k}{k!}$$

Remarkably, infinite series of elements of a group (whose sum is not even defined within the group structure) is an element into an associated algebra, while another infinite series of matrices of the algebra appears to be the natural way to going backward. A second door to passing from one structure to the other, when \mathbf{r} is little appears to be the following approximation:

$$\exp(\mathbf{r}) \simeq I + \mathbf{r} \quad \log(d\mathbf{r}) \simeq d\mathbf{r} - I$$

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

xxx this may deserve an investigation about the errors in the approximations error!

³If first-kind Bernoulli number is used then each term of the summation must be multiplied for $(-1)^n$, as did for example inKlarsfeld.

⁴If first-kind Bernoulli number is used then each term of the summation must be multiplied for $(-1)^n$, as did for example inKlarsfeld.

Chapter 3

Numerical computation of the Log-composition for 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

3.1 The Group of Rigid Body Transformations

In the previous chapter we have introduced some fundamental tools from differential geometry commonly utilized in computational anatomy. The core object of the theory, exponential and logarithmic map, as well as pole ladder, are obviously different for each manifold and each metric, if there is one: practical implementations have to be determined case by case. This chapter is aimed to go through the details of the generalized theory for the cases of SE(2) and the Lie group of diffeomorphisms parametrized with stationary velocity fields.

3.1.1 Lie Logarithm, Lie Exponential and Log-compositions for SE(2)

A rigid body transformation in a normed vector space is a transformation that preserves distances. The set of rigid body transformations is constructed as any combination of rotations, translations and reflection, and forms the euclidean group $E(2)$. For 2d rigid registration usually reflections are not required and so we restrict our attention to the special euclidean group $SE(2)$. We are interested in two things about them: their expression in matrix form, and the Lie group and the Lie algebra structures involved.

We denote denoted with $M_3(\mathbb{R})$ the set of all of the 3×3 matrices with real entries. Its subset, defined by all the matrices with non-zero determinant, and thus by all the invertible matrices, is denoted with $GL_3(\mathbb{R})$. A *matrix group* is any proper or improper subgroup of $GL_3(\mathbb{R})$. The group of 2d rigid body transformation

$$\mathbb{G} = \{(\theta, tx, ty) \mid \theta \in [0, 2\pi), tx, ty \in \mathbf{R}^2\}$$

using matrices, so as a subgroup of $GL_3(\mathbb{R})$. Rotation in the plane can be expressed using matrix of the orthogonal group $SO(2)$, linear subgroup of $GL_2(\mathbb{R})$, so that rotations' actions

on planes' points are simply defined as a product:

$$SO(2) = \left\{ \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \mid \theta \in [0, 2\pi) \right\}$$

To include the translation we can add its $(tx, ty)^T$ parameter to the action of the rotation over the initial point $(x_i, y_i)^T$ to obtain the transformed $(x_t, y_t)^T$. So each element of the group \mathbb{G} act over \mathbf{R}^2 as

$$\begin{pmatrix} x_t \\ y_t \end{pmatrix} = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} x_i \\ y_i \end{pmatrix} + \begin{pmatrix} tx \\ ty \end{pmatrix}$$

Another way to express rigid body transformation group's elements is to include the translation in a bigger matrix, subgroup (not linear, since the translation is not linear) of $GL_3(\mathbb{R})$. This is defined as the group $SE(2)$:

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

Expressed in this way the matrices act on the point of the plane represented as the elements of the vector space $\{1\} \times \mathbf{R}^2$.

The passage between the restricted form \mathbb{G} and $SE(2)$ is defined by the injection:

$$\begin{aligned} \rho_{\mathbb{G}} : \mathbb{G} &\longrightarrow SE(2) \\ (\theta, tx, ty) &\longmapsto \begin{pmatrix} \cos(\theta) & -\sin(\theta) & tx \\ \sin(\theta) & \cos(\theta) & ty \\ 0 & 0 & 1 \end{pmatrix} \end{aligned}$$

We are now interested the Lie algebra of the Lie group $SE(2)$. It is defined as:

$$\mathfrak{se}(2) = \left\{ \begin{pmatrix} 0 & -\theta & dt_x \\ \theta & 0 & dt_y \\ 0 & 0 & 1 \end{pmatrix} \mid \theta \in [0, 2\pi), (tx, ty) \in \mathbf{R}^2 \right\}$$

Expressing $r \in SE(2)$ as:

$$\mathbf{r} = \begin{pmatrix} R(\theta) & t \\ 0 & 1 \end{pmatrix} \quad R(\theta) \in SO(2) \quad t \in \mathbb{R}^2$$

for t plane translation and $R(\theta)$ in $SO(2)$, then the element of the Lie algebra can be expressed as:

$$d\mathbf{r} = \begin{pmatrix} dR(\theta) & dt \\ 0 & 1 \end{pmatrix} \quad R(\theta) \in SO(2) \quad t \in \mathbb{R}^2$$

Both $SE(2)$ and $\mathfrak{se}(2)$ are in bijective correspondence with \mathbb{G} , and both are subset of the bigger algebra of, The algebra $\mathfrak{se}(2)$ do not form a group with the operation of composition, but it is provided with the lie bracket defined by the commutator:

$$[d\mathbf{r}, ds] = d\mathbf{r}ds - dsd\mathbf{r}$$

The Lie logarithm between Lie group and Lie algebra is given by:

$$\begin{aligned} \log : \mathfrak{se}(2) &\longrightarrow SE(2) \\ \begin{pmatrix} R(\theta) & t \\ 0 & 1 \end{pmatrix} &\longmapsto \begin{pmatrix} dR(\theta) & dt \\ 0 & 1 \end{pmatrix} \end{aligned}$$

Where

$$dR(\theta) = \begin{pmatrix} 0 & -\theta \\ \theta & 0 \end{pmatrix}$$

and $dt = L(\theta)t$ for

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

The inverse function, Lie exponential is given by:

$$\begin{aligned} \exp : SE(2) &\longrightarrow \mathfrak{se}(2) \\ \begin{pmatrix} dR(\theta) & dt \\ 0 & 1 \end{pmatrix} &\longmapsto \begin{pmatrix} R(\theta) & t \\ 0 & 1 \end{pmatrix} \end{aligned}$$

where $t = L(\theta)^{-1}dt$ for

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

The proposed exponential function is not well defined over all $\mathfrak{se}(2)$.

In fact the elements of \mathbb{G} can be identified with no risk with their matrices, while the same thing do not happen for the element of the Lie algebra \mathfrak{g} of \mathbb{G} . If we formalize the passage between \mathfrak{g} and $\mathfrak{se}(2)$ with the function:

$$\begin{aligned} \rho_{\mathfrak{g}} : \mathfrak{g} &\longrightarrow \mathfrak{se}(2) \\ (\theta, dtx, dty) &\longmapsto \begin{pmatrix} 0 & -\theta & dtx \\ \theta & 0 & dty \\ 0 & 0 & 1 \end{pmatrix} \end{aligned}$$

it is not an injection if we do not restrict its domain. In addition, given two elements (θ_0, dtx_0, dty_0) and (θ_1, dtx_1, dty_1) in \mathfrak{g} , with $\theta_1 \neq 0$, we have that for each $k \in \mathbb{Z}$, if

$$\theta_0 = \theta_1 + 2k\pi$$

and

$$(dtx_0, dty_0) = \frac{\theta_0}{\theta_1}(dtx_1, dty_1)$$

then

$$\exp(\theta_0, dtx_0, dty_0) = \exp(\theta_1, dtx_1, dty_1)$$

The exponential is then well defined only on the quotient of \mathfrak{g} over the relation \sim , defined by

$$(\theta_0, dtx_0, dty_0) \sim (\theta_1, dtx_1, dty_1) \iff \exp(\theta_0, dtx_0, dty_0) = \exp(\theta_1, dtx_1, dty_1)$$

3.1. THE GROUP OF RIGID BODY TRANSFORMATIONS

The quotient set \mathfrak{g}/\sim coincides the neighborhood U of the identity on which the function $\rho_{\mathfrak{g}}$ becomes an injection

$$\rho_{\mathfrak{g}/\sim} : \mathfrak{g} \longrightarrow \mathfrak{se}(2)$$

and \exp is a bijection having \log as its inverse. What said so far can be summarize in the following commutative diagram:

$$\begin{array}{ccc}
 \mathfrak{g} & \xrightarrow{\rho_{\mathfrak{g}}} & \mathfrak{se}(2) \\
 \log \uparrow & \searrow \pi & \nearrow \text{hook} \\
 & \mathfrak{g}/\sim & \xrightarrow{\rho_{\mathfrak{g}/\sim}} U \subset \mathfrak{se}(2) \\
 & \nearrow \exp & \searrow \exp \\
 \mathbb{G} & \xrightarrow{\rho_{\mathbb{G}}} & SE(2)
 \end{array}$$

We can see that the function $\rho_{\mathfrak{g}}$ is the inverse of a restriction of the general vectorization function that aligns column vector in a single vector. This will be particularly useful for our purposes.

xxx this part must be set after subsection 2.5 is done, to avoid repetitions and circular properties!

We can see that the function $\rho_{\mathfrak{g}}$ is the inverse of a restriction of the general vectorization function that aligns column vector in a single vector:

$$\begin{aligned}
 \text{Vect} : M_3(\mathbb{R}) &\longrightarrow \mathbb{R}^{3 \times 3} \\
 [A_1 | A_2 | A_3] &\longmapsto (A_1^t, A_2^t, A_3^t)
 \end{aligned}$$

Thanks to this adjoint action can be defined as an action over The vectorization, in combination with Lie bracket, Kronecker product, adjoint action and adjoint map, satisfies the following properties:

- $\text{Vect}([M, X]) = (I \otimes M - M^t \otimes I) \text{Vect}(X)$
- $\text{Vect}([X, M]) = (M^t \otimes I - I \otimes M) \text{Vect}(X)$

These are still valid for its restriction

$$\begin{aligned}
 \text{Vect}^{\sim} : M_3(\mathbb{R}) &\longrightarrow \mathbb{R}^3 \\
 [A_1 | A_2 | A_3] &\longmapsto (a_{2,1}, a_{3,1}, a_{3,2})
 \end{aligned}$$

that respects the Lie group operations between the restricted representation \mathfrak{g} and the matrix representation $SE(2)$:

and will be used in the next subsection to compute the log composition.

In the finite-dimensional case, investigate here the log-composition can be computed with a close formula:

$$d\mathbf{r}_1 \star d\mathbf{r}_2 = \log(\exp(d\mathbf{r}_1) \circ \exp(d\mathbf{r}_2))$$

which results

$$d\mathbf{r}_1 \star d\mathbf{r}_2 = xxx \text{On some lost paper... to be computed again!}$$

Chapter 4

Log-computation Algorithm using Log-composition

We believe that we know something about the things themselves when we speak of trees, colors, snow, and flowers; and yet we possess nothing but metaphors for things — metaphors which correspond in no way to the original entities.
-Nietzsche, *On Truth and Lies in extra-moral sense.*

zz write chapter intro.

The problem of the computation of the logarithm computation can be stated as follows: given $p \in \mathbb{G}$ the goal is to find \mathbf{u} such that $\exp(\mathbf{u})$ is the best possible approximation of p . This chapter is devote to the numerical computation of the logarithm, using an iterative algorithm based on the Log-composition. In this context each of the presented techniques are suitable to perform this computation.

Before we need to introduce the space of the approximation of the Lie algebra and the Lie group.

4.1 Space of approximations

xxx Space of the approximations, in connection with the small rotation chapter.

We emphasize the fact that if \mathfrak{g} and \mathbb{G} are subset of a bigger algebra, then \exp and \log can be considered as infinite series. Remarkable consequence is the approximation of $\exp(\mathbf{v})$ with $1 + \mathbf{v}$ if the transformation \mathbf{v} is small. This approximation is the base of what follows in this chapter.

In parallel with the log-composition $\mathbf{v}_1 \oplus \mathbf{v}_2 = \log(\exp(\mathbf{v}_1) \circ \exp(\mathbf{v}_2))$ we define two approximating functions:

$$\begin{aligned} \text{app} : \mathfrak{g} &\longrightarrow \mathfrak{g}^\sim \\ \mathbf{u} &\longmapsto \exp(\mathbf{u}) - 1 \end{aligned}$$

$$\begin{aligned} \text{App} : \mathbb{G} &\longrightarrow \mathbb{G}^\sim \\ \exp(\mathbf{u}) &\longmapsto 1 + \mathbf{u} \end{aligned}$$

Where \mathfrak{g}^\sim is a space of approximations of elements of \mathfrak{g} , and \mathbb{G}^\sim is a space of approximations of elements in \mathbb{G} (xxx that requires some more investigations and formal definition in

conjunction with truncated series).

Consequence of this definition is the fact that

$$\mathbf{u} \simeq \text{app}(\mathbf{u}) \quad \exp(\mathbf{u}) \simeq \text{App}(\exp(\mathbf{u}))$$

xxx errors can be investigated and maybe can become known elements in the computations! The two following straightforward properties, that holds for all \mathbf{u}, \mathbf{v} in the Lie algebra

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

lead us to consider the algorithm presented in [BO08], here called log-computation, with a new reformulation.

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:

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

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

4.2.1 BCH Strategy

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

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

thus, for the first degree we have

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

For the second degree we have:

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

Theorem 4.2.1 (Bossa). The iterative algorithm (4.2) converges to \mathbf{v} with error $\delta_n \in \mathbb{G}$, where

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

4.2.2 Parallel Transport Strategy

If we use the parallel transport for the computation of the log-composition, we obtain:

$$\begin{cases} \mathbf{u}_0 = \mathbf{0} \\ \mathbf{u}_t = \mathbf{u}_{t-1} + \exp(-\frac{\mathbf{u}_{t-1}}{2}) \circ \exp(\delta \mathbf{u}_{t-1}) \circ \exp(\frac{\mathbf{u}_{t-1}}{2}) - e \end{cases} \quad (4.3)$$

4.2.3 Symmetrization Strategy

The algorithm for the computation of the group logarithm can be improved considering a symmetric version of the underpinning strategy. In this version we use the first order approximation of the BCH formula (see equation (4.6) in the following proof), compensating with the fact that the symmetrization should decrease the error involved. It gives birth to the following algorithm:

$$\begin{cases} \mathbf{v}_0 = \mathbf{0} \\ \mathbf{v}_{t+1} = \mathbf{v}_t + \frac{1}{2}(\tilde{\delta} \mathbf{v}_t^L + \tilde{\delta} \mathbf{v}_t^R) \end{cases} \quad (4.4)$$

Where $\tilde{\delta} \mathbf{v}_t^R = \exp(\mathbf{v}) \circ \exp(-\mathbf{v}_t) - e$ and $\tilde{\delta} \mathbf{v}_t^L = \exp(-\mathbf{v}_t) \circ \exp(\mathbf{v}) - e$.

Proof. To show why it works we remind that the starting point was

$$p = \exp(\mathbf{v}) = \exp(\mathbf{v}_0) \circ \exp(\delta \mathbf{v}_0)$$

where $\exp(\delta \mathbf{v}_0) = \exp(-\mathbf{v}_0) \circ p$.

An equivalent starting point would have been $\exp(\mathbf{v}) = \exp(\delta \mathbf{v}) \circ \exp(\mathbf{v}_0)$ for $\exp(\delta \mathbf{v}) = p \circ \exp(-\mathbf{v}_0)$.

This idea leads to the definition of

$$\begin{aligned} \exp(\delta \mathbf{v}_t^R) &:= p \circ \exp(-\mathbf{v}_t) = \exp(\mathbf{v}) \circ \exp(-\mathbf{v}_t) \\ \exp(\delta \mathbf{v}_t^L) &:= \exp(-\mathbf{v}_t) \circ p = \exp(-\mathbf{v}_t) \circ \exp(\mathbf{v}) \end{aligned}$$

It follows that

$$\begin{aligned} \exp(\mathbf{v}) &= \exp(\mathbf{v}_0) \circ \exp(\delta \mathbf{v}_0^R) \\ \exp(\mathbf{v}) &= \exp(\delta \mathbf{v}_0^L) \circ \exp(\mathbf{v}_0) \end{aligned}$$

Using $\exp(\delta \mathbf{v}_t^R) \approx e + \delta \mathbf{v}_t^R$ and $\exp(\delta \mathbf{v}_t^L) \approx e + \delta \mathbf{v}_t^L$ we can use the following approximation to define the symmetric algorithm:

$$\begin{aligned} \exp(\delta \mathbf{v}_t^R) &= \exp(\mathbf{v}) \circ \exp(-\mathbf{v}_t) \\ e + \tilde{\delta} \mathbf{v}_t^R &= \exp(\mathbf{v}) \circ \exp(-\mathbf{v}_t) \\ \tilde{\delta} \mathbf{v}_t^R &= \exp(\mathbf{v}) \circ \exp(-\mathbf{v}_t) - e \end{aligned}$$

$$\begin{aligned}\exp(\delta \mathbf{v}_t^L) &= \exp(-\mathbf{v}_t) \circ \exp(\mathbf{v}) \\ e + \tilde{\delta} \mathbf{v}_t^L &= \exp(-\mathbf{v}_t) \circ \exp(\mathbf{v}) \\ \tilde{\delta} \mathbf{v}_t^L &= \exp(-\mathbf{v}_t) \circ \exp(\mathbf{v}) - e\end{aligned}$$

Which gives birth to iterative algorithm, for a given initial value V_0 :

$$\begin{cases} \mathbf{v}_0 \\ \mathbf{v}_{t+1} = \text{BCH}(\mathbf{v}_t, \tilde{\delta} \mathbf{v}_t^R) \end{cases} \quad \begin{cases} \mathbf{v}_0 \\ \mathbf{v}_{t+1} = \text{BCH}(\tilde{\delta} \mathbf{v}_t^L, \mathbf{v}_t) \end{cases} \quad (4.5)$$

It follows that

$$\mathbf{v}_{t+1} = \frac{1}{2}(\text{BCH}(\tilde{\delta} \mathbf{v}_t^L, \mathbf{v}_t) + \text{BCH}(\mathbf{v}_t, \tilde{\delta} \mathbf{v}_t^R))$$

Taking the first order approximation of the BCH formula:

$$\text{BCH}(\tilde{\delta} \mathbf{v}_t^L, \mathbf{v}_t) \approx \tilde{\delta} \mathbf{v}_t^L + \mathbf{v}_t \quad (4.6)$$

$$\text{BCH}(\mathbf{v}_t, \tilde{\delta} \mathbf{v}_t^R) \approx \mathbf{v}_t + \tilde{\delta} \mathbf{v}_t^R \quad (4.7)$$

we get

$$\mathbf{v}_{t+1} = \mathbf{v}_t + \frac{1}{2}(\tilde{\delta} \mathbf{v}_t^L + \tilde{\delta} \mathbf{v}_t^R)$$

□

We observe that the symmetric approach do not requires to use the BCH formula at each passage, having considered the approximation at the first order of the BCH.

We conclude with a formula that relates $\tilde{\delta} \mathbf{v}_t^L$ with $\tilde{\delta} \mathbf{v}_t^R$:

Theorem 4.2.2. Be $\tilde{\delta} \mathbf{v}_t^R = \exp(\mathbf{v}) \circ \exp(-\mathbf{v}_t) - e$ and $\tilde{\delta} \mathbf{v}_t^L = \exp(-\mathbf{v}_t) \circ \exp(\mathbf{v}) - e$ as before, then

$$\delta \mathbf{v}_t^L \approx \exp(-\mathbf{v}_t) \circ \delta \mathbf{v}_t^R \circ \exp(\mathbf{v}_t)$$

Proof. Since $\exp(\mathbf{v}_t) \circ \exp(\delta \mathbf{v}_t^R) \approx \exp(\delta \mathbf{v}_t^L) \circ \exp(\mathbf{v}_t)$ it follows

$$\exp(\delta \mathbf{v}_t^R) = \exp(-\mathbf{v}_t) \circ \delta \mathbf{v}_t^L \circ \exp(\mathbf{v}_t)$$

Using $\exp(\delta \mathbf{v}_t^R) = e + \delta \mathbf{v}_t^R$ and $\exp(\delta \mathbf{v}_t^L) = e + \delta \mathbf{v}_t^L$ we get

$$\begin{aligned}e + \delta \mathbf{v}_t^R &= \exp(-\mathbf{v}_t) \circ (e + \delta \mathbf{v}_t^L) \circ \exp(\mathbf{v}_t) \\ \delta \mathbf{v}_t^R &= \exp(-\mathbf{v}_t) \circ \delta \mathbf{v}_t^L \circ \exp(\mathbf{v}_t)\end{aligned}$$

□

Symmetric-Parallel Transport Strategy

If we are not satisfied to having take only the first order approximation of the BCH in the equation (4.6) we use at this stage the parallel transport in the method presented in this subsection. Going back to the algorithm 4.4 we can apply to

$$\mathbf{v}_{t+1} = \frac{1}{2}(\text{BCH}(\tilde{\delta} \mathbf{v}_t^L, \mathbf{v}_t) + \text{BCH}(\mathbf{v}_t, \tilde{\delta} \mathbf{v}_t^R))$$

the parallel transport to get

$$\begin{aligned}\mathbf{v}_{t+1} &= \frac{1}{2}((\tilde{\delta}\mathbf{v}_t^L)^\parallel + \mathbf{v}_t + \mathbf{v}_t + (\tilde{\delta}\mathbf{v}_t^R)^\parallel) \\ &= 2\mathbf{v}_t + \frac{1}{2}((\tilde{\delta}\mathbf{v}_t^L)^\parallel + (\tilde{\delta}\mathbf{v}_t^R)^\parallel)\end{aligned}$$

Applying the definition of parallel transport we get

$$(\tilde{\delta}\mathbf{v}_t^L)^\parallel + (\tilde{\delta}\mathbf{v}_t^R)^\parallel = \exp(-\frac{\mathbf{v}_t}{2}) \circ (\tilde{\delta}\mathbf{v}_t^L + \tilde{\delta}\mathbf{v}_t^R) \circ \exp(\frac{\mathbf{v}_t}{2})$$

where

$$\begin{aligned}\tilde{\delta}\mathbf{v}_t^L &= \exp(\mathbf{v}) \circ \exp(-\mathbf{v}_t) - e \\ \tilde{\delta}\mathbf{v}_t^R &= \exp(-\mathbf{v}_t) \circ \exp(\mathbf{v}) - e\end{aligned}$$

Then a new improvement of the algorithm ?? is

$$\begin{cases} \mathbf{v}_0 = 0 \\ \mathbf{v}_t = 2\mathbf{v}_{t-1} + \frac{1}{2}(\exp(-\frac{\mathbf{v}_{t-1}}{2}) \circ (\tilde{\delta}\mathbf{v}_{t-1}^L + \tilde{\delta}\mathbf{v}_{t-1}^R) \circ \exp(\frac{\mathbf{v}_{t-1}}{2})) \end{cases} \quad (4.8)$$

(This must be investigated!)

Chapter 5

Experimental Results

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

xxx Sum up what has been done
xxx Explored tools for statistics of diffeomorphisms.
xxx Statistics on anatomies:

xxx It is of fundamental importance to have the possibility to going from an element of a group of spatial transformations to a tangent space, in which each vector corresponds to the tangent vector field that this transformation causes on the space. It makes possible to lean on the group structure a structure of vector space, which implies the possibility to compute statistics on the group of transformation as well as compose velocity fields in the tangent space passing through the corresponding transformation (both of them are made possible thanks to the local bijection between the Lie group and the Lie algebra).

5.1 Group composition at the Service of Image Registration

xxx Sum up: log-composition in diffeomorphic image registration.

5.2 Experimental Results

5.2.1 Log-Compositions Performance for Toy examples and Patient Images

5.2.2 Logarithm Computation using Log-composition

5.3 Further Research and Conclusion

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

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