Constrained Optimization on Manifolds

Von der Universität Bayreuth
zur Erlangung des Grades eines
Doktors der Naturwissenschaften (Dr. rer. nat.)
genehmigte Abhandlung

von

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Tag der Einreichung: 23.07.2020
Tag des Kolloquiums: 26.11.2020

Zusammenfassung

Optimierungsprobleme sind Bestandteil vieler mathematischer Anwendungen. Die herausforderndsten Optimierungsprobleme ergeben sich dabei, wenn hoch nichtlineare Probleme gelöst werden müssen. Daher ist es von Vorteil, gegebene nichtlineare Strukturen zu nutzen, wofür die Optimierung auf nichtlinearen Mannigfaltigkeiten einen geeigneten Rahmen bietet. Es ergeben sich zahlreiche Anwendungsfälle, zum Beispiel bei nichtlinearen Problemen der Linearen Algebra, bei der nichtlinearen Mechanik etc. Im Fall der nichtlinearen Mechanik ist es das Ziel, Spezifika der Struktur zu erhalten, wie beispielsweise Orientierung, Inkompressibilität oder Nicht-Ausdehnbarkeit, wie es bei elastischen Stäben der Fall ist. Außerdem können sich zusätzliche Nebenbedingungen ergeben, wie im wichtigen Fall der Optimalsteuerungsprobleme. Daher sind für die Lösung solcher Probleme neue geometrische Tools und Algorithmen nötig.

In dieser Arbeit werden Optimierungsprobleme auf Mannigfaltigkeiten und die Konstruktion von Algorithmen für ihre numerische Lösung behandelt. In einer abstrakten Formulierung soll eine reelle Funktion auf einer Mannigfaltigkeit minimiert werden, mit der Nebenbedingung einer C^2-Submersionsabbildung zwischen zwei differenzierbaren Mannigfaltigkeiten. Für Anwendungen der Optimalsteuerung wird diese Formulierung auf Vektorbündel erweitert. In der Literatur finden sich bereits Optimierungsalgorithmen auf Mannigfaltigkeiten, meist ohne Berücksichtigung von Nebenbedingungen [AMS09]. Dabei ist der Einsatz von Retraktionen maßgeblich. Retraktionen, die eine bedeutende Rolle bei der Schrittberechnung von Optimierungsalgorithmen spielen, erlauben es, die involvierten Abbildungen auf lineare Räume zurückzuziehen, und machen somit einige Ergebnisse aus dem linearen Fall nutzbar. Insbesondere sind über Retraktionen die KKT-Bedingungen und Optimalitätsbedingungen zweiter Ordnung erreichbar. In dieser Arbeit wird das Konzept der Retraktionen auf Vektorbündel erweitert, auf denen Konsistenzbedingungen erster und zweiter Ordnung definiert sind. Andererseits ergibt sich auf jedem Punkt der Mannigfaltigkeit ein 1-Form Lagrange-Multiplikator als Lösung des Sattelpunktproblems. Wir beweisen, dass die Existenz einer Potentialfunktion für den Lagrange-Multiplikator von der Integrierbarkeit (im Sinne von Frobenius) der horizontalen Verteilung, d.h. der orthogonalen Komponente der linearisierten Nebenbedingung, abhängt.

Für die algorithmische Lösung beschränkter Optimierungsprobleme auf Mannigfaltigkeiten wird die affine kovariante Composite-Step-Methode, wie dargestellt in [LSW17], auf diese Räume erweitert und somit lokale superlineare Konvergenz des Algorithmus für Retraktionen erster Ordnung erreicht. Zuerst wird der Algorithmus an einem beschränkten Eigenwert-Problem getestet. Dann werden numerische Experimente in der Mechanik von elastischen nicht dehnbaren Stäben betrachtet. In letzterem Fall wird der Gleichgewichtszustand eines elastischen nicht dehnbaren Stabes unter Eigengewicht berechnet. Der Fall, dass der Stab in Kontakt mit einer oder mehreren Flächen kommt, wird in Betracht gezogen. Dabei wird die Riemannsche Struktur des positiven Kegels im $\mathbb{R}^3$, wie in [NT$^+$02] dargestellt genutzt. Zusätzlich wird ein Optimalsteuerungsproblem eines elastischen nichtdehnbaren Stabs gelöst als Anwendungsfall beschränkter Optimierungsprobleme auf Vektorbündeln. Schließlich werden Retraktionen auf dem Raum von Orientierung erhaltenden Tetraedern für finite Elastizitätsprobleme genutzt.

Abstract

Optimization problems are present in many mathematical applications, and those that are particularly challenging arise when it comes to solving highly nonlinear problems. Hence, it is of benefit exploiting available nonlinear structure, and optimization on nonlinear manifolds provides a general and convenient framework for this task. Applications arise, for instance, in nonlinear problems for linear algebra, nonlinear mechanics, and many more. For the case of nonlinear mechanics, the aim is to preserve some specific structure, such as orientability, incompressibility or inextensibility, as in the case of elastic rods. Moreover, additional constraints can occur, as in the important case of optimal control problems. Therefore, for the solution of such problems, new geometrical tools and algorithms are needed.

This thesis deals with the setting of constrained optimization problems on manifolds and with the construction of algorithms for their numerical solution. In the abstract formulation, we seek to minimize a real function on a manifold, where the constraint is given by a submersion that is a C^2-map between two differentiable manifolds. Furthermore, for optimal control applications, we extend this formulation to vector bundles. Optimization algorithms on manifolds are available in the literature, mostly for the unconstrained case [AMS09], and the usage of retraction maps is an indispensable tool for this purpose. Retractions, which play a fundamental role in the updating of the iterates in optimization algorithms, also allow us to pullback the involved maps to linear spaces, making possible the use of tools and results from the linear setting. In particular, KKT-theory and second-order optimality conditions are tractable thanks to such maps. In this work, we extend the concept of retraction to vector bundles, where first and second-order consistency conditions are also defined. On the other hand, at each point in the manifold, a 1-form Lagrange multiplier arises as a solution of a saddle point problem. We prove that the existence of a potential function for this Lagrange multiplier depends on the integrability, in the sense of Frobenius, of the horizontal distribution, i.e., the orthogonal complement of the linearized constraint map.

For the algorithmic solution of constrained optimization problems on manifolds, we generalize the affine covariant composite step method presented in [LSW17] to these spaces, and local superlinear convergence of the algorithm for first-order retractions is obtained. First, we test the algorithm in a constrained eigenvalue problem. Then, we consider numerical experiments on the mechanics of elastic inextensible rods. There, we compute the final configuration of an elastic inextensible rod under dead load. The case in which the rod enters in contact with one, or several planes, is considered. Hence, we exploit the Riemannian structure of the positive cone in $\mathbb{R}^3$, as pointed out

in [NT$^+$02]. In addition, we solve an optimal control problem of an elastic inextensible rod, as an application to constrained optimization problems on vector bundles. Finally, we use retractions on the space of orientation preserving tetrahedra for finite elasticity problems.

Acknowledgments

Firstly, I would like to thank my supervisor Prof. Dr. Anton Schiela, not only for giving me the opportunity of working on this exciting and challenging topic but also for his consistent support and guidance throughout the project. All my gratitude and admiration for him.

I thank Prof. Dr. Oliver Sander for agreeing to review the present work. I also want to thank Prof. Dr. Lars Grüne and Prof. Dr. Thomas Kriecherbauer for being members of the examination committee.

Likewise, I would like to thank all the people from the chair of Applied Mathematics of the University of Bayreuth with whom I had the opportunity to share time. Special thanks to Dr. Robert Baier, Sigrid Kinder, Dr. Philipp Braun, Dr. Marleen Stieler, Dr. Georg Müller, Arthur Fleig, Tobias Sproll, Manuel Schaller, Dr. Simon Pirkelmann, Matthias Stöcklein - I will never forget the days spent in this place with such wonderful people.

Finally, I thank my family: Flor, Javier, and Cristian, for always being there even in the distance. To Isadora, thanks for all your support, care, love and for filling my days with joy.

Contents

Chapter 1

Introduction

In an important variety of fields, optimization problems benefit from a formulation on nonlinear manifolds. For instance, applications to numerical linear algebra like invariant subspace computations, or low-rank approximation problems can be tackled using this approach [AMS09]. Optimization problems for Machine learning [SH16, Bis06], are carried over structured spaces. Nonlinear partial differential equations, in which the configuration space is given by maps where the domain and target consist of nonlinear manifolds, are found in many applications. Further examples are Cosserat materials [BS89, SS14, JLLO11, San12], where configurations are maps into the space $\mathbb{R}^3 \times SO(3)$, which are particularly relevant for shell and rod mechanics. Liquid crystal physics [Pro95, DGP93, HK87, LL89], where molecules are described as little rod- or plate-like objects; in a PDE setting, a liquid Crystal configuration is a field with values in the unit sphere, or, depending on the symmetry of the molecules, in the projective plane or the special orthogonal group. Various numerical approaches to simulate liquid crystals and related problems from micro-magnetics can be found in the literature [Alo97, AKT12, BP07, KVBP$^+$14]. Numerical computations with shapes, such as shape analysis [BHM10, RW12, You10] and shape optimization [Sch14, SZ92, You10, SO19] are done using the inherent structure of the space of shapes. This structure originates from the fact that deformations, i.e., diffeomorphisms, form a nonlinear manifold, rather than a vector space. Similar insights have been successfully exploited in the analysis of finite strain elasticity and elastoplasticity [Bal02, Mie02]. Applications of fields with nonlinear codomain are models of topological solitions [MS04, Kam82], image processing [TSC00], and the treatment of diffusion-tensor imaging [PFA06, LBMP$^+$01]. Further instances can be found in [SS00, GG17] on geometric wave maps, or [EL78, SY97, Ham06] on harmonic maps.

Unconstrained optimization on manifolds is by now well established, as can be seen in [AMS09, Lue72, TSC00, HHLM07, ABG07], where theory and applications are covered. One of the aims of this work is to extend well known SQP-methods from the linear setting [CGT11, Deu11, CGT00, NW06, Sch17, NP06], to the manifold case. In fact, many things run in parallel to algorithmic approaches on linear spaces. In particular, local (usually quadratic) models are minimized at the current iterate, allowing the computation of optimization corrections. The main difference between optimization algorithms on manifolds and linear spaces is how to update the iterates for a given search direction. If the manifold is linear, its tangent space coincides with the manifold itself and the current iterate can be added to the search direction to obtain the update. If the manifold is nonlinear, the additive update has to be replaced by a suitable generalization. A natural idea on Riemannian manifolds would be to compute an update via the exponential map, i.e., via geodesics, but in many cases, such exponential can be expensive to compute, therefore the use of cheaper surrogates, so-called *retractions* is advocated in [AMS09]. These retractions have to satisfy certain consistency conditions and the weaker these conditions are, the more flexibly the retractions can be chosen. Based on these ideas, many algorithms of unconstrained optimization have been carried over to Riemannian manifolds, and have been analyzed in this framework [HT04, Lue72]. In general, the use of nonlinear retractions enables to exploit the given nonlinear problem structure within an optimization algorithm. While this is true in particular for nonlinear manifolds, it may also sometimes be beneficial to use nonlinear retractions even in the case of linear spaces.

In coupled problems, mixed formulations, or optimal control of the above listed physical models, additional equality constraints occur, and thus one is naturally led to equality constrained optimization on manifolds. Up to now, optimization algorithms on manifolds have mainly been considered for the unconstrained case, in contrast, less research has been conducted on the construction of algorithms for equality constrained optimization on manifolds. Recently, however, the study on the constrained case has emerged. For instance in [YZS14, BH18, LB19], optimization problems on manifolds with equality and inequality constraints are considered. There, the domain space of the mappings describing the constraints is a known manifold. More specifically, in [YZS14], necessary optimality conditions for these kinds of problems are discussed. In [LB19], algorithmic methods for the numerical solution of such problems are proposed, and, in particular, augmented Lagrangian and the exact penalty method on Riemannian manifolds are considered. Also, in the work [BH18], the extension of a set of constraint qualifications from the Euclidean setting to the manifold setting is presented. Further approaches can be found, for instance in [KGB16], where the alternating direction method of multipliers to the Riemannian case is presented with applications to dimensionality reduction, data analysis, and manifold learning.

This thesis develops methods for the solution of equality constrained optimization problems on manifolds. Throughout this work, we consider the problem:

$$\min_{x\in M} f(x) \quad \text{s.t.} \quad c(x) = y$$

where $f : M \to \mathbb{R}$ and $c : M \to N$ are C^2-maps, and c is a submersion. In our setting, the objective function maps from a manifold to the real numbers, and the constraint mapping, has manifolds as domain and target. In addition, for optimal control problems, we consider the case in which the constraint maps into a cotangent bundle space, which is an instance of a special manifold, called vector bundle. For this reason, new theory over this structure has to be developed. In [AMS09], suitable mappings for optimization algorithms on manifolds are introduced. These maps, called retractions, serve as a way to pullback, both objective and constraint maps, to linear spaces and compute optimization corrections. Afterwards, retractions can also be used to update the iterates. For the case of vector bundles, we define suitable retractions operating over this structure, and new consistency conditions are also introduced.

Concerning the algorithmic part, the employed approach is a generalization of an affine covariant composite step method as in [LSW17], to the manifold case. This method was successfully used in challenging applications to finite elasticity, including optimal control problems. In this work, the resulting algorithm is tested in a nonlinear eigenvalue problem, as considered in [GGvM89], and in applications to finite elasticity, as in [GLT89, AR78, Ped00]. Finally, as an application to constrained optimization problems on vector bundles, we solve an optimal control problem of an elastic inextensible rod. There, the optimization process is performed on a specific instance of a vector bundle, namely, the co-tangent bundle. This space arises, due to that, the constraint is a minimizer of the elastic energy over the manifold. Finally, we introduce and test retractions on the space of oriented tetrahedra. In Finite elasticity, the discretization of an elastic body into tetrahedra is often used to solve numerical problems in mechanics. We consider an elastic body $\Omega \subset \mathbb{R}^3$, which is in turn subdivided into several tetrahedra. There, we aim to minimize an elastic energy in the discrete setting, and optimization corrections are computed. Here, the configuration is updated using the retraction over the space of oriented tetrahedra. In this way, the updates are done in a nonlinear way over this space, thus, preserving the structure, and avoiding self-penetration. We show the convenience of using such nonlinear updates in comparison to the linear ones.

1.1 Outline

Regarding the mathematical tools for the development of the thesis, and intending to make this work as self-contained as possible, we start in Chap.2 with the necessary preliminaries on differential geometry. We take as main references [Lan12a, Kli11, Mic08, Lee13, Spi70, DC16, JJ08, Car92, Hel79], where the basic differential geometry theory is developed. In Chap.2, the concepts of differential manifold, tangent bundle, co-tangent bundle, vector bundle, Riemannian manifold, submersions, transversality, integrability of distributions, sprays, and covariant derivatives are introduced. With this, we have the prerequisites needed for our purposes.
We start Chap.3, with a review of the fundamental ideas for unconstrained optimization problems on manifolds following the work of [AMS09]. We continue Chap.3, with an important tool for optimization algorithms on manifolds, which was introduced in [AMS09] and whose use has become customary, namely, the concept of local retraction. Nonlinear retractions play a crucial role in the implementation of algorithms. A retraction R_x^M on a manifold M is a mapping:

$$R_x^M : T_xM \longrightarrow M$$

from the tangent space T_xM at $x \in M$ to the manifold, that is first order consistent with the exponential map. Retractions play two roles in optimization algorithms. They serve as a way to pullback through composition the involved mappings into the tangent space at each point. Given that the tangent space is linear, it allows the computation of optimization corrections. Once an optimization correction $\delta x \in T_xM$ is computed, the update of the iterates will be performed by the formula $x_+ = R_x^M(\delta x) \in M$, which is again a point in M. Among others, examples for the n-sphere are shown, and we introduce retractions over the space of orientation preserving tetrahedra, as well as the space of volume preserving tetrahedra. These are important tools for the implementation of the numerical applications performed in Chap.6. For the actual implementation in the computer, and in order to increase manageability of the formulas, the notion of local parametrization is presented (Sec.3.2.2). There, we use a representation of the tangent space through a map $\Theta_{TM} : \mathbb{E} \to T_xM$, where $\mathbb{E}$ is the linear model space of the manifold M. In this way, a parametrization

$$\begin{aligned} \mu_x^M(\vartheta) :& \mathbb{E} \longrightarrow T_xM \\ & \vartheta \longrightarrow \mu_x^M(\vartheta) = (R_x^M \circ \Theta_{TM})(\vartheta) \end{aligned}$$

will be defined as the composition of a retraction, with a linear map Θ_{TM} (Sec.3.2.2). Further manifolds with additional structure, such as vector bundles $p : E \to M$, are also considered. This class of manifolds, which contains the distinguished cases of tangent and co-tangent bundles, will be of importance for optimal control problems. We introduce retractions, $R^E : TE \to E$ acting over this specific structure (Sec.3.3). A vector bundle $p : E \to M$, can locally be regarded as a product $U \times \mathbb{F}$, where $U \subset M$ and $\mathbb{F}$, the so-called fiber space, is a topological linear space. Assuming the existence of a vector bundle connection κ_E (Sec.2.8), a retraction on a vector bundle is defined in (Sec.3.3), as:

$$\begin{aligned} R^E_{x_0,e_0} : & T_{x_0,e_0}E \longrightarrow E \\ & (\xi, \eta) \longrightarrow (R^M_{x_0}(\xi), (A \circ R^M_{x_0})(\xi)(e_0 + \eta)) \end{aligned}$$

where $R^M_{x_0}$ is a retraction on the base manifold M, and $A : E_{x_0} \to E_x$ is a linear isomorphism between the fibers, in this case, the vector spaces, E_{x_0} and E_x. As in the previous case, pullbacks and updates can be done through retractions over this structure. Using the concept of vector bundle connection, we define first and second-order vector bundle retractions (Sec.3.3.1). In a similar fashion, as in the plain manifold case, we define parametrizations for the vector bundle context (Sec.3.88).
In Chap.4, the equality constrained optimization problem on manifolds is formulated (Sec.4.1). Performing pullbacks to the cost and constraint mappings, at each point $x \in M$, solutions to a block linear system are found, obtaining, in particular, a 1-form Lagrange multiplier $\lambda_x \in T_{c(x)}N^*$. We study the existence of a potential function $\Lambda : M \to \mathbb{R}$, such that $d\Lambda = \lambda_x$ (Sec.4.4). The answer (Sec.4.4.2), which is intimately related to the integrability of the horizontal subbundle $(\ker c'(x))^\perp$, is positive for some special cases (Sec.4.4.1), and relates to the structure of M. Additionally, with the help of retractions, KKT-conditions (Sec.4.2) and corresponding second order optimality conditions (Sec.4.3) are derived. The framework of constrained optimization problems on vector bundles is discussed (Sec.4.5), and an adequate setting of the problem, which involves the concept of transversality, is developed.
In Chap.5, the affine covariant composite step method as presented in [LSW17], is generalized from the linear setting to the manifold case. In the pure linear setting (Sec.5.1), the way the composite step method copes with the double aim of feasibility and optimality, is done by splitting the optimization step δx into a normal step δn and a tangential step δt

$$\delta x = \delta n + \delta t : \qquad \delta t \in \ker c'(x), \qquad \delta n \in (\ker c'(x))^\perp,$$

where δn is a minimal norm Gauss-Newton step for the solution of the underdetermined problem $c(x) = 0$, and δt aims to minimize f on the current space of the linearized constraints. The generalization to manifolds (Sec.5.2), is done by performing the pullback of both, cost and constraint mappings to linear spaces, their respective tangent spaces. The pullbacked mappings $\mathbf{f}$ and $\mathbf{c}$, now with linear spaces as domain and codomain, yield the problem:

$$\min_{u \in T_x X} \mathbf{f}(u) \quad \text{s.t.} \quad \mathbf{c}(u) = 0$$

where $\mathbf{f} : T_xM \to \mathbb{R}$ and $\mathbf{c} : T_xM \to T_{c(x)}N$. Normal, tangential and simplified normal steps δn, δt and δs are computed as elements of T_xM (Sec.5.2.1), and subsequently updated using the formula:

$$x_+ = R^M_x(\delta n + \delta t + \delta s).$$

Local superlinear convergence for first order retractions is obtained with the introduction of a second order modified model (Sec.5.2.3). After this, the extension of the algorithm to the case in which the co-domain N is a vector bundle is also considered (Sec.5.5).
In Chap.6, applications and numerical results are presented. We start with a constrained eigenvalue problem, as treated in [GGvM89]. There, we consider:

$$\min_{x \in \mathbb{R}^{n+m}} x^T A x \quad \text{s.t.} \quad \begin{aligned} Cx &= t \\ x^T x &= 1. \end{aligned}$$

where A is a symmetric matrix, C^T is a matrix with full rank and t a vector. The problem is re-formulated as:

$$\min_{x\in\mathbb{S}^{n+m}} x^T A x \quad \text{s.t.} \quad Cx = t$$

obtaining a constrained optimization problem on the manifold $\mathbb{S}^{n+m}$, where the composite step method is applicable.
After that, in the context of finite elasticity, we consider the problem of finding equilibrium configurations of elastic inextensible rods under different prescribed conditions. We consider three cases: First, the forward problem of finding the final configuration of an inextensible elastic rod under a prescribed force. For the second case, the mentioned rod can enter in contact with either one or several planes, and, for the last case, we consider the optimal control problem.
For the forward problem (Sec.6.2), the stable equilibrium position of an inextensible transversely isotropic elastic rod under dead load is searched. To this end, the optimization problem [GLT89]

$$\min_{\substack{y\in H^2([0,1];\mathbb{R}^3)\\ \|y'\|=1}} \frac{1}{2}\int_0^1 \left\langle y'', y''\right\rangle \, ds - \int_0^1 \langle g, y\rangle \, ds$$

is considered, and through a mixed formulation:

$$\min_{Y\times V} J(y,v) = \frac{1}{2}\int_0^1 \left\langle v', v'\right\rangle \, ds - \int_0^1 \langle g, y\rangle \qquad \text{s.t.} \quad y' = v,$$

where $Y = H^2([0,1];\mathbb{R}^3)$ and $V = H^1([0,1],\mathbb{S}^2)$, we land in the framework of a constrained optimization problem on manifolds. Here, J is the total potential energy, and the requirement $v \in \mathbb{S}^2$, enforces the inextensibility condition of the rod. Next, we consider the case in which the rod can enter in contact with one of the planes that delimit the first octant in $\mathbb{R}^3$. We do this by considering the space:

$$K_+ = \{x \in \mathbb{R}^3 |\, x_i > 0,\ i = 1,2,3\}$$

together with the Riemannian metric

$$\langle \xi, \xi\rangle_x = \sum_{i=1}^{3} \frac{\mu}{x_i^2} \xi_i \, \xi_i$$

for $x \in K_+$, $\xi \in \mathbb{R}^3$, and $\mu \in \mathbb{R}$. This set, endowed with this metric, becomes a Riemannian manifold without boundary [NT+02]. Here, we solve the following problem:

$$\begin{aligned}\min_{Y\times V\times\mathcal{K}_+} J(y,v,s) = \frac{1}{2}\int_0^1 \left\langle v', v'\right\rangle \, ds - \int_0^1 \langle g, y\rangle - \mu\int_0^1 \sum_{i=1}^{3} \log(\sigma_i)\, ds \qquad \text{s.t.} \quad & y' = v,\\ & y = s,\end{aligned}$$

with $\mathcal{K}_+ = H^2([0,1],K_+)$. In the above regularized problem, the barrier function:

$$b(\mu,\sigma) = -\mu\int_0^1 \sum_{i=1}^{3} \log(\sigma_i)\, ds$$

is as introduced in [Gül96], and the solution of the problem is found when the homotopy parameter $\mu \to 0$ is decreased. Suitable retractions for this space are used, avoiding the need for checking feasibility of the iterates.
Finally, using the abstract setting for the optimal control of energy minimizers as presented in (Sec.4.5.1), we consider the optimal control problem of elastic inextensible rods (Sec.6.4). There, we consider the problem:

$$
\begin{aligned}
\min_{Y\times U} \frac{1}{2}\|y-y_d\|_{L_2([0,1];\mathbb{R}^3)} + \frac{\alpha}{2}\|u\|^2_{L_2([0,1];\mathbb{R}^3)} \\
s.t. \quad \min_{Y\times V\times U} J(y,v,u) := \frac{1}{2}\int_0^1 \langle v', v'\rangle\, ds - \int_0^1 \langle u, y\rangle \\
\text{s.t.} \quad c(y,v) = y' - v = 0.
\end{aligned}
$$

which, through a KKT-reformulation, yields:

$$
\begin{aligned}
\min_{Y\times V\times\Lambda\times U} \frac{1}{2}\|y-y_d\|_{L_2([0,1];\mathbb{R}^3)} + \frac{\alpha}{2}\|u\|^2_{L_2([0,1];\mathbb{R}^3)} + \frac{\gamma}{2}\|\lambda\|^2_{L_2([0,1];\mathbb{R}^3)} \\
\text{s.t.} \quad J'(y,v,u) + \lambda c'(y,v) - Bu = 0 \\
c(y,v) = 0.
\end{aligned}
$$

The latter, can be regarded as a constrained optimization problem on vector bundles:

$$
\begin{aligned}
\min_{Y\times V\times\Lambda\times U} f(y,v,u,\lambda) \quad \text{s.t} \quad c_F(y,v,\lambda,u) = 0 \\
c(y,v) = 0
\end{aligned}
$$

where

$$c_F : Y \times V \times \Lambda \times U \longrightarrow Y^* \times TV^* \times \Lambda^*$$

and $\lambda \in \Lambda = L^2([0,1];\mathbb{R}^3)$. We observe that the derivative of the elastic energy, which is a map that belongs to the co-tangent space $Y^*\times TV^*\times\Lambda^*$, defines the new constraint c_F. This is an instance of a constrained optimization problem, where the constraint maps on a vector bundle. For the numerical solution of this problem, we implement the theory developed for vector bundle retractions (Sec.3.3).
We end Chap.6, by testing the nonlinear updates for the space of oriented tetrahedra (Sec.3.2) in finite elasticity problems. There, we proceed in the following way: the discretization of a body $\Omega \subset \mathbb{R}^3$ into tetrahedra is performed. Then, we compute a correction vector field δx that lies at each node of each tetrahedron, using the linear retraction. This is followed by a nonlinear update using the formulas introduced in (Sec.3.2), for the space of oriented tetrahedra. By construction, this procedure avoids self penetration of each tetrahedron. Besides, further structure such are rotations are exploited, making the updates more efficient. We show the impact of these updates on numerical simulations (Sec.6.5).

Chapter 2

Concepts of Differential Geometry

In this chapter, we do a review of the fundamental concepts of differential geometry (manifolds, tangent spaces, vector bundles, Lie groups, differential forms, distributions, integrability, sprays, covariant derivatives, exponential map) needed for the development of this work. Central to the topic is the concept of differential manifold. In a broad sense, manifolds are sets possessing additional structure with the property that locally, they resemble a linear space, the model space, which can be finite or infinite-dimensional, Hilbert or even a Banach space. We start with the definition of a manifold, followed by some examples. We continue with a rather succinct overview of the differential geometric objects needed in subsequent sections. For a complete presentation on the topic, we refer the reader to [Kli11, Lan12a, Mic08, RS11, Lee13, AMR12, Spi70, KN63, Hel01, Ste99], which are part of the vast literature on the field. Among the needed tools, we deal with mappings between manifolds, and in particular, those that are submersions. We show the construction of such maps, their differentials, and main properties. We also mention theorems concerning integrability of bundles, results that will be needed in Chapter 4, where we study the existence of a potential function for the Lagrange multiplier when it is considered as a 1-form on the target manifold of the constraint mapping. We close this section with a central concept on differential geometry, that of connection. Throughout connections, splitting of the double tangent bundle and the tangent space of a vector bundle is possible. This provides a way to define a proper differentiation of vector fields. The latter will be of importance for the construction of suitable mappings for optimization on manifolds, which includes vector bundles.

2.1 Manifolds

We start by defining the central concept in differential geometry, namely, that of a differentiable manifold. As we already mentioned, a manifold can be understood as a topological set that locally resembles a euclidean space. We write this in a more precise way.

Definition 2.1.1. *Let be M a topological space. An atlas of class (C^p) $p \geq 0$ on M is a collection of pairs $(U_i, \phi_i)_{i \in I}$, satisfying the following conditions:*

i) Each U_i is a subset of M and the U_i cover M.

ii) *Each ϕ_i is a bijection of U_i onto an open subset $\phi_i U_i$ of some topological vector space $\mathbb{E}_i$, and for any i, j, $\phi_i(U_i \cap U_j)$ is open in $\mathbb{E}_i$.*

iii) *The map*

$$\phi_j \phi_i^{-1} : \phi_i(U_i \cap U_j) \longrightarrow \phi_j(U_i \cap U_j)$$

is a C^p-isomorphism for each pair of indices i, j.

Each pair (U_i, ϕ_i) is called a chart of the atlas, and for any point $x \in U_i$, it is said that (U_i, ϕ_i) is a chart at x.

Remark 2.1.1. *If all the topological vector spaces $\mathbb{E}_i$ are all equal to $\mathbb{E}$, then we say that the atlas is an $\mathbb{E}$ atlas and that the manifold M is modeled on $\mathbb{E}$. The model manifold can be either a Hilbert space, a Banach space, a Fréchet space or a convenient locally convex vector space. For more details see [Lan12a, Mic08].*

Remark 2.1.2. *If M is modeled on $\mathbb{R}^n$ for some fixed n, then we say that the manifold is n-dimensional. There, the function ϕ maps from U to $\mathbb{R}^n$ and is given by n coordinate functions $\phi_1, ..., \phi_n$.*

It is possible to add more structure to a manifold, giving rise to a wide number of them. We mention some examples that are oriented to our specific applications to optimization algorithms. Before that, we define another central notion in differential geometry, that of a tangent vector.

Definition 2.1.2. *Let M be a manifold of class C^p $(p \geq 1)$. Let x be a point of M. We call a tangent vector to the equivalence class $[U, \phi, \xi]$, where (U, ϕ) is a chart at x and ξ is an element of the vector space where ϕU lies. Two triples (U, ϕ, ξ), (V, ψ, η) are equivalent if:*

$$(\psi\phi^{-1})'(\phi x)\xi = \eta.$$

Where the usual derivative $(\psi\phi^{-1})'$ between topological vector spaces is defined in A.2. The set of such tangent vectors is called the tangent space of M at x and is denoted by $T_x M$.

A new manifold can be constructed by gluing in a special way all the tangent spaces $T_x M$ for $x \in M$. This manifold receives the name of tangent bundle, and, as we will see later, is a special case of a more general structure called vector bundle.

Definition 2.1.3. *Let be a manifold M of class C^p with $p \geq 1$. We call the tangent bundle to*

$$TM := \bigsqcup_{x \in M} T_x M$$

i.e., the disjoint union of the tangent spaces $T_x M$, which is a family of vector spaces parameterized by M, with projection $\pi : TM \longrightarrow M$ given by $\pi(T_x M) = x$.

Approach via curves An alternative equivalent definition of tangent vector can be given using equivalent classes of curves realizing the same derivation at a point.

Definition 2.1.4. *Let be M a manifold. A smooth curve in M is a map*

$$\gamma : I \to M$$

from an open interval $I \subset \mathbb{R}$ into M.

Definition 2.1.5. *Let be M a manifold and let be $x \in M$ a point. A tangent vector of M at x is defined as the equivalent class of curves on M*

$$[\gamma(t)] = \{\hat{\gamma}(t) \,|\, x = \hat{\gamma}(0) = \gamma(0) \text{ and } (\phi \circ \hat{\gamma})'(0) = (\phi \circ \gamma)'(0)\}$$

with $\gamma(t)$ and $\hat{\gamma}(t)$ curves on M and (U, ϕ) a chart around x. It can be seen that there is bijection between tangency classes of curves and the tangent space T_xM of M at x. For more details, see $[Lan12a, IV, \S 2]$.

It is possible to go further and define the second-order tangent bundle.

Definition 2.1.6. *Let M be a manifold and let $x \in M$ be a point. The second order tangent bundle of M at $x \in M$, denoted by $T_x^2 M$, is the set of all classes of curves on M*

$$[\gamma(t)] = \{\hat{\gamma}(t) | \, x = \hat{\gamma}(0) = \gamma(0), \ (\phi \circ \hat{\gamma})'(0) = (\phi \circ \gamma)'(0) \text{ and } (\phi \circ \hat{\gamma})''(0) = (\phi \circ \gamma)''(0)\}$$

where $\hat{\gamma}(t) : I_1 \to M$ and $\gamma(t) : I_2 \to M$ are curves on M, I_1 and I_2 are intervals containing the zero, and (U, ϕ) is a chart around x. This means that the second order tangent bundle consists of classes of curves that agree up to their second derivative.

Definition 2.1.7. *Let be M a manifold of class C^p with $p \geq 2$. The tangent bundle of order two is given by:*

$$T^2 M := \bigsqcup_{x \in M} T_x^2 M.$$

The union of all tangent spaces of order two.

Remark 2.1.3. *Let us consider a curve $\gamma(t) : I \to M$, where $I \subset \mathbb{R}$ is an interval that contains the zero, with $\gamma(0) = x \in M$. Let be (U, ϕ) and (V, ψ) two charts around x. We observe the following:*

$$\begin{aligned}(\phi \circ \gamma)(t) &= (\phi \circ \psi^{-1} \circ \psi \circ \gamma)(t) \\ &= (\Phi \circ \psi \circ \gamma)(t),\end{aligned}$$

where $\Phi = (\phi \circ \psi^{-1}) : \psi(U \cap V) \to \phi(U \cap V)$, is the transition of charts map. Taking first and second derivative at zero we get:

$$(\phi \circ \gamma)'(0) = \Phi'(0)(\psi \circ \gamma)'(0) \tag{2.1}$$

$$(\phi \circ \gamma)''(0) = \Phi''(0)((\psi \circ \gamma)'(0))^2 + \Phi'(0)(\psi \circ \gamma)''(0) \tag{2.2}$$

In (2.1), we observe that a tangent vector is transformed in a linear way under the derivative of the coordinate transformation. In contrast, we observe in (2.2), that the second derivative does not transform linearly anymore, and depends on the choice of charts. This shows the nonlinear nature of the second order tangent bundle.

One can go further and consider the dual space of the tangent bundle giving rise to a new manifold structure, the co-tangent bundle $TM^* \to M$ associated with M. For each $x \in M$, let T_xM^* be the dual of T_xM. From there, the construction of the co-tangent bundle is done similarly as for the case of the tangent bundle.

Definition 2.1.8. *Let be a manifold M of class C^p with $p \geq 1$. Let us consider the space T_xM^*, the dual of T_xM, for each $x \in M$. The co-tangent bundle is given by:*

$$TM^* := \bigsqcup_{x \in M} T_xM^*$$

the disjoint union of the co-tangent spaces T_xM^*, which is a family of vector spaces parameterized by M. The projection $\pi^* : TM^* \longrightarrow M$, is such that $\pi^*(T_xM)^* = x$, i.e., maps into the base point.

In the tangent and co-tangent bundles, we see how, out of the manifold M, modeled on $\mathbb{E}$, two new manifolds were constructed, namely, the tangent bundle TM, which is a manifold modeled on $\mathbb{E} \times \mathbb{E}$, and the co-tangent bundle, which is a manifold modeled on the space $\mathbb{E} \times \mathbb{E}^*$. Now, we define curves on the tangent bundle, that lie above curves on the manifold.

Definition 2.1.9. *Let be $\pi : TM \to M$ the tangent bundle, and let be $\gamma : I \to M$ with $I \subset \mathbb{R}$ a differentiable curve. We say that the curve $\gamma_L : I \to TM$ is a lift of γ if $\pi\gamma_L = \gamma$. The set of lifts of γ is denoted by* $\mathrm{Lift}(\gamma)$.

Example 2.1.1. *In particular, if $\gamma : I \to M$ is a differentiable curve, then, the derivative curve $\gamma_L(t) = \gamma'(t)$ is a lift of γ, called the canonical lift of $\gamma(t)$.*

Riemannian Manifold We can have more structure, and for many purposes, it is needed a notion of length that applies to tangent vectors at each point x in a manifold M. We can do that by endowing every tangent space T_xM with an inner product

$$\langle \cdot, \cdot \rangle_x : T_xM \times T_xM \longrightarrow \mathbb{R}$$

this is, a bilinear, symmetric positive-definite form that smoothly varies on M, which we will call, Riemannian metric.

Definition 2.1.10. *A Riemannian manifold is a couple $(M, \langle \cdot, \cdot \rangle_x)$, where M is a manifold modeled on a Hilbert space, and $\langle \cdot, \cdot \rangle_x$ is a Riemannian metric on M.*

The symmetric positive definite form $\mathbf{M}(x)$, denotes the Riesz isomorphism between the spaces TM and TM^*, i.e., at $x \in M$, the isomorphism is given by:

$$\begin{aligned} \mathbf{M}(x) : T_xM &\longrightarrow T_xM^* \\ \xi &\longrightarrow \mathbf{M}(x)\xi \end{aligned} \tag{2.3}$$

hence, $\mathbf{M}(x)\xi \in T_xM^*$ is an element of the dual, endowed with the dual pair $\langle \mathbf{M}(x)\xi, \eta \rangle$, where $\langle , \rangle : \mathbb{E} \times \mathbb{E} \to \mathbb{R}$, is the inner product on the Hilbert space $\mathbb{E}$. We use the notation

$$\langle \mathbf{M}(x)\xi, \eta \rangle = \langle \xi, \mathbf{M}(x)\eta \rangle = \langle \xi, \eta \rangle_x$$

for $\xi, \eta \in T_xM$, to denote the inner product of two tangent vectors.

2.2 Examples of Manifolds

We now provide some examples of manifolds that will be particularly useful in the subsequent development of this work. For instance, we define the sphere, which will play a role in the mechanics of flexible rods, describing the inextensibility condition. We also mention some examples of matrix Lie groups, which are closely related to nonlinear mechanics.

The n-Sphere Let be $\|\cdot\|_2 = \sqrt{\langle\cdot,\cdot\rangle}$ the 2-norm on $\mathbb{R}^{n+1}$. The n-Sphere

$$\mathbb{S}^n = \{x \in \mathbb{R}^{n+1} \mid \|x\|_2 = 1\},$$

is a manifold. Let be $N = \{0,..,0,1\}$ and $S = \{0,..,0,-1\}$ then we consider the stereographic projections:

$$\phi_N : U_N \longrightarrow \mathbb{R}^n \quad \text{and} \quad \phi_S : U_S \longrightarrow \mathbb{R}^n$$

where $U_N = \mathbb{S}^n \setminus \{N\}$ and $U_S = \mathbb{S}^n \setminus \{S\}$ and they are given by:

$$\phi_N(x_1,..,x_{n+1}) = \frac{1}{1-x_{n+1}}(x_1,...,x_n) \quad \text{and} \quad \phi_S(x_1,..,x_{n+1}) = \frac{1}{1+x_{n+1}}(x_1,...,x_n)$$

with inverses

$$\phi_N^{-1}(x_1,...,x_n) = \frac{1}{\left(\sum_{i=1}^n x_i^2\right)+1}\left(2x_1,...,2x_n,\left(\sum_{i=1}^n x_i^2\right)-1\right)$$

and

$$\phi_S^{-1}(x_1,...,x_n) = \frac{1}{\left(\sum_{i=1}^n x_i^2\right)+1}\left(2x_1,...,2x_n,\left(\sum_{i=1}^n x_i^2\right)+1\right)$$

Thus, we see that U_N and U_S are two open subsets covering $\mathbb{S}^n$, and that the transition maps $\phi_{NS} = \phi_N \circ \phi_S^{-1}$, $\phi_{SN} = \phi_S \circ \phi_N^{-1}$ where $\phi_{NS} = \phi_{SN}$

$$\phi_{NS} : \phi_N(U_N \cap U_S) \longrightarrow \phi_S(U_N \cap U_S)$$

are given by:

$$(x_1,...,x_n) \longrightarrow \frac{1}{\sum_{i=1}^n x_i^2}(x_1,...,x_n).$$

Finally, its tangent space is given by:

$$T_x\mathbb{S}^n = \{v \in \mathbb{R}^{n+1} | \langle v, x\rangle = 0\}.$$

The Positive Cone Let be the positive cone

$$K_+ = \{x \in \mathbb{R}^n \mid x_i \geq 0, \text{ i=1,...,n}\}. \tag{2.4}$$

Then, for $x \in K_+$, if we consider the metric:

$$\langle \xi, \eta\rangle_x = \sum_{i=1}^n \frac{1}{x_i^2}\langle \xi_i, \eta_i\rangle \tag{2.5}$$

for $\xi, \eta \in \mathbb{R}^n$. The set K_+, together with $\langle\cdot,\cdot\rangle_x$ becomes a Riemannian manifold without boundary. For more details see e.g., [NT$^+$02].

Lie Groups We now introduce Lie groups, which are manifolds that possess a group structure and where the group operation is differentiable. A group manifold, or a Lie group G, is a manifold with a group structure, such that

$$\begin{aligned} G \times G &\longrightarrow G \\ (g, h) &\longrightarrow gh^{-1} \end{aligned}$$

is differentiable. For more material on the vast theory of Lie groups, see e.g., [Ada82, BR58, Tay02, Mil84, Che18, Nom56]. Next, we show some important examples of matrix Lie groups.

The General Group The general linear group $GL(n)$, is the set of all real $n \times n$ invertible matrices. $GL(n)$ is a Lie group of dimension n^2, and its tangent space at the neutral element $\hat{x}$ is given by:

$$T_{\hat{x}}GL(n) = \mathcal{M}_n(\mathbb{R})$$

which is the vector space of all $n \times n$ matrices as defined in A.4.

The Special Linear Group The special linear group $SL(n)$, is the set of all real $n \times n$ invertible matrices with determinant equals to one

$$SL(n) = \{x \in GL(n) | \det(x) = 1\}$$

and its tangent space at the neutral element $\hat{x}$, is given by:

$$T_{\hat{x}}SL(n) = \{x \in \mathbb{R}^{n \times n} | \operatorname{tr}(x) = 0\}$$

the space of traceless matrices.

The Orthogonal Group The orthogonal group $O(n)$, is the subgroup of $GL(n)$ given by:

$$O(n) = \{x \in GL(n) | x^T x = I_d\}.$$

$O(n)$ is a Lie group of dimension $\frac{n(n-1)}{2}$. The tangent space at the neutral element $\hat{x}$ is given by:

$$T_{\hat{x}}O(n) = \{x \in \mathbb{R}^{n \times n} | x^T + x = 0\}.$$

The Special Orthogonal Group The Special orthogonal group is defined as:

$$SO(n) = \{x \in O(n) | \det(x) = 1\}.$$

The tangent space at the neutral element $\hat{x}$ is:

$$T_{\hat{x}}SO(n) = T_{\hat{x}}SL(n) \cap T_{\hat{x}}O(n).$$

The Real Projective Space On the space $R^{m+1} \setminus \{0\}$, we define the equivalence relation $\sim$ by: $v \sim w$ if and only if, there exists a $\lambda \in \mathbb{R} \setminus \{0\}$ such that $v = \lambda w$. Then, the projective space $\mathbb{R}P^m := (\mathbb{R}^{m+1}/\sim)$ is a manifold of dimension m. For $k \in \{1, ..., m+1\}$ we define the open subset $U_k \subset \mathbb{R}P^m$ by:

$$U_k = \{[p] \in \mathbb{R}P^m \,|\, p_k \neq 0\}$$

and the local chart $\phi_k : U_k \to \mathbb{R}^m$ as:

$$\phi_k : [p] \to (\frac{p_1}{p_k}, ..., \frac{p_{k-1}}{p_k}, 1, \frac{p_{k+1}}{p_k}, ..., \frac{p_{m+1}}{p_k}). \tag{2.6}$$

In particular, we have that:

$$\mathbb{R}P^m = \bigcup_{k=1}^{m+1} U_k.$$

For more details, see e.g., [Gud04, LCC$^+$09, O'n14, CCL99, Küh15, Apé13].

The Space of Orientation Preserving Tetrahedra Consider a tetrahedron $\tilde{\mathrm{T}}$ in $\mathbb{R}^3$ with nodes $\{v_1, v_2, v_3, v_4\}$, and with non-zero volume. We embed each vector $v_i \in \mathbb{R}^3$, into the projective plane $\mathbb{R}P^4$, i.e.,

$$v_i \longrightarrow \begin{bmatrix} v_i \\ 1 \end{bmatrix}.$$

Next, we arrange the embedded nodes as an element of $GL(4)$, which we denote by x, namely:

$$x = \begin{bmatrix} | & | & | & | \\ v_1 & v_2 & v_3 & v_4 \\ | & | & | & | \\ 1 & 1 & 1 & 1 \end{bmatrix} \tag{2.7}$$

and denote by $\mathcal{T}$, the set of all tetrahedra as defined above. It can be checked that $\det(x) \neq 0$. We denote by $\mathcal{T}_{pos}$, the sub-manifold:

$$\mathcal{T}_{pos} = \{x \in \mathcal{T} \subset GL(4) \mid \det(x) > 0\}. \tag{2.8}$$

Concerning the tangent space of $\mathcal{T}_{pos}$, we use the characterization given in Definition 2.1.5 for tangent vectors. We take a curve $\gamma(t) : (-\varepsilon, \varepsilon) \to \mathcal{T}_{pos}$ contained in this manifold, with $\gamma(0) = x$. The curve $\gamma(t)$ has the form:

$$\gamma(t) = \begin{bmatrix} | & | & | & | \\ v_1(t) & v_2(t) & v_3(t) & v_4(t) \\ | & | & | & | \\ 1 & 1 & 1 & 1 \end{bmatrix}.$$

Now, we consider the derivative $\gamma'(t) : (-\varepsilon, \varepsilon) \to T(\mathcal{T}_{pos})$. We see that:

$$\gamma'(t) = \begin{bmatrix} | & | & | & | \\ v_1'(t) & v_2'(t) & v_3'(t) & v_4'(t) \\ | & | & | & | \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

which, evaluated at $t = 0$, becomes

$$\gamma'(0) = \begin{bmatrix} | & | & | & | \\ v_1'(0) & v_2'(0) & v_3'(0) & v_4'(0) \\ | & | & | & | \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{2.9}$$

therefore, the tangent space of $\mathcal{T}_{pos}$ denoted by $\mathfrak{t}_{pos}$, is given by the 4×4 matrices such that the last row is filled with zeros. In (2.9), each $v_i'(0) \in \mathbb{R}^3$ represents a perturbation vector attached to the vertex v_i, for $i = 1, 2, 3, 4$ respectively.

The Space of Volume Preserving Tetrahedra We now consider the space of oriented tetrahedra $\tilde{\mathrm{T}}$ with fixed volume. Let be $\rho > 0$, we define the space of volume preserving tetrahedra by:

$$\mathcal{T}_\rho = \{x \in \mathcal{T}_{pos} \mid \operatorname{vol}(\tilde{\mathrm{T}}) = \rho\}. \tag{2.10}$$

Recall that $\tilde{\mathrm{T}}$ denotes the tetrahedra, and $x \in \mathcal{T}_{pos}$, its representation as in (2.7). In fact, given that each $x \in \mathcal{T}_{pos}$ is as defined in (2.7), then we have that $\operatorname{vol}(\tilde{\mathrm{T}}) = \frac{1}{6}\det(x)$. Therefore, for given $x \in \mathcal{T}_\rho$, in order to characterize the tangent space $T_x(\mathcal{T}_\rho)$, we consider a curve contained in this manifold, i.e., $\hat{\gamma}(t) : (-\varepsilon, \varepsilon) \to \mathcal{T}_\rho$, with $\hat{\gamma}(0) = x$. We know that $\operatorname{vol}(\hat{\gamma}(t)) = \frac{1}{6}\det(\hat{\gamma}(t)) = \rho$, we differentiate this expression, obtaining:

$$\frac{d}{dt}\det(\hat{\gamma}(t)) = 0 \tag{2.11}$$

and using Jacobi's Identity (see, e.g., A.4.6):

$$\frac{d}{dt}\det(\hat{\gamma}(t)) = \operatorname{tr}\left(\operatorname{Adj}(\hat{\gamma}(t))\hat{\gamma}'(t)\right) \tag{2.12}$$

where, $\operatorname{Adj}(\hat{\gamma}(t))$ denotes the adjugate of the matrix $\hat{\gamma}(t)$, and $\operatorname{tr}(\cdot)$ the trace operator. Then, we get that:

$$\operatorname{tr}\left(\operatorname{Adj}(\hat{\gamma}(t))\hat{\gamma}'(t)\right) = 0 \tag{2.13}$$

which, evaluating at $t = 0$, becomes:

$$\begin{aligned} \operatorname{tr}\left(\operatorname{Adj}(\hat{\gamma}(0))\hat{\gamma}'(0)\right) &= 0 \\ \operatorname{tr}\left(\operatorname{Adj}(x)\hat{\gamma}'(0)\right) &= 0. \end{aligned}$$

Therefore, the tangent space to $\mathcal{T}_\rho$ at x is given by:

$$T_x(\mathcal{T}_\rho) := \mathfrak{t}_{x,\rho} = \{\xi \in \mathfrak{t}_{pos} \mid \operatorname{tr}(\operatorname{Adj}(x)\xi) = 0\}. \tag{2.14}$$

The following manifold example, which is central in Hydrodynamics, is used to describe the motion of a fluid in a compact manifold.

The Group of Diffeomorphisms of a Manifold Let be M a n-dimensional compact manifold. The group of diffeomorphisms

$$\mathrm{Diff}(M) = \{\phi \in W^{s,2}(M,M) \mid \phi \text{ is one-one, orientation preserving and } \phi^{-1} \in W^{s,2}(M,M)\}, \tag{2.15}$$

where, $W^{s,2}$ is the Sobolev space as defined in A.3, is a manifold, for $s > \frac{n}{2} + 1$. For more details, see e.g.,[Mar74].

2.3 Vector Bundles

We introduce the concept of vector bundles. These manifolds possess a special structure, locally, they are a product of an open set and a topological vector space. Vector bundles will be relevant for us, in particular when we consider the case of optimal control of energy minimizers. The tangent bundle, which is an instance of a vector bundle, was constructed by gluing the tangent spaces as the base point varies along the manifold. This procedure can be used to construct more general manifolds.

Definition 2.3.1. *Let be M a C^p manifold and let be $p : E \longrightarrow M$ be a mapping. Let be $\{U_i\}$ be a open covering of M, and for each i, suppose we are given a mapping*

$$\tau_i : p^{-1}(U_i) \longrightarrow U_i \times \mathbb{E}$$

satisfying the conditions:

VB1. The map τ_i is a fiber respecting C^p-isomorphism, i.e., the diagram

$$\begin{tikzcd} p^{-1}(U_i) \arrow[rr, "\tau_i"] \arrow[dr, "p"'] & & U_i \times \mathbb{E} \arrow[dl, "pr_1"] \\ & U_i & \end{tikzcd}$$

commutes. In particular, we get an isomorphism τ_i^x on each fiber

$$\tau_i^x : p^{-1}(x) \longrightarrow \{x\} \times \mathbb{E}.$$

VB2. For each pair U_i and U_j of open sets, the map

$$\tau_{ji}^x := (\tau_j^x) \circ (\tau_i^x)^{-1} : \mathbb{E} \longrightarrow \mathbb{E}$$

is a fiber linear C^p isomorphism, which receives the name of transition map associated with the covering.

VB3. If U_i and U_j are members of the covering, then the map of $U_i \cap U_j$ into $L(\mathbb{E}, \mathbb{E})$ given by

$$x \longrightarrow \tau_{ji}^x$$

is a morphism. (This condition is needed for the infinite dimensional case, otherwise, VB2 implies VB3). This means that, for $i \neq j$, the map τ_{ji}^x has the form

$$(x, e) \rightarrow (x, g_{ji}(x)e) \tag{2.16}$$

wherever it is defined, and in addition, the transition maps

$$g_{ji} : U_i \cap U_j \rightarrow L(\mathbb{E}, \mathbb{E}) \tag{2.17}$$

are all C^p-maps.

Here, $\{(U_i, \tau_i)\}$ is called a trivializing covering for p, and the τ_i are the trivializing maps. A vector bundle (E, p, M), consists of the total space manifold E, the base space manifold M, a smooth mapping $p : E \longrightarrow M$ and an equivalent class of trivializing coverings. In this case, we say that the vector bundle has fiber $\mathbb{E}$ or is modeled on $\mathbb{E}$.
We say that a vector bundle is trivial if it is isomorphic to a product $M \times \mathbb{E}$. This is relatively rare although, by definition, it is always trivial locally. If we restrict ourselves to the finite-dimensional case, this is, if we assume that E has dimension n, then a trivialization is equivalent to the existence of sections $\xi_1, ..., \xi_n$, such that for each $x \in M$, the vectors $\xi_1(x), ..., \xi_n(x)$ form a basis of E_x. This choice of sections is called a frame of the bundle.
Next, we see how the tangent bundle is a particular case of a vector bundle.

Example 2.3.1. *Let be a manifold M of class C^p, $p \geq 1$ with atlas $(U_i, \phi_i)_{i \in I}$, then the tangent bundle TM, is a vector bundle of class C^{p-1}, where the trivializing maps:*

$$\tau_{ji} : \phi_i(U_i \cap U_j) \times \mathbb{E} \longrightarrow \phi_j(U_i \cap U_j) \times \mathbb{E}$$

are given by the formula

$$\tau_{ji}^x(x, v) = (\phi_{ji}(x), D\phi_{ji}(x)\ v)$$

for $x \in U_i \cap U_j$, $v \in \mathbb{E}$ and $\phi_j \phi_i^{-1} = \phi_{ji}$.

Example 2.3.2. *Let be $p : E \rightarrow M$ a vector bundle. For each $x \in M$, consider the fiber E_x at x, then, the dual bundle of E denoted by E^*, is given by:*

$$E^* = \bigsqcup_{x \in M} E_x^* \tag{2.18}$$

i.e., the disjoint union of E_x^*, where is E_x^* the dual space of the fiber E_x. Therefore, the dual bundle is given by $p^* : E^* \rightarrow M$, where $p^*(E_x^*) = x$. For more details on the construction of the dual bundle see [Lan12a, III, §4].

Remark 2.3.1. *The second order tangent bundle T^2M as defined in 2.1.6, fails to be a vector bundle over M, in contrast to the previous case of the tangent bundle TM. Incompatibilities between the nonlinearity of the second tangent map and vector bundle structure, arise as shown in Remark 2.1.3.*

A very useful operation between vector bundles is the direct sum or Whitney sum, which takes as fiber, the direct product of the bundles.

Definition 2.3.2. *Let be $p : E \to M$ and $p' : E' \to M$ two vector bundles over M. The Whitney sum, or the direct sum bundle of the bundles p and p', is a vector bundle $E \oplus E'$ over M whose fiber at $x \in M$ is the direct sum $E_x \oplus E'_x$ of the vector spaces E_x and E'_x.*

We now show, how maps between vector bundles are defined in the correct way.

Definition 2.3.3. *Let $p_1 : E_1 \to M_1$ and $p_2 : E_2 \to M_2$ be two vector bundles. A vector bundle morphism $p_1 \to p_2$, consists of two mappings*

$$f_b : M_1 \to M_2 \quad \text{and} \quad f : E_1 \to E_2$$

satisfying the following conditions.

i) The diagram

$$\begin{tikzcd} E_1 \arrow[r, "f"] \arrow[d, "p_1"] & E_2 \arrow[d, "p_2"] \\ M_1 \arrow[r, "f_b"] & M_2 \end{tikzcd}$$

is commutative, and each map between fibers $f_x : E_{1,x} \to E_{2,x}$, is linear and continuous.

ii) There exist trivializing maps

$$\tau_1 : p_1^{-1}(U_1) \to U_1 \times \mathbb{E}_1$$
$$\tau_2 : p_2^{-1}(U_2) \to U_2 \times \mathbb{E}_2$$

for each $x_0 \in M_1$ and $f(x_0)$ respectively, such that $f_b(U_1)$ is contained in U_2, and such that the map of U_1 into $L(\mathbb{E}_1, \mathbb{E}_2)$, given by:

$$x \to \tau_{2,f_b(x)} \circ f_x \circ \tau_1^{-1}$$

where

$$\tau_{2,f_b(x)} \circ f_x \circ \tau_1^{-1} : U_1 \times \mathbb{E}_1 \to U_2 \times \mathbb{E}_2$$

is a well defined bundle map.

Proposition 2.3.1. *Let $p_1 : E_1 \to M_1$ and $p_2 : E_2 \to M_2$ be two vector bundles. Let $f_b : M_1 \to M_2$ be a map between M_1 and M_2, and suppose that we are given for each $x \in M_1$ a continuous linear map*

$$f_x : p_{1,x} \to p_{2,f_b(x)}$$

such that, for each x_0, condition ii) in the previous definition is satisfied. Then the map f form p_1 to p_2 defined by f_x on each fiber is a vector bundle morphism.

Proof. The proof, which we remit to [Lan12a, III, §1], defines the map f as

$$(x, v) \to (f_b(x), f_x(v))$$

as the required vector bundle morphism. $\square$

The Pullback of a Vector Bundle We now introduce the notion of the pullback of a vector bundle. This is an object that is a vector bundle itself and will be useful for the splitting of bundles of order two. Let $p : E \to M$ be a vector bundle, and let be $g : N \to M$ a map from the manifold N to M. The pullback g^* of $p : E \to M$, is a vector bundle $g^*p : g^*E \to N$ satisfying the following properties:

i) For each $x \in M$, we have $(g^*E)_x = E_{g(x)}$.

ii) The diagram

$$\begin{tikzcd}
g^*(E) \arrow[r] \arrow[d, "g^*(p)"'] & E \arrow[d, "p"] \\
N \arrow[r, "g"] & M
\end{tikzcd}$$

is commutative and the top horizontal map is the identity on each fiber.

iii) If $E = M \times \mathbb{F}$, i.e., if E is trivial, then $g^*(E) = N \times \mathbb{F}$ and $g^*(p)$ is the projection.

iv) If V is an open subset of M and $U = g^{-1}(V)$, then

$$g^*(E_V) = (g^*E)_U,$$

and we have the commutative diagram:

$$\begin{tikzcd}
g^*E_V \arrow[rr] \arrow[dr] \arrow[dd] & & E_V \arrow[dr] \arrow[dd] & \\
& g^*E \arrow[rr] \arrow[dd] & & E \arrow[dd] \\
U \arrow[rr] \arrow[dr] & & V \arrow[dr] & \\
& N \arrow[rr] & & M
\end{tikzcd}$$

Examples

Tangent Bundle If we apply this concept to the tangent bundle $p = \pi : TM \to M$, and if we choose $g = \pi$, then we may take the pullback:

$$\begin{tikzcd} \pi^*(TM) \arrow[r, "\pi^*(\pi)"] \arrow[d] & TM \arrow[d, "\pi"] \\ TM \arrow[r, "\pi"] & M \end{tikzcd}$$

In a chart U of M, for $\xi \in \mathbb{E}$, a point of TU consists of a pair (x, ξ). Then we may identify the fiber $(\pi^*TM)_{x,\xi}$ with $(TM)_x = T_xM$. Then, we have that:

$$\begin{tikzcd} (\pi^*TM)_U \arrow[r, leftrightarrow, "\approx"] \arrow[d] & (U \times \mathbb{E}) \times \mathbb{E} \arrow[d, "\pi"] \\ (TM)_U \arrow[r, leftrightarrow] & U \times \mathbb{E} \end{tikzcd}$$

shows the vector bundle chart for the pullback, meaning that a point of π^*TM in the chart is a triple

$$(x, \xi, \eta) \in (U \times \mathbb{E}) \times \mathbb{E}.$$

General Vector Bundle We consider a vector bundle $p : E \to M$, and we choose $g = p$. Then, we take the pullback:

$$\begin{tikzcd} p^*(E) \arrow[r, "p^*(p)"] \arrow[d] & E \arrow[d, "p"] \\ E \arrow[r, "p"] & M \end{tikzcd}$$

Therefore, we now consider a point $(x, e) \in U \times \mathbb{F}$ in a vector bundle chart. For this case, we identify the fiber $(p^*E)_{(x,e)}$ with E_x and we get the pullback:

$$\begin{tikzcd} (p^*E)_U \arrow[r, leftrightarrow, "\approx"] \arrow[d] & (U \times \mathbb{F}) \times \mathbb{F} \arrow[d, "p"] \\ E_U \arrow[r, leftrightarrow] & U \times \mathbb{F} \end{tikzcd}$$

so that a point of p^*E in the chart is given by the triple:

$$(x, e, \eta) \in (U \times \mathbb{F}) \times \mathbb{F}.$$

2.4 Immersions, Submersions and Submanifolds

This work aims to consider constrained optimization problems on manifolds, where the constraint mapping is a submersion. We introduce this concept and recall its main properties. First, we define maps between manifolds and the corresponding differentiation, which is done through charts. The concept of immersion is also introduced in order to define subsets of manifolds with manifold structure, i.e., submanifolds.

Definition 2.4.1. *Let M, N be two manifolds. We say that g is a C^p-map between the manifolds M and N, if for given $x \in M$, there exists a chart (U, ϕ) at x and a chart (V, ψ) at $g(x)$ such that $g(U) \subset V$, and the map*

$$g_{V,U} = \psi \circ g \circ \phi^{-1} : \phi U \longrightarrow \psi V$$

is C^p-continuously differentiable.

Remark 2.4.1. *Let be $g : M \longrightarrow N$ a map from the manifold M to the manifold N. Then at $x \in M$, we can interpret the derivative of g by means of charts, i.e., the derivative on each chart at x is a mapping*

$$g'(x) = T_x g : T_x M \longrightarrow T_{g(x)} N \tag{2.19}$$

with the property that, if (U, ϕ) is a chart at x and (V, ψ) is a chart at $g(x)$ such that $g(U) \subset V$ and $\hat{v}$ is a tangent vector at x represented by v in the chart (U, ϕ), then $T_x g(\hat{v})$ is the tangent vector at $g(x)$ represented by $Dg_{V,U}(x)v$.

Remark 2.4.2. *Let be $g : M \to N$ a C^p-mapping between the manifolds M and N. We can define*

$$Tg : TM \to TN$$

to be $T_x g$ on each fiber $T_x M$. Locally, the map Tg takes the form:

$$Tg(x, v) = (g(x), g'(x)v) \tag{2.20}$$

for $x \in M$ and $v \in \mathbb{E}$, with $\mathbb{E}$ the model space of M. This mapping is known as the tangent map, and will be of importance for the computation of derivatives of maps between manifolds.

Immersions and embeddings are special kinds of maps between manifolds, which, in particular, are useful to define subsets of a manifold that posses manifold structure.

Definition 2.4.2. *Let be $h : M \to N$ a smooth map between the smooth manifolds M and N, and let $x \in M$. We say that h is an immersion at x, if its derivative $T_x h$ is injective. The map h is called an immersion, if it is an immersion at every point.*

Definition 2.4.3. *Let be $h : M \to N$ be an immersion. Then the map h is called an embedding if $h : M \to h(M)$ is an homeomorphism, i.e., h is bijective, continuous and with inverse $h^{-1} : h(M) \to M$ continuous.*

Definition 2.4.4. *Let be $\tilde{M}$ a manifold, and M a subset of $\tilde{M}$. If M can be given the structure of differentiable manifold such that the inclusion $i : M \to \tilde{M}$ is an embedding, then M is called a submanifold of $\tilde{M}$.*

Next we show a characterization for submanifolds.

Theorem 2.4.1. *A subset M of a manifold $\tilde{M}$ modeled on $\mathbb{E}$ is a submanifold if and only if the following condition holds:*
There exists a splitting $\mathbb{E} = \mathbb{E}_1 \times \mathbb{E}_2$, and, for every $x \in M$, there exists a chart (U, ϕ) of $\tilde{M}$ around x of the form

$$\phi : U \to (U_1 \times U_2)$$

with $\phi(x) = (0, 0)$, and where U_j is an open neighborhood of $0 \in \mathbb{E}_j$, $j = 1, 2$. In addition the restriction $\phi_{|_{U \cap M}}$ is given by

$$\phi_{|_{U \cap M}} : U \cap M \to U_1 \times \{0\}.$$

Proof. See e.g., [Kli11, I,§3], [Lan12a, II,§2]. □

Definition 2.4.5. *Given a vector bundle $p : E \to M$, we say that $p|_D : D \to M$ is a subbundle of E if the restriction $p|_D : D \to M$ is a vector bundle, and D is an embedded submanifold in E. We denote by D_x the subbundle at the point $x \in M$.*

Next, we define the concept of submersion.

Definition 2.4.6. *A map $g : M \longrightarrow N$ will be called a submersion at a point $x \in M$, if there exists a chart (U, ϕ) at x, and a chart (V, ψ) at $g(x)$ such that ϕ gives an isomorphism of U on a products $U_1 \times U_2$ (U_1 and U_2 open on the model spaces), and such that the map*

$$\psi g \phi^{-1} = g_{V,U} = g : U_1 \times U_2 \longrightarrow V \tag{2.21}$$

is a projection. We say that g is a submersion if it is a submersion at every point.

Proposition 2.4.1. *Let be M, N manifolds and let be $g : M \longrightarrow N$ a mapping between M and N. We say that g is a submersion at $x \in M$ if there exists a chart (U, ψ) at x and (V, ϕ) at $g(x)$ such that $g'_{V,U} = T_x g$ is surjective and its kernel splits.*

Proof. See [Lan12a, II,§2]. □

Definition 2.4.7. *We say that $g : M \to N$ is a submersion if g is a submersion for every $x \in M$.*

Example 2.4.1. *Let be (E, p, M) a vector bundle, then the projection p is a submersion.*

Finally, we introduce the concept of Riemannian submersion.

Definition 2.4.8. *Let be M, N Riemannian manifolds, we say that g is a Riemannian submersion, if for each $x \in M$, the differential*

$$Tg(x) : T_x M \to T_{g(x)} N$$

is an orthogonal projection.

For more details on the study of submersion maps see [Bes07, Lan12a, Mic08, PT06].

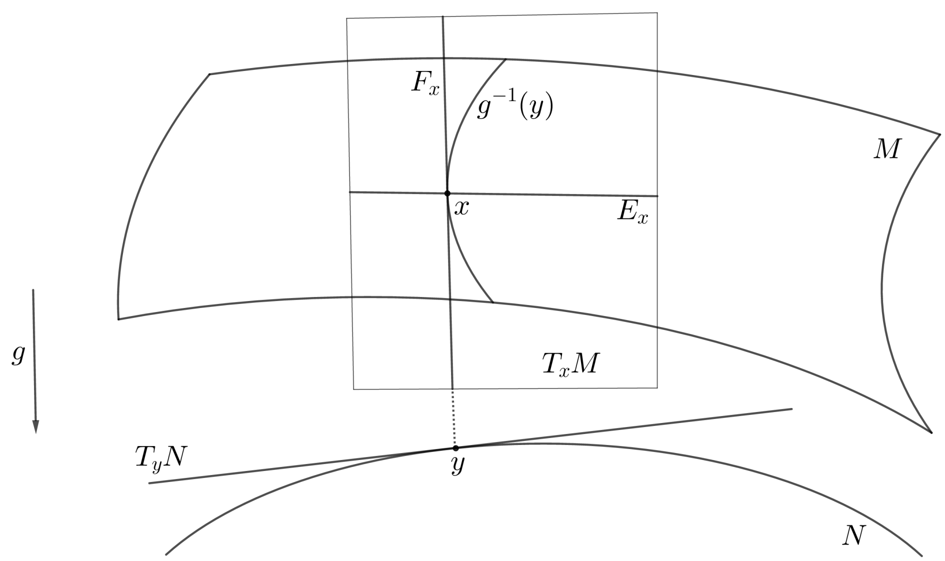


Figure 2.1: *Submersion*

2.5 Transversality

The notion of transversal maps will be used, in our context, for the setting of optimization problems over more structured manifolds.

Definition 2.5.1. *Let N be a submanifold of the manifold M, and let $g : R \longrightarrow M$ be a mapping from the manifold R to M. We say that g is transversal over the submanifold N of M if the following condition is satisfied:*
Let $x \in R$ such that $g(x) \in N$. Let (W, ψ) be a chart at $g(x)$ such that $\psi : W \longrightarrow W_1 \times W_2$ is a diffeomorphism on a product, with

$$\psi(g(x)) = (0, 0) \quad \text{and} \quad \psi(N \cap W) = W_1 \times 0.$$

Then, there exists an open neighborhood U of x such that the composite map

$$U \xrightarrow{g} W \xrightarrow{\psi} W_1 \times W_2 \xrightarrow{pr} W_2$$

is a submersion.

We say that g is transversal over the submanifold N of M if the condition stated above holds and it will be denoted as $g \pitchfork N$. As a consequence, we can split the space into the direct sum $T_{g(x)}M = (T_{g(x)}N) \oplus (T_{g(x)}M/T_{g(x)}N)$. In particular we have the following proposition.

Proposition 2.5.1. *Let be $g : R \longrightarrow M$ a mapping between the manifolds R and M, and let be N a submanifold of the manifold M. The map g is transversal over N if and only if for each $x \in R$ with $g(x) \in N$, the map*

$$T_xR \xrightarrow{T_xg} T_{g(x)}M \longrightarrow (T_{g(x)}M/T_{g(x)}N)$$

is surjective and its kernel splits.

Proof. See [Lan12a, II,§2]. □

The following theorem characterizes manifolds as pre-image of transversal maps.

Theorem 2.5.1. *Let be N a submanifold of M, and $g : R \to M$ be transversal to N. In addition if $S = g^{-1}(N) \neq \emptyset$, then S is a submanifold of R.*

Proof. See [Kli11, I, §3]. □

2.6 Vector Fields, Differential Forms and Integrability

Definition 2.6.1. *Let M be a manifold of class C^p with $p \geq 2$. A vector field ξ on M is a map of class C^{p-1}*

$$\xi : M \longrightarrow TM$$

such that $\xi(x)$ lies in the tangent space T_xM for each $x \in M$, i.e., $\pi\xi = id_M$.

Definition 2.6.2. *We denote by ΓTM the $\mathbb{R}$-vector space of vector fields over M.*

Let be $\xi : M \longrightarrow TM$ a vector field. If TM is trivial, this is, if $TM = M \times \mathbb{E}$, then ξ is completely determined by its projection onto the second factor, $\xi(x) = (x, \xi_2(x))$ and this projection will be called the local representation of ξ. We say that $\xi(x)$ is represented locally by ξ_2 if we are working over an open set U of M where the tangent bundle admits a trivialization, more frequently, we will use the ξ itself to denote this representation.
We can regard vector fields as derivations on real functions over a manifold, as we see in the next proposition.

Proposition 2.6.1. *Let be $\xi : M \longrightarrow TM$ a vector field, and let be $\phi : U \longrightarrow \mathbb{R}$ a differentiable function defined on an open set U of M. Then, there exists a unique function $\xi\phi$ on U such that if ξ denotes the local representation of the vector field on U, then*

$$(\xi\phi)(x) = \phi'(x)\xi(x).$$

Proof. See [Lan12a, V, §1]. □

For given two vector fields ξ, η on M, we define a new vector field $[\xi, \eta]$, known as the bracket product of ξ and η.

Proposition 2.6.2. *Let be ξ, η two vector fields of class C^{p-1} on M. Then, there exists a unique vector field $[\xi, \eta]$ of class C^{p-2}, such that for each open set U, and a function φ on U we have:*

$$[\xi, \eta]\varphi = \xi(\eta(\varphi)) - \eta(\xi(\varphi)). \tag{2.22}$$

and the local representation of $[\xi, \eta]$ is given by

$$[\xi, \eta](x) = \eta'(x)\xi(x) - \xi'(x)\eta(x). \tag{2.23}$$

Proof. See [Lan12a, V,§1]. □

We see how the tangent map of a Riemannian submersion $g : M \to N$, acts on the bracket product of two horizontal vector fields ξ, $\eta \in \ker(T_x g)^\perp$.

Remark 2.6.1. *Let be g a Riemannian submersion between the Riemannian manifolds M and N. Its differential, gives an isomorphism at each point between the spaces $\ker g'(x)^\perp$ and $T_{g(x)}N$, namely:*

$$g'(x) : \ker g'(x)^\perp \longrightarrow T_{g(x)}N, \tag{2.24}$$

with its corresponding inverse, denoted by:

$$g'^{-}(x) : T_{g(x)}N \longrightarrow \ker g'(x)^\perp. \tag{2.25}$$

We say that a vector field ξ on N lifts uniquely to a horizontal field ξ_M, i.e., a vector field such that

$$\xi_M(x) \in \ker g'(x)^\perp \quad \text{and} \quad g'(x)\xi_M(x) = \xi(g(x)),$$

at each point $x \in M$.
In addition, for given η_1, η_2 vector fields on N, if we consider η_{1_M}, η_{2_M}, their corresponding liftings, then:

$$\begin{aligned} g'(x)\eta_{1_M} &= \eta_1(g(x)) \\ g'(x)\eta_{2_M} &= \eta_2(g(x)) \end{aligned}$$

then taking derivatives of the first in direction η_{2_M} and the second in direction η_{1_M}, we get that:

$$\begin{aligned} g''(x)(\eta_{2_M}\eta_{1_M}) + g'(x)\eta'_{1_M}\eta_{2_M} &= \eta'_1(g(x))g'(x)\eta_{2_M} \\ g''(x)(\eta_{1_M}\eta_{2_M}) + g'(x)\eta'_{2_M}\eta_{1_M} &= \eta'_2(g(x))g'(x)\eta_{1_M} \end{aligned}$$

subtracting the last two equations we obtain

$$g'(x)\eta'_{1_M}\eta_{2_M} - g'(x)\eta'_{2_M}\eta_{1_M} = \eta'_1(g(x))g'(x)\eta_{2_M} - \eta'_2(g(x))g'(x)\eta_{1_M}$$

implying

$$\begin{aligned} g'(x)[\eta_{2_M}, \eta_{1_M}] &= \eta'_1(g(x))\eta_2(g(x)) - \eta'_2(g(x))\eta_1(g(x)) \qquad (2.26)\\ &= [\eta_2, \eta_1]. \qquad (2.27) \end{aligned}$$

Finally, we point out the induced isomorphism:

$$g'(x)^* : (T_{g(x)}N)^* \longrightarrow (\ker g'(x)^\perp)^*$$

between the adjoint spaces.

We now turn our attention to differential forms. We know that tangent vectors are elements that belong to the tangent space of a manifold M. Differential 1-forms, on the other hand, are elements that belong to the dual of the tangent space. These objects will be used in section 4.4, there we study the existence of a potential function of the Lagrange multiplier when defined as a section of the co-tangent bundle. A vector field ξ, is a section of the tangent bundle $\pi : TM \to M$, i.e., it is a map $\xi : M \longrightarrow TM$, satisfying $\pi \circ \xi = id_M$. In a similar way, we say that a section $\hat{\eta}$ of the co-tangent bundle $\hat{\pi} : TM^* \to M$, is a map $\hat{\eta} : M \to TM^*$, that satisfies $\hat{\pi} \circ \hat{\eta} = id_M$. The object $\hat{\eta}$ is also known as a 1-form, and at $x \in M$, we have that $\hat{\eta}_x : T_xM \to \mathbb{R}$. This can be generalized to the set of r-multilinear alternating continuous maps. For $x \in M$, an r-form on M at x is a continuous, multilinear, alternating map $\hat{\eta} : T_xM \times ... \times T_xM \longrightarrow \mathbb{R}$, which we denote by $\hat{\eta} \in L^r_a(T_xM)$ (see A.1.8).

Definition 2.6.3. *A differential form of degree r, or an r-form on a manifold M, is a section of $L^r_a(TM)$, alternating multilinear forms on TM.*

For our purposes, we need to differentiate on the latter space. We have that, for a function $g : M \to \mathbb{R}$, its differential $T_xg(x) : T_xM \to \mathbb{R}$, is a continuous linear map, i.e., $T_xg \in L^1_a(T_xM)$. It is a 1-form which will be denoted by dg. Then dg, is the unique 1-form such that for every vector field ξ we have $\langle dg, \xi\rangle = T_xg(x)\xi$. We extend the definition of d to forms of higher degree, this operator, receives the name of exterior derivative.

Proposition 2.6.3. *Let η be an r-form of class C^{p-1} on M. Then there exists a unique $(r+1)$-form $d\eta$ on M of class C^{p-2} such that, for any open set U of M and vector fields $\xi_0, ..., \xi_r$ on U we have*

$$\begin{aligned} \langle d\eta, \xi_0 \times ...\xi_r\rangle =& \sum_{i=0}^{r}(-1)^i \xi_i \left\langle \eta, \xi_0 \times ... \times \hat{\xi}_i \times ... \times \xi_r \right\rangle \\ &+ \sum_{i<j}^{r}(-1)^{i+j} \left\langle \eta, [\xi_i, \xi_j] \times \xi_0 \times ... \times \hat{\xi}_i \times ...\hat{\xi}_j \times ... \times \xi_r \right\rangle . \end{aligned} \tag{2.28}$$

where $[\xi_i, \xi_j]$ is the bracket product between ξ_i and ξ_j.

Proof. See [Lan12a, V, §3] □

Pullbacks of differential forms by maps, and their differentials, will be of importance for our needs.

Definition 2.6.4. *Let be $g : M \longrightarrow N$ a mapping, and let be η a differential form on N. Then, we get a differential form $g^*(\eta)$ on M, which is given at a point $x \in M$, by the formula:*

$$\langle g^*\eta(x), \xi_1(x) \times ... \times \xi_r(x)\rangle = \left\langle \eta(g(x)), g'(x)\xi_1(x) \times ... \times g'(x)\xi_r(x)\right\rangle \tag{2.29}$$

if $\xi_1(x), ..., \xi_r(x)$ are vector fields. In particular, if η is a differential 1-form on N, then we obtain a differential 1-form $g^*(\eta)$ on M, which is given at a point $x \in M$ by the formula

$$g^*(\eta)_x = \eta_{g(x)} \circ (T_xg)$$

with the corresponding local representation formula

$$\langle g^*\eta(x), \xi(x)\rangle = \left\langle \eta(g(x)), g'(x)\xi(x)\right\rangle$$

where ξ is a vector field.

A differential r-form η that satisfies $d\eta = 0$ is called closed, and if there exists an $(r-1)$-form ψ such that $\eta = d\psi$, then we say that η is exact. The Poincaré Lemma asserts that locally, every closed form is exact.

Theorem 2.6.1 (Poincaré Lemma)**.** *Let U be an open ball in $\mathbb{E}$ and let η be a differential form of degree ≥ 1 on U such that $d\eta = 0$. Then, there exists a differential form ψ on U such that $d\psi = \eta$.*

Proof. See [Lan12a, V, §4]. □

Distributions and Integrability

Let be ξ a vector field on M and a point $x_0 \in M$. An integral curve for the vector field ξ with initial condition x_0, is a curve $\gamma : I \to M$, mapping an open interval of $\mathbb{R}$ containing 0 into M, such that $\gamma(0) = x_0$ and $\gamma'(t) = \xi(\gamma(t))$. Those curves, which are solutions to the previous problem, are called integral curves. Theorems for the existence and uniqueness of integral curves are famous in the literature, see for instance [Lan12a, IV]. We can generalize this idea, from curves to higher dimensional submanifolds. If we consider a subbundle of the tangent bundle TM, which we call a distribution on M, we formulate the following question: Is there a submanifold whose tangent space at each point, is the given subbundle at the point x? If the answer is affirmative, we say that this submanifold is the integral manifold of the distribution. For smooth sections $\xi \in D$ and $\eta \in D$, defined in a subbundle D of TM, we say that D is involutive if $[\xi, \eta] \in D$. It turns out that the condition of being involutive will be necessary and sufficient for a distribution to be integrable. In other words, we say that a subbundle of the tangent bundle to a smooth manifold is integrable if its space of sections is closed under the bracket operation.

Definition 2.6.5. *Let be D a tangent subbundle of TM. A nonempty immersed submanifold $\hat{M} \subset M$ is called an integral submanifold of D, if $T_x\hat{M} = D_x$, at each point $x \in \hat{M}$.*

The theorem of Frobenius, which is the fundamental base for the theory of foliations, see e.g., [Ton12b, CN13, MC88, HH81, Ton12a, MM03, Rei12, Her60, Bot72], gives us conditions for integrability of distributions.

Theorem 2.6.2 (Frobenius)**.** *Let be M a manifold of class C^p $p \geq 2$, and let be E a tangent subbundle over M. Then, E is integrable if and only if, for each point $x \in M$ and vector fields ξ, η, at x which lie in E, the bracket $[\xi, \eta]$ also lies in E.*

Proof. See [Lan12a, VI, §1]. □

The distribution given by $\ker g'(x)$, for a submersion $g : M \to N$, is integrable.

Example 2.6.1. *Let be $g : M \longrightarrow N$ a smooth submersion. For each $x \in M$, we call the subbundle $\ker g'(x)$ the vertical distribution. At every $x \in M$, we have that the vertical distribution is integrable. Indeed, let be ξ_t, $\eta_t \in \ker g'(x)$, we get that, $[\xi_t, \eta_t] \in \ker g'(x)$. In fact, we have that:*

$$g'(x)\xi_t'\eta_t = g''(x)(\xi_t, \eta_t) = g'(x)\eta_t'\xi_t$$

yielding

$$g'(x)[\xi_t, \eta_t] = 0.$$

Therefore, by Theorem 2.6.2*, we have that this subbundle is integrable, which illustrates that indeed, each fiber $g^{-1}(y)$ is a submanifold of M, for every $y \in N$. As an alternative, it is also consequence of Theorem* 2.5.1*.*

It turns out that, in general, subbundles of the tangent bundle are not always integrable, or isomorphic to an integrable one. See e.g., [Bot68].

2.7 Sprays, Exponential Map and Covariant Derivatives on the Tangent Bundle

We go further and define special kinds of second-order vector fields, which are vector fields over the tangent bundle TM, that are homogeneous of degree two, called sprays. These objects give rise to the notion of connection over a manifold, and henceforth the notion of geodesics, concepts that we use as references for the construction of suitable mappings for optimization algorithms on manifolds.

Definition 2.7.1. *A second-order vector field S over M is a vector field on the tangent bundle such that:*

$$T\pi S(v) = v, \quad \textit{for all } v \in TM$$

where $\pi : TM \longrightarrow M$, is the canonical projection of TM on M.

Remark 2.7.1. *The representation in charts of the above statement is as follows. Let be U open in the model space $\mathbb{E}$, so that $TU = U \times \mathbb{E}$, then, $T(T(U)) = (U \times \mathbb{E}) \times (\mathbb{E} \times \mathbb{E})$. The map π is the projection $\pi : U \times \mathbb{E} \to U$, and the tangent map of π is given by:*

$$\begin{aligned} T\pi : (U \times \mathbb{E}) \times (\mathbb{E} \times \mathbb{E}) &\to (U \times \mathbb{E}) \\ (x, v, u, w) &\to (x, u) \end{aligned}$$

which means that locally, if the vector field S has representation $S(x, v) = (S_1(x, v), S_2(x, v))$, then the condition $T\pi S(v) = v$ implies $S_1(x, v) = v$.

We define Sprays as in [Lan12a, IV, §3] and [APS60], i.e., as second-order vector fields which satisfies an homogeneous quadratic condition.

Definition 2.7.2. *Let be S a second-order vector field, and $S : U \times \mathbb{E} \longrightarrow \mathbb{E} \times \mathbb{E}$ its local representation in the chart $U \times \mathbb{E}$ with $S = (S_1, S_2)$. We say that the mapping S represents a spray if:*

$$S_2(x, tv) = t^2 S_2(x, v)$$

for all $t \in \mathbb{R}$.

If we define $S_2(x,v) := B(x;v,v)$, then S_2 is quadratic in its second variable, and the map S defined by:

$$S(x,v) = (v, B(x;v,v)) = (v, S_2(x,v))$$

represents the spray over U. B is the symmetric bilinear map associated with the spray. In particular, we say that a curve γ on M is a geodesic, if and only if, is a solution to the differential equation:

$$\gamma''(t) = B(\gamma(t);\gamma'(t),\gamma'(t)) \text{ for all } t.$$

With geodesics, we can define the concept of exponential map.

Definition 2.7.3. *Let be S an spray over M. Let be β_v the integral curve of the spray with initial condition v. We define the exponential map*

$$\exp : TM \longrightarrow M$$

as

$$\exp(v) = \pi\beta_v(1)$$

where $v \in T_xM$ is such that β_v is defined at least on the interval $[0,1]$.

If $x \in M$ and 0_x is the zero vector in T_xM, then $S(0_x) = 0$ therefore, $\exp(0_x) = x$. And $\exp_x$ will be the restriction of exp to the tangent space T_xM, Thus

$$\exp_x : T_xM \longrightarrow M.$$

We return to sprays and give the transformation rule for the quadratic part of a spray under change of charts. Let be (U,ϕ) and (V,ψ) charts on M, and let be $h : U \to V$, the corresponding change of charts maps, which is and isomorphism. The derivative, Th is represented by:

$$H : U \times \mathbb{E} \to \mathbb{E} \times \mathbb{E},$$

and it is given by:

$$H(x,v) = (h(x), h'(x)v). \tag{2.30}$$

Taking one more derivative, this is, a lift to the double tangent bundle TTU, we get that

$$(H, H') : (U \times \mathbb{E}) \times (\mathbb{E} \times \mathbb{E})$$

is given by:

$$H'(x,v)\begin{bmatrix} u \\ w \end{bmatrix} = \begin{bmatrix} h'(x) & 0 \\ h''(x)v & h'(x) \end{bmatrix}\begin{bmatrix} u \\ w \end{bmatrix}$$

which is the Jacobian matrix operating on $[u,w]^T$, with $u, w \in \mathbb{E}$. Therefore, we have that

$$(H,H') : (x,v,u,w) \to \left(h(x), h'(x)v, h'(x)u, h''(x)(u,v) + h'(x)w\right).$$

Thus, if S_U is the second-order vector field representing the spray on the chart U, we get that its first component, is such that $S_{U,1}(x,v) = v$, and its second component is given by $S_{U,2}(x,v) = w$. Finally, if S_V is the vector field on the chart V, then we get that S_U and S_V are related by:

$$S_V(h(x), h'(x)v) = (h'(x)v, h''(x)(v,v) + h'(x)S_{U,2}(x,v)).$$

With the previous considerations we get:

Proposition 2.7.1. *Let be (U,ϕ), (V,ψ) two charts around $x \in M$, and $h = (\phi \circ \psi^{-1})$ the corresponding change of charts map. Then, the quadratic part of a spray transforms in the following way:*

$$B_V(h(x); h'(x)v, h'(x)w) = h''(x)(v,w) + h'(x)B_U(x; v, w). \tag{2.31}$$

We need to define a proper way to differentiate vector fields. The main difficulty lies in the fact that the tangent map, or derivative of a vector field, is mapped into T^2M, which is not a vector bundle over M. The following theorem shows an isomorphism between the double tangent bundle T^2M and the direct product $\pi^*TM \oplus_{TM} \pi^*TM$, which is a vector bundle over M. This is done through a spray on M.

Theorem 2.7.1 (Tensorial Splitting Theorem)**.** *Let be given a spray on the differential manifold M and its corresponding quadratic part B. For the map*

$$\kappa_{TM} : TTM \to \pi^*TM \oplus_{TM} \pi^*TM$$

which, in the chart

$$(TTM)_U = (U \times \mathbb{E}) \times (\mathbb{E} \times \mathbb{E})$$

is given by:

$$\kappa_{TM,U}(x,v,z,w) = (x,v,z,w - B_U(x;v,z)). \tag{2.32}$$

We have that κ_{TM} is a vector bundle isomorphism over TM.

Proof. We compute $\kappa_{TM,V} \circ (H,H')$ with the notation used in (2.30), obtaining

$$\begin{aligned}\kappa_{TM,V} \circ (H,H')(x,v,z,w) &= (h(x), h'(x)v, h'(x)z, h''(x)(v,z) + h'(x)w - B_V(h(x); h'(x)v, h'(x)z)) \\ &= (h(x), h'(x)v, h'(x)z, h'(x)(w - B(x;v,z)))\end{aligned} \tag{2.33}$$

where the transformation rule (2.31) has been used. The family $\{\kappa_{TM,U}\}$ defines a vector bundle morphism over TM, and in addition, the expression (2.33) of the map κ_{TM} over a chart is a vector bundle isomorphism. $\square$

Remark 2.7.2. *The last component of the map defined in* (2.32)*, can be seen as the 2×2 matrix acting on $[z,w]^T$, given by:*

$$\begin{bmatrix} id & 0 \\ -B_U(x;v,\cdot) & id \end{bmatrix} \begin{bmatrix} z \\ w \end{bmatrix}.$$

Covariant Derivatives on the Tangent Bundle

Differentiation of vector fields presents some difficulties. As we have mentioned, by taking the derivative of a vector field $\xi : M \to TM$, we get that $T\xi : TM \to TTM$, i.e., it takes values in TTM, which is not a vector bundle over M. Therefore, in order to define a proper derivative, we need some additional structure that yields the covariant derivation $\nabla\xi$ of a vector field ξ with values on a vector bundle over M. This can be done via sprays or with the help of a Riemannian metric in case that such a structure is available. First, we mention the properties of a covariant derivative, then, we see how from a spray a covariant derivative can be obtained. In the case of the manifold being Riemannian, we can get the corresponding spray from the metric, also called, the canonical spray.

Definition 2.7.4. *A covariant derivative ∇ on a manifold M is a mapping*

$$\nabla : \Gamma TM \times \Gamma TM \longrightarrow \Gamma TM$$

which is denoted by $(\xi, \eta) \longrightarrow \nabla_\xi \eta$ and satisfies the following conditions:

i) *$\mathfrak{F}$-linearity in η:* $\nabla_{f\eta + g\nu}\xi = f\nabla_\eta \xi + g\nabla_\nu \xi, \qquad f, g \in \mathfrak{F}.$

ii) *$\mathbb{R}$-linearity in ξ :* $\nabla_\eta(a\xi + b\nu) = a\nabla_\eta \xi + b\nabla_\eta \nu, \qquad a, b \in \mathbb{R}.$

iii) *Product rule:* $\nabla_\eta(f\xi) = (\eta f)\xi + f\nabla_\eta \xi,$

iv) *Symmetry:* $\nabla_\eta \xi - \nabla_\xi \eta = [\eta, \xi].$

Where $\mathfrak{F}$ is the space of C^∞-real functions over M.

Given a spray, we can define a covariant derivative satisfying the previous conditions.

Theorem 2.7.2. *Let be given a spray over M, together with its corresponding quadratic part B. Then, there exists a unique covariant derivative ∇, such that in a chart U, the derivative is given by the formula:*

$$\nabla_\xi \eta(x) = \eta'(x)\xi(x) - B(x; \xi(x), \eta(x)) \tag{2.34}$$

where η and ξ denote the local representatives of the vector fields in the chart.

Proof. See [Lan12a, X, §4]. □

If in addition, if we suppose that the manifold M is Riemannian, with metric $\mathbf{M}$, and product

$$\langle \xi, \eta \rangle_x = \langle \xi, \mathbf{M}(x)\eta \rangle = \langle \mathbf{M}(x)\xi, \eta \rangle$$

then we can obtain a spray, the canonical spray.

Proposition 2.7.2. *In a chart U, let be $B = (B_1, B_2)$ the vector field representing the one form dK, where $K(\eta) = \frac{1}{2}\langle v, v \rangle_x$ is the kinetic energy functional, then $B_2(x, v)$ given by:*

$$\langle B_2(x, v), \boldsymbol{M}(x)w_1 \rangle = \frac{1}{2}\left\langle \boldsymbol{M}'(x)w_1\, v, v \right\rangle - \left\langle \boldsymbol{M}'(x)\, v\, v, w_1 \right\rangle$$

represents a spray.

Proof. see [Lan12a, VII, §7]. □

The Covariant Derivative on a Submanifold

We need to make some observations concerning covariant derivatives and connections on submanifolds. In the following, we assume that M is a Riemannian manifold, and N is a submanifold of M, with the induced Riemannian structure. At a point $x \in N$, we have the following orthogonal decomposition:

$$T_xM = T_xN + (T_xN)^{\perp}$$

where $(T_xN)^{\perp}$ is the orthogonal complement of T_xN in T_xM, called the normal bundle. We denote by:

$$P_{TN} : T_xM \to T_xN \qquad \text{and} \qquad P_{TN}^{\perp} : T_xM \to (T_xN)^{\perp} \tag{2.35}$$

the orthogonal projections from TM to TN and $(TN)^{\perp}$ respectively. In this way, a section over N has two components (v, ν), where v is a vector field over N, and ν is a normal field, i.e., a section of the normal bundle. We have the following theorem.

Theorem 2.7.3. *Let be v_M, ν_M extensions of v, ν to M, and let ζ a vector field over N. The covariant derivatives of v_M and ν_M on N can be expressed in the form:*

$$\nabla_{\zeta}^{M} v_M = \nabla_{\zeta}^{N} v + h_{12}(\zeta, v) \tag{2.36}$$

$$\nabla_{\zeta}^{M} \nu_M = \nabla_{\zeta}^{\perp} \nu + h_{21}(\zeta, \nu), \tag{2.37}$$

where:

∇^M *is the covariant derivative on* M

h_{12} *is a symmetric bilinear bundle map* $TN \times TN \to (TN)^{\perp}$

h_{21} *is a bilinear bundle map* $TN \times (TN)^{\perp} \to TN$.

$\nabla_{\zeta}^{N} v = P_{TN} \nabla_{\zeta}^{M} v$.

$\nabla_{\zeta}^{\perp} \nu = P_{TN}^{\perp} \nabla_{\zeta}^{M} \nu$ *is independent of the extension* ν_M *of* ν.

Proof. See [Lan12a, XIV,§1]. □

In the literature, the map h_{12} is known as the second fundamental form on the manifold N, see e.g., [Lan12a, XIV,§1], [RS11, II,§4], and it will be relevant for us, in particular, for the construction of connections and vector bundle retractions for optimization algorithms on submanifolds. In order to illustrate Theorem 2.7.3, and thinking in our applications, we consider the particular case where $M = \mathbb{R}^3$ with the euclidean product and $N = \mathbb{S}^2$.

Example 2.7.1. *Let be the 2-sphere $\mathbb{S}^2$ regarded as a Riemannian submanifold of the Euclidean space $\mathbb{R}^3$, in which $B_{\mathbb{R}^3} = 0$, i.e., the spray is zero everywhere. Then, in Theorem 2.7.3 making $M = \mathbb{R}^3$ and $N = \mathbb{S}^2$, for $x \in \mathbb{S}^2$, we have that:*

$$v'\zeta = P_{T_x\mathbb{S}^2}(v'\zeta) + (I - P_{T_x\mathbb{S}^2})(v'\zeta) \tag{2.38}$$

$$= \nabla_{\zeta}^{\mathbb{S}^2} v + h_{12}(\zeta, v) \tag{2.39}$$

where:

$$\begin{aligned} P_{T_x\mathbb{S}^2} : \mathbb{R}^3 &\to T_x\mathbb{S}^2 \\ \xi &\to (I - xx^T)\xi \end{aligned} \tag{2.40}$$

is the projection from $T_x\mathbb{R}^3 \simeq \mathbb{R}^3$ *to* $T_x\mathbb{S}^2$*, and* $(I - P_{T_x\mathbb{S}^2}) = xx^T$*, maps from* $\mathbb{R}^3$ *into* $(T_x\mathbb{S}^2)^\perp$*.*

The formula (2.39) is known as the Gauss-Weingarten formula, see e.g.[RS11, II,§4], [Lan12a, XIV,§1]. In addition, in example 2.7.1, we observe that:

$$\nabla^{\mathbb{S}^2}_\zeta v = v'\zeta - h_{12}(\zeta, v). \tag{2.41}$$

Therefore, we obtain the spray on the submanifold $\mathbb{S}^2$, given by $B_{T\mathbb{S}^2}(\zeta, v) = h_{12}(\zeta, v)$. In fact, if $\gamma(t) : (-\varepsilon, \varepsilon) \to \mathbb{S}^2$ is a geodesic, then $\nabla^{\mathbb{S}^2}_{\gamma'(0)}\gamma'(0) = 0$, yielding in (2.41) that:

$$\gamma''(0) = h_{12}(\gamma'(0), \gamma'(0)). \tag{2.42}$$

We also observe that differentiating the equality:

$$P_{T_x\mathbb{S}^2} v = v \tag{2.43}$$

in direction $\zeta \in T_x\mathbb{S}^2$, we get that

$$P'_{T_x\mathbb{S}^2}(\zeta, v) + P_{T_x\mathbb{S}^2} v'\zeta = v'\zeta \tag{2.44}$$

which implies:

$$P'_{T_x\mathbb{S}^2}(\zeta, v) = (I - P_{T_x\mathbb{S}^2})v'\zeta. \tag{2.45}$$

Meaning that the second fundamental form can be expressed as:

$$h_{12}(\zeta, v) = P'_{T_x\mathbb{S}^2}(\zeta, v). \tag{2.46}$$

Splitting for $T\mathbb{S}^2$ We now provide a connection map for the sphere $\mathbb{S}^2$ as a submanifold $\mathbb{R}^3$. Let be $(x, \xi) \in T\mathbb{S}^2$, for perturbations $(\delta\xi, \delta\eta)$, we observe that, if we apply the tangent map to

$$\begin{aligned} (U \times \mathbb{E}) &\to (U \times \mathbb{E}) \\ (x, \xi) &\to (x, P_{T_x\mathbb{S}^2}\xi) \end{aligned} \tag{2.47}$$

we get:

$$\begin{aligned} (U \times \mathbb{E}) \times (\mathbb{E} \times \mathbb{E}) &\to (U \times \mathbb{E}) \times (\mathbb{E} \times \mathbb{E}) \\ (x, \xi, \delta\xi, \delta\eta) &\to (x, P_{T_x\mathbb{S}^2}\xi, \delta\xi, P'_{T_x\mathbb{S}^2}(\delta\xi, \xi) + P_{T_x\mathbb{S}^2}\delta\eta) \\ &\to (x, \xi, \delta\xi, h_{12}(\delta\xi, \xi) + P_{T_x\mathbb{S}^2}\delta\eta). \end{aligned} \tag{2.48}$$

With that, as a consequence of Theorem 2.7.3, we get a splitting of $T(T\mathbb{S}^2)$ as in Theorem 2.7.1, via the connection map:

$$\kappa_{T\mathbb{S}^2}(x, \xi, \delta\xi, \delta\eta) = (x, \xi, \delta\xi, P_{T_x\mathbb{S}^2}\delta\eta + h_{12}(\xi, \delta\xi)). \tag{2.49}$$

Second Tensorial Derivatives For SQP-algorithms on manifolds, second-order information is needed, making necessary the concept of second tensorial derivatives.

Definition 2.7.5. *Let be M a manifold with covariant derivative ∇. For vector fields η, ξ we define the second tensorial derivative $Q(\eta, \xi)$ as:*

$$Q(\eta, \xi) = \nabla_\eta \nabla_\xi - \nabla_{\nabla_\eta \xi}. \tag{2.50}$$

We now address the discussion on derivatives of real functions on manifolds. Let be $f : M \to \mathbb{R}$ a differentiable function. Then, we say that the first derivative of f in direction ξ is given by the formula:

$$\nabla_\xi f = f'(x)\xi.$$

The Hessian of f, denoted by Hf, is given by:

$$Hf(\eta, \xi) = Q(\eta, \xi)f. \tag{2.51}$$

Let be η, ξ the representations of the vector fields in a chart U, and let be B the quadratic part of the spray on M. Then we have that:

$$Hf(x)(\eta, \xi) = f''(x)(\eta(x), \xi(x)) + f'(x)B(x; \eta(x), \xi(x)). \tag{2.52}$$

which is symmetric, by the symmetry of f'' and the symmetry of the bilinear map B. For more details on the tensorial Hessian, see [Lan12a, XIII, §1].

Proposition 2.7.3. *Let be $x \in M$ and let be $v \in T_xM$. Let α be a geodesic with $\alpha(0) = x$ and $\alpha'(0) = v$. Then*

$$Hf(v, v) = \left(\frac{d}{dt}\right)^2 f(\alpha(t))|_{t=0}. \tag{2.53}$$

Proof. This follows by applying the operator

$$Q(\alpha', \alpha') = \nabla_{\alpha'} \nabla_{\alpha'} - \nabla_{\nabla_{\alpha'}\alpha'}$$

to f, recalling that α is a geodesic i.e., $\nabla_{\alpha'}\alpha' = 0$. □

In a similar way, through the operator Q as introduced in (2.50), we define the second tensorial derivative of a twice differentiable function g. Let be $g : M \to N$ a C^2 function, then we define the tensorial second derivative of g as:

$$(D^2 g)(\eta, \xi) = Q(\eta, \xi)g. \tag{2.54}$$

Again, if η, ξ are representations of the vector fields in a chart, then the local representation of $D^2 g$ is given by:

$$D^2 g(x)(\eta, \xi) = g''(x)(\eta(x), \xi(x)) + g'(x)B(x; \eta(x), \xi(x)). \tag{2.55}$$

And finally, a similar formula for the derivative through geodesics.

Proposition 2.7.4. *Let be $g : M \to N$ a C^2 function and $x \in M$. Let be $v \in T_xM$ and α a geodesic in M with $\alpha(0) = x$ and $\alpha'(0) = v$. Then*

$$D^2 g(v, v) = \left(\frac{d}{dt}\right)^2 g(\alpha(t))|_{t=0}. \tag{2.56}$$

Proof. We use the property for geodesics $\nabla_{\alpha'}\alpha' = 0$ and the chain rule. □

2.8 Connections and Covariant Derivatives on General Vector Bundles

So far, we have defined connections on manifolds through bilinear maps $B : \mathbb{E} \times \mathbb{E} \to \mathbb{E}$, where $\mathbb{E}$ is the model space of the manifold M, satisfying certain transformation conditions. We generalize the concept of connections, to the case where the manifold is a vector bundle $p : E \to M$, with fiber $\mathbb{F}$. Here, we do it through bilinear maps, that are of the form $B_E : \mathbb{F} \times \mathbb{E} \to \mathbb{F}$, i.e., mapping into the fiber space. Through these maps, we will be able to define propper differentiation on the more general context of vector bundles, as mappings from the direct sum $E \oplus TM$ to TE.

Definition 2.8.1. *Let be $p : E \longrightarrow M$ a vector bundle over a manifold M, and consider the tangent bundles $\pi_E : TE \longrightarrow E$ and $T(p) : TE \longrightarrow TM$. A connection is a mapping from the direct sum $E \oplus TM$ into TE:*

$$H : E \oplus TM \longrightarrow TE$$

such that

$$(\pi_E, T(p)) \circ H = id_{E \oplus TM}.$$

The latter means that, if we consider a chart U on M, and if we suppose that M is modeled on $\mathbb{E}$ and that the vector bundle fiber is the space $\mathbb{F}$, then:

$$TU = U \times \mathbb{E} \quad \text{ and } \quad T(U \times \mathbb{F}) = (U \times \mathbb{F}) \times (\mathbb{E} \times \mathbb{F}).$$

Then H maps as:

$$H(x, e, \xi) = (x, e, H_1(x, e, \xi), H_2(x, e, \xi)) \qquad \text{for } (x, e, \xi) \in M \times \mathbb{F} \times \mathbb{E}.$$

The condition $(\pi_E, T(p)) \circ H = id_{E \oplus TM}$ implies that $H_1(x, e, \xi) = \xi$. Additionally, for fixed x, the map

$$H_2(x, e, \xi) : \mathbb{F} \times \mathbb{E} \longrightarrow \mathbb{F} \tag{2.57}$$

is bilinear, and if we denote the latter bilinear map by B_E, then, in charts, it takes the form:

$$H(x, e, \xi) = (x, e, \xi, B_E(x)(e, \xi)) \, . \tag{2.58}$$

With this, we can define the covariant derivative of a section $v(x) : M \to E$ of the vector bundle in the direction of $w \in TM$, as:

$$\nabla^E v(x) w = v'(x) w - B_E(x)(v(x), w).$$

As a final remark, we see that if we take the special case $E = TM$, and if the map B_E is symmetric, then we land on the case of a spray on M. For more details on vector bundle connections see [Kli11, E$^+$67, Lan12a, PT06, JJ08, Dom62, V$^+$67, KN63, Kow71, Sas58, Sas62, YL64, Hus66]. For simplicity, we will refer to B_E as the spray for the vector bundle $p : E \to M$, where in fact $B_E = H_2$ as in (2.58).

We now define the map $K_2 : TE \to p^* E$ with the help of a spray

$$B_E : \mathbb{F} \times \mathbb{E} \to \mathbb{F}$$

as follows:

$$K_2 : TE \to p^*E \tag{2.59}$$
$$(x, e, \xi, \eta) \to (x, e, \eta - B_E(x)(e, \xi)). \tag{2.60}$$

It is important to observe that K_2 defines a mapping from TE, which is a vector bundle over E but not over M, to p^*E, which is a vector bundle over M. The above representation is given locally, with respect to charts, but it can be verified that it transforms correctly and thus gives rise to a global mapping. This observation follows from the fact that if we consider a change of charts on E, namely:

$$U \times \mathbb{F} \xrightarrow{(h_M, h_E)} V \times \mathbb{F}$$

such that, for $(x, e) \in U \times \mathbb{F}$, it maps:

$$(x, e) \xrightarrow{H_E := (h_M, h_E)} (h_M(x), h_E(x)e)$$

the derivative of the previous map is represented by:

$$\begin{bmatrix} h'_M(x)\cdot & 0 \\ h'_E(x)\cdot e & h_E(x)\cdot \end{bmatrix} \begin{bmatrix} \xi \\ \eta \end{bmatrix}$$

this means that, for $(\xi, \eta) \in \mathbb{E} \times \mathbb{F}$ we get the transformation rule for TE:

$$(H_E, H'_E)(x, e, \xi, \eta) = (h_M(x), h_E(x)e, h'_M(x)\xi, h'_E(x)(\xi, e) + h_E(x)\eta). \tag{2.61}$$

Concatenation with the map K_2 yields:

$$(x, e, \xi, \eta) \to (h_M(x), h_E(x)e, h'_E(x)(\xi, e) + h_E(x)\eta - B_{E,V}(h_E(x)e, h'_M(x)\xi)). \tag{2.62}$$

In a similar fashion, as in the tangent bundle case, from (2.61), we see that a vector bundle spray B_E over E obeys the transformation rule:

$$B_{E,V}(h_E(x)e, h'_M(x)\xi) = h'_E(x)(\xi, e) + h_E(x)B_{E,U}(e, \xi) \tag{2.63}$$

and thus, in (2.62), we obtain:

$$(x, e, \xi, \eta) \to (h_M(x), h_E(x)e, h_E(x)(\eta - B_{E,U}(e, \xi))). \tag{2.64}$$

Thus, a change of charts in the preimage space yields a matching change of charts in the image space. We now make use of the map K_2 to construct an isomorphism over the vector bundle that splits the space TE.
First of all, we have the canonical mapping:

$$Tp : TE \to TM$$
$$(x, e, \xi, \eta) \to (x, \xi).$$

Gathering Tp and K_2 into one mapping, we obtain the following splitting of TE:

$$\begin{aligned}\kappa_E := (K_2, Tp) : TE \to \tilde{E} := TM \oplus p^*E \\ (x, e, \xi, \eta) \to (x, e, \xi, \eta - B_E(x)(e, \xi)).\end{aligned} \tag{2.65}$$

This is the desired splitting of TE into a vector bundle $\tilde{p} : \tilde{E} \to M$ over M that consist of a direct product of TM and p^*E. We now state the vector bundle version of Theorem 2.7.1.

Theorem 2.8.1. *Let be $B_E : \mathbb{F} \times \mathbb{E} \to \mathbb{F}$ a vector bundle connection on the vector bundle $p : E \to M$. And let be p^*E the pullback of the vector bundle. Then the map:*

$$\kappa_E : TE \to TM \oplus p^*E$$

is s a vector bundle isomorphism over E, where in the vector bundle chart

$$(TE)_U = (U \times \mathbb{F}) \times \mathbb{E} \times \mathbb{F}$$

this map is given by

$$\kappa_{E,U}(x, e, \xi, \eta) = (x, e, \xi, \eta - B_{E,U}(e, \xi)). \tag{2.66}$$

Proof. Similarly as in the tangent bundle case, using the formula for (H_E, H'_E) given in (2.61), and the transformation rule (2.66) for B_E, we have that:

$$\kappa_{E,V} \circ (H_E, H'_E)(x, e, \xi, \eta) = (h_1(x), h_2(x)e, h'_1(x)\xi, h_2(x)(\eta - B_{E,U}(e, \xi))) \tag{2.67}$$

obtaining a family of vector bundle morphisms $\{\kappa_{E,U}\}$ over E, and the expression of the map in a chart, yields a vector bundle isomorphism. $\square$

In particular, the splitting of Theorem 2.8.1 will allow us to define suitable mappings for optimization algorithms on vector bundles in an invariant way under change of charts.

Remark 2.8.1. *We observe that the last component of the map* (2.66) *can be expressed as:*

$$\begin{bmatrix} id_{TM} & 0 \\ -B_E(e, \cdot) & id_E \end{bmatrix} \begin{bmatrix} \xi \\ \eta \end{bmatrix}. \tag{2.68}$$

2.8.1 Splitting of (double) Tangent Bundles

Let us consider a vector bundle $p : E \to M$, where the base manifold M is modeled on $\mathbb{E}$ and the vector bundle has as fiber space $\mathbb{F}$. In a chart, let be $(x, e) \in U \times \mathbb{F}$. Our aim is to split TE, a vector bundle over E, into a product of vector bundles over M. Once this is done, we proceed to split TTE into a product of vector bundles over the base manifold M. We assume the existence of sprays B_{TM} for M and B_E for the vector bundle E, which are associated to covariant derivatives ∇^{TM} and ∇^E respectively. We make use of p^*E, the pullback of E via p, which adds to each element of E at x another fiber E_x. Finally, TE can be represented in charts by $(x, e, \xi, \eta) \in U \times \mathbb{F} \times \mathbb{E} \times \mathbb{F}$. Here (ξ, η) represent perturbations of (x, e).
In the following, we use the notation to write down mappings between manifolds, giving their algebraic definition with respect to charts.
We use the following notation:

- The representation of $\tilde{E}$ in charts is $U \times \tilde{\mathbb{F}} = U \times (\mathbb{F} \times \mathbb{E} \times \mathbb{F})$.
- There is a spray $B_{\tilde{E}} : \tilde{\mathbb{F}} \times \mathbb{E} \to \tilde{\mathbb{F}}$ that consists of three components:

$$B_{\tilde{E}}(x)(\tilde{e}, \delta x) := (B_E(x)(e, \delta x), B_{TM}(x)(\xi, \delta x), B_E(x)(\eta, \delta x)), \text{ where } \tilde{e} = [e, \xi, \eta] \in \mathbb{F} \times \mathbb{E} \times \mathbb{F}. \tag{2.69}$$

Application to a Section $F : Z \to E$. Let be Z a differentiable manifold, and with it, consider a differentiable section, which locally in charts is given by:

$$\begin{aligned} F : Z &\to E \\ z &\to (F_x(z), F_e(z)) \end{aligned} \tag{2.70}$$

where $(p \circ F)(z) = F_x(z)$, so $F_e(z) \in E_{F_x(z)}$ is in the right fiber. Then, the tangent map of F is given by:

$$\begin{aligned} TF : TZ &\to TE \\ (z, \zeta) &\to ([F_x(z), F_e(z)], [F_x'(z)\zeta, F_e'(z)\zeta]) = (F(z), (T_z F)\zeta). \end{aligned} \tag{2.71}$$

And composition with κ_E yields:

$$\begin{aligned} \nabla^E F := \kappa_E \circ TF : TZ \to \tilde{E} \\ (z, \zeta) &\to ([F_x(z)], [F_e(z), F_x'(z)\zeta, F_e'(z) - B_E(F_x(z))(F_e(z), F_x'(z)\zeta)]) \\ &= (F_x(z), [F_e(z), (T_z F_x \zeta), \nabla^E_\zeta F_e(z)]) = (F_x(z), \tilde{F}_e(z, \zeta)) \end{aligned} \tag{2.72}$$

where the map $\tilde{F}_e(z, \zeta)$ is given by:

$$\tilde{F}_e(z, \zeta) = (F_e(z), T_z F_x \zeta, \nabla^E_\zeta F_e(z)).$$

The mapping $\kappa_E \circ TF$, yields in the last component a proper way to differentiate sections on general vector bundles, of course, for the case of the tangent bundle $E = TM$, we get that B_{TM} is the bilinear map mapping from $\mathbb{E} \times \mathbb{E}$ to $\mathbb{E}$. Thanks to the transformation property of the map B_E given in (2.63), we get that the last component transforms in a covariant way under change of charts see [Lan12a, VIII, §2]. In this way, the last component of the above defined map ∇F, defines the covariant derivative of a section F in direction ζ, which is represented as:

$$\nabla^E_\zeta F_e(z) := F_e'(z)\zeta - B_E(F_x(z))(F_e(z), F_x'(z)\zeta). \tag{2.73}$$

We go one step higher and consider the second derivative.

Computation of the Second Derivative From now on, we use [...] to group variables. This is just notation to make things more readable. Also for $\tilde{E}$, we have a mapping $\kappa_{\tilde{E}}$ that is just defined as before:

$$\begin{aligned} \kappa_{\tilde{E}} : T\tilde{E} &\to TM \oplus p^* \tilde{E} \\ (x, [\tilde{e}], \delta x, [\delta \tilde{e}]) &\to (x, [\tilde{e}], \delta x, [\delta \tilde{e} - B_{\tilde{E}}(x)(\tilde{e}, \delta x)]). \end{aligned} \tag{2.74}$$

In detail this yields:

$$\begin{aligned}
&\kappa_{\tilde{E}} : T\tilde{E} \to TM \oplus p^*\tilde{E}\\
&\qquad (x,[e,\xi,\eta],\delta x,[\delta e,\delta\xi,\delta\eta])\\
&\qquad\quad \to (x,[e,\xi,\eta],\delta x,[\delta e - B_E(x)(e,\delta x),\delta\xi - B_{TM}(x)(\xi,\delta x),\delta\eta - B_E(x)(\eta,\delta x)]).
\end{aligned} \tag{2.75}$$

If we apply $\kappa_{\tilde{E}} \circ T$ to $\kappa_E \circ TF$ we obtain:

$$\begin{aligned}
&\nabla^{2,E}F := \kappa_{\tilde{E}} \circ T \circ \kappa_E \circ TF : TTZ \to TM \oplus \tilde{p}^*\tilde{E}\\
&\qquad\qquad (z,\zeta,\delta z,\delta\zeta) \to (F_x(z),\tilde{F}_e(z,\zeta),(T_{(z,\zeta)}F_x)(\delta z,\delta\zeta),\nabla^{\tilde{E}}_{(\delta z,\delta\zeta)}\tilde{F}_e(z,\zeta))
\end{aligned} \tag{2.76}$$

In particular, we obtain (using the structure of $\tilde{F}_e$) that:

$$\begin{aligned}
&(T_{(z,\zeta)}F_x)(\delta z,\delta\zeta) = (T_zF_x)\delta z + 0\delta\zeta\\
&\nabla^{\tilde{E}}_{(\delta z,\delta\zeta)}\tilde{F}_e(z,\zeta) = [\nabla^E_{\delta z}F_e(z) + 0\delta\zeta, \nabla^{TM}_{\delta z}((T_zF_x)\zeta) + (T_zF_x\delta\zeta), \nabla^E_{\delta z}(\nabla^E_\zeta F_e(z)) + \nabla^E_{\delta\zeta}F_e(z)].
\end{aligned}$$

We can write these relations in matrix form:

$$M_1(z)\zeta = \begin{bmatrix} (T_zF_x)(\cdot) \\ \nabla^E_{(\cdot)}F_e(z) \end{bmatrix}[\zeta] \quad M_2(z,\zeta)\begin{bmatrix} \delta z \\ \delta\zeta \end{bmatrix} = \begin{bmatrix} (T_zF_x(z))(\cdot) & 0 \\ \nabla^E_{(\cdot)}F_e(z) & 0 \\ \nabla^{TM}_{(\cdot)}((T_zF_x)\zeta) & (T_zF_x)(\cdot) \\ \nabla^E_{(\cdot)}(\nabla^E_\zeta F_e(z)) & \nabla^E_{(\cdot)}F_e(z) \end{bmatrix}\begin{bmatrix} \delta z \\ \delta\zeta \end{bmatrix}. \tag{2.77}$$

It can be seen from the block structure of these matrices, that the following quantities fully characterize the first and second derivative:

$$(T_zF_x)v,\ \ \nabla^E_v F_e(z),\ \ \nabla^{TM}_v((T_zF_x)\zeta),\ \ \nabla^E_v(\nabla^E_\zeta F_e(z))\ \ v \in T_zZ$$

We can even go further and write:

$$M_2(z,\zeta) = \begin{bmatrix} M_1(z) & 0 \\ M_{12}(z,\zeta) & M_1(z) \end{bmatrix},\ \ M_{12}(z,\zeta) = \begin{bmatrix} \nabla^{TM}_{(\cdot)}(T_zF_x(z)\zeta) \\ \nabla^E_{(\cdot)}(\nabla^E_\zeta F_e(z)) \end{bmatrix}. \tag{2.78}$$

In the above approach, we were able to define covariant derivatives ∇^E of sections on general vector bundles, making use of the composition $\kappa_E \circ T$. Moreover, by iterating the process and by performing the composition map $\kappa_{\tilde{E}} \circ T \circ \kappa_E \circ T$, we got the iterated covariant derivative $\nabla^{2,E}$. These considerations will be useful for our work, in particular when we define consistency properties for suitable optimization mappings on vector bundles.

2.9 Derivative Along A Curve

Here, we return to the tangent bundle context. One can consider covariant differentiation applied not only to vector fields but also to curves, with this, we can define the important concept of parallelism. Let be $I \subset \mathbb{R}$ an interval, and let be the curve $\gamma : I \to M$, we wish to define $\nabla_{\gamma'}\gamma_L$, where $\gamma_L : I \to TM$ is a lift of γ as in defined in 2.1.9. The next theorem assures the existence of such operation.

Theorem 2.9.1. *Let be B_U the bilinear map associated to the spray in a chart U. Then there exists a unique linear map*

$$\nabla_{\gamma'} : \mathrm{Lift}(\gamma) \to \mathrm{Lift}(\gamma)$$

which in a chart U has the expression

$$(\nabla_{\gamma'}\gamma_L)(t) = \gamma_L'(t) - B_{\gamma(t)}(\gamma'(t), \gamma_L(t)). \tag{2.79}$$

Definition 2.9.1. *Let be $\gamma : I \to M$ a differentiable curve. We say that a lift $\gamma_L : I \to TM$ of γ is γ-parallel if $\nabla_{\gamma'}\gamma_L = 0$. This means that in a chart U we have that:*

$$\begin{aligned} \gamma_L'(t) &= B_{\gamma(t)}(\gamma'(t), \gamma_L(t)) && (2.80)\\ &= B(\gamma(t); \gamma'(t), \gamma_L(t)) && (2.81) \end{aligned}$$

In particular, we have that, a curve is a geodesic for the spray if and only if $\nabla_{\gamma'}\gamma' = 0$, that is, if and only if the canonical lift γ' is γ-parallel. The next theorem assures that for every curve $\gamma : I \to M$ and a vector on the curve at a point $t_0 \in I$, there exists a lift that is γ-parallel and takes the value of the vector at the point t_0.

Theorem 2.9.2. *Let be $\gamma : I \to M$ a differentiable curve in M. Let $t_0 \in I$. For given $\xi \in T_{\gamma(t_0)}M$, there exists a unique lift $\gamma_L : I \to TM$ which is γ-parallel and such that $\gamma_L(t_0) = \xi$.*

Proof. The existence and uniqueness follows from the existence and uniqueness of solutions of differential equations. For more details see [Lan12a, VIII, §3]. □

Theorem 2.9.3. *Let be $\gamma : I \to M$ a curve and $t_0 \in I$ fixed. The map*

$$P^t_{t_0,\gamma} = P^t : T_{\gamma(t_0)}M \to T_{\gamma(t)}M$$

defined by

$$P^t(\xi) = \gamma_L(t, \xi)$$

where $\gamma_L(t, \xi)$ is the unique curve in TM which is γ-parallel and $\gamma(t_0, \xi) = \xi$, is a linear isomorphism.

Proof. See [Lan12a, VIII, §3] □

The map P^t defined above is called parallel translation along γ.

Chapter 3

Optimization on Manifolds and Retractions

With the previous background on differential geometry, we go on with an overview of optimization on manifolds and especially the tools needed for this purpose. In this section, we consider the concept of retractions, mappings that can be understood as approximations of the exponential mapping. Retractions will play a crucial role in the implementation of algorithms and the consequent numerical solution of optimization problems on manifolds. For constrained optimization problems, the idea is to pullback cost and constraint maps to linear vector spaces through retractions, and use optimization methods to get corrections, which lie in linear spaces. After that, the updates are performed in a nonlinear way via retractions. Thus, the use of such mappings is then, twofold. In the literature [AMS09], the concept of nonlinear retraction is introduced and its use has become customary. We remind this concept as defined there. Several examples are shown, we remind the well known retractions for the sphere, and we construct retractions for the space of orientation and volume preserving tetrahedra, which are useful in the context of finite elasticity and for the numerical solution of mechanical problems on the space of volume preserving diffeomorphims. After this, we introduce the concept of vector bundle retraction, as well as corresponding consistency properties. Specifically thinking in our applications, we construct retractions for the bundles $T\mathbb{S}^2$ and $(T\mathbb{S}^2)^*$. For implementation purposes, and in order to work with representations of the tangent spaces, we introduce the concept of local parametrizations, which will be of special importance in Chapter 6 when numerical applications are discussed. We begin with a very short overview of unconstrained optimization on manifolds motivated from [AMS09], as a prelude to the subsequent section on the constrained case.

3.1 Unconstrained Optimization on Manifolds

In the present section, we do a short review of optimization on manifolds for the unconstrained case, and for the sake of presentation, we recall the most important concepts and ideas. For a detailed exposition, we refer the reader to [AMS09]. In the following, we consider the problem:

$$\min_{x \in M} f(x) \tag{3.1}$$

where M is a differentiable manifold and $f(x)$ is a real differentiable function on M. In linear spaces, iterative methods for minimization are based on the update formula:

$$x_{k+1} = x_k + t_k \delta x_k$$

where δx_k is the search direction, and t_k is the step size. If we try to perform this procedure on manifolds we find some differences. If δx_k is found as a correction by using gradient or Newton's method, then δx_k must belong to a linear space $\mathbb{E}$. On manifolds, we encounter the problem of updating the actual point $x_k \in M$ on the manifold, to the correction $\delta x_k \in \mathbb{E}$, which belongs to a linear space. To overcome this problem, we need a suitable generalization of the sum, assuring that we can update the iterates in a nonlinear way, and such that the new iterate belongs to the manifold. The proposed generalization in [AMS09], is to take δx_k as a tangent vector to the manifold at the point x_k and perform a search along a curve contained in M in the direction of δx_k. This can be done by using the concept of *retraction* mapping as defined in section 3.2. Roughly speaking, a retraction R_x^M at the point $x \in M$, is a mapping $R_x^M : T_xM \to M$ that is first order consistent with the exponential map $\exp_x$. Optimization algorithms can also be constructed by using the map $\exp_x$ as a way to update iterates along its flow, however, often $\exp_x$ is hard or very expensive to evaluate, this is why in the optimization literature [AMS09], the notion of *retractions* has become customary, which can be seen as an efficient surrogate for $\exp_x$. We show how to use retractions in optimization algorithms for the unconstrained case.

3.1.1 Optimization Algorithms on Manifolds

The retraction mapping R_x^M can play two roles, R_x^M not only transforms points of T_xM into points on M, it also transforms the cost function defined in a neighborhood of $x \in M$ into a cost function defined on the linear space T_xM. Let be $f : M \to \mathbb{R}$, we achieve this by performing the pullback of the function f through R^M, this is, at $x \in M$, we have

$$\mathbf{f} := f \circ R_x^M : T_xM \to \mathbb{R}.$$

We note that $\mathbf{f}$ defined in this way is a real valued function on a linear space. This makes possible to compute derivatives locally, in the usual way, and corrections can be computed by gradient, Newton's method or even as minimizers of quadratic models of $\mathbf{f}$ within some trust-region defined over the model tangent space. The latter means that with the help of the pullback, we can construct local models for $\mathbf{f}$ leading to the implementation of SQP-methods for the solution of the optimization problems.

3.1.2 Computation of Corrections

In Algorithm 1, the correction step δx can be computed in different ways and depending on the method, and the retraction employed, the algorithm will experience a different behavior. It is, of course, well know from the linear setting, that second-order methods are more efficient for this task, but the effect of the employed retractions on the algorithm is a new effect that has to be considered. Advantages and disadvantages known from the linear case, will be inherited to the manifold case (for the case of second order retractions). In the following, we show how the steps can be computed, and we mention some properties of the algorithm corresponding to the method employed, for more details see [AMS09].

Algorithm 1 Unconstrained Optimization on Manifolds

Require: initial iterate x_0
  repeat// *NLP loop*
    Choose a retraction R_x^M at x
    repeat// *step computation as usual*
      compute $\delta x \in T_x M$
    until trial correction δx accepted
    $x \leftarrow R_x^M(\delta x)$
  until converged

Gradient Method Let us suppose that M is a Riemannian manifold with metric $\mathbf{M}$. Then, the gradient vector field $\operatorname{grad} f(x) \in T_x M$ of $f(x)$ is defined as

$$\langle \operatorname{grad} f(x), v \rangle_x = \mathbf{f}'(0_x)v \quad \text{for all} \quad v \in T_x M.$$

The latter makes sense, indeed $\mathbf{f}'(0_x) \in (T_x M)^*$, and given that the metric can be interpreted as a map

$$\mathbf{M}(x) : T_x M \longrightarrow (T_x M)^*$$

then $(M(x))^{-1}\mathbf{f}'(0_x) \in T_x M$. Therefore, in Algorithm 1, the search direction $\delta x \in T_x M$ is chosen as

$$\delta x = -\operatorname{grad} f(x).$$

Newton's Method In Newton's method, second-order information on the cost function is used, and the zeros of the gradient vector field are searched. In Newton's method, the corresponding search direction δx, is picked as the solution to

$$Hf(x)\delta x = -\operatorname{grad} f(x)$$

where, the general Hessian operator Hf is as defined in (2.51). The case in which the retraction satisfies $\nabla_\xi DR^M(0_x) = 0$, then:

$$Hf(x) = H(f \circ R_x^M)(0_x)$$

as it is shown in formula (2.53).

Trust-Region Methods For the case of vector spaces, in trust-region methods, the correction δx_k is chosen as a minimizer of the quadratic Taylor expansion of the function f around an iterate x_k, subject to norm bound constraints. In [AMS09], the proposed generalization to the case of a Riemannian manifold, takes the pullback of the cost function using a retraction around the current iterate. After that, the local quadratic model is constructed and minimized over the current tangent space subjected to bound constraints. The norm is induced by the Riemannian metric over the tangent space of the current iterate. This is how we get the desired correction, which will be updated using the retraction map. Of course, the quality of the model will depend on how good the model approximates the true function, this, in turn, will depend on the quality of the retraction.

Therefore, in [AMS09], the proposed trust region method algorithm on Riemannian manifolds, aims to find a correction δx as a solution to the trust-region subproblem:

$$\min_{\delta x \in T_x M} \mathbf{m}_x(\delta x) = \mathbf{f}(0_x) + \langle \mathbf{f}'(0_x), \delta x\rangle + \frac{1}{2}\langle A\delta x, \delta x\rangle$$
$$\text{s.t} \quad \langle \delta x, \delta x\rangle_x \leq \Delta^2,$$

where $\langle\cdot,\cdot\rangle_x$ denotes the Riemannian metric and A is some symmetric operator on T_xM. A possible choice for A, is the Riemannian Hessian $H\mathbf{f}(0_x)$.
In a nutshell, as stated in [AMS09], in order to apply a Riemannian trust-region method to optimize a function $f : M \to \mathbb{R}$, we need the following:

i) Tractable numerical numerical representation for points x in M, for tangent spaces T_xM and for the inner products $\langle\cdot,\cdot\rangle$ in T_xM .

ii) A retraction $R_x^M : T_xM \to M$.

iii) Formulas for $f(x)$, $\operatorname{grad} f(x)$ and the Hessian Hf, or at least a good approximation of it.

An exact formula for the Hessian Hf is not needed, and we could choose $A = H(f \circ R_x^M)$ for any retraction R_x^M.
As we saw, retractions are a central tool for the implementation of numerical methods for optimization on manifolds. We define this important concept as it is done in [AMS09], and as a new feature, we extend the definition to the case where the manifold has the structure of a vector bundle.

3.2 Retractions and their Consistency

As we already mentioned, we need suitable mappings for optimization algorithms that maps the tangent bundle into the manifold, namely:

$$\begin{aligned} R_x^M : T_xM &\to M \\ \xi &\to R_x^M(\xi). \end{aligned}$$

for $x \in M$ and $\delta x \in T_xM$.
For our purposes, we need to take first and second derivatives T_xR^M and $T^2R_x^M$ of this map. For the tangent map, and its representation in a chart we obtain:

$$\begin{aligned} TR_x^M : T(T_xM) &\to TM \\ (\xi, \delta\xi) &\to (R_x^M(\xi), DR_x^M(\xi)\delta\xi). \end{aligned} \tag{3.2}$$

Note, however, that $DR_x^M(0_x)$ does not depend on the choice of chart on M and can thus be interpreted as a mapping

$$DR_x^M(0_x) : T_xM \to T_xM.$$

Definition 3.2.1. *A (first order) C^k-retraction ($k \geq 1$) on a manifold M, is a mapping R^M from the tangent bundle TM onto M with the following properties: Let R_x^M denote the restriction of R^M to T_xM, then* *i)* $R_x^M(0_x) = x$, *where* 0_x *denotes the zero element of* T_xM.

ii) R_x^M *is k-times continuously differentiable.*

iii) *With the canonical identification* $T_{0_x}T_xM \simeq T_xM$, R_x^M *satisfies*

$$DR_x^M(0_x) = id_{T_xM}, \tag{3.3}$$

where id_{T_xM} *denotes the identity mapping on* T_xM.

For the second tangent map of the retraction, we take perturbations $(\delta^2\xi_1, \delta^2\xi_2)$ of $(\xi, \delta\xi)$, obtaining the second tangent map and its representation in a chart:

$$\begin{aligned} &T_x^2 R^M : T^2(T_xM) \to T^2M \\ &(\xi, \delta\xi, \delta^2\xi_1, \delta^2\xi_2) \to (R_x^M(\xi), DR_x^M(\xi)\delta\xi, DR_x^M(\xi)\delta^2\xi_1, D^2R_x^M(\xi)(\delta^2\xi_1, \delta\xi) + DR_x^M(\xi)\delta^2\xi_2). \end{aligned} \tag{3.4}$$

As we observe, the latter formula tells us that the second-order derivative, in particular $D^2R_x^M(\xi)$, depends on the choice of charts. We define the second-order consistency of retractions in a way that is independent of such choice of charts, following the results from section 2.7.

Second-Order Retractions Using the map introduced in (2.72), we make $Z = TM$ and $E = TM$, the tangent bundle. If we define $F(\xi, \delta\xi) := (R_x^M(\xi), DR_x^M(\xi)\delta\xi)$, we can compute its covariant derivative, for perturbations $(\delta^2\xi_1, \delta^2\xi_2)$ of $(\xi, \delta\xi)$, obtaining:

$$\nabla^{TM} F(0, \delta\xi)(\delta^2\xi_1, \delta^2\xi_2) = (x, \delta\xi, \delta^2\xi_1, \nabla^{TM}_{\delta^2\xi_1}(DR_x^M(0)\delta\xi) + \delta^2\xi_2).$$

We say that a retraction is of second order if:

$$\nabla^{TM} F(0, \delta\xi)(\delta^2\xi_1, \delta^2\xi_2) = (x, \delta\xi, \delta^2\xi_1, \delta^2\xi_2),$$

which can be written in short (suppressing the first two components) as

$$\nabla^{TM} F(0, \delta\xi) = Id_{(TM)^2}.$$

This means that, in addition to the first order consistency condition $DR_x^M(0) = id_{T_xM}$, we impose:

$$\nabla^{TM}_{\delta\xi^2}(DR_x^M(0)\delta\xi) = 0 \quad \forall \delta\xi, \delta\xi^2 \in T_xM.$$

or in short

$$\nabla^{TM}(DR_x^M(0)\delta\xi) = 0, \quad \forall\, \delta\xi \in T_xM$$

for the linear mapping: $\nabla^{TM}(DR_x^M(0)\delta\xi) : T_xM \to T_xM$.
Certainly, the exponential map $R_x^M = \exp_x$ is the most prominent retraction of second order. Often, first order retractions are easier to construct and compute than second order retractions. It is thus of interest, in how far algorithmic quantities depend on the choice of retraction. In the context of unconstrained optimization, it is known (cf. e.g., [HT04, AMS09]), that first order retractions are sufficient in many aspects.

Remark 3.2.1. *If* M *is an embedded submanifold of a linear space* $\mathbb{E}$, *then we can consider* T_xM *as a subspace of* $T_x\mathbb{E} \simeq \mathbb{E}$. *In particular, for* $x \in M$ *and* $\xi \in T_xM$, *where* $\xi \in T_x\mathbb{E} \simeq \mathbb{E}$, *the element* $x + \xi \in \mathbb{E}$ *is well defined. Therefore, the projection of the element* $x + \xi$ *onto the manifold* M *yields a retraction on* M, *as we see in the next example.*

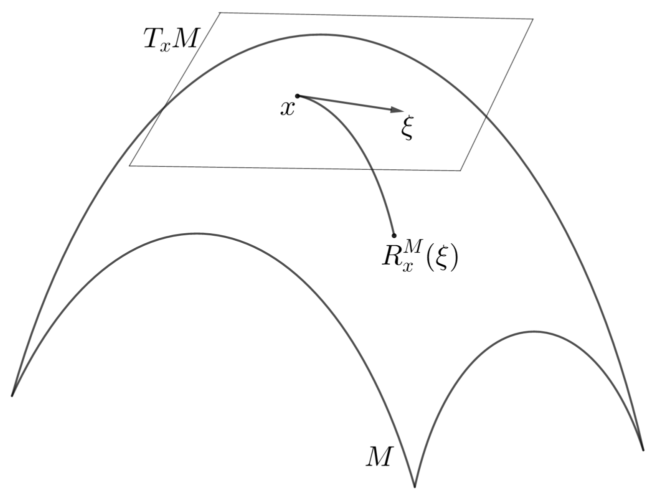


Figure 3.1: *Retraction map*

3.2.1 Examples

The n-Sphere Let be $M = \mathbb{S}^n \subseteq \mathbb{R}^{(n+1)}$ the n-Sphere. Then, the mapping

$$R^{\mathbb{S}^n}_{x,1}(\xi) = \frac{x+\xi}{\|x+\xi\|} \tag{3.5}$$

is a retraction for $\mathbb{S}^n$. For details see e.g., [AMS09, IV,§1].

The Positive Cone Let be $(K_+, \langle\cdot,\cdot\rangle_x)$ as defined in (2.5). Then, for $x \in K_+$ and $\xi \in \mathbb{R}^n$, the map:

$$R^{K_+}_x(\xi) = \begin{bmatrix} x_1 \exp(\frac{1}{x_1}\xi_1) \\ \vdots \\ x_i \exp(\frac{1}{x_i}\xi_i) \\ \vdots \\ x_n \exp(\frac{1}{x_n}\xi_n) \end{bmatrix} \tag{3.6}$$

is a retraction for K_+, with $\exp(\cdot) : \mathbb{R} \to \mathbb{R}^+$ the real exponential map. Observe that $T_xK_+ \simeq \mathbb{R}^n$.

Using Matrix exponential Let be $M = \mathbb{S}^2 \subseteq \mathbb{R}^3$ the 2-sphere. The following alternative parametrization uses a characterization of $T_x\mathbb{S}^2$ via the space of skew-symmetric matrices

$$\mathfrak{so}(3) = \{H \in \mathbb{R}^{3\times 3} | H = -H^T\}$$

by:

$$T_x\mathbb{S}^2 = \{Hx : H \in \mathfrak{so}(3)\}.$$

This follows from $\langle Hx, x\rangle = -\langle x, Hx\rangle = 0$ by the fact that Hx can be written as $w \times x$, which is non-zero if $0 \neq w \perp x$.
Using the matrix exponential matrix operator, and setting $\xi = Hx$ we can define the following retraction:

$$R_{x,2}^{\mathbb{S}^2}(\xi) = \exp(H)x.$$

where

$$\exp : \mathfrak{so}(3) \longrightarrow SO(3)$$

is as defined in (A.40), with $SO(3) = \{Q \in \mathbb{R}^{3\times 3} | QQ^T = Q^TQ = Id_3, \det(Q) = 1\}$, the special orthogonal group as defined in A.4 . We remark that the retraction is well defined: if $H_0x = 0$, then $\exp(H_0)x = x$ as can be seen by the series expansion of the matrix exponential, and thus $\exp(H + H_0)x = \exp(H)x$.

The special orthogonal group For the special orthogonal group $SO(n)$, we have the retraction

$$R_x^{SO(n)}(\xi) = \exp(\xi)x, \quad \text{with } \xi = -\xi^T. \tag{3.7}$$

where $\exp(\cdot)$ is the matrix exponential map.
The next two retractions over the space of oriented tetrahedra and volume preserving tetrahedra as defined in (2.8) and (2.10), can be used for structure preservation in the discretized versions of problems in nonlinear mechanics. In finite elasticity, for instance, one seeks to avoid self penetration, therefore, we must preserve the orientation of the tetrahedra that are part of the discretization, thus we pick $\mathcal{T}_{pos}$ as the space to work in. On the other hand, if one seeks to preserve the volume, as in the case of Hydrodynamics of incompressible fluids, the space $\mathcal{T}_\rho$ becomes a potential candidate to use in the discretized version. We construct retractions over the spaces $\mathcal{T}_{pos}$ and $\mathcal{T}_\rho$ that can be used for structure preservation algorithms.

The Space of Orientation Preserving Tetrahedra Let be $x \in \mathcal{T}_{pos}$ as defined in (2.8), where

$$x = \begin{bmatrix} | & | & | & | \\ v_1 & v_2 & v_3 & v_4 \\ | & | & | & | \\ 1 & 1 & 1 & 1 \end{bmatrix} \tag{3.8}$$

and the v_i, $i = 1, 2, 3, 4$, are the vertices of the tetrahedra $\tilde{\mathrm{T}}$. Then, the map

$$R_x^{\mathcal{T}_{pos}}(\xi) = \exp(\xi x^{-1})x \tag{3.9}$$

is a retraction for $\mathcal{T}_{pos}$, where $\xi \in \mathfrak{t}_{pos}$, i.e., ξ has the form

$$\xi = \begin{bmatrix} \xi_{11} & \xi_{12} & \xi_{13} & \xi_{14} \\ \xi_{21} & \xi_{22} & \xi_{23} & \xi_{24} \\ \xi_{31} & \xi_{32} & \xi_{33} & \xi_{34} \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{3.10}$$

and $\exp(\cdot)$ is the matrix exponential map. In fact, by the structure of ξ which has zeros in the last row, we observe that ξx^{-1} is such that the last row is also filled with zeros, as well as the matrix $(\xi x^{-1})^n$, for every $n \in \mathbb{N}$. Indeed, the matrix $\exp(\xi x^{-1})$ has the form:

$$\begin{aligned} e := \exp(\xi x^{-1}) &= Id_{4\times 4} + \sum_{k=1}^{\infty} \frac{(\xi x^{-1})^k}{k!} \\ &= \begin{bmatrix} e_{11} & e_{12} & e_{13} & e_{14} \\ e_{21} & e_{22} & e_{23} & e_{24} \\ e_{31} & e_{32} & e_{33} & e_{34} \\ 0 & 0 & 0 & 1 \end{bmatrix} \end{aligned}$$

and the matrix $\exp(\xi x^{-1})x$ is given by:

$$\begin{aligned} y := \exp(\xi x^{-1})x &= \begin{bmatrix} e_{11} & e_{12} & e_{13} & e_{14} \\ e_{21} & e_{22} & e_{23} & e_{24} \\ e_{31} & e_{32} & e_{33} & e_{34} \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_{11} & x_{12} & x_{13} & x_{14} \\ x_{21} & x_{22} & x_{23} & x_{24} \\ x_{31} & x_{32} & x_{33} & x_{34} \\ 1 & 1 & 1 & 1 \end{bmatrix} \\ &= \begin{bmatrix} y_{11} & y_{12} & y_{13} & y_{14} \\ y_{21} & y_{22} & y_{23} & y_{24} \\ y_{31} & y_{32} & y_{33} & y_{34} \\ 1 & 1 & 1 & 1 \end{bmatrix}. \end{aligned}$$

Therefore, the last row of the matrix $\exp(\xi x^{-1})x$ is filled with ones. Additionally, we observe that the orientation of the tetrahedra is preserved

$$\det(R_x^{\mathcal{T}_{pos}}(\xi)) = \det(\exp(\xi x^{-1}))\det(x) > 0$$

given that $\det(\exp(\xi x^{-1})) > 0$, therefore $R_x^{\mathcal{T}_{pos}}(\xi) \in \mathcal{T}_{pos}$. Observe that

$$\begin{aligned} DR_x^{\mathcal{T}_{pos}}(\xi) &= \exp(\xi x^{-1})x^{-1}x \\ &= \exp(\xi x^{-1}) \end{aligned}$$

which, evaluating at $\xi = 0$, yields:

$$DR_x^{\mathcal{T}_{pos}}(0) = id.$$

Finally, the new updated tetrahedra T_+ has vertices

$$v_1^+ = \begin{bmatrix} y_{11} \\ y_{21} \\ y_{31} \end{bmatrix}, \quad v_2^+ = \begin{bmatrix} y_{12} \\ y_{22} \\ y_{32} \end{bmatrix}, \quad v_3^+ = \begin{bmatrix} y_{13} \\ y_{23} \\ y_{33} \end{bmatrix}, \quad v_4^+ = \begin{bmatrix} y_{14} \\ y_{24} \\ y_{34} \end{bmatrix}. \tag{3.11}$$

The Space of Volume Preserving Tetrahedra Let us consider the space of volume preserving tetrahedra as defined in (2.10). We construct a retraction for this space. Let be given $x \in \mathcal{T}_\rho$, where:

$$x = \begin{bmatrix} | & | & | & | \\ v_1 & v_2 & v_3 & v_4 \\ | & | & | & | \\ 1 & 1 & 1 & 1 \end{bmatrix} \tag{3.12}$$

and the $v_i \in \mathbb{R}^3$, $i = 1, 2, 3, 4$, are the vertices of the tetrahedra $\tilde{\mathrm{T}}$, with $\mathrm{vol}(\tilde{\mathrm{T}}) = \rho$. Let us consider a perturbation $\xi \in \mathfrak{t}_{pos}$, from (2.9), we have that ξ has the form

$$\xi = \begin{bmatrix} \xi_{11} & \xi_{12} & \xi_{13} & \xi_{14} \\ \xi_{21} & \xi_{22} & \xi_{23} & \xi_{24} \\ \xi_{31} & \xi_{32} & \xi_{33} & \xi_{34} \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{3.13}$$

And let be $\mathrm{Adj}(x)$, the adjugate matrix of x:

$$\mathrm{Adj}(x) = \begin{bmatrix} m_{11} & m_{12} & m_{13} & m_{14} \\ m_{21} & m_{22} & m_{23} & m_{24} \\ m_{31} & m_{32} & m_{33} & m_{34} \\ m_{41} & m_{42} & m_{43} & m_{44} \end{bmatrix} \tag{3.14}$$

whose entries are specified in $(A.37)$. We consider the vectors $N, \tilde{\xi} \in \mathbb{R}^{12}$ given by:

$$N = \begin{bmatrix} m_{11} \\ m_{21} \\ m_{31} \\ m_{41} \\ m_{12} \\ m_{22} \\ m_{32} \\ m_{42} \\ m_{13} \\ m_{23} \\ m_{33} \\ m_{43} \end{bmatrix}, \qquad \tilde{\xi} = \begin{bmatrix} \xi_{11} \\ \xi_{12} \\ \xi_{13} \\ \xi_{14} \\ \xi_{21} \\ \xi_{22} \\ \xi_{23} \\ \xi_{24} \\ \xi_{31} \\ \xi_{32} \\ \xi_{33} \\ \xi_{34} \end{bmatrix}. \tag{3.15}$$

Note that N is formed by stacking the three first columns of $\mathrm{Adj}(x)$ on top of one another and $\tilde{\xi}$ is formed by stacking the first three rows of ξ on top of each other. Due to the invertibility of x we get that $\|N\| \neq 0$. We consider $n = \frac{1}{\|N\|}N$, and the projection matrix:

$$P = \left(I - nn^T\right). \tag{3.16}$$

We apply the projection to the vector $\tilde{\xi}$, obtaining

$$P\tilde{\xi} = q_\xi = \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \\ q_5 \\ q_6 \\ q_7 \\ q_8 \\ q_9 \\ q_{10} \\ q_{11} \\ q_{12} \end{bmatrix} \tag{3.17}$$

and re-arrange q_ξ as the matrix:

$$Q_\xi = \begin{bmatrix} q_1 & q_2 & q_3 & q_4 \\ q_5 & q_6 & q_7 & q_8 \\ q_9 & q_{10} & q_{11} & q_{12} \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{3.18}$$

With this, we define the retraction for the space of volume preserving tetrahedra as

$$R_x^{\mathcal{T}_\rho}(\xi) = \exp(Q_\xi x^{-1})x. \tag{3.19}$$

We observe that for any given $\xi \in \mathfrak{t}_{pos}$, thanks to the previous construction, we get that $Q_\xi \in \mathfrak{t}_{x,\rho}$, the tangent space to $\mathcal{T}_\rho$ at x, as given in (2.14). The matrix Q_ξ satisfies:

$$\operatorname{tr}(Q_\xi \ \mathrm{Adj}(x)) = 0. \tag{3.20}$$

Indeed, note that $\operatorname{tr}(Q_\xi \ \mathrm{Adj}(x)) = \langle q_\xi, N\rangle$, with $\langle\cdot,\cdot\rangle$ the usual euclidean product in $\mathbb{R}^{12}$, then we have that:

$$\begin{aligned} \operatorname{tr}(Q_\xi \ \mathrm{Adj}(x)) &= \langle q_\xi, N\rangle \\ &= \|N\| \langle q_\xi, n\rangle \\ &= \|N\| \left\langle (I - nn^T)\tilde{\xi}, n \right\rangle \\ &= 0. \end{aligned}$$

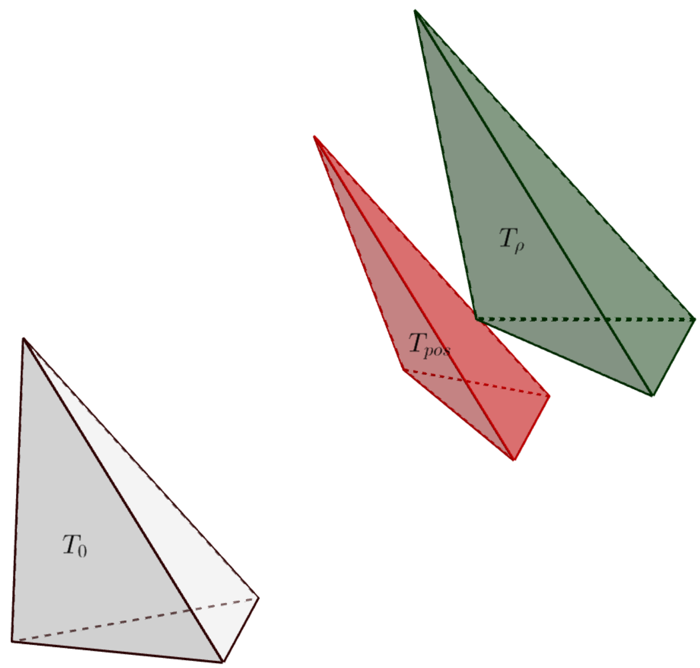


Figure 3.2: *Different updates of the Tetrahedra T_0 using the same perturbation ξ: $T_{pos} = R^{\mathcal{T}_{pos}}(\xi)$ preserves orientation, and $T_\rho = R^{\mathcal{T}_\rho}(\xi)$ preserves the volume.*

The tetrahedra $\tilde{\mathrm{T}}_+$ obtained by the update $R_x^{\mathcal{T}_\rho}(\xi)$, is such that:

$$\begin{aligned}
\mathrm{vol}(\tilde{\mathrm{T}}_+) &= \frac{1}{6}\det(\exp(Q_\xi x^{-1})x) \\
&= \frac{1}{6}\det(\exp(Q_\xi x^{-1}))\det(x) \\
&= \frac{1}{6}\exp(\mathrm{tr}(Q_\xi x^{-1}))\det(x) \\
&= \frac{1}{6}\exp\left(\frac{1}{\det(x)}\mathrm{tr}(Q_\xi\,\mathrm{Adj}(x))\right)\det(x) \\
&= \frac{1}{6}\exp(0)\det(x) \\
&= \frac{1}{6}\det(x) \\
&= \mathrm{vol}(\tilde{\mathrm{T}}) \\
&= \rho
\end{aligned}$$

where the identity $\det(\exp(Q_\xi x^{-1})) = \exp(\mathrm{tr}(Q_\xi x^{-1}))$ has been used (see e.g., A.4.6). Therefore, the volume has been preserved. As we know, the update $R_x^{\mathcal{T}_\rho}(\xi)$ has the form:

$$R_x^{\mathcal{T}_\rho}(\xi) = \begin{bmatrix} | & | & | & | \\ v_1^+ & v_2^+ & v_3^+ & v_4^+ \\ | & | & | & | \\ 1 & 1 & 1 & 1 \end{bmatrix} \tag{3.21}$$

and the vertices of the updated tetrahedra $\tilde{\mathrm{T}}_+$ are the v_i^+, for $i = 1, 2, 3, 4$.

The group of diffeomorphisms of a manifold Let $\mathrm{Diff}(M)$ be the group of diffeomorphisms of the manifold M as defined in (2.15). Then, for $\varphi \in \mathrm{Diff}(M)$ and $\xi \in T_\varphi \mathrm{Diff}(M)$ we have that

$$R_\varphi^{\mathrm{Diff}(M)}(\xi) = \varphi + \varepsilon\xi,$$

is a retraction, for a given sufficiently small $\varepsilon > 0$.
More generally, it would be sufficient and appropriate to define a retraction only on a neighborhood $U \subset T_xM$ of 0_x and not on all of T_xM. However, this would add additional technicalities to our study. For practical implementation in an optimization algorithm, retractions should have a sufficiently large domain of definition, so that $R_x^M(\delta x)$ is defined for reasonable trial corrections δx. If necessary, $\delta x \in U$ can be enforced by additional scaling.

Retractions: Basic Properties

Let be $R_x^M : T_xM \to M$ a retraction as in definition 3.2.1, in particular, by the inverse mapping theorem, R_x^M is locally continuously invertible and:

$$D(R_x^M)^{-1}(x) = (DR_x^M(0_x))^{-1} = id_{T_xM}.$$

As we will see, the construction of an SQP method involves a pair of retractions. One of them (e.g., the exponential map) is used to establish a quadratic model of the problem on the tangent space. The other retraction is used to compute the update $x_+ = R_x^M(\delta x)$. These two retractions can be *consistent* of first or second order. This frees us from the requirement to establish a Riemannian metric or compute covariant derivatives.

Definition 3.2.2. *On a smooth manifold M, consider a pair of C^k-retractions at $x \in M$*

$$R_{x,i}^M : T_xM \to M \qquad i = 1, 2$$

and their local transformation mapping:

$$\Phi_M := (R_{x,1}^M)^{-1} \circ R_{x,2}^M : T_xM \to T_xM. \tag{3.22}$$

The pair $(R_{x,1}^M, R_{x,2}^M)$ of C^k-retractions is called first order consistent, if $k \geq 1$ and $\Phi_M'(0_x) = id_{T_xM}$ and second order consistent, if in addition $k \geq 2$ and $\Phi_M''(0_x) = 0$.

Lemma 3.2.1. *Let be retractions* $(R^M_{x,1}, R^M_{x,2})$ *and* Φ_M *the local transformation mapping as before. Then, if the pair* $(R^M_{x,1}, R^M_{x,2})$ *is a* C^1 *pair of first order consistent retractions, we get:*

$$\Phi_M(0_x) = 0_x \qquad \Phi'_M(0_x) = id_{T_xM},$$

and for C^2*-retractions we have in addition:*

$$(\Phi_M^{-1})''(0_x) = -\Phi''_M(0_x).$$

Proof. The first result for first order consistent C^1-retractions follows from chain rule. For the second case, we get that

$$(\Phi_M^{-1})''(0_x) = [(\Phi'_M)^{-1}]'(0_x)$$

and using the formula for the derivative of the inverse of a map

$$[(\Phi'_M)^{-1}]'(0_x) = -(\Phi'_M)^{-1}(0_x)\Phi''_M(0_x)(\Phi'_M)^{-1}(0_x)$$

and by first order consistency, $(\Phi'_M(0_x))^{-1} = id_{T_xM}$, we get

$$-(\Phi'_M)^{-1}(0_x)\Phi''_M(0_x)(\Phi'_M)^{-1}(0_x) = -\Phi''_M(0_x).$$

therefore

$$(\Phi_M^{-1})''(0_x) = -\Phi''_M(0_x).$$

□

As a special case, a retraction R^M_x is of first (second) order in the sense of Definition 3.2.1, if it is consistent of first (second) order with $\exp_x$. To prove this, we start with a formula.

Lemma 3.2.2. *Let be* $(R^M_{x,1}, R^M_{x,2})$ *a pair of retractions that are first order consistent, then for the transformation map* $\Phi_M := (R^M_{x,1})^{-1} \circ R^M_{x,2}$ *we have that:*

$$\nabla^{TM}_{\delta^2\xi_1} DR^M_{x,2}(0)\delta\xi - \nabla^{TM}_{\delta^2\xi_1} DR^M_{x,1}(0)\delta\xi = \Phi''_M(0)(\delta^2\xi_1, \delta\xi) \tag{3.23}$$

for all $\xi, \delta\xi, \delta^2\xi_1 \in TM$.

Proof. We first define the maps:

$$F_2(\xi, \delta\xi) = (R^M_{x,2}(\xi), DR^M_{x,2}(\xi)\delta\xi)$$
$$F_1(\xi, \delta\xi) = (R_{x,1}(\Phi_M(\xi)), DR^M_{x,1}(\Phi_M(\xi))\Phi'_M(\xi)\delta\xi)$$

observing that:

$$F_2(\xi, \delta\xi) = F_1(\xi, \delta\xi). \tag{3.24}$$

The maps DR^M_1 and DR^M_2 are regarded as lifts of R^M_1 and R^M_2 to the tangent bundle, meaning that the maps F_1 and F_2 represent sections of the tangent bundle as in (2.70). Therefore, applying the map ∇^{TM} defined in (2.72), to both sides of (3.24) in direction $(\delta^2\xi_1, \delta^2\xi_2)$ at $\xi = 0$, we get that:

$$DR^M_{x,2}(0)\delta\xi = DR^M_{x,1}(0)\delta\xi$$
$$\nabla^{TM}_{\delta^2\xi_1} DR^M_{x,2}(0)\delta\xi + DR^M_{x,2}(0)\delta^2\xi_2 = \nabla^{TM}_{\delta^2\xi_1} DR^M_{x,1}(0)\delta\xi + DR^M_{x,1}(0)\delta^2\xi_2 + DR^M_{x,1}(0)\Phi''_M(0)(\delta^2\xi_1, \delta\xi)$$

where, the first order consistency condition $\Phi'_M(0) = id_{TM}$ has been used. Finally, from the last line of the previous equations, and using $DR^M_1(0) = DR^M_2(0) = id_{TM}$, we obtain:

$$\nabla^{TM}_{\delta^2\xi_1} DR^M_{x,2}(0)\delta\xi = \nabla^{TM}_{\delta^2\xi_1} DR^M_{x,1}(0)\delta\xi + \Phi''_M(0)(\delta^2\xi_1, \delta\xi)$$

obtaining the result. □

From the latter, we get that if a retraction is second order consistent with the exponential map $\exp_x$, in the sense of Definition 3.2.2, then the retraction is of second order.

Proposition 3.2.1. *Let be $R^M_{x,1}$ a retraction that is second order consistent with the exponential $\exp_x$. Then $R^M_{x,1}$ is a second order retraction.*

Proof. If we assume that $R^M_{x,2} = \exp_x$ in formula (3.23), and given that the two retractions are second order consistent, i.e., $\Phi''_M = 0$, we get that $\nabla_\xi DR^M_{x,1} = 0$, therefore, $R^M_{x,1}$ is a second order retraction, from definition 3.2.1. □

The following results also hold:

Lemma 3.2.3.

i) Every pair of first (second) order retractions is first (second) order consistent.

ii) $(R^M_{x,1}, R^M_{x,2})$ is first (second) order consistent iff $(R^M_{x,2}, R^M_{x,1})$ is.

3.2.2 Local Parametrizations

Manifolds are locally described as linear spaces through bijective maps called charts. With the help of these charts, one can also define pullbacks of functions over manifolds to linear vector spaces and many concepts from the linear setting can now be transferred into this approach. For optimization algorithms, where functions have to be represented in the computer, such chart maps can be rather cumbersome to implement. Due to that, the complexity of such representations can be reduced and more manageable formulas can be attained using, for instance, the concept of retractions. In fact, for the actual implementation of retractions on a computer, we need to represent them with respect to a basis of the tangent space. We do this using the concept of local parametrization. Local parametrizations use local representations of the tangent space through a basis to map open sets of $\mathbb{R}^n$ into a local neighborhood on the manifold. We define this concept and show some examples that are oriented to the applications in section 6.

Definition 3.2.3. *Let $R_x^M : T_xM \longrightarrow M$ be a retraction on the n-dimensional manifold M modeled on $\mathbb{E} = \mathbb{R}^n$. In addition, at $x \in M$ let be*

$$\Theta_{T_xM} : \mathbb{E} \to T_xM \tag{3.25}$$

given by:

$$\Theta_{T_xM} = \begin{bmatrix} | & | & | & | \\ \xi_1(x) & \xi_2(x) & \cdots & \xi_n(x) \\ | & | & | & | \end{bmatrix}$$

where the vectors $\{\xi_1(x), \cdots, \xi_n(x)\}$ constitute a basis for the tangent space T_xM. Then, we define the local parametrization $\mu_x^M : \mathbb{E} \to M$ around x as:

$$\mu_x^M(\zeta) = (R_x^M \circ \Theta_{T_xM})(\zeta). \tag{3.26}$$

Proposition 3.2.2. *Let be μ_x^M a local parametrization around $x \in M$ as in the previous definition. Then we have that:*

i) $\mu_x^M(0) = x$.

ii) $D\mu_x^M(0) = \Theta_{T_xM}$.

Proof. This result follows from the properties of retractions and the chain rule, indeed, given that $\Theta_{T_xM}\, 0 = 0_x$ maps the $0 \in \mathbb{R}^n$ into $0_x \in T_xM$, then *i)* follows. For *ii)*, we use the chain rule:

$$\begin{aligned} D\mu_x^M(\zeta)_{|\zeta=0} &= D(R_x \circ \Theta_{T_xM})(\zeta)_{|\zeta=0} \\ &= (DR_x(\Theta_{T_xM}\,\zeta)\,\Theta_{T_xM})_{|\zeta=0} \\ &= DR_x(0_x)\Theta_{T_xM} \\ &= id_{T_xM}\,\Theta_{T_xM} \\ &= \Theta_{T_xM}. \end{aligned}$$

given that $DR_x(0_x) = id_{T_xM}$. □

Here we provide some examples of parametrizations, specially oriented to the applications in section 6.

3.2.3 Examples

The n-sphere Let be $M = \mathbb{S}^n \subset \mathbb{R}^{n+1}$, the n-sphere, considered as a submanifold of $\mathbb{R}^{n+1}$, and let be

$$\Theta_{T_x\mathbb{S}^n} = \begin{bmatrix} | & | & & | \\ \xi_1 & \xi_2 & \ldots & \xi_n \\ | & | & & | \end{bmatrix}$$

the matrix whose columns constitute a basis $\{\xi_1, \xi_2, ..., \xi_n\}$ for the tangent space $T_x\mathbb{S}^n$, then, for $\zeta \in \mathbb{R}^n$:

$$\mu_{x,1}^{\mathbb{S}^n}(\zeta) = \frac{x + \Theta_{T_x\mathbb{S}^n}\,\zeta}{\|x + \Theta_{T_x\mathbb{S}^n}\,\zeta\|} \tag{3.27}$$

is a parametrization around x, where first and second derivatives, using the linear connections, are given by the formulas:

$$D\mu_{x,1}^{\mathbb{S}^n}(0)v_1 = \Theta_{T_x\mathbb{S}^n} v_1 \tag{3.28}$$

$$D^2\mu_{x,1}^{\mathbb{S}^n}(0)(v_2, v_1) = -x\,\langle \Theta_{T_x\mathbb{S}^n} v_2, \Theta_{T_x\mathbb{S}^n} v_1\rangle \tag{3.29}$$

for $v_i \in \mathbb{R}^n$, and $i = 1, 2$.

Matrix exponential Let be $M = \mathbb{S}^2 \subset \mathbb{R}^3$. For any given $x \in \mathbb{S}^2$, we consider the matrix

$$\Theta_{T_x\mathbb{S}^2} = \begin{bmatrix} | & | \\ C_1x & C_2x \\ | & | \end{bmatrix} \tag{3.30}$$

whose columns constitute a basis for the tangent space $T_x\mathbb{S}^2$, where $C_j \in \mathfrak{so}(3)$ are chosen in a way that $C_jx \neq 0$ for $j = 1, 2$. For $\zeta \in \mathbb{R}^2$, such that, $\zeta = [\zeta_1, \zeta_2]^T$, the map:

$$\mu_{x,2}^{\mathbb{S}^2}(\zeta) = \exp\left(\zeta_1 C_1 + \zeta_2 C_2\right) x. \tag{3.31}$$

is a parametrization on the sphere $\mathbb{S}^2$. From the formula above, we can check that:

$$\left\langle \mu_{x,2}^{\mathbb{S}^2}(\zeta), \mu_{x,2}^{\mathbb{S}^2}(\zeta)\right\rangle = 1 \text{ and } \mu_{x,2}^{\mathbb{S}^2}(0) = x.$$

which means that $\mu_{x,2}^{\mathbb{S}^2}(\zeta) \in \mathbb{S}^2$. First and second derivatives are given by the formulas:

$$D\mu_{x,2}^{\mathbb{S}^2}(\zeta)_{|\zeta=0}v = (v_1C_1 + v_2C_2)x \tag{3.32}$$

$$D^2\mu_{x,2}^{\mathbb{S}^2}(\zeta)_{|\zeta=0}(v, w) = (v_1C_1 + v_2C_2)(w_1C_1 + w_2C_2)x. \tag{3.33}$$

where $v = [v_1, v_2]^T \in \mathbb{R}^2$ and $w = [w_1, w_2]^T \in \mathbb{R}^2$.

3.3 Vector Bundle Retractions

For some interesting problems such as optimal control of energy minimizers on manifolds, optimization algorithms are carried out on vector bundles, which are, as we know, manifolds endowed with special structure. In a vector bundle chart, there is a product in terms of a usual manifold chart and a linear topological vector space. Consequently, vector bundle retractions have to be defined acting over this specific structure. Let be $p : E \to M$ a vector bundle, using trivializing maps, the vector bundle E can be written as:

$$\tau(p^{-1}U) = U \times \mathbb{F}$$

for U open in M, and $\mathbb{F}$ the vector bundle fiber. Thus, locally, TE looks like the following product:

$$T(U \times \mathbb{F}) = (U \times \mathbb{F}) \times (\mathbb{E} \times \mathbb{F})$$

where $\mathbb{E}$ is the space where M is modeled. In the following, for $(x_0, e_0) \in U \times \mathbb{F}$, we need to define a vector bundle retraction mapping $R^E_{x_0,e_0} : T_{x_0,e_0}E \to E$. Our construction requires a splitting of TE into a "tangential component" ξ and a "fiber component" η to define it. While ξ can be defined via $Tp : TE \to TM$, there is no natural way to find η, except for the case e_0, which means that e_0 is the zero element of the vector space $E_{p(e_0)}$. To overcome this gap, we need a connection. To be precise, κ_E yields the required η in its last component, as done in (2.66).
We are now ready to define suitable retractions for vector bundles.

Definition 3.3.1. *Let be $p : E \to M$ a vector bundle endowed with a connection κ_E as defined in* (2.65)*. Let be $(x_0, e_0) \in M \times E_{x_0}$, and let be $(\xi, \eta) \in T_{x_0,e_0}E$ defined via the splitting of TE through κ_E. Then a vector bundle retraction $R^E_{x_0,e_0}$ is a mapping of the form:*

$$\begin{aligned} R^E_{x_0,e_0} &: T_{x_0,e_0}E \to E \\ &(\xi, \eta) \to (x, e) = (R^M_{x_0}(\xi), A(R^M_{x_0}(\xi))(e_0 + \eta)) \end{aligned} \tag{3.34}$$

where $e = A(x)(e_0 + \eta) \in E_x$, $A(x) \in L(E_{x_0}, E_x)$ is an isomorphism, and $R^M : TM \to M$ is a retraction on the manifold M. These mappings satisfy the following conditions:

$$R^M_{x_0}(0_{x_0}) = x_0, \tag{3.35}$$

and

$$DR^M(0_{x_0}) = id_{T_{x_0}M}, \quad A(x_0) = id_{E_{x_0}}. \tag{3.36}$$

Additionally, we have that its inverse is given by

$$\begin{aligned} (R^E_{x_0,e_0})^{-1} &: E \to T_{x_0,e_0}E \\ &(x, e) \to (\xi, \eta) = ((R^M_{x_0})^{-1}(x), A(x)^{-1}e - e_0). \end{aligned} \tag{3.37}$$

With the above definition of vector bundle retraction, we operate over the specific structure of this class of manifolds. The first component of $R^E_{x_0,e_0}$ is such that $p(R^E_{x_0,e_0}) = R^M_{x_0}$ is a retraction on the base manifold, and the second component of $R^E_{x_0,e_0}$ is linear mapping in $E_{x_0} \to E_x$ between fibers.

Remark 3.3.1. *Retractions on vector bundles consist of two parts: an ordinary retraction R^M on the base manifold and a vector transport A, which maps vectors from fiber to fiber. If the vector bundle is the particular case of the tangent bundle, i.e., if $E = TM$, and if a Riemannian metric is given on the base manifold, then, we can use the canonical spray as given in Proposition 2.7.2 and the corresponding exponential map* exp*, together with the parallel transport P^t along geodesics as defined in Theorem 2.9.3. With this, we can define a retraction on the tangent bundle, with $R^M_{x_0} = \exp$ and $A = P^t$, where:*

$$\exp_{x_0} : T_{x_0}M \to M \quad \textit{and} \quad P^t : T_{x_0}M \to T_xM.$$

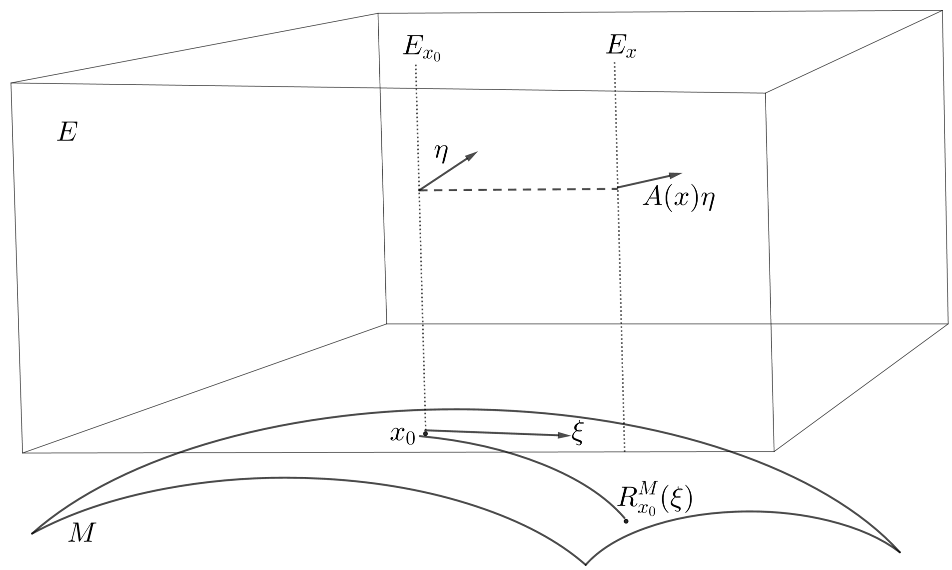


Figure 3.3: *Vector bundle retraction*

A vector bundle retraction $R^E : TE \to E$, induces a retraction $R^{E^*} : TE^* \to E^*$ on the dual bundle $p^* : E^* \to M$ as described in Example 2.3.2. This is done by using the same retraction on the base manifold R^M, and the contragradient isomorphism (i.e., the inverse transposed) determined by $A(x) \in L(E_{x_0}, E_x)$, as we describe in the next example.

Example 3.3.1. *Let be $p : E \to M$ a vector bundle, and let be $R^E_{x_0,e_0} T_{x_0,e_0}E \to E$ a vector bundle retraction as described in definition 3.3.1. For $(x_0, \tilde{e}_0) \in M \times E^*_{x_0}$, the map*

$$\begin{aligned} R^{E^*}_{x_0,\tilde{e}_0} &: T_{x_0,\tilde{e}_0}E^* \to E^* \\ &(\xi, \tilde{\eta}) \to (x, \tilde{e}) = (R^M_{x_0}(\xi), (A(x)^{-1})^*(\tilde{e}_0 + \tilde{\eta})) \end{aligned} \tag{3.38}$$

is a vector bundle retraction for the dual bundle $p^* : E^* \to M$. First of all, with the help of a connection κ_{E^*} on E^*, we can recover $\tilde{\eta} \in E^*_{x_0}$. In addition, observe that, the isomorphism $A(x) \in L(E_{x_0}, E_x)$ induces the map $(A(x)^{-1})^* \in L(E^*_{x_0}, E^*_x)$, obtaining that $(A(x)^{-1})^*(\tilde{e}_0 + \tilde{\eta}) \in E^*_x$. It can be seen that conditions (3.35) *and* (3.36)*, are also satisfied. The corresponding inverse is given by:*

$$\begin{aligned} (R^{E^*}_{x_0,\tilde{e}_0})^{-1} &: E^* \to T_{x_0,\tilde{e}_0}E^* \\ &(x, \tilde{e}) \to (\xi, \tilde{\eta}) = ((R^M_{x_0})^{-1}(x), A(x)^*\tilde{e} - \tilde{e}_0). \end{aligned} \tag{3.39}$$

We discuss the quality of vector bundle retractions, i.e., we define first and second-order retractions for the case of a vector bundle. Due to that vector bundles carry additional structure, the properties that these mappings should have, are, as well, more structured.

3.3.1 Quality of Vector Bundle Retractions

We use the considerations of section 2.8.1, specially for the map $F : Z \to E$ as in (2.70) with $z = (\xi, \eta)$ and

$$F(z) = (F_x(z), F_e(z)) := R^E_{x_0,e_0}(\xi, \eta) = (R^M_{x_0}(\xi), A(R^M_{x_0}(\xi))(e_0 + \eta)).$$

We require different orders of consistency:

- $R^E_{x_0,e_0}(0, 0) = (x_0, e_0)$: basic consistency.
- $\nabla^E R^E_{x_0,e_0}(0, 0) = Id_{T_{x_0}M\times E_{x_0}}$: first order consistency.
- $\nabla^{2,E} R^E_{x_0,e_0}(0, 0)(\delta\xi, \delta\eta) = Id_{(T_{x_0}M\times E_{x_0})^2}\ \forall\, (\delta\xi, \delta\eta) \in T_{x_0}M \times E_{x_0}$: second order consistency.

A comparison with general retractions of manifolds reveals that already for first order consistency we need to use covariant derivatives, and the discussion of second order consistency requires second covariant derivatives. This is a consequence of the fact that we needed a connection map κ_E to split TE and thus, define vector bundle retractions in an invariant way.
The computations performed in section 2.8.1 can be applied directly to obtain (splitting $\zeta = (\delta\xi, \delta\eta)$) and abbreviating $x = R^M_{x_0}(\xi)$:

$$\begin{aligned} T_z F_x \zeta &= DR^M_{x_0}(\xi)\delta\xi \\ \nabla^E_\zeta F_e(z) &= \nabla^E_{\delta\xi} A(x)(e_0 + \eta) + A(x)\delta\eta. \end{aligned}$$

For second derivatives, we split $\delta z = (\delta^2\xi_1, \delta^2\eta_1)$ and $\delta\zeta = (\delta^2\xi_2, \delta^2\eta_2)$

$$\begin{aligned} \nabla^{TM}((T_z F_x)\zeta) &= \nabla^{TM}_{\delta^2\xi_1}(DR^M_{x_0}(\xi)\delta\xi) \\ \nabla^E_{\delta z}(\nabla^E_\zeta F_e(z)) &= \nabla^E_{(\delta^2\xi_1,\delta^2\eta_1)}(\nabla^E_{\delta\xi} A(x)(e_0 + \eta) + A(x)\delta\eta) \\ &= \nabla^E_{\delta^2\xi_1}(\nabla^E_{\delta\xi} A(x)(e_0 + \eta) + A(x)\delta\eta) + \nabla^E_{\delta\xi} A(x)\delta^2\eta_1 \end{aligned}$$

Now, we evaluate these expressions at $(0, 0)$, imposing the requirements of basic consistency:

$$\begin{aligned} R^M_{x_0}(0) &= x_0 \\ A(x_0) &= Id_{E_{x_0}} \end{aligned}$$

obtaining

$$\begin{aligned} (T_0 F_x)\zeta &= DR^M_{x_0}(0) \\ \nabla^E_\zeta F_e(0) &= \nabla^E_{\delta\xi} A(x_0)e_0 + \delta\eta \\ \nabla^{TM}((T_z F_x(0))\zeta) &= \nabla^{TM}_{\delta^2\xi_1}(DR^M_{x_0}(0)\delta\xi) \\ \nabla^E_{\delta z}(\nabla^E_\zeta F_e(z)) &= \nabla^E_{\delta^2\xi_1}\nabla^E_{\delta\xi} A(x_0)e_0 + \nabla^E_{\delta^2\xi_1} A(x_0)\delta\eta + \nabla^E_{\delta\xi} A(x_0)\delta^2\eta_1 \end{aligned} \tag{3.40}$$

Writing down the matrices M_1 and M_2 as they appeared in (2.77), with the expressions above, we obtain:

$$M_1(0, 0) = \begin{bmatrix} DR^M_{x_0}(0) & 0 \\ \nabla^E_{(\cdot)} A(x_0)e_0 & Id_{E_{x_0}} \end{bmatrix} \tag{3.41}$$

$$M_{12}(0,0,\delta\xi,\delta\eta) = \begin{bmatrix} \nabla^{TM}_{(\cdot)}(DR^M_{x_0}(0)\delta\xi) & 0 \\ \nabla^E_{(\cdot)}\nabla^E_{\delta\xi}A(x_0)e_0 + \nabla^E_{(\cdot)}A(x_0)\delta\eta & \nabla^E_{\delta\xi}A(x_0)(\cdot) \end{bmatrix}. \tag{3.42}$$

To obtain a first order vector bundle retraction, we require that $M_1(0,0) = Id$. This holds, if and only if:

$$\begin{aligned} Id_{TM} &= DR^M_{x_0}(0) \\ 0 &= \nabla^E A(x_0)e_0. \end{aligned}$$

Then in (2.78) we obtain:

$$M_2(z,\zeta) = \begin{bmatrix} Id & 0 \\ M_{12}(z,\zeta) & Id \end{bmatrix}.$$

For a second order vector bundle retraction, we would like to achieve $M_2 = Id$, which holds, if and only if $M_{12} = 0$. This yields the additional conditions:

$$\begin{aligned} 0 &= \nabla^E A(x_0)\eta \quad \text{for all } \eta \in E_{x_0} \\ 0 &= \nabla^{TM}(DR^M_{x_0}(0)) \\ 0 &= \nabla^E(\nabla^E A(x_0)e_0). \end{aligned}$$

Consistency of Two retractions

We generalize the consistency conditions given in Lemma 3.2.2 to vector bundle retractions. Consider a transition mapping of the form:

$$\begin{aligned} \Theta_{1\to 2} : T_{x_0,e_0}E &\to T_{x_0,e_0}E \\ (\xi,\eta) &\to (\Phi(\xi), \Psi(R^M_2(\xi))(e_0+\eta) - e_0) \end{aligned} \tag{3.43}$$

where $R^M_2(\xi)$ is the inner retraction of the second retraction. We define:

$$\begin{aligned} \Phi(\xi) &= (R^M_1)^{-1}(R^M_2(\xi)) \\ \Psi(x) &= A_1^{-1}(x)A_2(x) \end{aligned}$$

and obtain indeed:

$$R^E_1(\Theta_{1\to 2}(\xi,\eta)) = (R^M_1(\Phi(\xi)), A_1(R^M_1(\Phi(\xi)))(\Psi(R^M_2(\xi))(e_0+\eta) - e_0)) = R^E_2(\xi,\eta). \tag{3.44}$$

First Order Consistency

We now define consistency conditions for our vector bundle retractions. By applying the tangent map to (3.43), we obtain (using $R^M(\xi) = R^M_2(\xi)$) that:

$$\begin{aligned} T\Theta_{1\to 2} : TT_{x_0,e_0}E &\to TT_{x_0,e_0}E \\ (\xi,\eta,\delta\xi,\delta\eta) &\to (\Phi(\xi), \Psi(x)(e_0+\eta) - e_0, \Phi'(\xi)\delta\xi, \Psi'(x)DR^M(\xi)\delta\xi(e_0+\eta) + \Psi(x)\delta\eta) \end{aligned} \tag{3.45}$$

as first order conditions, we require $T_{0,0}\Theta_{1\to 2} = Id$. This yields apart from the basic conditions $\Phi(0) = 0$ and $\Psi(x_0) = Id$, the first order consistency conditions:

$$\begin{aligned} Id_{TM} &= \Phi'(0) \\ 0 &= \Psi'(x_0)(\cdot)e_0 \end{aligned}$$

Theorem 3.3.1. *A vector bundle retraction is first order consistent to a first order retraction if and only if it is a first order retraction.*

Proof. We consider the formula (3.44), where:

$$R_1^E(\Theta_{1\to 2}(\xi,\eta)) = R_2^E(\xi,\eta)$$

and apply the tangent map to both sides of this equality followed by application of the operator κ_E as described in (2.65) to compute ∇^E. From the chain rule we get that

$$TR_1^E T\Theta_{1\to 2}(\xi,\eta)(\cdot) = TR_2^E(\xi,\eta)(\cdot)$$

and applying the map κ_E to both sides, yields:

$$\nabla^E(R_1^E(\Theta_{1\to 2}(\xi,\eta))) = \nabla^E(R_2^E(\xi,\eta)).$$

We make use of the equalities provided in (3.40) in direction $(\delta\xi,\delta\eta)$, which evaluated at $(\xi,\eta) = (0,0)$, yields:

$$DR_1^M(0)\Phi'(0)\delta\xi = DR_2^M(0)\delta\xi \tag{3.46}$$

$$\nabla^E_{\delta\xi}A_1(x_0)e_0 + A_1(x_0)\Psi'(x_0)(DR_2^M(0)\delta\xi, e_0) + A_1(x_0)\Psi(x_0)\delta\eta = \nabla^E_{\delta\xi}A_2(x_0)e_0 + A_2(x_0)\delta\eta \tag{3.47}$$

from the latter, if the pair is first order consistent, i.e., if $\Phi'(0) = id_{TM}$ and $\Psi'(x_0)(\cdot)e_0 = 0$, we get:

$$\nabla^E_{\delta\xi}A_1(x_0)e_0 = \nabla^E_{\delta\xi}A_2(x_0)e_0. \tag{3.48}$$

Since $\kappa_E \circ T$ is invertible, the converse follows as well. □

In the important case $e_0 = 0$, first order consistency already follows from $id_{TM} = \Phi'(0)$.

Second Order Consistency

We now derive second-order consistency conditions. As for the second derivative of $\Theta_{1\to 2}$, we apply the tangent map to (3.45), obtaining:

$$\begin{aligned} &T^2\Theta_{1\to 2} : T^2T_{x_0,e_0}E \to T^2T_{x_0,e_0}E \\ &(\xi,\eta,\delta\xi,\delta\eta,\delta^2\xi_1,\delta^2\eta_1,\delta^2\xi_2,\delta^2\eta_2) \\ &\to \big(\Phi(\xi), \Psi(x)(e_0+\eta) - e_0, \Phi'(\xi)\delta\xi, \Psi'(x)DR^M(\xi)\delta\xi(e_0+e) + \Psi(x)\delta\eta, \\ &\Phi'(\xi)\delta^2\xi_1, \Psi'(x)(DR^M(\xi)\delta^2\xi_1,(e_0+\eta)) + \Psi(x)\delta^2\eta_1, \Phi''(\xi)(\delta^2\xi_1,\delta\xi) + \Phi'(\xi)\delta^2\xi_2, \\ &\Psi''(x)(DR^M(\xi)\delta\xi, DR^M(\xi)\delta^2\xi_1,(e_0+\eta)) + \Psi'(x)D^2R^M(\xi)(\delta\xi,\delta^2\xi_1)(e_0+\eta) + \\ &\Psi'(x)(DR^M(\xi)\delta\xi,\delta^2\eta_1) + \Psi'(x)(DR^M(\xi)\delta^2\xi_1,\delta\eta) + \Psi'(x)(DR^M\delta^2\xi_2,(e_0+\eta)) + \Psi(x)\delta^2\eta_2\big) \end{aligned} \tag{3.49}$$

Using the conditions for first order consistency, we obtain the simplifications:

$$\begin{aligned}(0,0,\delta\xi,\delta\eta,\delta^2\xi_1,\delta^2\eta_1,\delta^2\xi_2,\delta^2\eta_2) \to (0,0,\delta\xi,\delta\eta,\delta^2\xi_1,\delta^2\eta_1,\Phi''(0)(\delta^2\xi_1,\delta\xi)+\delta^2\xi_2,\\ \Psi''(x_0)(\delta\xi,\delta^2\xi_1,e_0)+\delta^2\eta_2)\end{aligned}$$

where $(\xi,\eta,\delta\xi,\delta\eta,\delta^2\xi_1,\delta^2\eta_1,\delta^2\xi_2,\delta^2\eta_2) \in (U\times\mathbb{F})\times(\mathbb{E}\times\mathbb{F})\times(\mathbb{E}\times\mathbb{F})\times(\mathbb{E}\times\mathbb{F})$. Thus, we obtain the additional conditions for second order consistent retractions:

$$\begin{aligned}0 &= \Psi'(x_0)(\cdot)\delta\eta \text{ for all } \delta\eta \in E_{x_0}\\ 0 &= \Phi''(0)(\cdot,\cdot)\\ 0 &= \Psi''(x_0)(\cdot,\cdot)e_0.\end{aligned}$$

Theorem 3.3.2. *A first order retraction is second order consistent to a second order retraction if and only if it is a second order retraction.*

Proof. We consider again the formula:

$$R_2^E(\xi,\eta) = R_1^E(\Theta_{1\to 2}(\xi,\eta))$$

and apply the map $\nabla^{2,E} = \kappa_{\tilde{E}}\circ T\circ\kappa_E\circ T$ introduced in (2.76) to both sides of the previous equation in direction $(\xi,\eta,\delta\xi,\delta\eta,\delta^2\xi_1,\delta^2\eta_1,\delta^2\xi_2,\delta^2\eta_2)$ at $(\xi,\eta)=(0,0)$. Using the formulas given (3.40) and, in addition to the formula (3.47), we get:

$$\begin{aligned}&\nabla^{TM}_{\delta^2\xi_1}DR_2^M(0)\delta\xi + DR_2^M(0)\delta^2\xi_2 = \nabla^{TM}_{\delta^2\xi_1}DR_1^M(0)\delta\xi + DR_1^M(0)\Phi''(0)(\delta^2\xi_1,\delta\xi) + DR_1^M(0)\delta^2\xi_2\\ &\nabla^E_{\delta^2\xi_1}(\nabla^E_{\delta\xi}A_2(x_0)e_0 + A_2(x_0)\delta\eta) + \nabla_{\delta\xi}A_2(x_0)\delta^2\eta_1 = \nabla^E_{\delta^2\xi_1}(\nabla^E_{\delta\xi}A_1(x_0)e_0 + A_1(x_0)\delta\eta)\\ &\qquad\qquad + \nabla_{\delta\xi}A_1(x_0)\delta^2\eta_1 + C(\Phi''(0),\Psi'(x_0),\Psi''(x_0)).\end{aligned}$$

Where the basic conditions $DR_1^M(0) = DR_2^M(0) = id_{TM}$, $A_1(x_0)=A_2(x_0)=id_{E_{x_0}}$ and the first order consistency condition for the base manifold $\Phi'(0)=id_{TM}$ have been used. We observe that the term $C(\Phi''(0),\Psi'(x_0),\Psi''(x_0))$, which is given by:

$$\begin{aligned}C(\Phi''(0),\Psi'(x_0),\Psi''(x_0)) =& DA_1(x_0)\Phi''(0)(\delta^2\xi_1,\delta\xi)e_0 + DA_1(x_0)\delta\xi\Psi'(x_0)(\delta^2\xi_1,e_0)\\ &+ DA_1(x_0)\delta^2\xi_1\Psi'(x_0)(\delta\xi,e_0) + \Psi''(x_0)(\delta^2\xi_1,\delta\xi,e_0)\\ &+ \Psi'(x_0)D^2R^M(0)(\delta^2\xi_1,\delta\xi)e_0 + \Psi'(x_0)(\delta^2\xi_1,\delta\eta)\\ &- B_E(e_0,\Phi''(0)(\delta^2\xi_1,\delta\xi)) + \Psi'(x_0)(\delta\xi,\delta^2\eta_1) + \Psi'(x_0)(\delta^2\xi_2,e_0)\\ &- B_E(\Psi'(x_0)(\delta\xi,e_0),\delta^2\xi_1) - B_E(\Psi'(x_0)(\delta^2\xi_1,e_0),\delta\xi)\end{aligned}$$

vanishes when the conditions $\Phi''(0)=0$, $\Psi'(x_0)=0$ and $\Psi''(x_0)=0$ are satisfied. Therefore, if the pair (R_1^E,R_2^E) is second order consistent, we get:

$$\begin{aligned}\nabla^{TM}_{\delta^2\xi_1}DR_2^M(0)\delta\xi =& \nabla^{TM}_{\delta^2\xi_1}DR_1^M(0)\delta\xi\\ \nabla^E_{\delta\xi}A_2(x_0)e_0 =& \nabla^E_{\delta\xi}A_1(x_0)e_0\\ \nabla^E_{\delta^2\xi_1}(\nabla^E_{\delta\xi}A_2(x_0)e_0 + A_2(x_0)\delta\eta) + \nabla_{\delta\xi}A_2(x_0)\delta^2\eta_1 =& \nabla^E_{\delta^2\xi_1}(\nabla^E_{\delta\xi}A_1(x_0)e_0 + A_1(x_0)\delta\eta) + \nabla_{\delta\xi}A_1(x_0)\delta^2\eta_1.\end{aligned}$$

On the other hand, since $\kappa_{\tilde{E}}\circ T\circ\kappa_E\circ T$ is invertible, the converse follows as well. □

3.3.2 Retractions for the Tangent and the Co-Tangent Bundle

For our applications, we will be particularly interested in the cases where the vector bundles are the tangent and the co-tangent bundle over the manifold. In this section, we construct vector bundle retractions for these special cases. We begin with the construction of a vector transport on the tangent bundle using a retraction on the base space as proposed in [AMS09]. Then, with the knowledge of transports on the tangent bundle, we proceed with the construction of retractions for the co-tangent bundle. Different alternatives are shown, and we make use of the adjoint operator or the Riesz isomorphism as ways to map into the dual space of the tangent bundle.

Tangent Bundle Retraction Let us consider the case where the vector bundle $p : E \to M$ is the tangent bundle, i.e., $E = TM$ endowed with a connection κ_{TM} as in (2.32). Let be $R^M : TM \to M$, a retraction for the base manifold M, then we define the retraction on the tangent bundle

$$R^{TM}_{x_0,e_0} : T_{x_0,e_0}(TM) \to TM \tag{3.50}$$

given by the map:

$$\begin{aligned} R^{TM}_{x_0,e_0}(\xi,\eta) &= \left(R^M_{x_0}(\xi), \frac{d}{dt} R^M_{x_0}(\xi + t(e_0+\eta))\Big|_{t=0} \right) &(3.51)\\ &= \left(R^M_{x_0}(\xi), DR^M_{x_0}(\xi)(e_0+\eta) \right) &(3.52)\\ &= (x,e). &(3.53) \end{aligned}$$

The second component of the above retraction mapping corresponds to the vector transport of $(e_0 + \eta)$ along ξ, induced by the retraction R^M on the base manifold. This transport is given by the map:

$$\mathcal{T}_\xi(e_0+\eta) : TM \oplus TM \longrightarrow TM$$

defined by:

$$\begin{aligned} \mathcal{T}_\xi(e_0+\eta) :&= DR^M_{x_0}(\xi)(e_0+\eta) \\ &= \frac{d}{dt} R^M_{x_0}(\xi + t(e_0+\eta))\Big|_{t=0}. \end{aligned}$$

From $DR^M_{x_0} = id_{TM}$, we get that $\mathcal{T}_{0_{x_0}}(e_0+\eta) = (e_0+\eta)$, and $\mathcal{T}_\xi(e_0+\eta) \in T_{R^M_{x_0}(\xi)}M$. Therefore, the isomorphism $A(x) \in L(T_{x_0}M, T_xM)$ is given by

$$A(x) = DR^M_{x_0}(\xi). \tag{3.54}$$

In addition, using the considerations from section 3.3.1, we have that this retraction is of first order if:

$$\begin{aligned} Id_{T_{x_0}M} =& DR^M_{x_0}(0) &(3.55)\\ 0 =& \nabla^{TM} DR^M_{x_0}(0)e_0 &(3.56) \end{aligned}$$

and the retraction is of second order, if additionally, we have that:

$$\begin{aligned} 0 =& \nabla^{TM} DR^M_{x_0}(0)\eta \qquad \text{for all} \quad \eta \in T_{x_0}M &(3.57)\\ 0 =& \nabla^{TM}(\nabla^{TM} DR^M_{x_0}(0)e_0). &(3.58) \end{aligned}$$

Co-Tangent Bundle Retractions We turn our attention to the co-tangent bundle, and we construct transport operators on this space, for this, we follow the idea for the construction of retractions on the dual bundle, as in example 3.3.1. As we know, the co-tangent space is the dual of the tangent space, therefore, we construct transport operators through the adjoint operator and the Riesz isomorphism. In the following, we assume that $R^M_{x_0} : T_{x_0}M \to M$ is a retraction on M, and that we have in hand a connection κ_{TM^*} for the co-tangent bundle.

Retraction Induced by the Adjoint.

Let be $A \in L(T_{x_0}M, T_xM)$ a transport map on the tangent bundle:

$$A(x) : T_{x_0}M \longrightarrow T_xM. \tag{3.59}$$

From the latter, we construct a transport

$$((A^{-1})^* \in L((T_{x_0}M)^*), (T_xM)^*).$$

We use the adjoint of the inverse of the primal vector transport, indeed we note that:

$$A(x)^{-1} : T_xM \longrightarrow T_{x_0}M$$

therefore its adjoint maps

$$(A(x)^{-1})^* : (T_{x_0}M)^* \longrightarrow (T_xM)^*$$

and this map has the property that, for given $\hat{\eta} \in (T_{x_0}M)^*$ and $\hat{\vartheta} \in T_xM$ then:

$$((A(x)^{-1})^*\hat{\eta})\hat{\vartheta} = \hat{\eta}(A(x)^{-1}\hat{\vartheta}).$$

The latter, induces the vector bundle retraction

$$R^{TM^*}_{x_0,\tilde{e}_0} : T_{x_0,\tilde{e}_0}(TM^*) \to TM^* \tag{3.60}$$

given by:

$$R^{TM^*}_{x_0,\tilde{e}_0}(\hat{\xi}, \hat{\eta}) = (R^M_{x_0}(\hat{\xi}), (A(x)^{-1})^*(\tilde{e}_0 + \hat{\eta})). \tag{3.61}$$

where

$$R^M_{x_0} : T_{x_0}M \to M \qquad \text{and} \qquad (A(x)^{-1})^* : (T_{x_0}M)^* \to (T_xM)^* \tag{3.62}$$

with $x = R^M_{x_0}(\hat{\xi})$, $\hat{\xi} \in T_{x_0}M$ and $\hat{\eta} \in (T_{x_0}M)^*$. Observe that we may choose $A(x) = DR^M_{x_0}(\hat{\xi})$ as in the previous section. The inverse of the previous retraction is needed for optimal control applications. This map, which was defined in (3.37), for this particular case:

$$(R^{TM^*}_{x_0,\tilde{e}_0})^{-1} : TM^* \to T_{x_0,\tilde{e}_0}(TM^*) \tag{3.63}$$

is given by:

$$(R^{TM^*}_{x_0,\tilde{e}_0})^{-1}(x, \tilde{e}) = \left((R^M_{x_0})^{-1}(x), A(x)^*\tilde{e} - \tilde{e}_0\right). \tag{3.64}$$

Retraction Through the Riesz Isomorphism.

We continue assuming that we are given a vector transport $A(x) \in L(T_{x_0}M, T_xM)$, a retraction $R^M : TM \to M$ on the base manifold, and a connector map κ_{TM^*} for the space TM^*. We construct a vector transport mapping from $(T_{x_0}M)^*$ to $(T_xM)^*$ using the Riesz Isomorphism. Here, we assume that the base manifold M is Riemannian with metric $\mathbf{M}_x$. At any $x \in M$, we have the isomorphism:

$$\mathbf{M}_x : T_xM \longrightarrow (T_xM)^*.$$

Based on this, for $x_0, x \in M$ and $\hat{\xi} \in T_{x_0}M$, with $x = R^M_{x_0}(\hat{\xi})$, we introduce the transport:

$$\mathbf{M}_x A(x) \mathbf{M}_{x_0}^{-1} : (T_{x_0}M)^* \longrightarrow (T_xM)^*.$$

We see that $\mathbf{M}_x A(x) \mathbf{M}_{x_0}^{-1} \in L((T_{x_0}M)^*, (T_xM)^*)$ induces the vector bundle retraction on the cotangent bundle

$$R^{TM^*}_{x_0,e_0} : T_{x_0,e_0}(TM^*) \to TM^*$$

which is given by:

$$R^{TM^*}_{x_0,e_0}(\hat{\xi}, \hat{\eta}) = (R^M_{x_0}(\hat{\xi}), \mathbf{M}_x A(x) \mathbf{M}_{x_0}^{-1}(e_0 + \hat{\eta})) \tag{3.65}$$

where

$$R^M_{x_0} : T_{x_0}M \to M \qquad \text{and} \qquad \mathbf{M}_x A(x) \mathbf{M}_{x_0}^{-1} : (T_{x_0}M)^* \longrightarrow (T_xM)^*$$

for $\hat{\eta} \in (T_{x_0}M)^*$ and $x = R^M_{x_0}(\hat{\xi})$. We may also choose $A(x) = DR^M_{x_0}(\hat{\xi})$ as in (3.54).

3.3.3 Retraction for the Tangent Bundle $T\mathbb{S}^2$

For our specific applications, the special case of the bundle $T\mathbb{S}^2$ is considered, and we write explicit formulas for this retraction. In the following, we consider the 2-sphere $\mathbb{S}^2$, as a Riemannian submanifold of $\mathbb{R}^3$. Thus, we follow the considerations made in Theorem 2.7.3 and the Example 2.7.1, where the connection $\kappa_{T\mathbb{S}^2}$ is given in terms of the second fundamental form h_{12}. In the following, we first write formulas for the map h_{12} as defined in (2.39), when $P_{T_x\mathbb{S}^2} = (I - xx^T)$ and $x = R^{\mathbb{S}^2}_{x_0}(\xi)$, for a given retraction $R^{\mathbb{S}^2} : T\mathbb{S}^2 \to \mathbb{S}^2$.

Proposition 3.3.1. *Let be $\mathbb{S}^2$ the 2-sphere regarded as a submanifold of the space $\mathbb{R}^3$ endowed with the usual euclidean product. In addition, for $x_0 \in \mathbb{S}^2$ and $\xi \in T_{x_0}\mathbb{S}^2$, let be*

$$\begin{aligned} R^{\mathbb{S}^2}_{x_0} &: T_{x_0}\mathbb{S}^2 \to \mathbb{S}^2 \\ &\quad \xi \to x = R^{\mathbb{S}^2}_{x_0}(\xi) \end{aligned}$$

a retraction for $\mathbb{S}^2$. For each $x \in \mathbb{S}^2$ as defined above, consider the projection map

$$\begin{aligned} P_{T_x\mathbb{S}^2} &: \mathbb{R}^3 \to T_x\mathbb{S}^2 \\ &\quad \eta \to (I - xx^T)\eta. \end{aligned}$$

Then, at x_0, for $\delta\xi, \delta\eta \in T_{x_0}\mathbb{S}^2$, we have that:

$$h_{12}(\delta\xi, \delta\eta) = -x_0 \langle \delta\xi, \delta\eta \rangle. \tag{3.66}$$

Proof. We use the characterization of the second fundamental form h_{12} given in formula (2.46). For given $\delta\xi \in T_{x_0}\mathbb{S}^2$, by differentiating the expression:

$$P_{T_x\mathbb{S}^2}\delta\xi = (I - xx^T)\delta\xi \tag{3.67}$$

$$= (I - (R_{x_0}^{\mathbb{S}^2}(\xi))(R_{x_0}^{\mathbb{S}^2}(\xi))^T)\delta\xi \tag{3.68}$$

in direction $\delta\eta \in T_{x_0}\mathbb{S}^2$, we get:

$$P'_{T_x\mathbb{S}^2}(\delta\eta, \delta\xi) = -DR_{x_0}^{\mathbb{S}^2}(\xi)\delta\eta(R_{x_0}^{\mathbb{S}^2}(\xi))^T)\delta\xi - (R_{x_0}^{\mathbb{S}^2}(\xi))(DR_{x_0}^{\mathbb{S}^2}(\xi))^T)\delta\eta\delta\xi \tag{3.69}$$

we use that at $\xi = 0$, we get $R_{x_0}^{\mathbb{S}^2}(0) = x_0$ and $DR_{x_0}^{\mathbb{S}^2}(0) = id_{T_{x_0}\mathbb{S}^2}$. Then the formula for (3.66) follows from the fact that $\delta\xi \in T_{x_0}\mathbb{S}^2$, i.e., $\delta\xi \perp x_0$. $\square$

We now provide a tangent bundle retraction for $T\mathbb{S}^2$, namely:

$$\begin{aligned} R_{x_0,e_0}^{T\mathbb{S}^2} &: T_{x_0,e_0}T\mathbb{S}^2 \to T\mathbb{S}^2 \\ &(\xi, \eta) \to (x, e) = (R_{x_0}^{\mathbb{S}^2}(\xi), (A \circ R_{x_0}^{\mathbb{S}^2})(\xi)(e_0 + \eta)). \end{aligned} \tag{3.70}$$

Where $R^{\mathbb{S}^2}$ is a retraction on $\mathbb{S}^2$, and the transport operator $A : \mathbb{R}^3 \to T_x\mathbb{S}^2$, is given by:

$$A(x) = I - xx^T \tag{3.71}$$

with $x = R_{x_0}^{\mathbb{S}^2}(\xi)$. The corresponding inverse is:

$$\begin{aligned} (R_{x_0,e_0}^{T\mathbb{S}^2})^{-1} &: T\mathbb{S}^2 \to T_{x_0,e_0}T\mathbb{S}^2 \\ &(x, e) \to (\xi, \eta) = ((R_{x_0}^{\mathbb{S}^2})^{-1}(x), A(x)^{-1}e - e_0). \end{aligned} \tag{3.72}$$

Observe that $A(x) = P_{T_x\mathbb{S}^2}$ is the projection onto the tangent space $T_x\mathbb{S}^2$, as introduced in (2.40), and the splitting given in (2.48) applies. Indeed, we see that the tangent map $TR_{x_0,e_0}^{T\mathbb{S}^2}$ in direction $(\delta\xi, \delta\eta)$ is given by:

$$\begin{aligned} &TR_{x_0,e_0}^{T\mathbb{S}^2} : T(T_{x_0,e_0}T\mathbb{S}^2) \to T(T\mathbb{S}^2) \\ &(\xi, \eta, \delta\xi, \delta\eta) \to (R^{\mathbb{S}^2}(\xi), (A \circ R^{\mathbb{S}^2})(\xi)(e_0 + \eta), DR^{\mathbb{S}^2}(\xi)\delta\xi, D(A \circ R^{\mathbb{S}^2})(\xi)\delta\xi(e_0 + \eta) + (A \circ R^{\mathbb{S}^2})(\xi)\delta\eta) \end{aligned} \tag{3.73}$$

which evaluated at $(\xi, \eta) = (0, 0)$ takes the form

$$TR_{x_0,e_0}^{T\mathbb{S}^2}(0, 0)(\delta\xi, \delta\eta) = (x_0, e_0, \delta\xi, DA(x_0)(\delta\xi, e_0) + A(x_0)\delta\eta) \tag{3.74}$$

$$= (x_0, e_0, \delta\xi, P'_{T_{x_0}\mathbb{S}^2}(\delta\xi, e_0) + P_{T_{x_0}\mathbb{S}^2}\delta\eta) \tag{3.75}$$

$$= (x_0, e_0, \delta\xi, h_{12}(\delta\xi, e_0) + P_{T_{x_0}\mathbb{S}^2}\delta\eta) \tag{3.76}$$

which coincides with the connector map $\kappa_{T\mathbb{S}^2}$ given in (2.49), yielding a splitting for $T(T\mathbb{S}^2)$. For implementation purposes, we now show explicit computations of first and second derivatives of the transport $A(x) : \mathbb{R}^3 \to T_x\mathbb{S}^2$ as a map defined on a linear space. From

$$A(x)\eta = (I - xx^T)\eta$$

we get:

$$DA(x)(\eta_1,\eta) = -\eta_1 x^T\eta - x\eta_1^T\eta \tag{3.77}$$

$$D^2A(x)(\eta_2,\eta_1,\eta) = -\eta_1\eta_2^T\eta - \eta_2\eta_1^T\eta \tag{3.78}$$

for $\eta,\eta_1,\eta_2 \in \mathbb{R}^3$. As in definition (3.34), the composition with the retraction $R^{\mathbb{S}^2}(\xi)$ yields with $x = R^{\mathbb{S}^2}_{x_0}(\xi)$:

$$D(A\circ R^{\mathbb{S}^2}_{x_0})(\xi) = DA(x)DR^{\mathbb{S}^2}_{x_0}(\xi)$$

$$D^2(A\circ R^{\mathbb{S}^2}_{x_0})(\xi) = D^2A(x)(DR^{\mathbb{S}^2}_{x_0}(\xi), DR^{\mathbb{S}^2}_{x_0}(\xi)) + DA(x)D^2R^{\mathbb{S}^2}_{x_0}(\cdot,\cdot).$$

at $\xi = 0$ we obtain, using that $DR^{\mathbb{S}^2}_{x_0}(0) = Id_{T_{x_0}\mathbb{S}^2}$:

$$D(A\circ R^{\mathbb{S}^2}_{x_0})(0) = DA(x_0)$$

$$D^2(A\circ R^{\mathbb{S}^2}_{x_0})(0) = D^2A(x_0)(\cdot,\cdot) + DA(x_0)D^2R^{\mathbb{S}^2}_{x_0}(0)(\cdot,\cdot).$$

Which implies that:

$$\begin{aligned} D(A\circ R^{\mathbb{S}^2}_{x_0})(0)(\eta_1,\eta) &= -DR^{\mathbb{S}^2}_{x_0}(0)\eta_1 x_0^T\eta - x_0 DR^{\mathbb{S}^2}_{x_0}(0)\eta_1^T\eta \\ &= -\eta_1 x_0^T\eta - x_0\eta_1^T\eta \end{aligned}$$

and for the special case in which $R^{\mathbb{S}^2}_{x_0}(\xi) = \frac{x_0+\xi}{\|x_0+\xi\|}$, where

$$D^2R^{\mathbb{S}^2}_{x_0}(0)(\eta_2,\eta_1) = \langle\eta_2,\eta_1\rangle\, x_0$$

we get that:

$$D^2(A\circ R^{\mathbb{S}^2}_{x_0})(0)(\eta_2,\eta_1,\eta) = -\eta_2\eta_1^T\eta - \eta_1\eta_2^T\eta + 2\eta_2^T\eta_1 x_0 x_0^T\eta.$$

Finally, for $\eta \in T_{x_0}\mathbb{S}^2$, i.e, $\eta \perp x_0$, we get:

$$D(A\circ R^{\mathbb{S}^2}_{x_0})(0)(\eta_1,\eta) = -x_0\eta_1^T\eta \tag{3.79}$$

$$D^2(A\circ R^{\mathbb{S}^2}_{x_0})(0)(\eta_2,\eta_1,\eta) = -(\eta_2\eta_1^T + \eta_1\eta_2^T)\eta. \tag{3.80}$$

Where in (3.79), the term $D(A\circ R^{\mathbb{S}^2}_{x_0})(0)(\eta_1,\eta)$ coincides with $h_{12}(\eta_1,\eta)$, the second fundamental form on $\mathbb{S}^2$ at x_0, just as in (3.66).

Retraction for the co-tangent Bundle $(T\mathbb{S}^2)^*$ In our applications, we consider equality constrained problems where the constraint map is a minimizer of a real function on a submanifold of a linear space. This means that we consider a constrained problem, where the constraint map has as codomain, the co-tangent space of the submanifold. In the numerical experiments for elastic inextensible rods, in the discretized version, the co-domain space of the constraint map is a product of $(T\mathbb{S}^2)^*$. A retraction for this space easily follows from the previous construction and the induced bundle retraction as defined in example 3.3.1 and (3.61). Let be $R^{T\mathbb{S}^2}_{x_0,e_0} : T_{x_0,e_0}T\mathbb{S}^2 \to T\mathbb{S}^2$, a retraction for $T\mathbb{S}^2$, as given in (3.70). Then, for $(x_0, \tilde{e}_0) \in \mathbb{S}^2 \times (T_{x_0}\mathbb{S}^2)^*$, we define the induced retraction on $(T\mathbb{S}^2)^*$ as:

$$\begin{aligned} R^{(T\mathbb{S}^2)^*}_{x_0,\tilde{e}_0} &: T_{x_0,\tilde{e}_0}(T\mathbb{S}^2)^* \to (T\mathbb{S}^2)^* \\ &(\xi, \tilde{\eta}) \to (x, \tilde{e}) = (R^{\mathbb{S}^2}_{x_0}(\xi), (A(x)^{-1})^*(\tilde{e}_0 + \tilde{\eta})). \end{aligned} \tag{3.81}$$

where $A(x)$ is as in (3.71). The corresponding inverse map is then given by:

$$\begin{aligned} (R^{(T\mathbb{S}^2)^*}_{x_0,\tilde{e}_0})^{-1} &: (T\mathbb{S}^2)^* \to T_{x_0,\tilde{e}_0}(T\mathbb{S}^2)^* \\ &(x, \tilde{e}) \to (\xi, \tilde{\eta}) = ((R^{\mathbb{S}^2}_{x_0})^{-1}(x), A(x)^*\tilde{e} - \tilde{e}_0). \end{aligned} \tag{3.82}$$

In the context of constraints defined as differentials of real functions over the manifold $\mathbb{S}^2$ regarded as a submanifold of $\mathbb{R}^3$, and using the connection provided in example 2.7.1, we show the expression of such constraint map and its derivative.

Example 3.3.2. *Let be $\mathbb{S}^2$ the 2-sphere regarded as a Riemannian submanifold of $\mathbb{R}^3$. If we consider*

$$J : \mathbb{S}^2 \to \mathbb{R}$$

a real function on $\mathbb{S}^2$, then we define the map

$$\begin{aligned} c : \mathbb{S}^2 &\to (T_x\mathbb{S}^2)^* \\ x &\to J'(x). \end{aligned}$$

For a given retraction $R^{\mathbb{S}^2}_x : T_x\mathbb{S}^2 \to \mathbb{S}^2$, and the vector transport $A(x) = (I - xx^T)$ as defined in (3.71), *we get that*

$$Tc : T\mathbb{S}^2 \to T(T_x\mathbb{S}^2)^* \tag{3.83}$$

which, locally in charts is given by:

$$\begin{aligned} T_xc : U \times T_x\mathbb{S}^2 &\to U \times (T_x\mathbb{S}^2)^* \times (T_x\mathbb{S}^2) \times (T_x\mathbb{S}^2)^* \\ (x, \xi) &\to (x, J'(x), \xi, (A^*(x)J''(x))\xi + (DA(x)\xi)^*J'(x)). \end{aligned} \tag{3.84}$$

To obtain this, we use the connection given in (2.49) *and the dual pairing*

$$\langle \ , \ \rangle : (T_x\mathbb{S}^2)^* \times (T_x\mathbb{S}^2) \to \mathbb{R}$$

induced by the euclidean structure on $\mathbb{R}^3$. Therefore, for $\eta \in T_x\mathbb{S}^2$, by differentiating the expression

$$\left\langle A(x)^*J'(x), \eta \right\rangle = \left\langle J'(x), A(x)\eta \right\rangle$$

in direction $\xi \in T_x\mathbb{S}^2$, we get:

$$\begin{aligned} \left\langle J'(x), A(x)\eta \right\rangle' \xi &= \left\langle J''(x)\xi, A(x)\eta \right\rangle + \left\langle J'(x), DA(x)(\xi, \eta) \right\rangle \\ &= \left\langle A(x)^*J''(x)\xi + (DA(x)\xi)^*J'(x), \eta \right\rangle. \end{aligned} \tag{3.85}$$

obtaining the last component of (3.84).

3.3.4 Vector Bundle Parametrizations.

Following the observations made in section 3.2.2, where we stated the convenience of working with local parametrizations on manifolds, we extend this concept to the case of vector bundles. We have already shown some examples of retractions on vector bundles, and for our concrete applications in section 6.4, we require the specific expressions of vector bundle parametrizations. These parametrizations use the local representation basis of the tangent space at each point on the base manifold as shown in Definition 3.2.3, as well as the corresponding representation of the basis for the fibers. We use the transport operation on the fibers, but now composed with the parametrizations of the base manifold, in contrast to formula (3.34), where the composition is performed with a retraction. In the following, we assume that the vector bundle $p : E \to M$ is finite dimensional.

Definition 3.3.2. *Let be $p : E \to M$ a vector bundle endowed with a connection κ_E. Let also be $\mu^M : \mathbb{E} \to M$ a parametrization on the base manifold M as in Definition 3.2.3. In addition, for $x, x_0 \in M$, let be $A(x) \in L(E_{x_0}, E_x)$, a transport operator between the fibers E_{x_0} and E_x, which are modeled on $\mathbb{F}$. We consider the linear operators $\Theta_{E_{x_0}}$ and Θ_{E_x}, such that:*

$$\Theta_{E_{x_0}} : \mathbb{F} \to E_{x_0} \quad \textit{and} \quad \Theta_{E_x} : \mathbb{F} \to E_x \tag{3.86}$$

are the matrices containing bases for the linear spaces E_{x_0} and E_x respectively, together with their respective (pseudo)inverses:

$$\Theta^-_{E_{x_0}} : E_{x_0} \to \mathbb{F} \quad \textit{and} \quad \Theta^-_{E_x} : E_x \to \mathbb{F}. \tag{3.87}$$

We define the vector bundle parametrization around (x_0, e_0), as:

$$\mu^E_{x_0,e_0}(\vartheta, \hat{\eta}) = \big((\mu^M_{x_0})(\vartheta), (\Theta^-_{E_x}(A \circ \mu_{x_0})(\vartheta))\Theta_{E_{x_0}}(\hat{e}_0 + \hat{\eta})\big) \tag{3.88}$$

where $\vartheta \in \mathbb{E}$, $(x, \hat{e}) = \mu^E_{x_0,e_0}(\vartheta, \hat{\eta})$ and $\hat{e}_0, \hat{\eta} \in \mathbb{F}$, with $e_0 = \Theta_{E_{x_0}}\hat{e}_0$. Observe that:

$$\mu^M_{x_0} : \mathbb{E} \to M \qquad \textit{and} \qquad (\Theta^-_{E_x}(A \circ \mu_{x_0})(\vartheta))\Theta_{E_{x_0}} : \mathbb{F} \to \mathbb{F}.$$

The inverse, which we need for optimal control applications, is given by:

$$(\mu^E_{x_0,e_0})^{-1}(x, \hat{e}) = \Big((\mu^M_{x_0})^{-1}(x), \Theta^-_{E_{x_0}} A(x)^{-1}\Theta_{E_x}\hat{e} - \hat{e}_0\Big). \tag{3.89}$$

Parametrization for the Tangent Bundle $T\mathbb{S}^2$

We construct parametrizations for the tangent bundle $T\mathbb{S}^2$. To this end, we use the formula (3.88), together with the parametrization for $\mathbb{S}^2$ and the transport A, as defined in (3.71). Let be $\mathbb{S}^2$ the 2-sphere, regarded as a Riemannian submanifold of $\mathbb{R}^3$. Let us consider $\mu^{\mathbb{S}^2}_{x_0} : \mathbb{R}^2 \to \mathbb{S}^2$, given by:

$$\mu^{\mathbb{S}^2}_{x_0}(\vartheta) = \frac{x_0 + \Theta_{T_{x_0}\mathbb{S}^2}\vartheta}{\|x_0 + \Theta_{T_{x_0}\mathbb{S}^2}\vartheta\|}$$

a parametrization for the sphere $\mathbb{S}^2$ around $x_0 \in \mathbb{S}^2$. Furthermore, let be

$$\Theta_{T_{x_0}\mathbb{S}^2} : \mathbb{R}^2 \to T_{x_0}\mathbb{S}^2 \qquad \text{and} \qquad \Theta_{T_x\mathbb{S}^2} : \mathbb{R}^2 \to T_x\mathbb{S}^2$$

given by:

$$\Theta_{T_{x_0}\mathbb{S}^2} = \begin{bmatrix} | & | \\ \xi_1^{x_0} & \xi_2^{x_0} \\ | & | \end{bmatrix} \qquad \text{and} \qquad \Theta_{T_x\mathbb{S}^2} = \begin{bmatrix} | & | \\ \xi_1^{x} & \xi_2^{x} \\ | & | \end{bmatrix}$$

the matrices whose columns $\xi_1^{x_0}, \xi_2^{x_0} \in \mathbb{R}^3$ and $\xi_1^x, \xi_2^x \in \mathbb{R}^3$, constitute bases for the tangent spaces $T_{x_0}\mathbb{S}^2$ and $T_x\mathbb{S}^2$ respectively, with $x = \mu_{x_0}^{\mathbb{S}^2}(\vartheta)$.
We consider the vector bundle parametrization on $T\mathbb{S}^2$ around (x_0, e_0), given by:

$$\mu_{x_0,e_0}^{T\mathbb{S}^2}(\vartheta, \hat{\eta}) = \Big((\mu_{x_0}^{\mathbb{S}^2})(\vartheta), (\Theta_{T_x\mathbb{S}^2}^{-}(A \circ \mu_{x_0})(\vartheta))\Theta_{T_{x_0}\mathbb{S}^2}(\hat{e}_0 + \hat{\eta}) \Big) \tag{3.90}$$

with $\hat{e}_0, \hat{\eta} \in \mathbb{R}^2$, and $\Theta_{T_{x_0}\mathbb{S}^2}\hat{e}_0 = e_0$. Here, we set $\Theta_{T_x\mathbb{S}^2}^{-} := (\Theta_{T_x\mathbb{S}^2}^T \Theta_{T_x\mathbb{S}^2})^{-1}\Theta_{T_x\mathbb{S}^2}^T$, as the left pseudo-inverse of $\Theta_{T_x\mathbb{S}^2}$. We take as transport, the operator

$$A(x) = I - xx^T$$

as defined in (3.71). Next, we compute first and second derivatives of $(A \circ \mu_{x_0}^{\mathbb{S}^2})\Theta_{T_{x_0}\mathbb{S}^2} : \mathbb{R}^2 \to T_x\mathbb{S}^2$, using the connection on this linear space. Let be $\hat{\eta} \in \mathbb{R}^2$, from:

$$(A \circ \mu_{x_0}^{\mathbb{S}^2})(\vartheta)\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta}$$

differentiating in direction $\hat{\eta}_1 \in \mathbb{R}^2$, we get that:

$$D(A \circ \mu_{x_0}^{\mathbb{S}^2})(\vartheta)(\hat{\eta}_1, \hat{\eta}) = DA(x)D\mu_{x_0}^{\mathbb{S}^2}(\vartheta)\hat{\eta}_1\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta} \tag{3.91}$$

and differentiating the latter, in direction $\hat{\eta}_2 \in \mathbb{R}^2$, we obtain:

$$D^2(A \circ \mu_{x_0}^{\mathbb{S}^2})(\vartheta)(\hat{\eta}_2, \hat{\eta}_1, \hat{\eta}) = D^2A(x)D\mu_{x_0}^{\mathbb{S}^2}(\vartheta)\hat{\eta}_2 D\mu_{x_0}^{\mathbb{S}^2}(\vartheta)\hat{\eta}_1\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta} + DA(x)D^2\mu_{x_0}^{\mathbb{S}^2}(\vartheta)(\hat{\eta}_2, \hat{\eta}_1)\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta}. \tag{3.92}$$

Evaluating (3.91) and (3.92) at $\vartheta = 0$, and using that $D\mu_{x_0}^{\mathbb{S}^2}(0) = \Theta_{T_{x_0}\mathbb{S}^2}$, we get:

$$\begin{aligned} D(A \circ \mu_{x_0}^{\mathbb{S}^2})(0)(\hat{\eta}_1, \hat{\eta}) &= DA(x_0)\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta}_1\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta} \\ D^2(A \circ \mu_{x_0}^{\mathbb{S}^2})(0)(\hat{\eta}_2, \hat{\eta}_1, \hat{\eta}) &= D^2A(x_0)\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta}_2\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta}_1\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta} + DA(x_0)D^2\mu_{x_0}^{\mathbb{S}^2}(0)(\hat{\eta}_2, \hat{\eta}_1)\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta}. \end{aligned}$$

Using formulas (3.29), (3.79) and (3.80), plus the condition $x_0 \perp \Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta}$, we obtain:

$$D(A \circ \mu_{x_0}^{\mathbb{S}^2})(0)(\hat{\eta}_1, \hat{\eta}) = -x_0(\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta}_1)^T(\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta}) \tag{3.93}$$

$$D^2(A \circ \mu_{x_0}^{\mathbb{S}^2})(0)(\hat{\eta}_2, \hat{\eta}_1, \hat{\eta}) = -((\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta}_2)(\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta}_1)^T + (\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta}_1)(\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta}_2)^T)(\Theta_{T_{x_0}\mathbb{S}^2}\hat{\eta}). \tag{3.94}$$

Therefore, the matrix representations for the operators given above are:

$$D(A \circ \mu_{x_0}^{\mathbb{S}^2})(0)\Theta_{T_{x_0}\mathbb{S}^2} = -x_0\Theta_{T_{x_0}\mathbb{S}^2}^T\Theta_{T_{x_0}\mathbb{S}^2} \tag{3.95}$$

$$D^2(A \circ \mu_{x_0}^{\mathbb{S}^2})(0)\Theta_{T_{x_0}\mathbb{S}^2} = -2(\Theta_{T_{x_0}\mathbb{S}^2}\Theta_{T_{x_0}\mathbb{S}^2}^T)\Theta_{T_{x_0}\mathbb{S}^2}. \tag{3.96}$$

Parametrization for the co-tangent Bundle $(T\mathbb{S}^2)^*$

Similarly as done in (3.61), we construct vector bundle parametrization for the co-tangent bundle $(T\mathbb{S}^2)^*$ induced by the adjoint map. We will use the inverse of such retraction in our applications for optimal control problems.

Let be $p : T\mathbb{S}^2 \to \mathbb{S}^2$ the tangent bundle to $\mathbb{S}^2$ endowed with a connection $\kappa_{T\mathbb{S}^2}$. Let also be $\mu^{\mathbb{S}^2} : \mathbb{E} \to \mathbb{S}^2$ a parametrization on the base manifold $\mathbb{S}^2$ as in (3.27), for $\mathbb{E} = \mathbb{R}^2$. In addition, for $x, x_0 \in \mathbb{S}^2$, let be $A(x) \in L(T_{x_0}\mathbb{S}^2, T_x\mathbb{S}^2)$, as in (3.71), a transport operator between the fibers $T_{x_0}\mathbb{S}^2$ and $T_x\mathbb{S}^2$, which are also modeled on $\mathbb{E}$. We consider the linear operators $\Theta^*_{T_{x_0}\mathbb{S}^2}$ and $\Theta^*_{T_x\mathbb{S}^2}$ such that:

$$\Theta^*_{T_{x_0}\mathbb{S}^2} : \mathbb{E}^* \to (T_{x_0}\mathbb{S}^2)^* \quad \text{and} \quad \Theta^*_{T_x\mathbb{S}^2} : \mathbb{E}^* \to (T_x\mathbb{S}^2)^* \tag{3.97}$$

are the matrices containing bases for the dual linear spaces $(T_{x_0}\mathbb{S}^2)^*$ and $(T_x\mathbb{S}^2)^*$ respectively, together with their respective (pseudo)inverses:

$$(\Theta^*_{T_{x_0}\mathbb{S}^2})^- : (T_{x_0}\mathbb{S}^2)^* \to \mathbb{E}^* \quad \text{and} \quad ((\Theta_{T_x\mathbb{S}^2})^*)^- : (T_x\mathbb{S}^2)^* \to \mathbb{E}^*. \tag{3.98}$$

Where $\mathbb{E}^*$ denotes the dual of the fiber space $\mathbb{E}$. Using the operator

$$(A(x)^{-1})^* : (T_{x_0}\mathbb{S}^2)^* \to (T_x\mathbb{S}^2)^*$$

we have that the map:

$$\mu^{(T\mathbb{S}^2)^*}_{x_0,e_0}(\vartheta, \hat{\eta}) = \Big((\mu^{\mathbb{S}^2}_{x_0})(\vartheta), ((\Theta^*_{T_x\mathbb{S}^2})^- \ ((A \circ \mu_{x_0})(\vartheta))^{-1})^* \ \Theta^*_{T_{x_0}\mathbb{S}^2}(\hat{e}_0 + \hat{\eta}) \Big) \tag{3.99}$$

is a co-tangent bundle parametrization for $(T\mathbb{S}^2)^*$ around (x_0, e_0), where $\vartheta \in \mathbb{E}$, $(x, \hat{e}) = \mu^{(T\mathbb{S}^2)^*}_{x_0,e_0}(\vartheta, \hat{\eta})$ and $\hat{e}_0, \hat{\eta} \in \mathbb{E}^*$, with $e_0 = \Theta^*_{T_{x_0}\mathbb{S}^2}\hat{e}_0$. Observe that:

$$\mu^{\mathbb{S}^2}_{x_0} : \mathbb{E} \to \mathbb{S}^2 \qquad \text{and} \qquad ((\Theta^*_{T_x\mathbb{S}^2})^- \, ((A \circ \mu_{x_0})(\vartheta))^{-1})^* \, \Theta^*_{T_{x_0}\mathbb{S}^2} : \mathbb{E}^* \to \mathbb{E}^*.$$

Finally, the inverse is given by:

$$(\mu^{(T\mathbb{S}^2)^*}_{x_0,e_0})^{-1}(x, \hat{e}) = \Big((\mu^{\mathbb{S}^2}_{x_0})^{-1}(x), (\Theta^*_{T_{x_0}\mathbb{S}^2})^- A(x)^* \Theta^*_{T_x\mathbb{S}^2}\hat{e} - \hat{e}_0 \Big). \tag{3.100}$$

Chapter 4

Equality Constrained Optimization on Manifolds

Central to this work is the construction of algorithms for equality constrained optimization on manifolds. We start this section with the problem formulation, this is, minimizing a function subject to constraints, where the domain and target spaces are manifolds. In this way, we generalize the usual setting of a constrained optimization problem for the linear case, see e.g., [Lue97, IT09]. The problem is locally transformed into a problem on vector spaces with the help of retractions, and, as we will see, the already available theory on constrained optimization on vector spaces can be used, in particular, KKT-conditions and second order optimality conditions are derived. In addition, as a consequence of the Brezzi splitting theorem [Bre74], at every point there exists a Lagrange multiplier which is a 1-form on the target space of the constraint mapping. We study the existence of a potential function for this co-vector, i.e., we study the integrability of this 1-form Lagrange multiplier in the sense of Frobenius. We close this section by setting the constrained optimization problem on more general manifolds. For instance, vector bundles, which will be of importance to get the proper formulation for the optimal control problem of energy minimizers. To achieve this, we pose the optimization problem by requiring the constraint map to satisfy a transversality condition.

4.1 Problem Formulation

We consider the equality constrained optimization problem:

$$\min_{x\in X} f(x) \quad s.t. \quad c(x) = y_*. \tag{4.1}$$

Where $f : X \longrightarrow \mathbb{R}$ and $c : X \longrightarrow Y$. Here, X and Y are manifolds modeled on Hilbert spaces, and f and c are C^2-maps. The constraint map c is bounded, C^2 and is a submersion.

We pullback the problem to the tangent spaces with the help of retractions, as defined in section 3.2. Let be R^X_x a retraction for X at $x \in X$ and R^Y_y a retraction for Y at $y = c(x) \in Y$, then we write the problem 4.1 as:

$$\min_{u \in T_x X} \mathbf{f}(u) \quad s.t. \quad \mathbf{c}(u) = 0. \tag{4.2}$$

The pullbacks are performed in the following way:

$$(f \circ R_x^X)(u) = \mathbf{f}(u) \tag{4.3}$$

and

$$\left((R_y^Y)^{-1} \circ c \circ R_x^X\right)(u) - (R_y^Y(y_*))^{-1} = \mathbf{c}(u). \tag{4.4}$$

where $u \in T_x X$. We have used bold letters to represent the pullbacked quantities, and this notation will be kept throughout this work. We present a sketch of the situation. For the objective functional we have:

$$\begin{tikzcd}
X \arrow[r, "f"] & \mathbb{R} \\
T_x X \arrow[u, "R_x^X"] \arrow[ur, "\mathbf{f}"] &
\end{tikzcd}$$

The pullback of the constraint map, which maps from $T_x X$ to $T_y Y$, is such that:

$$\begin{tikzcd}
X \arrow[r, "c"] & Y \\
T_x X \arrow[u, "R_x^X"] \arrow[r, "\mathbf{c}"] & T_y Y \arrow[u, "R_y^Y"']
\end{tikzcd}$$

Example 4.1.1. *Let be $\mathcal{S}$ the space of shapes. For each $\phi \in \mathcal{S}$, there is a given Hilbert space $H(\phi)$ such that the set $E = \{(\phi, H(\phi)) | \phi \in \mathcal{S}\}$ is a vector bundle $(E, \pi, \mathcal{S})$. Over this structure, we define the mappings:*

$$\begin{aligned}
f(\phi, y, u) &= \int_\phi (y(x) - y_d(x))^2 \, dx, \\
c(\phi, y, u) &= \int_\phi \nabla y(x) \nabla v(x) \, dx - u(x) v(x) \, dx, \quad \textit{for all } v \in H^1(\Omega).
\end{aligned}$$

where ∇ refers to the usual gradient in $\mathbb{R}^n$. This is an example of an equality constrained optimization on manifolds, in particular posed on vector bundles. See, e.g., [SSW15].

Proposition 4.1.1. *Let be (R^X, R^Y) a pair of retractions for the manifolds X and Y. Let be $x \in X$, we consider the pullbacked mappings $\boldsymbol{f}$ as in (4.3), and $\mathbf{c}$ as in (4.4). Then, the system*

$$\begin{pmatrix} \boldsymbol{M} & \boldsymbol{c}'(0_x)^* \\ \boldsymbol{c}'(0_x) & 0 \end{pmatrix} \begin{pmatrix} v \\ \lambda \end{pmatrix} + \begin{pmatrix} \boldsymbol{f}'(0_x) \\ 0 \end{pmatrix} = 0 \tag{4.5}$$

has a unique solution if $\boldsymbol{M}$ *is positive on* $\ker \boldsymbol{c}'(0_x)$*. It means that for any* $w \in T_xX$ *we have*

$$\begin{aligned} \boldsymbol{M}vw + \lambda\boldsymbol{c}'(0_x)w + \boldsymbol{f}'(0_x)w = 0 \quad \forall\ w \in T_xM \\ \boldsymbol{c}'(0_x)v = 0. \end{aligned} \tag{4.6}$$

Proof. We have that $\mathbf{c}'(0_x)$ is bounded and surjective, and $\mathbf{M}$ is elliptic on $\ker \mathbf{c}'(0_x)$ and continuous, then, the result is a consequence of the Brezzi splitting theorem, cf. [Bra07, Bre74], applied to the functionals $\mathbf{f}$ and $\mathbf{c}$ at $0_x \in T_xX$. □

Remark 4.1.1. *From* (4.6)*, we see that at each point* $x \in U$*, with* U *an open subset of* X*, there exists the Lagrange multiplier* $\lambda \in (T_{\boldsymbol{c}(0_x)}Y)^*$*. In particular at* $c(x) \in Y$*, for any* $w \in T_xX$*,* $\lambda\boldsymbol{c}'(0_x)w \in \mathbb{R}$*, this means that:*

$$\lambda : Y \longrightarrow (T_{\boldsymbol{c}(0_x)}Y)^*$$

which can be considered as a section of the co-tangent bundle or, equivalently as a 1-form on Y*.*

Definition 4.1.1. *We call the element* $\lambda \in (T_{\boldsymbol{c}(0_x)}Y)^*$ *from* (4.6)*, the Lagrange multiplier of the problem* (4.1) *at* x*.*

Using Defintion 2.6.4, we can consider the pullback of λ by $\mathbf{c}$.

Definition 4.1.2. *We define the* 1-*form* $\hat{\lambda}$ *on* X*, as the pullback of* λ *through* c*, namely:*

$$\hat{\lambda} := \boldsymbol{c}^*(\lambda) = \lambda(\boldsymbol{c}(0_x))\boldsymbol{c}'(0_x) \tag{4.7}$$

in this way $\hat{\lambda} \in (T_xX)^*$.

Remark 4.1.2. *From* (4.6)*, we observe the following:*

i) If we test the first line of (4.6) *with* $w \in \ker \boldsymbol{c}'(0_x)$*, then we have that:*

$$\begin{aligned} \boldsymbol{M}vw &= -\boldsymbol{f}'(0_x)w \\ \langle v, w\rangle_{\boldsymbol{M}} &= -\boldsymbol{f}'(0_x)w \end{aligned}$$

thus the vector field v *can be interpreted as the gradient vector* $\operatorname{grad} \boldsymbol{f}(0_x)$ *at the submanifold* $c^{-1}(x)$*.*

ii) If we test the first line of (4.6) *with* $w \in \ker \boldsymbol{c}'(u)^{\perp}$*, we obtain:*

$$\boldsymbol{f}'(0_x)w + \lambda\boldsymbol{c}'(0_x)w = 0 \tag{4.8}$$

this as a consequence of $v \in \ker \boldsymbol{c}'(x)$*, which implies that* $(\boldsymbol{M}v)w = 0$*.*

iii) Let us consider the submersion map c *through charts* (U, ϕ) *for* X *and* (W, ψ) *for* Y*, as described in* (2.19)*, where* $\boldsymbol{c} = \psi^{-1} \circ c \circ \phi$*. Let be* $v(x) \in \ker \boldsymbol{c}'(0_x)$ *the local representation of the vector field* v*. Differentiating the expression* $\boldsymbol{c}'(0_x)v(x) = 0$ *in the direction of* $w \in \ker \boldsymbol{c}'(0_x)$*, we get that:*

$$\boldsymbol{c}''(0_x)\big(w, v\big) + \boldsymbol{c}'(0_x)v'(x)w = 0. \tag{4.9}$$

We suppose the existence of a spray $B_X(\cdot,\cdot)$ for X. In addition, we use the same notation for v, w and their extensions to X. From (4.9), adding and subtracting the term $\boldsymbol{c}'(0_x)B(x;v,w)$, we get that:

$$\boldsymbol{c}''(0_x)\big(w,v\big) + \boldsymbol{c}'(0_x)(\nabla^X_w v) = -\boldsymbol{c}'(0_x)B_X(x;v,w) \tag{4.10}$$
$$\boldsymbol{c}''(0_x)\big(w,v\big) + \boldsymbol{c}'(0_x)h_{12}(v,w) = -\boldsymbol{c}'(0_x)B_X(x;v,w) \tag{4.11}$$

where in (4.11), the formula given in (2.36) is used. From (4.11), we get that:

$$-h_{12}(v,w) = B_X(x;v,w) + \boldsymbol{c}'^{-}(0_x)\boldsymbol{c}''(0_x)\big(w,v\big) \tag{4.12}$$

where $\boldsymbol{c}'^{-}(0_x) : TY \to \ker \boldsymbol{c}'(0_x)^{\perp}$, is as defined in (2.25). Here, we consider the case in which $X = \mathbb{E}$ is a linear space, implying $B_X \equiv 0$, and obtaining

$$h_{12}(v,w) = -\boldsymbol{c}'^{-}(0_x)\boldsymbol{c}''(0_x)\big(w,v\big). \tag{4.13}$$

We define the operator

$$-\boldsymbol{c}'^{-}(0_x)\boldsymbol{c}''(0_x)\big(w,v\big) := B_{c_x}\big(w,v\big). \tag{4.14}$$

In addition, if $w \in \ker \boldsymbol{c}'(0_x)$, then $\boldsymbol{c}'(0_x)w = 0$, and by differentiating in direction v and by

$$\boldsymbol{c}''(0_x)\big(w,v\big) + \boldsymbol{c}'(0_x)v'w = \boldsymbol{c}''(0_x)\big(v,w\big) + \boldsymbol{c}'(0_x)w'v$$

then, we conclude that $B_{c_x}(\cdot,\cdot)$ is symmetric on $\ker \boldsymbol{c}'(0_x)$.

iv) Let us take charts (U,ϕ) $(V,\hat{\phi})$ in X at x such that $\hat{\phi}(\boldsymbol{x}) = x$, and the change of charts mapping $h(\boldsymbol{x}) = (\hat{\phi}^{-1}\circ\phi)(\boldsymbol{x}) = \boldsymbol{x}$, together with a chart (W,ψ) at $c(x) = y$ where $\psi(\boldsymbol{y}) = y$. We check how the operator B_{c_x} defined in (4.14) transforms under the change of charts from U to V through $h(\boldsymbol{x})$. If we set

$$\boldsymbol{c}_{\psi\phi}(\boldsymbol{x}) := (\psi^{-1}\circ c\circ\phi)(\boldsymbol{x})$$

then

$$\boldsymbol{c}_{\psi\phi}(\boldsymbol{x}) = (\psi^{-1}\circ c\circ\hat{\phi}\circ\hat{\phi}^{-1}\circ\phi)(\boldsymbol{x}) = \boldsymbol{c}_{\psi\hat{\phi}}\circ h(\boldsymbol{x})$$

thus, taking derivative and testing at $w(\boldsymbol{x}) \in \ker{}'(x)$, we get

$$\boldsymbol{c}'_{\psi\phi}(\boldsymbol{x})w(\boldsymbol{x}) = \boldsymbol{c}'_{\psi\hat{\phi}}(h(\boldsymbol{x}))h'(\boldsymbol{x})w(\boldsymbol{x})$$

which is, in turn zero for $w(\boldsymbol{x}) \in \ker \boldsymbol{c}'$. Now taking one more derivative in direction $v \in T_xX$ we obtain

$$\begin{aligned}\boldsymbol{c}''_{\psi\phi}(\boldsymbol{x})\big(v,w(\boldsymbol{x})\big) + \boldsymbol{c}'_{\psi\phi}(\boldsymbol{x})w'(\boldsymbol{x})v =& \boldsymbol{c}''_{\psi\hat{\phi}}(\boldsymbol{x})\big(h'(\boldsymbol{x})v, h'(\boldsymbol{x})w(\boldsymbol{x})\big)\\ &+ \boldsymbol{c}'_{\psi\hat{\phi}}(\boldsymbol{x})\Big(h''(\boldsymbol{x})\big(v,w(\boldsymbol{x})\big) + h'(\boldsymbol{x})w'(\boldsymbol{x})v\Big)\end{aligned}$$

given that both sides of the above equation are zero, we have that

$$\boldsymbol{c}'_{\psi\phi}(\boldsymbol{x})w'(\boldsymbol{x})v = -\boldsymbol{c}''_{\psi\phi}\big(\boldsymbol{x})(v, w(\boldsymbol{x})\big)$$
$$\boldsymbol{c}'_{\psi\hat{\phi}}(\boldsymbol{x})\Big(h''(\boldsymbol{x})\big(v, w(\boldsymbol{x})\big) + h'(\boldsymbol{x})w'(\boldsymbol{x})v\Big) = -\boldsymbol{c}''_{\psi\hat{\phi}}(\boldsymbol{x})\big(h'(\boldsymbol{x})v, h'(\boldsymbol{x})w(\boldsymbol{x})\big)$$

or, in terms of the operator B_{c_x}, at each chart, we have

$$w'(\boldsymbol{x})v = B_{c_x,U}(\boldsymbol{x})\big(v, w(\boldsymbol{x})\big)$$
$$h''(\boldsymbol{x})\big(v, w(\boldsymbol{x})\big) + h'(\boldsymbol{x})u'(\boldsymbol{x})v = B_{c_x,V}\big(h'(\boldsymbol{x})v, h'(\boldsymbol{x})w(\boldsymbol{x})\big)$$

combining them, we end up with the transformation rule of B_{c_x} under change of charts

$$B_{c_x,V}(h(\boldsymbol{x}))\big(h'(\boldsymbol{x})v, h'(\boldsymbol{x})w(\boldsymbol{x})\big) = h''(\boldsymbol{x})\big(v, w(\boldsymbol{x})\big) + h'(\boldsymbol{x})B_{c_x,U}(\boldsymbol{x})\big(v, w(\boldsymbol{x})\big).$$

This shows that B_{c_x} as defined in (4.14)*, representing the second fundamental form, transforms as a spray.*

4.2 KKT-Conditions

In this section, we derive the KKT-conditions of the problem (4.1). We do this by performing the pullback of the problem to the spaces $T_{x_*}X$ and $T_{y_*}Y$ at the stationary point x_*. We use the usual KKT-theory for linear vector spaces in the new pullbacked problem. Second order conditions are also obtained, and we check that these results turn out to be invariant under change of retractions. We first define the Lagrangian function of the problem (4.1) through retractions.

4.2.1 The Lagrange Function of the Pulled-back Problem

We make the following assumption:

Assumption 4.2.1. *Consider for $x \in X$ and $y \in Y$ the following first order consistent pairs of retractions:*

$$R^X_{x,i} : T_xX \to X \qquad i = 1, 2$$

and

$$R^Y_{y,i} : T_yY \to Y \qquad i = 1, 2,$$

where R^X_1, R^X_2, R^Y_1 and R^Y_2 are C^2-retractions.

Their local transformation mappings read:

$$\Phi_X := (R^X_{x,1})^{-1} \circ R^X_{x,2} : T_xX \to T_xX$$
$$\Phi_Y := (R^Y_{y,1})^{-1} \circ R^Y_{y,2} : T_yY \to T_yY.$$

We define the pull-back of the cost functional via the retraction:

$$\mathbf{f}_i : T_xX \longrightarrow \mathbb{R}$$
$$\mathbf{f}_i(u) = (f \circ R^X_{x,i})(u)$$

Similarly, we may pull-back the equality constraint operator $c : X \to Y$ locally:

$$c \circ R^X_{x,i} : T_xX \to Y.$$

To obtain a mapping $\mathbf{c}_i : T_xX \to T_yY$ we have to define a push-forward via $R^Y_{y,i}$ as follows

$$\begin{aligned} \mathbf{c}_i : T_xX &\longrightarrow T_yY \\ \mathbf{c}_i(u) &:= (R^Y_{y,i})^{-1} \circ c \circ R^X_{x,i}(u). \end{aligned}$$

The pullbacked mappings $\mathbf{f}_i$ and $\mathbf{c}_i$ are maps with linear spaces as domain and co-domain, therefore we are allowed to take first and second order derivatives in the usual way. This will be used throughout this work. We note, however, that these derivatives are only defined locally and may depend on the choice of retraction.

We can now define pull-backs of the Lagrangian function:

Definition 4.2.1. *The Lagrangian function at the point x with retractions $R^X_{x,i}$ and $R^Y_{y,i}$ is given by:*

$$\begin{aligned} \boldsymbol{L}_i(u,p) &= \boldsymbol{f}_i(u) + p_x \boldsymbol{c}_i(u) \\ &= f \circ R^X_{x,i}(u) + p_x (R^Y_{y,i})^{-1} \circ c \circ R^X_{x,i}(u) \end{aligned} \tag{4.15}$$

for $u \in T_xX$ and $p_x \in (T_yY)^*$.

For our purpose, we need to compute first and second derivatives of the Lagrangian function:

$$\mathbf{L}_i'(0_x, p_x)v := \mathbf{f}_i'(0_x)v + p_x \mathbf{c}_i'(0_x)v \tag{4.16}$$

$$\mathbf{L}_i''(0_x, p_x)(v,v) := \mathbf{f}_i''(0_x)(v,v) + p_x \mathbf{c}_i''(0_x)(v,v). \tag{4.17}$$

We observe that our definition of $\mathbf{L}$ is again a local one that depends on the given pair of retractions. In particular, we have:

$$\begin{aligned} \mathbf{L}_2(u,p) &= \mathbf{f}_2(u) + p\mathbf{c}_2(u) = \mathbf{f}_1 \circ \Phi_X(u) + p\Phi_Y^{-1} \circ \mathbf{c}_1 \circ \Phi_X(u) \\ &= \mathbf{L}_1 \circ \Phi_X(u) + p(\Phi_Y^{-1} - id) \circ \mathbf{c}_1 \circ \Phi_X(u). \end{aligned} \tag{4.18}$$

Differentiating this expression at 0_x, using the chain rule, we obtain the identities:

$$\mathbf{f}_1'(0_x) = \mathbf{f}_2'(0_x), \qquad \mathbf{c}_1'(0_x) = \mathbf{c}_2'(0_x), \qquad \mathbf{L}_1'(0_x, p) = \mathbf{L}_2'(0_x, p). \tag{4.19}$$

Hence, we do not need to distinguish and thus we use the notation $\mathbf{f}'(0_x)$, $\mathbf{c}'(0_x)$, $\mathbf{L}'(0_x, p)$. However, concerning $\mathbf{L}_i''$ we obtain different expressions.

Lemma 4.2.1.

$$(\mathbf{L}_2''(0_x,p_x) - \mathbf{L}_1''(0_x,p_x))(v,w) = \mathbf{L}'(0_x,p_x)\Phi_X''(0_x)(v,w) - p_x\Phi_Y''(0_y)(\mathbf{c}'(0_x)v, \mathbf{c}'(0_x)w). \tag{4.20}$$

In particular:

i) if $(R^X_{x,1}, R^X_{x,2})$ *is second order consistent, or* $\mathbf{L}'(0_x, p_x) = 0$, *then* $\mathbf{L}''_1(0_x, p_x) = \mathbf{L}''_2(0_x, p_x)$ *on* $\ker \mathbf{c}'(0_x)$.

ii) if $(R^X_{x,1}, R^X_{x,2})$ *and* $(R^Y_{y,1}, R^Y_{y,2})$ *are second order consistent, then* $\mathbf{L}''_1(0_x, p_x) = \mathbf{L}''_2(0_x, p_x)$ *on* T_xX.

Proof. We compute by the chain rule:

$$\begin{aligned} \mathbf{f}''_2(0_x)(v,w) - \mathbf{f}''_1(0_x)(v,w) &= \mathbf{f}'(0_x)\Phi''_X(0_x)(v,w) \\ \mathbf{c}''_2(0_x)(v,w) - \mathbf{c}''_1(0_x)(v,w) &= (\Phi_Y^{-1})''(0_y)(\mathbf{c}'(0_x)v, \mathbf{c}'(0_x)w) + \mathbf{c}'(0_x)\Phi''_X(0_x)(v,w) \\ &= -\Phi''_Y(0_y)(\mathbf{c}'(0_x)v, \mathbf{c}'(0_x)w) + \mathbf{c}'(0_x)\Phi''_X(0_x)(v,w). \end{aligned} \tag{4.21}$$

□

Remark 4.2.1. *Obviously,* $\mathbf{L}''_1(0_x, p_x)(v,w) = \mathbf{L}''_2(0_x, p_x)(v,w)$ *if x is a KKT-point, i.e.,* $\mathbf{L}'(0_x, p_x) = 0$ *and v or* $w \in \ker \mathbf{c}'(0_x)$. *Hence, second order optimality conditions are invariant under change of retractions. This is, of course, to be expected.*
Moreover, close to a KKT point, $\mathbf{L}''_1(0_x, p_x) - \mathbf{L}''_2(0_x, p_x)$ *is small on* $\ker \mathbf{c}'(0_x)$. *Thus, if x is an SSC point, we obtain invertibility of the Lagrange-Newton matrix in a neighborhood of x, regardless of the choice of retraction.*

With previous preparatory material, we are now ready to obtain the KKT-conditions to the problem (4.1).

Proposition 4.2.1. *Let be x_* a local minimum of the problem* (4.1). *Consider a pair of retractions* $(R^X_{x_*}, R^X_{y_*})$ *at x_* and suppose in addition that the pullbacked mappings,* $\boldsymbol{f}$ *and* $\boldsymbol{c}$ *are continuously differentiable at x_* and* $\boldsymbol{c}'(0_{x_*})$ *surjective. Then there exists a Lagrange multiplier* $p \in (T_yY)^* \cong T_yY$ *such that:*

$$\boldsymbol{f}'(0_{x_*})v + p\boldsymbol{c}'(0_{x_*})v = 0 \quad \forall\, v \in T_xX \tag{4.22}$$
$$\boldsymbol{c}(0_{x_*}) = 0. \tag{4.23}$$

Proof. We can apply Ljusternik's theorem (cf. e.g [IT09, 0,§2]) and the Lagrange multiplier rule (cf. e.g [IT09, 1,§1]) to the pullbacked problem in the space $T_{x_*}X$, and we obtain (4.22) and (4.23). □

Using the closed range theorem we can see that the condition 4.22 in $\ker \mathbf{c}'(0_{x_*})$ is equivalent to:

$$\mathbf{f}'(0_{x_*}) \in \text{ran } \mathbf{c}'(0_{x_*}) \Longleftrightarrow \mathbf{f}'(0_{x_*})v = 0 \ \ \forall v \in \ker \mathbf{c}'(0_{x_*}).$$

Actually, conditions 4.22 and 4.23 are invariant under change of charts, to see this we observe that:

$$\mathbf{f}'_1(0_{x_*})v + p\mathbf{c}'_1(0_{x_*})v = \mathbf{f}'_2(0_{x_*})\Phi'_X(0_{x_*})v + p\Phi'_Y\mathbf{c}'_2(0_{x_*})\Phi'_X(0_{x_*})v$$

and using that the pair of retractions (R^X_1, R^Y_1) and (R^X_2, R^Y_2) are first order consistent then $\Phi'_X = Id_{T_xX}$ and $\Phi'_Y = Id_{T_yY}$ implying that

$$\mathbf{f}'_2(0_{x_*})v + p\mathbf{c}'_2(0_{x_*})v = 0 \quad \forall\, v \in T_{x_*}X.$$

4.3 Second Order Optimality Conditions

We now derive second order necessary and sufficient conditions for a local minimizer x_*. First, we derive second order necessary optimality conditions.

Proposition 4.3.1. *Let be x_* a stationary point that is a local minimum for f, and consider a pair of retractions $(R^X_{x_*}, R^Y_{y_*})$, with $y_* = c(x_*)$, where in addition to that, $R^X_{x_*}$ is a retraction of the submanifold $c^{-1}(y_*) \subset X$, then:*

$$\boldsymbol{L}''(0_{x_*}, p_{x_*})(v, v) \geq 0 \quad \forall v \in \ker \boldsymbol{c}'(0_{x_*}).$$

Proof. We use the Taylor expansion of the pullback Lagrangian function $\mathbf{L}(0_{x_*}, p_{x_*})$ at x_* and we consider a vector $v \in \ker \mathbf{c}'(0_{x_*})$, for $t \geq 0$ then:

$$\begin{aligned}\mathbf{L}(0_{x_*} + tv, p_{x_*}) = \mathbf{f}(0_{x_*}) + p_{x_*}\mathbf{c}(0_{x_*}) + t(\mathbf{f}'(0_{x_*})v + p_{x_*}\mathbf{c}'(0_{x_*}))v \\ + \frac{1}{2}t^2(\mathbf{f}''(0_{x_*})v + p_{x_*}\mathbf{c}''(0_{x_*}))(v, v) + t^2\|v\|^2 r(0_{x_*}, tv)\end{aligned}$$

where $r(0_{x_*}, tv) \to 0$ as $t \to 0$. Since x_* is a stationary point then $\mathbf{f}'(0_{x_*})v + p_{x_*}\mathbf{c}'(0_{x_*})v = 0$, $\mathbf{c}(0_{x_*}) = 0$ and $\mathbf{c}(0_{x_*} + tv) = 0$, the latter is due to the assumption over $R^X_{x_*}$, therefore, we get:

$$\frac{\mathbf{f}(tv) - \mathbf{f}(0_{x_*})}{t^2} = \frac{1}{2}(\mathbf{f}''(0_{x_*})v + p_{x_*}\mathbf{c}''(0_{x_*}))(v, v) + \|v\|^2 r(0_{x_*}, tv)$$

but x_* is a local minimum, this means that $\mathbf{f}(tv) - \mathbf{f}(0_{x_*}) \geq 0$ for sufficiently small t, thus we get that

$$(\mathbf{f}''(0_{x_*})v + p_{x_*}\mathbf{c}''(0_{x_*}))(v, v) + \|v\|^2 r(0_{x_*}, tv) \geq 0$$

and taking the limit as $t \longrightarrow 0$ we get

$$\mathbf{L}''(0_{x_*}, p_{x_*})(v, v) \geq 0 \quad \text{for all } v \in \ker \mathbf{c}'(0_{x_*}).$$

Finally, we see that this property is invariant under change of retractions by Lemma 4.20 and Remark 4.2.1. □

We provide now, sufficient optimality conditions for a local minimum.

Proposition 4.3.2. *Consider a pair of retractions $(R^X_{x_*}, R^X_{y_*})$ at x_* and $y_* = c(x_*)$, where $R^X_{x_*}$ is a retraction for the submanifold $c^{-1}(y_*) \subset X$ and suppose that $\boldsymbol{f}$ and $\boldsymbol{c}$ are twice continuously differentiable at x_*. If $\boldsymbol{L}'(0_{x_*}, p) = 0$ and $\boldsymbol{L}''(0_{x_*}, p)(v, v) > 0$ for all $v \in \ker \boldsymbol{c}'(0_{x_*})$ then x_* is a local minimum.*

Proof. By contradiction let us assume that x_* is not a local minimizer. Then, there exists a sequence of feasible points $\{x_k\}_{k\in\mathbb{N}}$ such that $x_k \to x_*$ and $f(x_k) \leq f(x_*)$. If we define $v_k := (R^X_{x_*})^{-1}(x_k)$, in particular we have that $v_k \to 0_{x_*}$, by continuity of the retraction $R^X_{x_*}$ at x_*. We also observe that $\mathbf{c}(v_k) = 0$ for all $k \in \mathbb{N}$, which follows from the assumption made on the retraction $R^X_{x_*}$, and feasibility of the sequence x_k. We now define the sequence $w_k := \frac{v_k}{\|v_k\|}$, it can be shown that $(w_k)_{k\in\mathbb{N}}$ also converges to a $w \in \ker \mathbf{c}'(0_{x_*})$, with $w \neq 0$ ($\|w_k\| = 1$ for all $k \in \mathbb{N}$). Using Taylor's expansion and the formula $v_k = \|v_k\|w_k$, we get:

$$\mathbf{L}(0_{x_*} + v_k, p_{x_*}) = \mathbf{L}(0_{x_*}, p_{x_*}) + \|v_k\|\mathbf{L}'(0_{x_*}, p_{x_*})w_k + \frac{1}{2}\|v_k\|^2\mathbf{L}''(0_{x_*}, p_{x_*})(w_k, w_k) + \|v_k\|^2 r(0_{x_*}, \|v_k\|w_k)$$

where $r(0_{x_*}, \|v_k\|w_k) \to 0$ as $\|v_k\| \to 0$. Given that $\mathbf{c}(0_{x_*}) = 0$ and $\mathbf{c}(v_k) = 0$, we have that, for every $k \in \mathbb{N}$:

$$\mathbf{f}(v_k) - \mathbf{f}(0_{x_*}) = \|v_k\|\mathbf{L}'(0_{x_*}, p_{x_*})w_k + \frac{1}{2}\|v_k\|^2\mathbf{L}''(0_{x_*}, p_{x_*})(w_k, w_k) + \|v_k\|^2 r(0_{x_*}, \|v_k\|w_k) \leq 0$$

which implies

$$\|v_k\|\mathbf{L}'(0_{x_k}, p_{x_*})w_k + \frac{1}{2}\mathbf{L}''(0_{x_*}, p_{x_*})(w_k, w_k) + r(0_{x_*}, \|v_k\|w_k) \leq 0, \quad \forall\ k \in \mathbb{N},$$

and taking limit we get that

$$\frac{1}{2}\mathbf{L}''(0_{x_*}, p_{x_*})(w, w) = \lim_{k\to\infty}\left(\|v_k\|\mathbf{L}'(0_{x_*}, p_{x_*})w_k + \frac{1}{2}\mathbf{L}''(0_{x_*}, p_{x_*})(w_k, w_k) + r(0_{x_*}, \|v_k\|w_k)\right) \leq 0$$

thus

$$\mathbf{L}''(0_{x_*}, p_{x_*})(w, w) \leq 0$$

contradicting our assumption. Finally, by Lemma 4.20 and Remark 4.2.1, we have that for two pairs of retractions, $\mathbf{L}_1''(0_{x_*}, p)(v, v) = \mathbf{L}_2''(0_{x_*}, p)(v, v)$ for any $v \in \ker \mathbf{c}'(0_{x_*})$ with $\mathbf{L}'(0_{x_*}, p) = 0$, therefore the property is invariant under change of retractions. □

4.4 The Lagrange Multiplier on Manifolds

We now study the integrability of the 1-form Lagrange multiplier $\hat{\lambda}$ defined in (4.7). We show that the existence of a potential function $\Lambda : X \to \mathbb{R}$ satisfying $d\Lambda = \hat{\lambda}$, depends on the integrability of the horizontal distribution $(\ker T_x c)^{\perp}$ in the sense of Frobenius, as shown in Theorem 2.6.2. We specify under which conditions the horizontal subbundle $(\ker T_x c)^{\perp}$ is integrable. To this end, we introduce some preparatory material on integrability of the horizontal distribution. We will use these results to give criteria for the integrability of the Lagrange multiplier. In order to have deeper insight on the topic, we refer the reader to [Mic08, PT06, Bes07].

4.4.1 Integrability of the Horizontal Distribution

We take the following results on integrability from [PT06].

Definition 4.4.1. *Let be $g : M \longrightarrow N$ be a submersion. Then we define*

$$F = F(g) := \ker(g'(x))$$

as the vertical subbundle of TM. Additionally, if M is a Riemann manifold with metric $\boldsymbol{M}$, we define the horizontal subbundle of TM as:

$$E := F(g)^{\perp}.$$

If both M and N are Riemannian manifolds, we know that g a Riemann submersion if

$$T_x g = g'(x) : T_x M \longrightarrow T_{g(x)} N$$

is an orthogonal projection. We also recall that $Tg(x)$ induces a linear isomorphism

$$T_x g : E_x \longrightarrow T_{g(x)} N$$

between the horizontal subbundle, and the tangent space of the target manifold N.

Definition 4.4.2. *Let be $g : M \longrightarrow N$ a Riemann submersion, and let be ξ a vector field on M, we say that ξ is:*

- *vertical if $\xi(x) \in F_x(g)$ for all x (i.e., if $g'(x)\xi(x) = 0$),*
- *horizontal if $\xi(x) \in E_x(g)$ for all x (i.e., if $\xi(x) \perp E_x(g)$).*

We have that any vector field ξ on M can be uniquely decomposed as

$$\xi = \xi^F + \xi^E$$

into its vertical ξ^F and horizontal ξ^E components.

Definition 4.4.3. *A Riemann submersion $g : M \longrightarrow N$ is called integrable if $E(M) = (\ker g')^{\perp}$ is an integrable distribution.*

We define two special tensors introduced by O'Neill in [O+66]. Let be ξ_1, ξ_2 vector fields over M then, the O'Neill tensors are given by:

$$T(\xi_1, \xi_2) := \left(\nabla_{\xi_1^F} \xi_2^F\right)^E + \left(\nabla_{\xi_1^F} \xi_2^E\right)^F \tag{4.24}$$

$$A(\xi_1, \xi_2) := \left(\nabla_{\xi_1^E} \xi_2^E\right)^F + \left(\nabla_{\xi_1^E} \xi_2^F\right)^E . \tag{4.25}$$

The following theorem gives us conditions for the horizontal distribution to be integrable.

Theorem 4.4.1. *Let be $g : M \longrightarrow N$ be a Riemann submersion; then the following conditions are equivalent:*

i) g is integrable (that is, $E(g)$ is integrable).

ii) Every normal field $\eta \in E_x$ satisfying that $g'(x)\eta(x) = \hat{\eta}$ is the same for all $x \in g^{-1}(y)$, is such that $\nabla^E \eta = 0$.

iii) The O'Neill tensor A is zero.

Here the term ∇^E, is the normal connection as defined for subamnifold geometry given in Theorem 2.7.3, there denoted as $\nabla^\perp$.

Proof. See [PT06, V,§5]. □

Example 4.4.1. *Let $(M_1, \boldsymbol{M}_1)$, $(M_2, \boldsymbol{M}_2)$ be two Riemannian manifolds; then the product manifold $M = M_1 \times M_2$ has a product Riemannian metric $\boldsymbol{M}_1 \oplus \boldsymbol{M}_2$ on the tangent space $T_{(x_1,x_2)}(M_1 \times M_2) = T_{x_1}M_1 \times T_{x_2}M_2$ and thus both projections are Riemannian submersions. We also see that the subbundles TM_1 and TM_2 are both involutive and their leaves are the manifolds $\{x_1\} \times M_2$ and $M_1 \times \{x_2\}$. A Riemannian manifold isometric to a product will be called reducible.*

4.4.2 Existence of a Potential for the Lagrange Multiplier

We return to the problem setting (4.2). In what follows we assume that our domain space is simply connected and that the manifold X is Riemannian. With help of the Poincaré Lemma 2.6.1, we compute $d\hat{\lambda}$ to find the obstructions for the existence of a potential $\Lambda : X \to \mathbb{R}$ such that $d\Lambda = \hat{\lambda}$, with $\hat{\lambda}$ as defined in (4.7).

Proposition 4.4.1. *Let be ξ, η, vector fields at $x \in X$ and $\hat{\lambda}$ as in (4.7), then we have that*

$$d\hat{\lambda}(\xi, \eta) = -(\mathbf{f}'(0_x) + \lambda(\boldsymbol{c}(0_x))\boldsymbol{c}'(0_x))[\xi_n, \eta_n], \tag{4.26}$$

where ξ_n, η_n are the normal component of ξ and η, i.e., $\xi_n, \eta_n \in (\ker \boldsymbol{c}'(0_x))^\perp$.

Proof. We use the formula (2.28) to compute $d\hat{\lambda}$, obtaining:

$$d\hat{\lambda}(\xi, \eta) = d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi, \eta) = \xi(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\eta) - \eta(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\xi) - \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)[\xi, \eta]$$

First, we split the vectors into their tangential and normal part, i.e., $\xi = \xi_t + \xi_n$ and $\eta = \eta_t + \eta_n$, with $\xi_t, \eta_t \in \ker \mathbf{c}'(0_x)$ and $\xi_n, \eta_n \in \ker(\mathbf{c}'(0_x))^\perp$, from that we get

$$\begin{aligned} d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi, \eta) =& d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi_n, \eta_n) + d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi_t, \eta_n) \\ &+ d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi_n, \eta_t) + d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi_t, \eta_t), \end{aligned}$$

and we inspect each term separately. We start with the term $d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi_t, \eta_t)$. Using the equation defining the exterior derivative we get that:

$$\begin{aligned} d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi_t, \eta_t) &= (\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\eta_t)'\xi_t - (\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\xi_t)'\eta_t - \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)(\eta_t'\xi_t - \xi_t'\eta_t) \\ &= 0 \end{aligned}$$

due to that $\mathbf{c}'(0_x)\eta_t = \mathbf{c}'(0_x)\xi_t = 0$ and $\mathbf{c}'(0_x)\eta_t'\xi_t = -\mathbf{c}''(0_x)(\xi_t, \eta_t) = \mathbf{c}'(0_x)\xi_t'\eta_t$. Now for the term $d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi_n, \eta_n)$, we take $\eta_n, \xi_n \in \ker \mathbf{c}'(0_x)^\perp$, and we use the remark (4.8), namely, that $\mathbf{f}'(0_x) = -\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)$ in normal directions, obtaining:

$$\begin{aligned} d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi_n, \eta_n) &= (\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\eta_n)'\xi_n - (\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\xi_n)'\eta_n - \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)(\eta_n'\xi_n - \xi_n'\eta_n) \\ &= (-\mathbf{f}'(0_x)\eta_n)'\xi_n - (-\mathbf{f}'(0_x)\xi_n)'\eta_n - \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)(\eta_n'\xi_n - \xi_n'\eta_n) \\ &= -\mathbf{f}''(0_x)(\xi_n, \eta_n) - \mathbf{f}'(0_x)\eta_n'\xi_n + \mathbf{f}''(0_x)(\eta_n, \xi_n) + \mathbf{f}'(0_x)\xi_n'\eta_n \\ &\quad - \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)(\eta_n'\xi_n - \xi_n'\eta_n) \\ &= -(\mathbf{f}'(0_x) + \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))[\xi_n, \eta_n] \end{aligned}$$

Before we consider the mixed terms $d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi_n,\eta_t)$ and $d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi_t,\eta_n)$, we observe that for the expression

$$(\mathbf{f}'(0_x)\eta_n + \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\eta_n)'\xi_t = 0$$

using that $\mathbf{c}''(0_x)(\eta_n,\xi_t) = -\mathbf{c}(0_x)\xi_t'\eta_n$, we obtain

$$\begin{aligned}\mathbf{f}''(0_x)(\xi_t,\eta_n) + \mathbf{f}'(0_x)\eta_n'\xi_t + \lambda'(\mathbf{c}(0_x))\mathbf{c}'(0_x)\xi_t\mathbf{c}'(0_x)\eta_n + \lambda(\mathbf{c}(0_x))\mathbf{c}''(0_x)(\xi_t,\eta_n) + \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\eta_n'\xi_t = 0\\ \mathbf{f}''(0_x)(\xi_t,\eta_n) + \mathbf{f}'(0_x)\eta_n'\xi_t - \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\xi_t'\eta_n + \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\eta_n'\xi_t = 0\end{aligned}$$

observe that the term $\lambda'(\mathbf{c}(0_x))\mathbf{c}'(0_x)\xi_t\mathbf{c}'(0_x)\eta_n$ vanishes. Then, we get that:

$$\mathbf{f}''(0_x)(\xi_t,\eta_n) + \mathbf{f}'(0_x)\eta_n'\xi_t + \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)[\xi_t,\eta_n] = 0. \tag{4.27}$$

Now we compute $d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi_t,\eta_n)$. Using the formula for the exterior derivative, and the relation $\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\eta_n = -\mathbf{f}'(0_x)\eta_n$, we get:

$$\begin{aligned}d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi_t,\eta_n) &= (\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\eta_n)'\xi_t - (\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\xi_t)'\eta_n - \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)[\xi_t,\eta_n]\\ &= (-\mathbf{f}'(0_x)\eta_n)'\xi_t - \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)[\xi_t,\eta_n]\\ &= -\mathbf{f}''(0_x)(\xi_t,\eta_n) - \mathbf{f}'(0_x)\eta_n'\xi_t - \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)[\xi_t,\eta_n]\\ &= 0.\end{aligned}$$

Where the equation (4.27) has been used. Analogously, as done for (4.27), we have that:

$$\mathbf{f}''(0_x)(\eta_t,\xi_n) + \mathbf{f}'(0_x)\xi_n'\eta_t + \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)[\eta_t,\xi_n] = 0. \tag{4.28}$$

With this, we now compute $d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi_n,\eta_t)$, obtaining:

$$\begin{aligned}d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi_n,\eta_t) &= (\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\eta_t)'\xi_n - (\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\xi_n)'\eta_t - \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)[\xi_n,\eta_t]\\ &= (\mathbf{f}'(0_x)\xi_n)'\eta_t - \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)[\xi_n,\eta_t]\\ &= \mathbf{f}''(0_x)(\eta_t,\xi_n) + \mathbf{f}'(0_x)\xi_n'\eta_t - \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)[\xi_n,\eta_t]\\ &= \mathbf{f}''(0_x)(\eta_t,\xi_n) + \mathbf{f}'(0_x)\xi_n'\eta_t + \lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)[\eta_t,\xi_n]\\ &= 0.\end{aligned}$$

where the formula (4.28), and the relations $[\xi_n,\eta_t] = -[\eta_t,\xi_n]$ and $\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x)\xi_n = -\mathbf{f}'(0_x)\xi_n$ have been used. Therefore, we have proven that

$$d(\lambda(\mathbf{c}(0_x))\mathbf{c}'(0_x))(\xi,\eta) = -(\mathbf{f}'(0_x) + \lambda\mathbf{c}'(0_x))[\xi_n,\eta_n].$$

□

From Poincaré Lemma 2.6.1, we have that the 1-form $\hat{\lambda}$ is integrable if $d\hat{\lambda} = 0$ and, as we saw in the previous proposition, this condition is met if $(\mathbf{f}'(0_x) + \lambda\mathbf{c}'(0_x))[\xi_n,\eta_n] = 0$, for ξ_n, $\eta_n \in (\ker\mathbf{c}'(0_x))^{\perp}$. We know that the term $(\mathbf{f}'(0_x) + \lambda\mathbf{c}'(0_x))$ vanishes in normal directions, therefore, if $[\xi_n,\eta_n] \in (\ker\mathbf{c}'(0_x))^{\perp}$, i.e., if the horizontal distribution $(\ker\mathbf{c}'(0_x))^{\perp}$ is integrable, then $d\hat{\lambda} = 0$, implying the integrability of $\hat{\lambda}$.
We can use Theorem 4.4.1 to characterize the obstructions to the existence of a potential function for the Lagrange multiplier.

Proposition 4.4.2. *Let be $\hat{\lambda}$ as in* (4.7)*. Then, if one of the conditions of Theorem* 4.4.1 *is met, then, there exists a function $\Lambda : X \longrightarrow \mathbb{R}$ such that $d\Lambda = \hat{\lambda}$.*

In the general case the function Λ does not exist, due in part to the non-integrability of the horizontal distribution, as can be seen in the following example:

Example 4.4.2. *Let us consider the Hopf map, this is, the map $c : \mathbb{S}^3 \longrightarrow \mathbb{S}^2$, which maps points from the three sphere:*

$$\mathbb{S}^3 = \{(x_1, x_2, x_3, x_4) \in \mathbb{R}^4 |\, x_1^2 + x_2^2 + x_3^2 + x_4^2 = 1\}$$

to $\mathbb{S}^2$, and is defined by:

$$c(x_1, x_2, x_3, x_4) = \left[x_1^2 + x_2^2 - (x_3^2 + x_4^2), 2(x_1x_4 + x_2x_3), 2(x_2x_4 - x_1x_3)\right].$$

This map is also called the Hopf fibration, for more details on this special structure see [Lyo03]. This map, has the property that, locally is the product space of $\mathbb{S}^2 \times \mathbb{S}^1$, but not globally. For any given $y \in \mathbb{S}^2$ the corresponding fiber $c^{-1}(y)$ is the circle $\mathbb{S}^1$. We check that:

$$T_xc(x) = 2\begin{bmatrix} x_1 & x_2 & -x_3 & -x_4 \\ x_4 & x_3 & x_2 & x_1 \\ -x_3 & x_4 & -x_1 & x_2 \end{bmatrix}$$

and

$$\ker T_xc(x) = \begin{bmatrix} x_2 \\ -x_1 \\ -x_4 \\ x_3 \end{bmatrix}$$

therefore, a basis for the horizontal space is given by

$$E = (\ker T_xc(x))^{\perp} = \{\eta_1, \eta_2, \eta_3\} = \left\{ \begin{bmatrix} x_3 \\ -x_4 \\ x_1 \\ -x_2 \end{bmatrix}, \begin{bmatrix} x_4 \\ x_3 \\ x_2 \\ x_1 \end{bmatrix}, \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \right\}$$

and the Lie bracket yields that:

$$[\eta_2, \eta_1] = \eta_1'\eta_2 - \eta_2'\eta_1 = 2\begin{bmatrix} x_2 \\ -x_1 \\ x_4 \\ -x_3 \end{bmatrix}$$

therefore $[\eta_2, \eta_1] \notin E$ and the horizontal distribution cannot be integrable.

Remark 4.4.1. *In particular, proposition 4.4.2 says that a potential function for the one form $\hat{\lambda}$ exists:*

i) If the manifold X is flat, i.e., if $P[\xi_n, \eta_n] = 0$, where $\xi_n, \eta_n \in \ker \boldsymbol{c}'(x)^{\perp}$, and $P : T_xX \longrightarrow \ker(\boldsymbol{c}'(0_x))$ is the projection onto $\ker \boldsymbol{c}'(0_x)$.

ii) If X is reducible, i.e., X is isometric to products $X_1 \times X_2$, then the normal bundle is involutive and $[\xi_n, \eta_n] \in \ker \boldsymbol{c}'(0_x)^{\perp}$ for $\xi_n, \eta_n \in \ker \boldsymbol{c}'(0_x)^{\perp}$.

iii) By the De Rham decomposition theorem, see e.g., [DR52, Wu63, FL06, BH83, PAN92, EH98, Gau81], if the manifold is complete, simply connected and its holonomy representation is reducible, then the manifold is a product. And the horizontal distribution is integrable.

iv) If every normal field is c parallel, i.e., if $\boldsymbol{c}'(0_x)\eta(0_x) = \hat{\eta}$ with $\hat{\eta}$ fixed independent of x, see e.g., [PT06].

In the case that the form $\hat{\lambda}$ is integrable, we can define the Lagrange function for the problem (4.1) as:

$$L(x, \Lambda) = f(x) + (\Lambda \circ c)(x),$$

for $\Lambda : X \to \mathbb{R}$.
We now return to constrained optimization problems, and we set the problem on vector bundles.

4.5 Constrained Optimization on Vector Bundles

In some interesting situations, the setting of the problem contains cases where the manifold spaces have more structure. For instance, formulation on vector bundles is needed when it comes to applications to optimal control problems. In order to achieve a correct formulation of such problems, we use the notion of transversality as in Definition 2.5.1. We do not start directly with the formulation on vector bundles, instead, we begin by imposing conditions on the constraint, so that it maps accordingly on the vector bundle structure of the co-domain. In particular, we ensure that the vector bundle retraction and the constraint mapping are compatible with our formulation.
Let be $f : X \to \mathbb{R}$ and $c : X \to Y$. We consider the following problem:

$$\min_{x \in X} f(x) \quad \text{s.t.} \quad c(x) \in S_0 \tag{4.29}$$

where S_0 is a submanifold of the target space Y, and c is transversal over S_0. This implies that:

$$\operatorname{ran} T_x c + T_{c(x)} S_0 = T_{c(x)} Y \quad \text{for } c(x) \in S_0.$$

Let be $c(x) = y$. We assume that $T_y Y$ is split into two subspaces:

$$T_y Y = W_1 \times W_2, \qquad W_1 \cap W_2 = \{0\}$$

and a corresponding projection

$$P_2 : T_y Y \to W_2$$

with $\operatorname{ran} P_2 = W_2$ and $\ker P_2 = W_1$. For a vector bundle $p : Y \to M$, in the local decomposition, the projection P_2 maps into the fiber space of the vector bundle at a point. In particular, a vector bundle connection as given in Definition 2.8.1, provides a way to split the tangent space TY into two complementary subbundles, one of them given by the vertical subbundle $\ker Tp$ and the corresponding complementary horizontal subbundle determined by the connection.

At the solution x_* we assume that $W_1 = T_{c(x_*)}S_0$. For given retractions $R_x^X : T_xX \to X$ and $R_y^Y : T_yY \to Y$, we may define the local pullback of $c : X \to Y$ as

$$\mathbf{c} : T_xX \to T_{c(x)}Y$$
$$\mathbf{c} = (R_{c(x)}^Y)^{-1} \circ c \circ R_x^X.$$

At this point we stress that such a construction cannot be performed for arbitrary problems, but for problems, where the above local product structure arises naturally, in particular for vector bundles. This also means that S_0 has to have particularly simple structure. For example, S_0 may be the 0-section of a vector bundle.
If $c(x) \in S_0$, and by our splitting of $T_{c(x)}Y$, we obtain the splitting

$$\mathbf{c}(v) = \mathbf{c}_B(v) + \mathbf{c}_F(v) = (I - P_2)\mathbf{c}(v) + P_2\mathbf{c}(v)$$
$$\mathbf{c}'(0_x) = \mathbf{c}'_B(0_x) + \mathbf{c}'_F(0_x) = (I - P_2)\mathbf{c}'(0_x) + P_2\mathbf{c}'(0_x).$$

By transversality we have that $\mathbf{c}_F$ is a submersion.

Proposition 4.5.1. *Let be x_* a local minimum of the problem* (4.29). *Consider a pair of retractions $(R_{x_*}^X, R_{y_*}^X)$ at $x_* \in c^{-1}(S_0)$, and suppose in addition that $\boldsymbol{f}$ and $\mathbf{c}$ are continuously differentiable at x_* and c is transversal over S_0. Then there exists a Lagrange multiplier $p \in \left(T_{c(0_{x_*})}Y/T_{c(0_{x_*})}S_0\right)^*$ such that:*

$$\boldsymbol{f}'(0_{x_*})v + p\boldsymbol{c}'_F(0_{x_*})v = 0 \quad \textit{for all} \quad v \in T_{x_*}X.$$

Proof. We know that $\mathbf{c}'_F(0_{x_*}) : T_{x_*}X \longrightarrow T_{c(0_{x_*})}Y/T_{c(0_{x_*})}S_0$ is surjective, this as a consequence of proposition 2.5.1, by transversality of c over S_0. Additionally, $\mathbf{c}(0_{x_*}) \in S_0$, therefore, once again, we can apply Ljusternik's theorem (cf. e.g [IT09, 0,§2]) and the Lagrange multiplier rule (cf. e.g [IT09, 1,§1]) to the current setting. □

Before we set the constrained optimization problem over vector bundles, we do some remarks concerning sections.

Definition 4.5.1. *Let be $p : E \longrightarrow M$ a vector bundle, a section of E is a smooth map $s : M \longrightarrow E$ such that $p \circ s = id_M$.*

Next, we see how the image of a section is a submanifold of the total space, hence, we land in the framework of the problem setting (4.29), where, as constraint submanifold, we take the image of a section. For applications, we consider a special section, namely, the zero section of the vector bundle.

Proposition 4.5.2. *Let be $s : M \longrightarrow E$ a section of the vector bundle $p : E \longrightarrow M$. Then $s(M)$ is an embedded submanifold of E.*

Proof. We have to proof that s and T_xs are injective maps, but this follows from $p \circ s = id_M$, additionally by continuity of p the embedding property follows. □

We now pose the constrained optimization problem on vector bundles using the considerations made at the beginning of the present section, and taking advantage of the available product structure of these kinds of manifolds. In particular, we consider a constrained map $c : X \to Y$, where $p : Y \to M$ is a vector bundle over M.

Constrained Optimization Problem on a Vector Bundle Let be $p_Y : Y \longrightarrow M$ a vector bundle endowed with a connection κ_Y, and let X be a manifold. Let be s_0, the zero section

$$s_0 : M \to Y$$

with $(p_Y \circ s_0) = id_M$, and with local representation given by

$$s_0(y) = (y, 0).$$

Let be $S_0 := s_0(M)$ the image of M by s_0. Then, S_0 is a submanifold of Y. With this, we define the problem:

$$\min_{x \in X} f(x) \quad \text{s.t} \quad c(x) \in S_0 \tag{4.30}$$

where $c : X \longrightarrow Y$ is assumed to be transversal over the submanifold S_0.
With the help of a retraction $R_x^X : T_xX \longrightarrow X$ for the manifold X, and a vector bundle retraction $R_{y,e}^Y : T_{y,e}Y \longrightarrow Y$ for Y, we have that, in a chart W of $c(x) \in Y$, with $p_Y(c(x)) = y$, there exists a chart U for $x \in X$, such that:

$$(R_{y,e}^Y)^{-1} \circ c \circ R_x^X := \mathbf{c} = (\mathbf{c}_B, \mathbf{c}_F) : T_xX \to T_yM \times \mathbb{F}. \tag{4.31}$$

According to the formulation (4.29), we get that $T_{y,e}Y = W_1 \times W_2$, with, $T_yM = W_1$ and $W_2 = \mathbb{F}$, where $\mathbb{F}$ is the fiber space for the vector bundle. In addition, we see that the map $\mathbf{c}_F$ is such that, $\mathbf{c}_F : T_xX \longrightarrow \mathbb{F}$ and by transversality, is a submersion. In particular, observe that at solution point $x_* \in X$, we get that $\mathbf{c}_F(0_{x*}) = 0$.
With this formulation, and as a consequence of Proposition 4.5.1, we derive the KKT-conditions for the problem

$$\min_{u \in TX} \mathbf{f}(u) \quad \text{s.t.} \quad \mathbf{c}_F(u) = 0. \tag{4.32}$$

Proposition 4.5.3. *Let be x_* a local minimum of the problem* (4.32). *Consider a pair of retractions $(R_{x_*}^X, R_{y_*}^Y)$ at $x_* \in c^{-1}(S_0)$, suppose in addition that $\boldsymbol{f}$ and $\mathbf{c}$ are continuously differentiable at x_*, and that c is transversal over the submanifold S_0. Then, there exists a Lagrange multiplier $p_{x_*} \in \mathbb{F}^*$ such that:*

$$\boldsymbol{f}'(0_{x_*})v + p_{x_*}\boldsymbol{c}_F'(0_{x_*})v = 0 \quad \textit{for all} \quad v \in T_{x_*}X.$$

Proof. We use Proposition 4.5.1 applied to the formulation (4.32). □

As an application of the previous considerations, and as a preparatory material for the optimal control problem of inextensible rods, we proceed with the abstract setting of optimal control of energy minimizers.

4.5.1 Optimal Control of Energy Minimizers

Suppose that the map
$$J : Y \to \mathbb{R}$$
represents the stored energy functional of an elastic body. Additional constraints can be considered through the mapping
$$C : Y \to V$$
where Y and V are manifolds, and $C : Y \to V$ is a submersion. Let be $v \in V$, we consider the constrained energy minimization problem:

$$\min_{y \in Y} J(y) \text{ s.t. } C(y) = v.$$

To illustrate the situation, we start by working in charts together with tangent maps, and then we write the problem in terms of retractions. We define the Lagrangian function:

$$\begin{aligned} L' &: Y \times TV^* \to TY^* \\ L'(y, \lambda) &= T_y J + \lambda_{c(0_y)} T_y C, \end{aligned}$$

where, however, L' need not be the derivative of any real function, because the cotangent-vector field λ need not have a potential, as we saw in section 4.4. By $\lambda_{C(0_y)} \in T_{C(0_y)}V^*$, we denote λ at $C(0_y)$.

First order optimality conditions can then be written as:

$$\begin{aligned} 0 &= T_y J + \lambda_{C(0_y)} T_y C \text{ in } T_y Y \\ v &= C(0_y) \end{aligned} \tag{4.33}$$

for some $\lambda_{C(0_y)} \in T_{C(0_y)}V^*$.

Here, we denote by U the control space. For $u \in U$, we add a force-field $B(y)u \in TY^*$, and write the optimal control problem:

$$\min_{(y,u) \in Y \times U} f(y, u) \quad \text{s.t.} \quad \begin{aligned} 0 &= T_y J + \lambda_{C(0_y)} T_y C - B(y)u \\ v &= C(y). \end{aligned} \tag{4.34}$$

Where
$$f : Y \times U \longrightarrow \mathbb{R}$$
could be, for instance, a tracking type functional. We see that:

$$\begin{aligned} TJ &: Y \to TY^* \\ y &\mapsto T_y J \\ \lambda &: V \to TV^* \\ v &\mapsto \lambda_v \\ TC &: Y \times TV^* \to TY^* \\ (y, \lambda) &\mapsto \lambda_{C(0_y)} T_y C \\ B &: Y \times U \to TY^* \\ (y, u) &\mapsto B(y)u. \end{aligned}$$

Which implies that

$$T_yJ + \lambda_{C(0_y)}T_yC - B(y)u \in TY^* \tag{4.35}$$

and we define

$$\begin{aligned} c : Y \times V \times U &\to TY^* \\ (y, \lambda, u) &\to (T_yJ + \lambda_{C(0_y)}T_yC - B(y)u). \end{aligned} \tag{4.36}$$

We now write the optimal control problem as a constrained optimization problem on a vector bundle. Let us consider the zero-section over the cotangent bundle space

$$p_{Y^*} : TY^* \to Y$$

namely:

$$s_0 : Y \to TY^* \tag{4.37}$$

with $(p_{Y^*} \circ s_0) = id_Y$ and local representation $s_0(y) = (y, 0)$. Consider the submanifold $S_0 = s_0(Y)$, and the problem

$$\begin{aligned} \min_{(y,u)\in Y\times U} f(y, u) \quad \text{s.t} \quad & c(y, \lambda, u) \in S_0 \\ & C(y) = v. \end{aligned} \tag{4.38}$$

with $c : Y \times V \times U \to TY^*$ transversal over S_0. We now write the problem in terms of retractions. Let us denote $Z = Y \times V \times U$, and consider the retraction $R^Z : TZ \to Z$, where, for $z \in Z$ such that $z = (y, v, u)$ and $\delta z \in TZ$ with $\delta z = (\delta y, \delta v, \delta u)$, R^Z is defined by:

$$R^Z_z(\delta z) = (R^Y_y(\delta y), R^V_v(\delta v), R^U_u(\delta u)) \tag{4.39}$$

for given retractions $R^Y : TY \to Y$, $R^V : TV \to V$ and $R^U : TU \to U$. We consider the tangent bundle $p_Y : TY \to Y$, endowed with a connection κ_{TY}, and a corresponding tangent bundle retraction

$$R^{TY}_{y_0,e_0} : T_{y_0,e_0}(TY) \to TY$$

given by:

$$R^{TY}_{y_0,e_0}(\xi_y, \eta_y) = \big(R^Y_{y_0}(\xi_y), A(R^Y_{y_0}(\xi_y))(e_0 + \eta_y)\big) = (y, e) \tag{4.40}$$

From this, we construct a new retraction on the co-tangent bundle $p_{Y^*} : TY^* \to Y$ induced by the adjoint, as described in (3.61). Using the expression (3.61), and given that $A(y) \in L(T_{y_0}Y, T_yY)$, we define the retraction

$$R^{TY^*}_{y_0,\tilde{e}_0} : T_{y_0,\tilde{e}_0}(TY^*) \to TY^*$$

by

$$R^{TY^*}_{y_0,\tilde{e}_0}(\xi_y, \tilde{\eta}_y) = \big(R^Y_{y_0}(\xi_y), (A(y)^{-1})^*(\tilde{e}_0 + \tilde{\eta}_y)\big) = (y, \tilde{e}). \tag{4.41}$$

Using (3.64), the corresponding inverse

$$(R^{TY^*}_{y_0,\tilde{e}_0})^{-1} : TY^* \to T_{y_0,\tilde{e}_0}(TY^*)$$

is given by:

$$(R^{TY^*}_{y_0,\tilde{e}_0})^{-1}(y,\tilde{e}) = \left((R^{Y}_{y_0})^{-1}(y), A(y)^*\tilde{e} - \tilde{e}_0\right). \tag{4.42}$$

Given that $c : Y \times V \times U \to TY^*$, the pullback of c by R^Z and R^{TY^*} is given by:

$$(R^{TY^*})^{-1} \circ c \circ R^Z := \mathbf{c} = (\mathbf{c}_B, \mathbf{c}_F)$$

where, according to (4.39) and (4.42), we have that:

$$\mathbf{c}_B = (R^Y)^{-1} \circ c \circ R^Z \quad \text{and} \quad \mathbf{c}_F = A^* \circ c \circ R^Z. \tag{4.43}$$

In order to obtain $\mathbf{c}_F$, from (4.36), we first perform the pullback $c \circ R^Z$, obtaining:

$$c \circ R^Z = \mathbf{J}'(\xi_y) + \lambda_{C(\xi_y)}\mathbf{C}'(\xi_y) - \mathbf{B}(\xi_y)\xi_u$$

with $\mathbf{J} = J \circ R^Y$, $\mathbf{C} = (R^V)^{-1} \circ C \circ R^Y - (R^V)^{-1}v$ and $\xi_y \in TY$ and $\xi_u \in TU$. Finally, if we denote by $\langle \cdot, \cdot \rangle$, the dual pairing between TY and TY^*, then we have that, for any given $\delta\xi_y \in TY$, the term $\langle \mathbf{c}_F, \delta\xi_y \rangle = \left\langle A^* \circ c \circ R^Z, \delta\xi_y \right\rangle$, is given by:

$$\begin{aligned} \langle \mathbf{c}_F, \delta\xi_y \rangle &= \left\langle A(y)^* \left(\mathbf{J}'(\xi_y) + \lambda_{\mathbf{C}(\xi_y)}\mathbf{C}'(\xi_y) - \mathbf{B}(\xi_y)\xi_u\right), \delta\xi_y \right\rangle & (4.44) \\ &= \left\langle \mathbf{J}'(\xi_y) + \lambda_{\mathbf{C}(\xi_y)}\mathbf{C}'(\xi_y) - \mathbf{B}(\xi_y)u, A(y)\,\delta\xi_y \right\rangle. & (4.45) \end{aligned}$$

meaning that the problem (4.38) can be formulated as:

$$\begin{aligned} \min_{(\xi_y,\xi_u)\in TY\times TU} \mathbf{f}(\xi_y,\xi_u) \;\; \text{s.t.} \;\; & 0 = \langle \mathbf{c}_F, \delta\xi_y \rangle \quad \text{for all} \;\; \delta\xi_y \in TY \\ & 0 = \mathbf{C}(\xi_y). \end{aligned} \tag{4.46}$$

Chapter 5

An SQP-Method on Manifolds

In this chapter we show the construction of an algorithm for equality constrained optimization on manifolds, the content of this section can be found in [OS19]. In the problem setting, as in (4.1), we consider the Hilbert manifolds X, Y and the problem:

$$\min_{x\in X} f(x) \;\; s.t. \;\; c(x) = y_*. \tag{5.1}$$

Here, $f : X \longrightarrow \mathbb{R}$ is a twice differentiable functional with suitable smoothness properties. The twice differentiable operator $c : X \longrightarrow Y$ maps from the manifold X to the manifold Y, and is a submersion.

In this work, particular focus is put on ways to exploit problem structure, and on invariance properties of the algorithm, extending the ideas of affine invariant Newton methods [Deu11]. Our point of departure is an *affine covariant composite step method* [LSW17] which was used to solve optimal control problems, involving finite strain elasticity [LSW14]. Composite steps are a very popular class of optimization methods for equality constrained problems, as can be seen in [CGT00] and the references therein. In the linear setting, the algorithmic idea is to partition the optimization step δx into a normal step δn, that improves feasibility, and a tangential step δt, that improves optimality:

$$\delta x = \delta n + \delta t : \qquad \delta t \in \ker c'(x), \qquad \delta n \in (\ker c'(x))^\perp$$

Close to a solution, δn and δt add up to a Lagrange-Newton step, and fast local convergence is obtained. Far away, the two substeps are suitably scaled to achieve global convergence. The method in [LSW17] is such a composite step method. Its main feature is the invariance under affine transformations of the codomain space of c, known as affine covariance. The invariance properties are also important for algorithms on manifolds, since they render them in a natural way, at least approximately, invariant under the choice of local coordinates.

We generalize the composite step method to manifolds in the following way. At a current iterate x_k, we pullback both the objective f and the constraint mapping c to linear spaces through suitable retraction mappings, obtaining maps $\mathbf{f}$ and $\mathbf{c}$ with linear spaces T_xM and $T_{c(x)}N$ as domain and codomain, namely:

$$\mathbf{f} : T_xX \longrightarrow \mathbb{R} \qquad \mathbf{c} : T_xX \longrightarrow T_{c(x)}Y$$

this is followed by the computation of the normal $\delta n \in \ker \mathbf{c}'^{\perp}$ and tangential $\delta t \in \ker \mathbf{c}'$ steps, corrections that belong to linear spaces. A third correction $\delta s \in \ker \mathbf{c}'^{\perp}$ is computed and will serve as a way to avoid the Marathos effect. Once all corrections are computed, we update by using a retraction on the manifold X via:

$$x_+ = R_x^X(\delta t + \delta n + \delta s).$$

We study the influence of the retractions on the convergence of the algorithm. While the case of second order retractions is relatively straightforward to analyze, the analysis of first order retractions is more subtle, but still yields, after some algorithmic adjustments, local superlinear convergence of our algorithm.

5.1 An Affine Invariant Composite Step Method

In [LSW17] a composite step method for the solution of equality constrained optimization with partial differential equations has been proposed. We will briefly recapitulate its most important features. For details we refer to [LSW17]. There, in the problem setting, a Hilbert space $(X, \langle \cdot, \cdot \rangle)$ together with a reflexive Banach space P are considered in order to solve the following optimization problem

$$\min_{x \in X} f(x) \;\; s.t \;\; c(x) = 0. \tag{5.2}$$

The functional $f : X \longrightarrow \mathbb{R}$ is twice continuously Fréchet differentiable and the nonlinear operator $c : X \longrightarrow P^*$ maps into the dual space of P so it can model a differential equation in weak form:

$$c(x) = 0 \text{ in } P^* \iff c(x)v = 0 \text{ for all } v \in P. \tag{5.3}$$

The Lagrangian function L is given by

$$L(x, p) := f(x) + pc(x) \tag{5.4}$$

where the element p is the Lagrange multiplier at x. By $pc(x)$ we denote the dual pairing $P \times P^* \to \mathbb{R}$ with $pc(x) \in \mathbb{R}$. First and second derivatives of the Lagrangian function are:

$$L'(x, p) = f'(x) + pc'(x) \tag{5.5}$$

and

$$L''(x, p) = f''(x) + pc''(x). \tag{5.6}$$

In the *composite step method*, feasibility and optimality are carried out by splitting the full Lagrange-Newton step δx into a *normal step* δn and a *tangential step* δt. The normal step δn is a minimal norm Gauss-Newton step for the solution of the underdetermined problem $c(x) = 0$, and δt aims to minimize f on the current nullspace of the linearized constraints. For this, a *cubic regularization method* is employed. The following local problems are solved

$$\begin{aligned}
\min_{\delta x} f(x) + f'(x)\delta x + \frac{1}{2}L''(x,p)(\delta x, \delta x) + \frac{[\omega_f]}{6}\|\delta x\|^3 \\
s.t. \; \nu c(x) + c'(x)\delta x = & 0, \\
\frac{[\omega_c]}{2}\|\delta x\| \leq & \Theta_{aim},
\end{aligned}$$

where $\nu \in (0,1]$ is an adaptively computed damping factor, $[\omega_c]$ and $[\omega_f]$ are algorithmic parameters, and Θ_{aim} is a user provided desired contraction factor. The parameters $[\omega_c]$ and $[\omega_f]$ are used for globalization of this optimization algorithm. They are used to quantify the mismatch between the quadratic model to be minimized and the nonlinear problem to be solved.

5.1.1 Computation of Composite Steps

Here, we show how to compute the normal step Δn, the Lagrange multiplier p_x and the tangential step Δt, for the equality constrained problem in the linear setting. All these quantities are computed as solutions of certain saddle point problems. As a review, we present the way these quantities are computed, which also serves as a motivation for the manifold case, for more details see [LSW17]. In this section we suppose that $f : X \longrightarrow \mathbb{R}$ is twice continuously differentiable, X is a Hilbert space, $c(x) : X \longrightarrow P^*$ is a bounded, surjective twice differentiable mapping, and P is a reflexive space.

Normal Step. It is well known that the minimal norm problem

$$\min_{v \in X} \frac{1}{2} \langle v, v \rangle \quad s.t \quad c'(x)v + g = 0, \tag{5.7}$$

is equivalent to the linear system

$$\begin{pmatrix} M & c'(x)^* \\ c'(x) & 0 \end{pmatrix} \begin{pmatrix} v \\ q \end{pmatrix} + \begin{pmatrix} 0 \\ g \end{pmatrix} = 0 \tag{5.8}$$

for some $g \in P^*$. Then, as shown in [LSW17], $v \in \ker c'(x)^\perp$. If the solution of the latter system is denoted as $v = -c'(x)^- g$, then we define the full normal step via

$$\Delta n := -c'(x)^- c(x).$$

For globalization, a damping factor $\nu \in]0,1]$ is applied, setting $\delta n := \nu \Delta n$.

Lagrangian Multiplier. At a point $x \in X$ we first compute a Lagrange multiplier p_x as the solution to the system:

$$\begin{pmatrix} M & c'(x)^* \\ c'(x) & 0 \end{pmatrix} \begin{pmatrix} v \\ p_x \end{pmatrix} + \begin{pmatrix} f'(x) \\ 0 \end{pmatrix} = 0. \tag{5.9}$$

It has been shown in [LSW17] that p_x is given uniquely, if $c'(x)$ is surjective, and p_x satisfies

$$f'(x)w + p_x c'(x)v = 0 \;\; \forall v \, \in \, \ker c'(x)^\perp.$$

This p_x will be called the Lagrange multiplier of the problem (5.2) at x.

Tangential Step. With the help of p_x we define the quadratic model

$$q(\delta x) := f(x) + f'(x)\delta x + \frac{1}{2}L''(x, p_x)(\delta x, \delta x) \tag{5.10}$$

on $\ker c'(x)$. We solve the following quadratic problem in order to find the tangential step δt

$$\min_{\Delta t} q(\delta n + \Delta t) \quad \text{s. t.} \quad c'(x)\Delta t = 0. \tag{5.11}$$

which is equivalent to

$$\min_{\Delta t} \left(L'(x, p_x) + L''(x, p_x)\delta n\right) \Delta t + \frac{1}{2}L''(x, p_x)(\Delta t, \Delta t) \quad \text{s.t.} \quad c'(x)\Delta t = 0, \tag{5.12}$$

with corresponding first order optimality conditions

$$\begin{pmatrix} L''(x, p_x) & c'(x)^* \\ c'(x) & 0 \end{pmatrix} \begin{pmatrix} \Delta t \\ q \end{pmatrix} + \begin{pmatrix} L'(x, p_x) + L''(x, p_x)\delta n \\ 0 \end{pmatrix} = 0. \tag{5.13}$$

as long as L'' is positive definite on $\ker c'(x)$, which assures the existence of an exact minimizer. For the purpose of globalization, a cubic term is added to q, ensuring also existence of a minimizer, if positive definiteness fails. More details can be found in [LSW17].

Simplified Normal Step. For purpose of globalization and to avoid the Maratos effect, we compute a simplified normal step, which also plays the role of a second order correction.
The simplified Newton step is defined as

$$\delta s := -c'(x)^-(c(x + \delta x) - c(x) - c'(x)\delta x), \tag{5.14}$$

which amount in solving a system of type (5.8). It can be seen from (5.8) that $\delta s \in \ker c'(x)^\perp$, and thus $(f'(x) + p_x c'(x))\delta s = 0$. It has been shown in [LSW17] that $f(x + \delta x + \delta s) - q(\delta x) = o(\|\delta x\|^2)$ is asymptotically more accurate than $f(x + \delta x) - q(\delta x) = O(\|\delta x\|^2)$. We will extend this result to the case of manifolds.

Update of iterates. If δx satisfies some acceptance criteria (cf. [LSW17]), the next iterate is computed as:

$$x_+ = x + \delta x + \delta s.$$

Of course, computation is only possible, because X is a linear space. To generalize our algorithm to manifolds, we have to replace this update by something different.

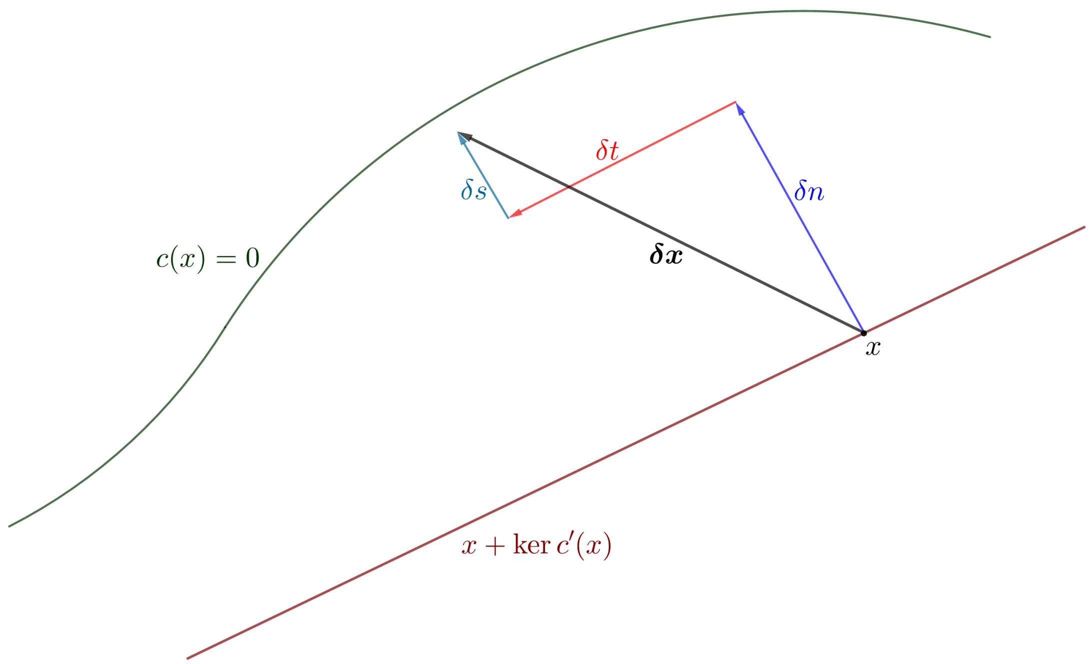


Figure 5.1: *Sketch of a composite step*

5.2 Composite Step Method on Manifolds

We generalize the *composite step method* from the setting of linear spaces, to the one in which the involved spaces are manifolds. Now, as in (4.1), we consider the problem

$$\min_{x \in X} f(x) \;\text{ s.t }\; c(x) = y_*. \tag{5.15}$$

where the twice differentiable functional $f : X \longrightarrow \mathbb{R}$ is defined over the manifold X and the twice differentiable submersion $c : X \longrightarrow Y$ maps from the manifold X to the manifold Y. Further, $y_* \in Y$ is the required point.

Classical SQP-methods on vector spaces introduce local quadratic models for f and c at a given iterate x. In addition, an SQP-method on a manifold has to provide local linear models for the nonlinear manifolds X and Y at x. From a differential geometric point of view, the tangent spaces T_xX and T_yY can be used for this purpose. Now, local linear models for f and c can be defined as $T_xf : T_xX \to \mathbb{R}$ and $T_xc : T_xX \to T_{c(x)}Y$. However, quadratic approximations cannot be defined canonically. In differential geometry there are several ways to introduce additional structure to solve this problem. One well known example among these structures is a Riemannian metric, which allows the definition of geodesics and of the exponential map:

$$\exp_x : T_xX \to X$$

that locally maps each tangent vector $v \in T_xX$ to a geodesic, starting in x in direction v. Now

pullbacks of f and c can be computed, and their corresponding first and second derivatives can be used to define quadratic models of f and c on T_xX and T_yY.
In this way, a quadratic optimization problem with linear constraints can be defined on T_xX and corresponding corrections δn, δt and p_x can be computed in a similar way as in Section 5.1.1 and also a trial step δx. By the exponential map a new iterate can be found via $x_+ = \exp_x(\delta x)$.
These considerations lay the ground for the following section. First, we describe how to derive local quadratic models with the help of retractions and how to compute the substeps δn and δt on T_xM. Then, with the introduced notion of consistency of a pair of retractions, we discuss the consequences for SQP-algorithms. In particular, we will derive a quadratic model that is useful for a first order pair of retractions.

Remark 5.2.1. *From a practical point of view, optimization algorithms on manifolds need not necessarily be based on the notion of tangent spaces and retractions. It is sufficient to define a local chart at each iterate, compute a local update in the chart with the help of a suitable quadratic model, and then perform the update by applying the local chart to the update.*

Next, we will extend our SQP-algorithm to the case of manifolds, using retractions. For a given iterate $x \in X$ with $y = c(x) \in Y$ we have to perform two tasks:

1. Construct a linear-quadratic model of f and c on T_xX and T_yY. This will be done, using C^2-retractions $R^X_{x,1}$ and $R^Y_{y,1}$, as for example the exponential maps. These retractions need not be implemented, but serve are a way to derive linear and quadratic terms that make up the model. With the help of this model, a trial direction δx can be computed just as in the vector space case.

2. Given δx, compute an update that generalizes $x + \delta x$. This will be done, using a retraction $R^X_{x,2}$ on X and a retraction $R^Y_{y,2}$ on Y. Only $R^X_{x,2}$ and $(R^Y_{y,2})^{-1}$ have to be implemented.

The assumptions 4.2.1 will be taken.

5.2.1 Computation of the Steps

The computation of the normal and tangential corrections, as well as the Lagrange multiplier, are done similarly as in the linear case. First, the mappings are pullbacked to linear spaces through the local retractions and there, we compute the quantities as solution of certain saddle point problems. We perform the pullbacks of the problem (5.15) as done in (4.2), through a pair of retractions (R^X_x, R^Y_y).

Normal Step. We note that the minimal norm problem

$$\min_{w \in T_xX} \frac{1}{2}\langle w, w\rangle \ s.t.\ \mathbf{c}'(0_x)w + g = 0, \tag{5.16}$$

is equivalent to finding $w \in \ker \mathbf{c}'(0_x)^\perp$ such that $\mathbf{c}'(0_x)w + g = 0$ and we write in short $w = -\mathbf{c}'(0_x)^- g$.

Let $\mathbf{M}_x : T_xX \to (T_xX)^*$ given via $(\mathbf{M}_x v)w = \langle v, w\rangle$ and thus symmetric and elliptic. Then the system:

$$\begin{pmatrix} \mathbf{M}_x & \mathbf{c}'(0_x)^* \\ \mathbf{c}'(0_x) & 0 \end{pmatrix} \begin{pmatrix} w \\ q \end{pmatrix} + \begin{pmatrix} 0 \\ g \end{pmatrix} = 0 \tag{5.17}$$

corresponds to the KKT-conditions for (5.16), and thus the solutions of (5.17) and (5.16) coincide. Now, we can define the full normal step as follows:

$$\Delta n := -\mathbf{c}'(0_x)^-(\mathbf{c}(0_x) - \mathbf{y}_*). \tag{5.18}$$

as solution of (5.17) and (5.16) with $g = \mathbf{c}(0_x) - \mathbf{y}_*$, where $\mathbf{y}_* = (R_y^Y)^{-1}(y_*)$. For globalization we will use damped normal steps $\delta n := \nu\Delta n$ with a damping factor $\nu \in]0, 1]$.

Lagrangian Multiplier. The Lagrange multiplier is the element p_x that solves

$$\begin{pmatrix} \mathbf{M}_x & \mathbf{c}'(0_x)^* \\ \mathbf{c}'(0_x) & 0 \end{pmatrix} \begin{pmatrix} w \\ p_x \end{pmatrix} + \begin{pmatrix} \mathbf{f}'(0_x) \\ 0 \end{pmatrix} = 0$$

and the latter, implies that p_x satisfies

$$\mathbf{f}'(0_x)v + p_x\mathbf{c}'(0_x)v = 0 \quad \forall v \in \ker \mathbf{c}'(0_x)^\perp. \tag{5.19}$$

Note that p_x is a linear function:

$$p_x : T_{\mathbf{c}(0_x)}Y \longrightarrow \mathbb{R}$$

i.e., $p_x \in T_{\mathbf{c}(0_x)}Y^*$. It can be easily observed that p_x is independent of the choice of first order retraction, as long as $\mathbf{M}_x$ does not change.

Tangential Step. Up to now, the computed quantities do not depend on the choice of retraction. However, the tangent step will. After computing Δn a damping factor ν, such that $\delta n = \nu\Delta n$, and an adjoint state p_x, we compute the tangential step $\delta t \in \ker \mathbf{c}'(0_x)$. Using (4.16) and (4.17), we define the quadratic model through a pair of retractions $(R_{x,1}^X, R_{y,1}^Y)$ as:

$$\mathbf{q}_1(\delta x) := \mathbf{f}(0_x) + \mathbf{f}'(0_x)\delta x + \frac{1}{2}\mathbf{L}_1''(0_x, p_x)(\delta x, \delta x),$$

if $\delta x := \delta n + \Delta t$ with $\Delta t \in \ker \mathbf{c}'(0)$ and $\delta n \in \ker \mathbf{c}'(0)^\perp$ then

$$\mathbf{q}_1(\delta x) = \mathbf{f}(0_x) + \mathbf{f}'(0_x)(\Delta t + \delta n) + \frac{1}{2}\mathbf{L}_1''(0_x, p_x)(\Delta t + \delta n, \Delta t + \delta n)$$

For given $\delta n = \nu\Delta n$ the tangential step δt is found by solving approximately the problem

$$\min_{\Delta t} \mathbf{q}_1(\delta n + \Delta t) \;\; s.t \;\; \mathbf{c}'(0_x)\Delta t = 0,$$

which, after adding the term $p_x\mathbf{c}'(0_x)\Delta t = 0$ and omitting terms that are independent of δt is equivalent to:

$$\begin{aligned} &\min_{\Delta t} \left(\mathbf{L}'(0_x, p_x) + \mathbf{L}_1''(0_x, p_x)\delta n\right)\Delta t + \frac{1}{2}\mathbf{L}_1''(0_x, p_x)(\Delta t, \Delta t) \\ &\text{s.t.} \quad \mathbf{c}'(0_x)\Delta t = 0. \end{aligned}$$

By assumption, since the pair (R_1^X, R_1^Y) is a sufficiently smooth pair of retractions, this yields a quadratic problem that can be solved by standard means. Of course, in the presence of non-convexity an exact solution does not always exist, but there are various algorithmic ways (e.g., truncated cg) to compute an appropriate surrogate.
Close to a solution satisfying the second order conditions ($\mathbf{L}_1''$ positive definite on $\ker \mathbf{c}'$) then the solution to the previous problem exists, and the first order optimality conditions are

$$\begin{pmatrix} \mathbf{L}_1''(0_x, p_x) & \mathbf{c}'(0_x)^* \\ \mathbf{c}'(0_x) & 0 \end{pmatrix} \begin{pmatrix} \Delta t \\ q \end{pmatrix} + \begin{pmatrix} \mathbf{L}'(0_x, p_x) + \mathbf{L}_1''(0_x, p_x)\delta n \\ 0 \end{pmatrix} = 0. \tag{5.20}$$

Again, for purpose of globalization we may compute a different tangent step δt (using, for example a line-search, a trust-regions, or cubic regularization), and set $\delta x = \delta n + \delta t$.

Simplified Normal Step. In the same way as above, a simplified normal step can be computed via

$$\delta s := -\mathbf{c}'(0_x)^- \left(\mathbf{c}_2(\delta x) - \mathbf{c}(0_x) - \mathbf{c}'(0_x)\delta x\right), \tag{5.21}$$

which is used for our globalization mechanism and as a second order correction. For the computation of δs, we have to evaluate $\mathbf{c}_2(\delta x)$. This is possible, because $R_{x,2}^X$ and $(R_{y,2}^Y)^{-1}$ are implemented. Since this is not the case for $R_{x,1}^X$ and $(R_{y,1}^Y)^{-1}$ it would not be possible to evaluate $\mathbf{c}_1(\delta x)$.

Updates of Iterates. As already noted before, new iterates are computed using $R_{x,2}^X$, namely:

$$x_+ := R_{x,2}^X(\delta x + \delta s).$$

Thus, for the new objective function value, we obtain:

$$f(x_+) = f(R_{x,2}^X(\delta x + \delta s)) = \mathbf{f}_2(\delta x + \delta s).$$

5.2.2 Consistency of Quadratic Models

To study invariance, we consider the case that our local model, depending on $\mathbf{f}$, $\mathbf{c}$, and its first and second derivatives, is computed with respect to the retractions R_1^X and R_1^Y, while the actual evaluation of f and c are performed with respect to the retractions R_2^X and R_2^Y. We assume only first order consistency of the first order retractions (R_1^X, R_2^X) and (R_1^Y, R_2^Y).

Lemma 5.2.1. *For a given perturbation $\delta x \in T_xX$, let $\delta s \in \ker \mathbf{c}'(0_x)^\perp$ be the simplified normal step given by the minimal norm solution of the equation:*

$$-\boldsymbol{c}'(0_x)\delta s = \boldsymbol{c}_2(\delta x) - \boldsymbol{c}(0_x) - \boldsymbol{c}'(0_x)\delta x. \tag{5.22}$$

Then the following identity holds:

$$\boldsymbol{f}_2(\delta x+\delta s)-\boldsymbol{q}_1(\delta x)=\boldsymbol{r}_2(\delta x)+\boldsymbol{s}_2(\delta x)+\frac{1}{2}\left(\boldsymbol{L}'(0_x,p_x)\Phi_X''(\delta x,\delta x)-p_x\Phi_Y''(\boldsymbol{c}'(0_x)\delta n,\boldsymbol{c}'(0_x)\delta n)\right). \tag{5.23}$$

where

$$\begin{aligned}\boldsymbol{r}_2(\delta x)&:=\boldsymbol{L}_2(\delta x,p_x)-\boldsymbol{L}(0_x,p_x)-\boldsymbol{L}'(0_x,p_x)\delta x-\frac{1}{2}\boldsymbol{L}_2''(0_x,p_x)(\delta x,\delta x)\\ \boldsymbol{s}_2(\delta x)&:=\boldsymbol{f}_2(\delta x+\delta s)-\boldsymbol{f}_2(\delta x)-\boldsymbol{f}'(0_x)\delta s.\end{aligned}$$

in addition, we have:

$$\delta s=\int_0^1 \boldsymbol{c}'(0_x)^-(\boldsymbol{c}_2'(\sigma\delta x)-\boldsymbol{c}'(0_x))\delta x\,d\sigma. \tag{5.24}$$

Proof. Using the fundamental theorem of calculus, from (5.22) we get (5.24). In order to proof (5.23), we start with

$$\begin{aligned}\mathbf{r}_2(\delta x)+\mathbf{q}_1(\delta x)&=\mathbf{L}_2(\delta x,p_x)-\mathbf{L}(0_x,p_x)-\mathbf{L}'(0_x,p_x)\delta x-\frac{1}{2}\mathbf{L}_2''(0_x,p_x)(\delta x,\delta x)\\ &\quad+\mathbf{f}(0_x)+\mathbf{f}'(0_x)\delta x+\frac{1}{2}\mathbf{L}_1''(0_x,p_x)(\delta x,\delta x)\\ &=\mathbf{f}_2(\delta x)+p_x[\mathbf{c}_2(\delta x)-\mathbf{c}(0_x)-\mathbf{c}'(0_x)\delta x]+\frac{1}{2}\left(\mathbf{L}_1''(0_x,p_x)-\mathbf{L}_2''(0_x,p_x)\right)(\delta x,\delta x)\\ &=\mathbf{f}_2(\delta x)-p_x\mathbf{c}'(0_x)\delta s-\frac{1}{2}\left(\mathbf{L}'(0_x,p_x)\Phi_X''(\delta x,\delta x)-p_x\Phi_Y''(\mathbf{c}'(0_x)\delta x,\mathbf{c}'(0_x)\delta x)\right),\end{aligned}$$

where the identity (4.20) has been used. Given that $\mathbf{f}'(0_x)\delta s=-p_x\mathbf{c}'(0_x)\delta s$ and adding and subtracting $\mathbf{f}_2(\delta x+\delta s)$, we obtain

$$\begin{aligned}\mathbf{r}_2(\delta x)+\mathbf{q}_1(\delta x)&=\mathbf{f}_2(\delta x+\delta s)-\mathbf{f}_2(\delta x+\delta s)+\mathbf{f}_2(\delta x)+\mathbf{f}'(0_x)\delta s\\ &\quad-\frac{1}{2}\left(\mathbf{L}'(0_x,p_x)\Phi_X''(\delta x,\delta x)-p_x\frac{1}{2}\Phi_Y''(\mathbf{c}'(0_x)\delta x,\mathbf{c}'(0_x)\delta x\right).\end{aligned}$$

Using finally $\mathbf{c}'(0_x)\delta x=\mathbf{c}'(0_x)\delta n$ we obtain (5.23). □

We observe that the difference of $\mathbf{f}_2$ to $\mathbf{q}_1$ is now second order, and not, as desired, of third order. There are two terms involved:

- The first term $\mathbf{L}'(0_x,p_x)\Phi_X''(\delta x,\delta x)$ is due to the lack of second order consistency of Φ_X. We observe, however, that $\mathbf{L}'(0_x,p_x)\Phi_X''(\delta x,\delta x)$ vanishes at a KKT point and is small in a neighborhood thereof.

- The second term $p_x\Phi_Y''(\mathbf{c}'(0_x)\delta x,\mathbf{c}'(0_x)\delta x)$ only affects normal directions, but it does not vanish at a KKT point. So it may affect the acceptance criteria of a globalization scheme and slow down local convergence.

5.2.3 A Second Order Quadratic Model for First Order Retractions

In the following, we consider again first order consistent pairs of first order retractions. Taking into account that Φ_Y does not influence the computation of the steps, but may have negative effects on the globalization scheme, we look for an alternative to the quadratic model $\mathbf{q}_1$ with better consistency properties. Here we have to keep in mind that $\mathbf{L}_2''(0_x, p_x)$ is not available.
If (R_1^Y, R_2^Y) is second order consistent, then we use $\mathbf{q}_1$ as a model. However, the case when (R_1^Y, R_2^Y) is only first order consistent, we propose to give the following surrogate model:

$$\begin{aligned}\tilde{\mathbf{q}}(\delta n)(\delta t) &:= \mathbf{L}_2(\delta n, p_x) - (1-\nu)p_x\mathbf{c}(0_x) + (\mathbf{f}'(0_x) + \mathbf{L}_1''(0_x, p)\delta n)\delta t + \frac{1}{2}\mathbf{L}_1''(0_x, p)(\delta t, \delta t)\\ &= \mathbf{f}_2(\delta n) + p_x(\mathbf{c}_2(\delta n) - (1-\nu)\mathbf{c}(0_x)) + (\mathbf{f}'(0_x) + \mathbf{L}_1''(0_x, p)\delta n)\delta t + \frac{1}{2}\mathbf{L}_1''(0_x, p)(\delta t, \delta t).\end{aligned} \tag{5.25}$$

With this, we will show below:

$$\mathbf{f}_2(\delta x + \delta s) - \tilde{\mathbf{q}}(\delta n)(\delta t) = \frac{1}{2}\mathbf{L}'(0_x, p_x)(\Phi_X''(\delta x, \delta x) - \Phi_X''(\delta n, \delta n)) + o(\|\delta x\|^2).$$

Close to a KKT-point, the remaining second order term is small. It turns out that such a model is sufficient to show local superlinear convergence. The evaluation of $\tilde{\mathbf{q}}(\delta n)(\delta t)$ requires the evaluation of $\mathbf{L}_2(\delta n, p_x)$ which has to be done once per outer iteration. If $\nu < 1$, which is the case far away from a feasible point, $\mathbf{q}_1$ is used as a model.

Lemma 5.2.2. *For the surrogate model $\tilde{\mathbf{q}}$, we have that:*

$$\tilde{\mathbf{q}}(0_x, \delta n)(\delta t) - \boldsymbol{q}_1(\delta x) = r_2(\delta n) + \frac{1}{2}\left(\boldsymbol{L}'(0_x, p_x)\Phi_X''(\delta n, \delta n) - p_x\Phi_Y''(\boldsymbol{c}'(0_x)\delta n, \boldsymbol{c}'(0_x)\delta n)\right). \tag{5.26}$$

In particular, for fixed δn:

$$\underset{\delta t \in \ker \mathbf{c}'(0_x)}{\operatorname{argmin}}\ \tilde{\mathbf{q}}(\delta n)(\delta t) = \underset{\delta t \in \ker \mathbf{c}'(0_x)}{\operatorname{argmin}}\ \mathbf{q}_1(\delta n + \delta t).$$

Proof. By definition of $\mathbf{q}_1(v)$ we obtain, using the fact that $\nu p_x\mathbf{c}(0_x) = -p_x\mathbf{c}'(0_x)\delta n = \mathbf{f}'(0_x)\delta n$

$$\begin{aligned}&\mathbf{L}_2(\delta n, p_x) - \mathbf{L}(0_x, p_x) + \mathbf{q}_1(\delta x) - \frac{1}{2}\mathbf{L}_1''(0_x, p_x)\delta n^2\\ &\qquad = \mathbf{L}_2(\delta n, p_x) - \mathbf{f}(0_x) - p_x\mathbf{c}(0_x) + \mathbf{f}(0_x) + \mathbf{f}'(0_x)\delta x + \frac{1}{2}\mathbf{L}_1''(0_x, p_x)\delta x^2 - \frac{1}{2}\mathbf{L}_1''(0_x, p_x)\delta n^2\\ &\qquad = \mathbf{L}_2(\delta n, p_x) + (\nu - 1)p_x\mathbf{c}(0_x) + \mathbf{f}'(0_x)\delta t + \frac{1}{2}\mathbf{L}_1''(0_x, p_x)(\delta x + \delta n, \delta t) = \tilde{\mathbf{q}}(\delta n)(\delta t).\end{aligned}$$

Taking into account

$$\mathbf{L}_2(\delta n, p_x) - \mathbf{L}(0_x, p_x) = \mathbf{r}_2(\delta n) + \mathbf{L}'(0_x, p_x)\delta n + \frac{1}{2}\mathbf{L}_2''(0_x, p_x)\delta n^2 = \mathbf{r}_2(\delta n) + \frac{1}{2}\mathbf{L}_2''(0_x, p_x)\delta n^2$$

and (4.20) we obtain (5.26). $\square$

Lemma 5.2.3. *For the surrogate model* $\tilde{\mathbf{q}}$*, we have the identity*

$$\boldsymbol{f}_2(\delta x + \delta s) - \tilde{\mathbf{q}}(\delta n)(\delta t) = \boldsymbol{r}_2(\delta x) - \boldsymbol{r}_2(\delta n) + \boldsymbol{s}_2(\delta x) + \frac{1}{2}\boldsymbol{L}'(0_x, p_x)(\Phi''_X(\delta x, \delta x) - \Phi''_X(\delta n, \delta n)). \tag{5.27}$$

Proof. By Lemma 5.2.1 and Lemma 5.2.2 we compute

$$\begin{aligned}
\mathbf{f}_2(\delta x + \delta s) - \tilde{\mathbf{q}}(\delta n)(\delta t) &= (\mathbf{f}_2(\delta x + \delta s) - \mathbf{q}_1(\delta x)) - (\tilde{\mathbf{q}}(\delta n)(\delta t) - \mathbf{q}_1(\delta x)) \\
&= \mathbf{r}_2(\delta x) + \mathbf{s}_2(\delta x) + \frac{1}{2}\left(\mathbf{L}'(0_x, p_x)\Phi''_X(\delta x, \delta x) - p_x\Phi''_Y(\mathbf{c}'(0_x)\delta n, \mathbf{c}'(0_x)\delta n)\right) \\
&\quad - \mathbf{r}_2(\delta n) - \frac{1}{2}\left(\mathbf{L}'(0_x, p_x)\Phi''_X(\delta n, \delta n) - p_x\Phi''_Y(\mathbf{c}'(0_x)\delta n, \mathbf{c}'(0_x)\delta n)\right) \\
&= \mathbf{r}_2(\delta x) + \mathbf{s}_2(\delta x) - \mathbf{r}_2(\delta n) + \frac{1}{2}\mathbf{L}'(0_x, p_x)\left(\Phi''_X(\delta x, \delta x) - \Phi''_X(\delta n, \delta n)\right).
\end{aligned}$$

The crucial observation is that $p_x\Phi''_Y(\mathbf{c}'(0_x)\delta n, \mathbf{c}'(0_x)\delta n)$ cancels out. □

To quantify the remainder terms, we have to use quantitative assumptions on the nonlinearity of the problem and the retractions.

Proposition 5.2.1. *Assume that there are constants* $\omega_{\boldsymbol{c}_2}$, $\omega_{\boldsymbol{f}'_2}$ *and* $\omega_{\boldsymbol{L}_2}$ *such that*

$$\|\boldsymbol{c}'(0_x)^-(\boldsymbol{c}'_2(v) - \boldsymbol{c}'(0_x))w\| \leq \omega_{\boldsymbol{c}_2}\|v\|\|w\|, \tag{5.28}$$

$$|(\boldsymbol{L}''_2(v, p_x) - \boldsymbol{L}''_2(0_x, p_x))(v, w)| \leq \omega_{\boldsymbol{L}_2}\|v\|^2\|w\|, \tag{5.29}$$

$$|(\boldsymbol{f}'_2(v) - \boldsymbol{f}'(0_x))w| \leq \omega_{\boldsymbol{f}'_2}\|v\|\|w\| \tag{5.30}$$

i.e., Lipschitz conditions holds for the pullback mappings with retraction R^X_2 *and* R^Y_2*, where* v *and* w *are arbitrary. Then for arbitrary* δx *and simplified normal step* δs *as defined in* (5.22) *we have the estimates:*

$$\begin{aligned}
\|\delta s\| &\leq \frac{\omega_{\boldsymbol{c}_2}}{2}\|\delta x\|^2 \\
|\boldsymbol{f}_2(\delta x + \delta s) - \tilde{\mathbf{q}}(0_x, \delta n)(\delta t)| &\leq \left(\frac{\omega_{\boldsymbol{L}_2}}{3} + \frac{\omega_{\boldsymbol{f}'_2}\omega_{\boldsymbol{c}_2}}{2}(1 + \frac{\omega_{\boldsymbol{c}_2}}{4}\|\delta x\|)\right)\|\delta x\|^3 + \frac{1}{2}|\boldsymbol{L}'(0_x, p_x)(\Phi''_X(\delta x^2) - \Phi''_X(\delta n^2))|
\end{aligned}$$

Proof. By Assumption 4.2.1 all stated derivatives exist. In particular $\mathbf{L}''_2(v, p_x)(v, w)$ exists as a directional derivative of $\mathbf{L}'_2(v, p_x)w$ in direction v, since R^X_2 is a C^2-retraction. This is all we need in the following.

From (5.24), setting $v = \sigma\delta x$, we have that

$$\|\delta s\| \leq \int_0^1 \frac{1}{\sigma}\|\mathbf{c}'(0_x)^-(\mathbf{c}'_2(\sigma\delta x) - \mathbf{c}'(0_x))\sigma\delta x\|\, d\sigma \leq \frac{\omega_{\mathbf{c}_2}}{2}\|\delta x\|^2$$

by Lemma 5.2.3 we get

$$|\mathbf{f}_2(\delta x + \delta s) - \tilde{\mathbf{q}}(\delta n)(\delta t)| \leq |\mathbf{r}_2(\delta x)| + |\mathbf{r}_2(\delta n)| + |\mathbf{s}_2(\delta x)| + \frac{1}{2}|\mathbf{L}'(0_x, p_x)(\Phi''_X(\delta x)^2 - \Phi''_X(\delta n)^2)|. \tag{5.31}$$

Assuming the affine covariant Lipschitz conditions, we get that

$$|\mathbf{r}_2(v)| \leq \int_0^1 \int_0^1 \frac{1}{\tau^2\sigma} |(\mathbf{L}_2''(\tau\sigma v, p_x) - \mathbf{L}_2''(0_x, p_x))(\tau\sigma v, \tau\sigma v)| \, d\tau d\sigma \leq \omega_{\mathbf{L}_2} \|v\| \int_0^1 \int_0^1 \tau\sigma^2 \, d\tau d\sigma = \frac{\omega_{\mathbf{L}_2}}{6} \|v\|^3$$

v is arbitrary, then the latter hold for $v = \delta x$ and $v = \delta n$

$$|\mathbf{r}_2(\delta x)| + |\mathbf{r}_2(\delta n)| \leq \frac{\omega_{\mathbf{L}_2}}{6} \|\delta x\|^3 + \frac{\omega_{\mathbf{L}_2}}{6} \|\delta n\|^3 \leq \frac{\omega_{\mathbf{L}_2}}{3} \|\delta x\|^3$$

and for $\mathbf{s}_2$ we obtain

$$\begin{aligned} |\mathbf{s}_2(\delta x)| &\leq \int_0^1 |(\mathbf{f}_2'(\delta x + \sigma \delta s) - \mathbf{f}'(0_x)\delta s)| d\sigma \leq \omega_{\mathbf{f}_2'} \|\delta s\| \int_0^1 \|\delta x + \sigma \delta s\| \, d\sigma \\ &\leq \omega_{\mathbf{f}'} \|\delta s\| \left(\|\delta x\| + \frac{1}{2} \|\delta s\| \right) \leq \frac{\omega_{\mathbf{f}'} \omega_{\mathbf{c}_2}}{2} \|\delta x\|^2 \left(\|\delta x\| + \frac{\omega_{\mathbf{c}_2}}{4} \|\delta x\|^2 \right) \end{aligned}$$

Adding all estimates up, we obtain the desired estimate. □

5.3 Globalization Scheme

In [LSW17, Section 4] a globalization scheme has been proposed for an affine covariant composite step method. In the following we will recapitulate its main features and adjust it to the case of manifolds, where necessary. Since our aim is to study local convergence of our algorithm, we concentrate on the aspects of our scheme that are relevant for local convergence.
Each step of the globalization scheme at a current iterate x will be performed on T_xX and T_yY, using $R^X_{x,i}$ and $R^Y_{y,i}$ as retractions to pull f and c back to T_xX and T_yY, as sketched in the previous section. Then the globalization scheme from [LSW17] can be used.
For given algorithmic parameters $[\omega_{\mathbf{f}}]$ and $[\omega_{\mathbf{c}}]$ and given damping-parameters ν, we compute the new trial correction δx as follows after Δn, p_x, Δt, ν have been computed.

$$\begin{aligned} \min_{\tau:\delta x = \nu\Delta n + \tau\Delta t} \mathbf{f}(0_x) + \mathbf{f}'(x)\delta x + \frac{1}{2}\mathbf{L}_1''(x,p)(\delta x, \delta x) + \frac{[\omega_{\mathbf{f}}]}{6}\|\delta x\|^3 & \\ s.t. \ \nu\mathbf{c}(x) + \mathbf{c}'(x)\delta x = 0&, \\ \frac{[\omega_{\mathbf{c}}]}{2}\|\delta x\| \leq \Theta_{\text{aim}}&, \end{aligned} \tag{5.32}$$

With the restriction $\delta x = \nu\Delta n + \tau\Delta t$. This problem is actually a scalar problem in τ, which is simple to solve. More sophisticated strategies to compute δt directly as an approximate minimizer of the cubic model are conceivable and have been described in the literature.
As elaborated in [LSW17], we use the algorithmic parameter $[\omega_{\mathbf{c}}]$ to capture the nonlinearity of c, while $[\omega_{\mathbf{f}}]$ models the nonlinearity of f. Initial estimates have to be provided.
After computation of Δn, we compute a maximal damping factor $\nu \in]0,1]$ and $\delta n := \nu\Delta n$, such that

$$\frac{[\omega_c]}{2}\|\delta n\| \leq \rho_{\text{ellbow}}\Theta_{\text{aim}}.$$

Algorithm 2 Outer and inner loop (inner loop simplified)

Require: initial iterate x, $[\omega_{\mathbf{c}}], [\omega_{\mathbf{f}}]$
  repeat// *NLP loop*
    choose retractions $R^X_{x,2}$, $R^Y_{y,2}$ at x and y
    compute quadratic models of f and c, based on $R^X_{x,1}$ and $R^Y_{y,1}$
    repeat// *step computation loop*
      compute Δn, p_x
      compute maximal $\nu \in]0,1]$, such that $\frac{[\omega_{\mathbf{c}}]}{2}\|\nu\Delta n\| \leq \rho_{\text{ellbow}}\Theta_{\text{aim}}$
      compute Δt via (5.20)
      compute trial correction δx, via (5.32)
      compute simplified correction δs, via (5.22)
      evaluate acceptance tests (5.33) and (5.35)
      compute new Lipschitz constants $[\omega_{\mathbf{c}}], [\omega_{\mathbf{f}}]$, using δs, $\mathbf{f}_2(\delta x + \delta s)$, and $\mathbf{q}_1(\delta x)$ or $\tilde{\mathbf{q}}(\delta n)(\delta t)$
    until trial correction δx accepted
    $x \leftarrow R^X_{x,2}(\delta x + \delta s)$
  until converged

Here $\Theta_{\text{aim}} \in]0,1[$ is a desired Newton contraction for the underdetermined problem $\mathbf{c}_2(x) = 0$ and $\rho_{\text{ellbow}} \in]0,1]$ provides some elbow space in view of the last line of (5.32), which can be seen as a trust-region constraint, governed by the nonlinearity of c.
Then, Δt is computed via (5.20). If $\mathbf{L}''_1$ is not positive definite on $\ker \mathbf{c}'(0_x)$, then a suitable modified solution (e.g., form truncated cg) is used. Then

$$\delta x := \delta n + \tau\Delta t$$

is computed via minimizing (5.32) over τ, and the simplified normal step δs is computed via (5.22). At this point updates for $[\omega_{\mathbf{c}}]$ and $[\omega_{\mathbf{f}}]$ can be computed. Just as in [LSW17] we define

$$[\omega_{\mathbf{c}}] := \frac{2\|\delta s\|}{\|\delta x\|^2}$$

as an affine covariant quantity that measures the nonlinearity of c. Concerning $[\omega_{\mathbf{f}}]$, the use of retractions requires a modification, compared to [LSW17]. We first define

$$\mathbf{q}(\delta x) := \begin{cases} \mathbf{q}_1(\delta x) & : \quad (R^Y_1, R^Y_2) \text{ is second order consistent} \\ \tilde{\mathbf{q}}(\delta n)(\delta t) & : \quad \text{otherwise} \end{cases}$$

and then set:

$$[\omega_{\mathbf{f}}]^{\text{raw}} := \frac{6}{\|\delta x\|^3}(\mathbf{f}_2(\delta x + \delta s) - \mathbf{q}(\delta x)).$$

This (potentially negative) estimate has to be augmented by some save-guard bounds of the form

$$[\omega_{\mathbf{f}}]^{\text{new}} = \min\{\rho_1[\omega_{\mathbf{f}}]^{\text{old}}, \max\{\rho_0[\omega_{\mathbf{f}}]^{\text{old}}, [\omega_{\mathbf{f}}]^{\text{raw}}\}\}$$

with $0 < \rho_0 < 1 < \rho_1$.

For acceptance of iterates, we perform a contraction test and a decrease test. The contraction test requires, just as in [LSW17],

$$\frac{\|\delta s\|}{\|\delta x\|} \leq \Theta_{\text{acc}} \tag{5.33}$$

for acceptance, with some parameter $\Theta_{\text{acc}} \in]\Theta_{\text{des}}, 1[$. For the decrease test we define

$$\mathbf{m}_{[\omega_{\mathbf{f}}]}(v) := \mathbf{q}(v) + \frac{[\omega_{\mathbf{f}}]}{6}\|v\|^3.$$

and require some ratio of actual decrease and predicted decrease condition. We choose $\underline{\eta} \in]0,1[$ and define:

$$\eta := \frac{\mathbf{f}_2(\delta x + \delta s) - \mathbf{m}_{[\omega_{\mathbf{f}}]}(\delta n)}{\mathbf{m}_{[\omega_{\mathbf{f}}]}(\delta x) - \mathbf{m}_{[\omega_{\mathbf{f}}]}(\delta n)}. \tag{5.34}$$

Then we require

$$\eta \geq \underline{\eta} \tag{5.35}$$

for acceptance of the step. As a further modification to [LSW17] we increase $[\omega_{\mathbf{f}}]$ at least by a fixed factor $\rho_2 \in]1, \rho_1]$ with respect to $[\omega_{\mathbf{f}}]^{\text{old}}$, if the decrease condition (5.34) fails. Moreover, $[\omega_{\mathbf{f}}]$ will not be increased, if $\eta \geq \hat{\eta}$, where $\hat{\eta} \in [\underline{\eta}, 1[$ is usually chosen close to 1.

5.4 Local Convergence Analysis

In this section, the transition of the method to fast local convergence is discussed. Throughout, we impose the following assumptions:

Assumption 5.4.1. *Let $x_* \in X$ be a local minimizer of f on $c(x) = y$ and $U \subset X$ a neighborhood of x_*. For $x \in U$ denote $\mathbf{x}_* := (R^X_{x,2})^{-1}x_*$.*

- *$\mathbf{c}'(0_x)$ is surjective and $\mathbf{L}''_1(0_x, p_x)$ is elliptic on $\ker \mathbf{c}'(0_x)$ with uniform constant $\alpha > 0$ and bounded with uniform constant Γ on $x \in U$.*

- *First order retractions $R^X_{x,i}$ and $R^Y_{c(x),i}$ exist for each $x \in U$ and $i = 1, 2$, and there are constants $\underline{c}, \overline{c} > 0$, such that for all $x, \tilde{x} \in U$:*

$$\underline{c}\|(R^X_{x_*,2})^{-1}\tilde{x} - 0_{x_*}\| \leq \|(R^X_{x,2})^{-1}\tilde{x} - (R^X_{x,2})^{-1}x_*\| \leq \overline{c}\|(R^X_{x_*,2})^{-1}\tilde{x} - 0_{x_*}\|. \tag{5.36}$$

  This is a local norm-equivalence condition on the charts.

- *The assumptions of Proposition 5.2.1 hold with uniform bounds on the constants $\omega_{\mathbf{c}_2}, \omega_{\mathbf{L}_2}, \omega_{\mathbf{f}'_2}$.*

- *There is a uniform bound γ, such that*

$$|\mathbf{L}'(0_x, p_x)\Phi''_{X,x}(0_x)(v, w)| \leq \gamma\|\mathbf{x}_* - 0_x\|\|v\|\|w\|. \tag{5.37}$$

  This can be seen as a Lipschitz condition on $\mathbf{L}'$, combined with a regularity assumption on Φ_X.

- *There is ω_* independent of x, such that with $\mathbf{x}_* := (R^X_{x,2})^{-1}x_*$:*

$$|\mathbf{f}_2'(\mathbf{x}_*)\mathbf{c}_2'(\mathbf{x}_*)^-(\mathbf{c}_2'(\mathbf{x}_*) - \mathbf{c}_2'(0_x))w| \le \omega_*\|\mathbf{x}_* - 0_x\|\|w\|.$$

  This is a variant of (5.28)*.*

In the following we consider a sequence x_k, generated by our algorithm. We will show that if x_0 is sufficiently close to x_*, then $x_k \to x_*$ quadratically. Mathematically, taking into account that $(R^X_{x_*,2})^{-1}x_* = 0_{x_*}$ this can be formulated as follows:

$$\exists C_N > 0 : \quad \|(R^X_{x_*,2})^{-1}x_{k+1} - 0_{x_*}\| \le C_N\|(R^X_{x_*,2})^{-1}x_k - 0_{x_*}\|^2. \tag{5.38}$$

We thus want to observe local quadratic convergence of the iterates, transformed to $T_{x_*}X$ via $R^X_{x_*,2}$.

Lemma 5.4.1. *Let $x = x_k$, δx the step, computed by our algorithm, and $\mathbf{x}_* := (R^X_{x,2})^{-1}x_*$. Assume that*

$$\exists \tilde{C}_N > 0 : \quad \|0_x + \delta x - \mathbf{x}_*\| \le \tilde{C}_N\|0_x - \mathbf{x}_*\|^2.$$

Then (5.38) *holds for $x_k = x$ and $x_{k+1} = R^X_{x,2}(0_x + \delta x)$.*

Proof. Let $x_+ = R^X_{x,2}(0_x + \delta x)$ describe one step of our algorithm. Computing

$$\underline{c}\|(R^X_{x_*,2})^{-1}x_+\| \le \|(R^X_{x,2})^{-1}x_+ - (R^X_{x,2})^{-1}x_*\| = \|0_x + \delta x - \mathrm{x}_*\| \le \tilde{C}_N\|0_x - \mathbf{x}_*\|^2 \le \overline{c}^2\tilde{C}_N\|(R^X_{x_*,2})^{-1}x\|^2,$$

yields

$$\|(R^X_{x_*,2})^{-1}x_+\| \le \tilde{C}_N\frac{\overline{c}^2}{\underline{c}}\|(R^X_{x_*,2})^{-1}x\|^2 = C_N\|(R^X_{x_*,2})^{-1}x\|^2$$

□

At a point $x \in X$ we denote $z = (v_x, p)$, $\mathbf{y}_* = (R^Y_{c(x),2})^{-1}y_* = \mathbf{c}_2(\mathbf{x}_*)$ and the nonlinear mapping

$$\mathbf{F}_2(z) = \mathbf{F}_2(v_x, p) = \begin{pmatrix} \mathbf{L}_2'(v_x, p) \\ \mathbf{c}_2(v_x) - \mathbf{y}_* \end{pmatrix} = \begin{pmatrix} \mathbf{L}_2'(v_x, p) \\ \mathbf{c}_2(v_x) - \mathbf{c}_2(\mathbf{x}_*) \end{pmatrix},$$

which results from a pull-back of our original problem via $R^X_{x,2}$ and $R^Y_{c(x),2}$. The full Lagrange-Newton Steps at an iterate $z_0 = (0_x, p)$ reads:

$$\Delta z := (\Delta x, \Delta p) := D_z\mathbf{F}_1(z_0)^{-1}\mathbf{F}_2(z_0), \tag{5.39}$$

which means in more detail:

$$\begin{pmatrix} \mathbf{L}_1''(0_x, p) & \mathbf{c}'(0_x)^* \\ \mathbf{c}'(0_x) & 0 \end{pmatrix}\begin{pmatrix} \Delta x \\ \Delta p \end{pmatrix} + \begin{pmatrix} \mathbf{L}'(0_x, p) \\ \mathbf{c}(0_x) - \mathbf{c}_2(\mathbf{x}_*) \end{pmatrix} = 0.$$

As before, $D_z\mathbf{F}_1(z_0)$ has been computed via the $R^X_{x,1}$ and $R^Y_{c(x),1}$.

Proposition 5.4.1. *Suppose that Assumption 5.4.1 holds close to x_*. Then the full-step variant of our method converges locally quadratically to x_*.*

Proof. We apply one Newton step Δz in T_xX at $z_0 = (0_x, p_x)$ to the following problem:

$$\mathbf{F}_2(z) = 0 \quad :\Leftrightarrow \quad \begin{pmatrix} \mathbf{L}_2'(v_x, p) \\ \mathbf{c}_2(v_x) - \mathbf{c}_2(\mathbf{x}_*) \end{pmatrix} = 0,$$

which results from a pullback of our original problem to T_xX via $R^X_{x,2}$ and $R^Y_{y,2}$. We obtain with $z_+ = z_0 + \Delta z$ and $z_* = (\mathbf{x}_*, p_*)$:

$$z_+ - z_* = z_0 - z_* + \Delta z = D_z\mathbf{F}_1^{-1}(z_0)(D_z\mathbf{F}(z_0)(z_0 - z_*) - \mathbf{F}_2(z_0))$$

Since we only use norms for the primal component, and p depends on x directly, our aim is to show:

$$\|x_+ - \mathbf{x}_*\| \leq C\|0_x - \mathbf{x}_*\|^2.$$

Writing the primal component $x_+ - \mathbf{x}_* = n_+ + t_+$ with $\mathbf{c}'(0_x)t_+ = 0$ and $n_+ \perp \ker \mathbf{c}'(0_x)$ we obtain:

$$n_+ = \mathbf{c}'(0_x)^-(\mathbf{c}'(0_x)(0_x - \mathbf{x}_*) - (\mathbf{c}(0_x) - \mathbf{c}_2(\mathbf{x}_*))).$$

Application of (5.28) yields via the fundamental theorem of calculus:

$$\|n_+\| \leq \frac{\omega_{\mathbf{c}_2}}{2}\|0_x - \mathbf{x}_*\|^2 = \frac{\omega_{\mathbf{c}_2}}{2}\|\mathbf{x}_*\|^2.$$

The tangential component t_+ is a minimizer of the problem:

$$\min_{v \in \ker \mathbf{c}'(0_x)} \frac{1}{2}\mathbf{L}_1''(0_x, p_x)(v, v) + (\mathbf{L}_1''(0_x, p_x)(0_x - \mathbf{x}_*) - \mathbf{L}'(0_x, p_x) + \mathbf{L}_1''(0_x, p_x)n_+)v$$

Due to the assumed uniform ellipticity of $\mathbf{L}_1''(0_x, p_x)$ it is sufficient to obtain an estimate for the linear part of this functional of the form:

$$(\mathbf{L}_1''(0_x, p_x)(0_x - \mathbf{x}_*) - \mathbf{L}'(0_x, p_x) + \mathbf{L}_1''(0_x, p_x)n_+)v \leq c\|\mathbf{x}_*\|^2\|v\|. \tag{5.40}$$

First, we observe that

$$\mathbf{L}_1''(0_x, p_x)(n_+, v) \leq \Gamma\|n_+\|\|v\| \leq \Gamma\frac{\omega_{\mathbf{c}_2}}{2}\|\mathbf{x}_*\|^2\|v\|.$$

Next, we telescope, subtracting $\mathbf{L}_2'(\mathbf{x}_*, p_*) = 0$,

$$\begin{aligned}(\mathbf{L}_1''(0_x, p_x)(0_x - \mathbf{x}_*) - \mathbf{L}'(0_x, p_x))v = {} & (\mathbf{L}_1''(0_x, p_x) - \mathbf{L}_2''(0_x, p_x))(0_x - \mathbf{x}_*, v) \\ & + (\mathbf{L}_2''(0_x, p_x)(0_x - \mathbf{x}_*) - (\mathbf{L}'(0_x, p_x) - \mathbf{L}_2'(\mathbf{x}_*, p_x)))v \\ & + (\mathbf{L}_2'(\mathbf{x}_*, p_x) - \mathbf{L}_2'(\mathbf{x}_*, p_*))v\end{aligned}$$

into a sum of three terms. The first term is estimated via (4.20) and (5.37), taking into account that $v \in \ker \mathbf{c}'(0_x)$:

$$|(\mathbf{L}_1''(0_x, p_x) - \mathbf{L}_2''(0_x, p_x))(0_x - \mathbf{x}_*, v)| = |\mathbf{L}'(0_x, p_x)\Phi''_{X,x}(0_x)(0_x - \mathbf{x}_*, v)| \leq \gamma\|\mathbf{x}_*\|^2\|v\|.$$

The second term is estimated via (5.29), using the fundamental theorem of calculus:

$$(\mathbf{L}_2''(0_x,p_x)(0_x-\mathbf{x}_*)-(\mathbf{L}'(0_x,p_x)-\mathbf{L}_2'(\mathbf{x}_*,p_x)))v \le \frac{\omega_{\mathbf{L}_2}}{2}\|\mathbf{x}_*\|^2\|v\|.$$

For the third term, we compute, using $v\in\ker\mathbf{c}'(0_x)$ and $\mathbf{c}'(0_x)\mathbf{c}'(0_x)^- = Id$:

$$(\mathbf{L}_2'(\mathbf{x}_*,p_x)-\mathbf{L}_2'(\mathbf{x}_*,p_*))v = (p_x-p_*)\mathbf{c}'(0_x)\mathbf{c}'(0_x)^-(\mathbf{c}_2'(\mathbf{x}_*)-\mathbf{c}'(0_x))v = (p_x-p_*)\mathbf{c}'(0_x)w.$$

With $w := \mathbf{c}'(0_x)^-(\mathbf{c}_2'(\mathbf{x}_*)-\mathbf{c}'(0_x))v \in \ker\mathbf{c}'(0_x)^\perp$ this yields $\|w\| \le \omega_{\mathbf{c}_2}\|\mathbf{x}_*\|\|v\|$. We continue, using $p_* = p_*\mathbf{c}_2'(x_*)\mathbf{c}_2'(x_*)^- = -\mathbf{f}_2'(x_*)\mathbf{c}_2'(x_*)^-$:

$$\begin{aligned}|(p_x-p_*)\mathbf{c}'(0_x)w| &= |p_*(\mathbf{c}_2'(\mathbf{x}_*)-\mathbf{c}'(0_x))w-(p_*\mathbf{c}_2'(\mathbf{x}_*)-p_x\mathbf{c}'(0_x))w|\\ &= |-\mathbf{f}_2'(\mathbf{x}_*)\mathbf{c}_2'(\mathbf{x}_*)^-(\mathbf{c}_2'(\mathbf{x}_*)-\mathbf{c}'(0_x))w+(\mathbf{f}_2'(\mathbf{x}_*)-\mathbf{f}'(0_x))w|\\ &\le \omega_*\|\mathbf{x}_*\|\|w\|+\omega_{\mathbf{f}_2}\|\mathbf{x}_*\|\|w\| \le c\|\mathbf{x}_*\|^2\|v\|.\end{aligned}$$

Adding all estimates yields (5.46), as desired. □

Close to an SSC point, we show that the computed, normal and tangential steps, approach to the full Lagrange-Newton steps asymptotically, and from the latter, they inherit local superlinear convergence. On one hand we have that $\delta t = \tau\Delta t$, where $\tau\in(0,1]$ is a damping factor, computed via minimizing

$$\mathbf{m}_{[\omega_\mathbf{f}]}(\delta x) = \mathbf{f}(0_x)+\mathbf{f}'(0_x)\delta x+\frac{1}{2}\mathbf{L}_1''(0_x,p_x)(\delta x,\delta x)+\frac{[\omega_\mathbf{f}]}{6}\|\delta x\|^3 \tag{5.41}$$

in the affine subspace $\delta n+\operatorname{span}\{\Delta t\}$. We have the relation between the optimization step and the full Lagrange-Newton step Δx:

$$\delta x = \delta n+\delta t = \nu\Delta n+\tau\Delta t, \quad \Delta x = \Delta n+\Delta t.$$

Theorem 5.4.1. *Assume that x_k converges to the SSC point x_* and assume that the Lipschitz conditions as in Proposition* 5.2.1 *hold in a neighborhood of x_*. Then we have superlinear convergence.*

Proof. We show that the damping factors ν_k and τ_k tend to 1 as $x\to x_*$. By boundedness of the algorithmic parameter $[\omega_\mathbf{c}]$ the normal damping factor ν_k becomes $\nu_k=1$ eventually, for details see [LSW17].

Concerning τ_k, using the minimizing property of δx_k along the direction Δt_k and by inserting this into the first order optimality conditions for (5.41), we get that:

$$\begin{aligned}0 &= \mathbf{m}_{[\omega_\mathbf{f}]}'(\delta x_k)\Delta t_k\\ &= (\mathbf{f}'(0_{x_k})+\mathbf{L}_1''(0_{x_k},p_{x_k})\delta n_k)\Delta t_k+\mathbf{L}_1''(0_{x_k},p_{x_k})(\delta t_k,\Delta t_k)+\frac{[\omega_\mathbf{f}]}{2}\|\delta x_k\|\langle\delta x_k,\Delta t_k\rangle\\ &= (\mathbf{f}'(0_{x_k})+\mathbf{L}_1''(0_{x_k},p_{x_k})\delta n_k)\Delta t_k+\tau_k\Big(\mathbf{L}_1''(0_{x_k},p_{x_k})(\Delta t_k,\Delta t_k)+\frac{[\omega_\mathbf{f}]}{2}\|\delta x_k\|\langle\Delta t_k,\Delta t_k\rangle\Big)\end{aligned}$$

The equation

$$\begin{aligned}0 = \mathbf{m}_0'(\delta x_k)\Delta t_k &= (\mathbf{f}'(0_{x_k})+\mathbf{L}_1''(0_{x_k},p_{x_k})\delta n_k)\Delta t_k+\mathbf{L}_1''(0_{x_k},p_{x_k})(\delta t_k,\Delta t_k)\\ &= (\mathbf{f}'(0_{x_k})+\mathbf{L}_1''(0_{x_k},p_{x_k})\delta n_k)\Delta t_k+\mathbf{L}_1''(0_{x_k},p_{x_k})\langle\Delta t_k,\Delta t_k\rangle\end{aligned}$$

holds for the full tangential step Δt_k, which minimizes the cubic model $\mathbf{m}_{[\omega_\mathbf{f}]}$ for $[\omega_\mathbf{f}] = 0$. Subtracting these two equations, we obtain

$$\mathbf{L}_1''(0_{x_k}, p_{x_k})(\Delta t_k, \Delta t_k) = \tau_k \left[\mathbf{L}_1''(0_{x_k}, p_{x_k})(\Delta t_k, \Delta t_k) + \frac{[\omega_\mathbf{f}]}{2}\|\delta x_k\| \langle \Delta t_k, \Delta t_k\rangle\right] \tag{5.42}$$

then

$$\tau_k = \frac{\mathbf{L}_1''(0_{x_k}, p_{x_k})(\Delta t_k, \Delta t_k)}{\mathbf{L}_1''(0_{x_k}, p_{x_k})(\Delta t_k, \Delta t_k) + \frac{[\omega_\mathbf{f}]}{2}\|\delta x_k\| \langle \Delta t_k, \Delta t_k\rangle} \tag{5.43}$$

With that we perform the following estimate, which holds sufficiently close to x_*:

$$\|0_{x_k} - \mathbf{x}_*\| \le \tilde{C}\|\Delta x_k\| \le \frac{\tilde{C}}{\tau_k}\|\delta x_k\| \le \tilde{C}\left(1 + \frac{[\omega_\mathbf{f}]}{2\alpha}\|\delta x_k\|\right)\|\delta x_k\| \le C(1 + [\omega_\mathbf{f}]\|\delta x_k\|)\|\delta x_k\|, \tag{5.44}$$

where α is the ellipticity constant of $\mathbf{L}_1''$.
Next, consider the acceptance test (5.34). Since $\mathbf{m}_{[\omega_\mathbf{f}]}(\delta x_k) < \mathbf{m}_{[\omega_\mathbf{f}]}(\delta n_k)$, (5.34) is certainly fulfilled with $\eta \ge 1$, if $\mathbf{f}(\delta x_k + \delta s_k) \le \mathbf{m}_{[\omega_\mathbf{f}]}(\delta x_k)$. To establish such an estimate, we compute from Proposition 5.2.1 and (5.44).

$$\mathbf{f}(\delta x_k + \delta s_k) - \mathbf{q}(\delta x_k) \le C\|\delta x_k\|^3 + C\gamma\|0_{x_k} - \mathbf{x}_*\|\|\delta x_k\|^2 \le C(1 + [\omega_\mathbf{f}]\|\delta x_k\|)\|\delta x_k\|^3$$

Since

$$\mathbf{m}_{[\omega_\mathbf{f}]}(\delta x_k) - \mathbf{q}(\delta x_k) = \frac{[\omega_\mathbf{f}]}{6}\|\delta x_k\|^3$$

we obtain $f(\delta x_k + \delta s_k) \le \mathrm{m}_{[\omega_\mathbf{f}]}(\delta x_k)$, if

$$6C(1 + [\omega_\mathbf{f}]\|\delta x_k\|) \le \frac{[\omega_\mathbf{f}]}{6}$$

For sufficiently small δx_k this is true, if

$$[\omega_\mathbf{f}] \ge \frac{6C}{1 - 6C\|\delta x_k\|}.$$

Thus, we conclude that close to a minimizer (5.34) always holds with $\eta \ge 1 > \hat{\eta}$, if $[\omega_\mathbf{f}]$ is above a certain bound that only depends on the problem and the chosen neighborhood around x_*. Consequently, by our algorithmic mechanism, $[\omega_\mathbf{f}]$ cannot become unbounded.
Hence, as $x_k \to x_*$, implies by (5.43) that $\tau_k \to 1$ taking ellipticity of $\mathbf{L}_1''$ close to x_* into account. Thus, we obtain local superlinear convergence of our algorithm. More accurately, by boundedness of $[\omega_\mathbf{f}]$ we obtain, using $\|\delta x_k\| \le \|\Delta x_k\|$ and (5.43):

$$\tau_k \ge \frac{1}{1 + C\|\Delta x_k\|} \quad \Rightarrow \quad 1 - \tau_k \le C\|\Delta x_k\|$$

and hence

$$\|\Delta x_k - \delta x_k\| \le (1 - \tau_k)\|\Delta x_k\| \le C\|\Delta x_k\|^2.$$

Since $\|\delta s_k\| \le C\|\Delta x_k\|^2$ as well, we have

$$\|\Delta x_k - (\delta x_k + \delta s_k)\| \le C\|\Delta x_k\|^2,$$

so quadratic convergence of the full Newton method carries over to our globalized version. □

5.4.1 An Extended Local Convergence Result

We study local convergence of the problem (4.29) in section 4.5. We recall the problem formulation. Let be $f : X \to \mathbb{R}$ and $c : X \to Y$, then we solve:

$$\min_{x \in X} f(x) \quad \text{s.t} \quad c(x) \in S_0$$

where S_0 is a submanifold of the target space Y and c is transversal over S_0. Here, the problem differs from the one in the previous section in that the desired value of the constraint mapping is unknown. At a point $x \in X$, we denote $z = (v_x, p)$, $\mathbf{y}_* = (R^Y_{c(x),2})^{-1} y_* = \mathbf{c}_2(\mathbf{x}_*)$ and the nonlinear mapping

$$\mathbf{F}_2(z) = \mathbf{F}_2(v_x, p) = \begin{pmatrix} \mathbf{L}_2'(v_x, p) \\ \mathbf{c}_2(v_x) - \mathbf{y}_x \end{pmatrix}$$

which results from a pull-back of our original problem via $R^X_{x,2}$ and $R^Y_{c(x),2}$. Since $\mathbf{c}_2(\mathbf{x}_*)$ is unknown, the estimate $\mathbf{y}_x$ is used instead. In particular, we cannot assume $\mathbf{F}_2(z_*) = 0$.
The full Lagrange-Newton Steps at an iterate $z_0 = (0_x, p)$ reads:

$$\Delta z := (\Delta x, \Delta p) := D_z \mathbf{F}_1(z_0)^{-1} \mathbf{F}_2(z_0), \tag{5.45}$$

which means in more detail:

$$\begin{pmatrix} \mathbf{L}_1''(0_x, p) & \mathbf{c}'(0_x)^* \\ \mathbf{c}'(0_x) & 0 \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta p \end{pmatrix} + \begin{pmatrix} \mathbf{L}'(0_x, p) \\ \mathbf{c}(0_x) - \mathbf{y}_x \end{pmatrix} = 0.$$

As before, $D_z \mathbf{F}_1(z_0)$ has been computed via $R^X_{x,1}$ and $R^Y_{c(x),1}$, and quantities that do not depend on the retraction are denoted without index.
Compared to the previous section, we weaken the assumptions in the following way. Earlier, we have assumed that $\mathbf{F}_2(z_*) = 0$, which means that the pull-back of the root gives us a zero of the pulled-back F. Now, let us assume instead that

$$\|D_z \mathbf{F}_1(z_0)^{-1} \mathbf{F}_2(z_*)\| \le \kappa \|0_x - \mathbf{x}_*\|^2.$$

Proposition 5.4.2. *Suppose that Assumption 5.4.1 holds close to x_*. Then the full-step variant of our method converges locally quadratically to x_*.*

Proof. We apply one Newton step Δz in $T_x X$ at $z_0 = (0_x, p_x)$ to the following problem:

$$\mathbf{F}_2(z) = 0 \quad \Leftrightarrow \quad \begin{pmatrix} \mathbf{L}_2'(v_x, p) \\ \mathbf{c}_2(v_x) - \mathbf{y}_x \end{pmatrix} = 0,$$

We obtain with $z_+ = z_0 + \Delta z$ and a solution $z_* = (\mathbf{x}_*, p_*)$:

$$\begin{aligned} z_+ - z_* = z_0 - z_* + \Delta z &= D_z \mathbf{F}_1(z_0)^{-1}(D_z \mathbf{F}_1(z_0)(z_0 - z_*) - \mathbf{F}_2(z_0) - \mathbf{F}_2(z_*) + \mathbf{F}_2(z_*)) \\ &= \underline{\Delta z} + D_z \mathbf{F}_1(z_0)^{-1} \mathbf{F}_2(z_*). \end{aligned}$$

Since we only use norms for the primal component, and p depends on x directly, our aim is to show:

$$\|x_+ - \mathbf{x}_*\| \leq C\|0_x - \mathbf{x}_*\|^2.$$

By our assumption this holds, if we can show

$$\|\underline{\Delta z}\| \leq C\|0_x - \mathbf{x}_*\|^2$$

since

$$\|x_+ - \mathbf{x}_*\| \leq \|\underline{\Delta z}\| + \|D_z\mathbf{F}_1(z_0)^{-1}\mathbf{F}_2(z_*)\| \leq (C+\kappa)\|0_x - \mathbf{x}_*\|^2.$$

Writing the primal component $\underline{\Delta x} = n_+ + t_+$ with $\mathbf{c}'(0_x)t_+ = 0$ and $n_+ \perp \ker \mathbf{c}'(0_x)$, we obtain:

$$n_+ = \mathbf{c}'(0_x)^-(\mathbf{c}'(0_x)(0_x - \mathbf{x}_*) - (\mathbf{c}(0_x) - \mathbf{c}_2(\mathbf{x}_*))).$$

Application of (5.28) yields via the fundamental theorem of calculus:

$$\|n_+\| \leq \frac{\omega_{\mathbf{c}_2}}{2}\|0_x - \mathbf{x}_*\|^2 = \frac{\omega_{\mathbf{c}_2}}{2}\|\mathbf{x}_*\|^2.$$

The tangential component t_+ is a minimizer of the problem:

$$\min_{v\in\ker\mathbf{c}'(0_x)} \frac{1}{2}\mathbf{L}_1''(0_x,p_x)(v,v) + (\mathbf{L}_1''(0_x,p_x)(0_x - \mathbf{x}_*) - \mathbf{L}'(0_x,p_x) + \mathbf{L}_1''(0_x,p_x)n_+)v.$$

Due to the assumed uniform ellipticity of $\mathbf{L}_1''(0_x,p_x)$, it is sufficient to obtain an estimate for the linear part of this functional of the form:

$$(\mathbf{L}_1''(0_x,p_x)(0_x - \mathbf{x}_*) - \mathbf{L}'(0_x,p_x) + \mathbf{L}_1''(0_x,p_x)n_+)v \leq c\|\mathbf{x}_*\|^2\|v\|. \tag{5.46}$$

First, we observe that

$$\mathbf{L}_1''(0_x,p_x)(n_+,v) \leq \Gamma\|n_+\|\|v\| \leq \Gamma\frac{\omega_{\mathbf{c}_2}}{2}\|\mathbf{x}_*\|^2\|v\|.$$

Next, we telescope, subtracting $\mathbf{L}_2'(\mathbf{x}_*,p_*) = 0$,

$$\begin{aligned}(\mathbf{L}_1''(0_x,p_x)(0_x - \mathbf{x}_*) - \mathbf{L}'(0_x,p_x))v &= (\mathbf{L}_1''(0_x,p_x) - \mathbf{L}_2''(0_x,p_x))(0_x - \mathbf{x}_*, v)\\ &\quad + (\mathbf{L}_2''(0_x,p_x)(0_x - \mathbf{x}_*) - (\mathbf{L}'(0_x,p_x) - \mathbf{L}_2'(\mathbf{x}_*,p_x)))v\\ &\quad + (\mathbf{L}_2'(\mathbf{x}_*,p_x) - \mathbf{L}_2'(\mathbf{x}_*,p_*))v\end{aligned}$$

into a sum of three terms. The first term is estimated via (4.20) and (5.37), taking into account that $v \in \ker \mathbf{c}'(0_x)$:

$$|(\mathbf{L}_1''(0_x,p_x) - \mathbf{L}_2''(0_x,p_x))(0_x - \mathbf{x}_*, v)| = |\mathbf{L}'(0_x,p_x)\Phi_{X,x}''(0_x)(0_x - \mathbf{x}_*, v)| \leq \gamma\|\mathbf{x}_*\|^2\|v\|.$$

The second term is estimated via (5.29), using the fundamental theorem of calculus:

$$(\mathbf{L}_2''(0_x,p_x)(0_x - \mathbf{x}_*) - (\mathbf{L}'(0_x,p_x) - \mathbf{L}_2'(\mathbf{x}_*,p_x)))v \leq \frac{\omega_{\mathbf{L}_2}}{2}\|\mathbf{x}_*\|^2\|v\|.$$

For the third term, we compute, using $v \in \ker \mathbf{c}'(0_x)$ and $\mathbf{c}'(0_x)\mathbf{c}'(0_x)^- = Id$:

$$(\mathbf{L}_2'(\mathbf{x}_*, p_x) - \mathbf{L}_2'(\mathbf{x}_*, p_*))v = (p_x - p_*)\mathbf{c}'(0_x)\mathbf{c}'(0_x)^-(\mathbf{c}_2'(\mathbf{x}_*) - \mathbf{c}'(0_x))v = (p_x - p_*)\mathbf{c}'(0_x)w.$$

With $w := \mathbf{c}'(0_x)^-(\mathbf{c}_2'(\mathbf{x}_*) - \mathbf{c}'(0_x))v \in \ker \mathbf{c}'(0_x)^\perp$ this yields $\|w\| \leq \omega_{\mathbf{c}_2}\|\mathbf{x}_*\|\|v\|$. We continue, using $p_* = p_*\mathbf{c}_2'(x_*)\mathbf{c}_2'(x_*)^- = -\mathbf{f}_2'(x_*)\mathbf{c}_2'(x_*)^-$:

$$\begin{aligned}
|(p_x - p_*)\mathbf{c}'(0_x)w| &= |p_*(\mathbf{c}_2'(\mathbf{x}_*) - \mathbf{c}'(0_x))w - (p_*\mathbf{c}_2'(\mathbf{x}_*) - p_x\mathbf{c}'(0_x))w| \\
&= |-\mathbf{f}_2'(\mathbf{x}_*)\mathbf{c}_2'(\mathbf{x}_*)^-(\mathbf{c}_2'(\mathbf{x}_*) - \mathbf{c}'(0_x))w + (\mathbf{f}_2'(\mathbf{x}_*) - \mathbf{f}'(0_x))w| \\
&\leq \omega_*\|\mathbf{x}_* - 0_x\|\|w\| + \omega_{\mathbf{f}_2}\|\mathbf{x}_* - 0_x\|\|w\| \leq c\|\mathbf{x}_* - 0_x\|^2\|v\|.
\end{aligned}$$

Adding all estimates yields (5.46), as desired. □

5.5 Extension to Vector Bundles

Here, we extend the setting of the SQP-method developed in the previous section to constrained problems on vector bundles. For this, we recall the problem formulation given in (4.30). Let be $f : X \to \mathbb{R}$ and $c : X \to Y$, we consider the problem:

$$\min_{x \in X} f(x) \quad \text{s.t.} \quad c(x) \in S_0 \tag{5.47}$$

where, $p_Y : Y \to M$ is a vector bundle endowed with a connection κ_Y and with typical fiber $\mathbb{F}$. In addition, the C^2-map c is transversal over the submanifold $S_0 \subset Y$. We also assume that $S_0 = s_0(M)$, where $s_0 : M \to Y$ is the zero section, i.e., it satisfies $(p_Y \circ s_0) = id_M$ and maps each point $y \in M$ to the zero vector in Y_y. In order to apply the composite step method for this formulation, some changes have to be made, in particular, we need to use vector bundle retractions for the target space Y. As a consequence, the pullbacked constraint map has a different form, thus, yielding a different structure for the quadratic models needed for the computation of corrections, we illustrate the corresponding changes.

Consider, for $x \in X$, the first order consistent C^2-retractions

$$R_{x,i}^X : T_xX \to X \qquad i = 1, 2 \tag{5.48}$$

for the manifold X. In addition, consider the pair of C^2-vector bundle retractions

$$R_{y,e,i}^Y : T_{y,e}Y \to Y \qquad i = 1, 2, \tag{5.49}$$

for the manifold Y, as defined in (3.34). Specifically, we have that

$$\begin{aligned}
&R_{y,e,i}^Y : T_{y,e}Y \to Y \\
&\qquad R_{y,e,i}^Y(\xi, \eta) = (R_{y,i}^M(\xi), A_i(R_{y,i}^M(\xi))(e + \eta)).
\end{aligned} \tag{5.50}$$

Furthermore, the local transformation map for the manifold X, is given by:

$$\Phi_X := (R_{x,1}^X)^{-1} \circ R_{x,2}^X : T_xX \to T_xX.$$

Also, for the vector bundle $p_Y : Y \to M$, we consider the transition map:

$$\begin{aligned} \Theta_{1\to 2} : T_{x,e}Y &\to T_{x,e}Y \\ (\xi, \eta) &\to (\Phi_M(\xi), \Psi(R_2^M(\xi))(e+\eta) - e) \end{aligned} \tag{5.51}$$

as described in (3.43), with

$$\begin{aligned} \Phi_M(\xi) &= (R_1^M)^{-1}(R_2^M(\xi)) \\ \Psi(y) &= A_1^{-1}(y)A_2(y). \end{aligned}$$

The pull-back of the cost functional via the retraction R_i^X, is given by:

$$\begin{aligned} \mathbf{f}_i : T_xX &\longrightarrow \mathbb{R} \\ \mathbf{f}_i(u) &= (f \circ R_{x,i}^X)(u) \end{aligned}$$

for $u \in T_xX$. Similarly, we pull-back the constraint operator $c : X \to Y$ locally, first through R_i^X, obtaining:

$$c \circ R_{x,i}^X : T_xX \to Y.$$

Then, to obtain a mapping $\mathbf{c}_i : T_xX \to T_{y,e}Y$, with $c(x) = (y, e)$, we pullback through $R_{y,e,i}^Y$, getting:

$$\begin{aligned} \mathbf{c}_i : T_xX &\longrightarrow T_{y,e}Y \\ \mathbf{c}_i(u) &:= (R_{y,e,i}^Y)^{-1} \circ c \circ R_{x,i}^X(u). \end{aligned}$$

Thanks to the connection κ_Y at each point on Y, we have a splitting of $T_{y,e}Y$ into the product $T_yM \times \mathbb{F}$. Therefore, the pullbacked constraint takes the form:

$$\begin{aligned} \mathbf{c}_i : T_xX &\to T_yM \times \mathbb{F} \\ \mathbf{c}_i(u) &= (\mathbf{c}_{B,i}(u), \mathbf{c}_{F,i}(u)) \end{aligned} \tag{5.52}$$

with

$$\begin{aligned} \mathbf{c}_{B,i} : T_xX &\to T_yM \\ \mathbf{c}_{B,i}(u) &= (R_{y,i}^M)^{-1} \circ c \circ R_{x,i}^X(u) \end{aligned} \tag{5.53}$$

and

$$\begin{aligned} \mathbf{c}_{F,i} : T_xX &\to \mathbb{F} \\ \mathbf{c}_{F,i}(u) &= A_i^{-1} \circ c \circ R_{x,i}^X(u). \end{aligned} \tag{5.54}$$

Observe that a solution point $x_* \in X$, we get $c(x_*) \in S_0$, which locally means that

$$\mathbf{c}_B(0_{x_*}) = 0_{y_*}, \quad \text{for some } \ y_* \in M \tag{5.55}$$

$$\mathbf{c}_F(0_{x_*}) = 0 \qquad \text{with } \ 0 \in \mathbb{F}, \tag{5.56}$$

where (5.55) implies that $c \circ R^X_{x_*} = R^M_{y_*}(0_{y_*}) = y_* \in M$. For this reason, in order to solve (5.47), we use the composite step method to solve the problem

$$\min_{u \in TX} \mathbf{f}(u) \quad \text{s.t.} \quad \mathbf{c}_F(u) = 0. \tag{5.57}$$

To achieve that, first of all, similarly as done in section 5.2, the Lagrangian function, as well as local quadratic models have to be defined. First, we consider the Lagrangian function and its derivatives.

Definition 5.5.1. *Given the retractions $R^X_{x,i}$ and $R^Y_{y,e,i}$ as in* (5.48) *and* (5.49)*, the Lagrangian function at the point $x \in X$ is defined as:*

$$\begin{aligned} \boldsymbol{L}_i(u,p) &= \boldsymbol{f}_i(u) + \mathbf{c}_{F,i}(u) \\ &= f \circ R^X_i(u) + p(A_i)^{-1} \circ c \circ R^X_{x,i}(u) \end{aligned} \tag{5.58}$$

with $u \in T_xX$ and $p \in \mathbb{F}^*$.

The corresponding first and second derivatives of the Lagrangian function are:

$$\mathbf{L}'_i(u,p)v = \mathbf{f}'_i(u)v + p\mathbf{c}'_{F,i}(u)v \tag{5.59}$$

and

$$\mathbf{L}''_i(u,p)(v,v) = \mathbf{f}''_i(u)(v,v) + p\mathbf{c}''_{F,i}(u)(v,v). \tag{5.60}$$

We see that the derivatives depend on the chosen retractions:

$$\begin{aligned} \mathbf{L}_2(u,p) &= \mathbf{f}_2(u) + p\mathbf{c}_{F,2}(u) \\ &= \mathbf{f}_1 \circ \Phi_X(u) + p\Psi^{-1} \circ \mathbf{c}_{F,1} \circ \Phi_X(u) \\ &= \mathbf{L}_1 \circ \Phi_X(u) + p(\Psi^{-1} - id) \circ \mathbf{c}_{F,1} \circ \Phi_X(u) \end{aligned}$$

and applying the chain rule, we get that

$$\mathbf{L}'_2(u,p)v = \mathbf{L}'_1(\tilde{u},p)\Phi'_X(u)v + p((\Psi^{-1})' - id)\mathbf{c}'_{F,1}(\tilde{u})\Phi'_X(u)v \tag{5.61}$$

for $\tilde{u} = \Phi_X(u)$, and for the second derivative we get:

$$\begin{aligned} \mathbf{L}''_2(u,p)(v,v) =& \mathbf{L}''_1(\tilde{u},p)(\Phi'_X(u)v)^2 + \mathbf{L}'_1(\tilde{u},p)\Phi''_X(u)v^2 + p(\Psi^{-1})''(\mathbf{c}'_{F,1}(\tilde{u})\Phi'_X(u)v)^2 + \\ &+ p((\Psi^{-1})' - id)\mathbf{c}''_{F,1}(\tilde{u})(\Phi'_X(u)v)^2 + p((\Psi^{-1})' - id)\mathbf{c}'_{F,1}(\tilde{u})\Phi''_X(u)v^2 \end{aligned} \tag{5.62}$$

therefore, evaluating at $u = 0$, and using $\Phi'_X = id$, we get that

$$\mathbf{L}'_2(0_x,p)v - \mathbf{L}'_1(0_x,p)v = p((\Psi^{-1})' - id)\mathbf{c}'_{F,1}(0_x)v \tag{5.63}$$

and

$$\begin{aligned} \mathbf{L}''_2(0_x,p)v^2 - \mathbf{L}''_1(0_x,p)v^2 =& \mathbf{L}'_1(0_x,p)\Phi''_X(0_x)v^2 + p(\Psi^{-1})''(\mathbf{c}'_{F,1}(0_x)v, \mathbf{c}'_{F,1}(0_x)v) \\ &+ p((\Psi^{-1})' - id)(\mathbf{c}''_{F,1}(0_x)v^2 + \mathbf{c}'_{F,1}(0_x)\Phi''_X(0_x)v^2). \end{aligned} \tag{5.64}$$

We observe that the term $(\Psi^{-1})'$ is not necessarily the identity map, as it happens with Φ'_X, therefore the dependency on the chosen transport is already visible in $\mathbf{L}'$ as we see in (5.63), and consequently in $\mathbf{L}''$, as seen in (5.64).
Next, similarly as done in (5.2.1), we show the computation of the steps δn, δt and δs. Given the dependency on the chosen retractions, we compute the corresponding corrections using the pair (R^X_1, R^Y_1).

Normal Step For $g \in \mathbb{F}$, consider the minimal norm problem

$$\min_{w \in T_x X} \frac{1}{2} \langle w, w \rangle \quad \text{s.t.} \quad \mathbf{c}'_{F,1}(0_x)w = g, \tag{5.65}$$

which, as we know, is equivalent to find $w \in \ker \mathbf{c}'_{F,1}(0_x)^\perp$, such that $\mathbf{c}'_{F,1}(0_x)w = g$. By assumption $\mathbf{c}'_{F,1}$ is surjective, therefore the pair (w, p) solves the problem

$$\begin{pmatrix} \mathbf{M}_x & \mathbf{c}'_{F,1}(0_x)^* \\ \mathbf{c}'_{F,1}(0_x) & 0 \end{pmatrix} \begin{pmatrix} w \\ p \end{pmatrix} + \begin{pmatrix} 0 \\ g \end{pmatrix} = 0 \tag{5.66}$$

where $\mathbf{M}_x : T_x X \to (T_x X)^*$ is symmetric and elliptic. The normal step is defined as the solution to (5.66), with $g = \mathbf{c}_{F,1}(0_x)$

$$\Delta n := -\mathbf{c}_{F,1}(0_x)^-(\mathbf{c}_{F,1}(0_x)). \tag{5.67}$$

Lagrange multiplier The lagrange multiplier p_x solves the system:

$$\begin{pmatrix} \mathbf{M}_x & \mathbf{c}'_{F,1}(0_x)^* \\ \mathbf{c}'_{F,1}(0_x) & 0 \end{pmatrix} \begin{pmatrix} w \\ p_x \end{pmatrix} + \begin{pmatrix} \mathbf{f}'(0_x) \\ 0 \end{pmatrix} = 0 \tag{5.68}$$

and p_x satisfies:

$$\mathbf{f}'(0_x)v + p_x \mathbf{c}_{F,1}(0_x)v = 0 \;\; \forall v \in \ker \mathbf{c}'_{F,1}(0_x)^\perp. \tag{5.69}$$

Tangential Step We define the quadratic model

$$\mathbf{q}_1(\delta x) := \mathbf{f}(0_x) + \mathbf{f}'(0_x)\delta x + \frac{1}{2}\mathbf{L}''_1(0_x, p_x)(\delta x, \delta x). \tag{5.70}$$

If $\delta x := \delta n + \Delta t$, with $\Delta t \in \ker \mathbf{c}'_{F,1}$ and $\delta n \in (\mathbf{c}'_{F,1})^\perp$, then the tangential step Δt is found by solving the problem

$$\min_{\Delta t} \mathbf{q}_1(\delta n + \Delta t) \quad \text{s.t.} \quad \mathbf{c}'_{F,1}(0_x)\Delta t = 0, \tag{5.71}$$

which is equivalent to solve

$$\begin{aligned} &\min_{\Delta t} \left(\mathbf{L}'_1(0_x, p_x) + \mathbf{L}''_1(0_x, p_x)\delta n\right)\Delta t + \frac{1}{2}\mathbf{L}''_1(0_x, p_x)(\Delta t, \Delta t) \\ &\text{s.t.} \;\; \mathbf{c}'_{F,1}(0_x)\Delta t = 0. \end{aligned} \tag{5.72}$$

So far, the quantities have been defined in similar way as done in section 5.2.1, the simplified normal step is however computed in a different fashion.

Simplified Normal Step in the Context of Vector Bundles Finally, we show the computation of the simplified normal step δs in the setting of constrained optimization on a vector bundle. We remind that the simplified normal step δs, is such that:

$$-\mathbf{c}'_F(0_x)\delta s = \mathbf{c}_F(\delta x) - \mathbf{c}_F(0_x) - \mathbf{c}'_F(0_x)\delta x. \tag{5.73}$$

If we denote $(p_Y \circ c)(x) = y$, $R_x^X(\delta x) = x_+$, $p \circ c \circ R_x^X(\delta x) = y_+$, and $(R_y^M)^{-1}(y_+) = \delta y$, we observe, that the residual term $\mathbf{c}_F(\delta x) \in Y_{y_+}$, despite the fact that $\mathbf{c}_F(0_{x_0}) \in Y_y$ and $\mathbf{c}'_F(0_{x_0})\delta x \in Y_y$. Then, in order to make the term (5.73) meaningful, we need to transport $\mathbf{c}_F(\delta x)$ back to Y_y. In this context, the simplified normal step is computed in the following way:

$$-\mathbf{c}'_{F,2}(0_x)\delta s = A_2(y_+)^{-1}\mathbf{c}_{F,2}(\delta x) - \mathbf{c}_{F,2}(0_x) - \mathbf{c}'_{F,2}(0_x)\delta x. \tag{5.74}$$

Above, similarly as in (5.21), we compute δs through $\mathbf{c}_{F,2}$, and again, this is possible because R_2^X and $(R_2^Y)^{-1}$ are implemented.
Concerning local convergence of the algorithm, and in order to use the results of section 5.4 in the current framework, we do the following assumption on the map Ψ'.

Assumption 5.5.1. *For the rest of this section, we assume that the retractions* $R^Y_{y,e,i} : T_{y,e}Y \to Y$, $i = 1, 2$ *as given in* (5.50)*, satisfy:*

$$\Psi'(y) = Id. \tag{5.75}$$

Assuming (5.75), we have that:

$$(\Psi(y)^{-1})' = Id \quad \text{and} \quad (\Psi(y)^{-1})'' = -\Psi''(y). \tag{5.76}$$

The latter implies that:

$$\mathbf{c}_{F,2}(u) = A_2^{-1} \circ c \circ R_2^X(u) = \Psi^{-1} \circ \mathbf{c}_{F,1} \circ \Phi_X(u) \tag{5.77}$$

which, differentiating and evaluating at $u = 0$, yields:

$$\mathbf{c}'_{F,2}(0_x) = (\Psi^{-1})'\mathbf{c}'_{F,1}(0_x)\Phi'_X(0) = \mathbf{c}'_{F,1}(0_x) \tag{5.78}$$
$$:= \mathbf{c}'_F(0_x) \tag{5.79}$$

therefore in equations (5.63) and (5.64), we have now:

$$\mathbf{L}'_2(0_x, p)v = \mathbf{L}'_1(0_x, p)v := \mathbf{L}'(0_x, p)v \tag{5.80}$$

and

$$\mathbf{L}''_2(0_x, p)v^2 - \mathbf{L}''_1(0_x, p)v^2 = \mathbf{L}'(0_x, p)\Phi''_X(0_x)v^2 - p_x\Psi''(y)(\mathbf{c}'_F(0_x)v, \mathbf{c}'_F(0_x)v) \tag{5.81}$$

just as in (4.19) and (4.20). With these assumptions and the next Lemma, we apply the convergence results of section 5.4 to the vector bundle case.

Lemma 5.5.1. *For a given perturbation* $\delta x \in T_xX$, *let* $\delta s \in \ker \mathbf{c}'_F(0_x)^\perp$ *be the simplified normal step given by the solution of the equation:*

$$-\boldsymbol{c}'_F(0_x)\delta s = A_2(y_+)^{-1}\boldsymbol{c}_{F,2}(\delta x) - \boldsymbol{c}_F(0_x) - \boldsymbol{c}'_F(0_x)\delta x. \tag{5.82}$$

as defined in (5.74)*, then, the following identity holds:*

$$\boldsymbol{f}_2(\delta x + \delta s) - \boldsymbol{q}_1(\delta x) = \boldsymbol{r}_{F,2}(\delta x) + \boldsymbol{s}_{F,2}(\delta x) + \frac{1}{2}\left(\boldsymbol{L}'(0_x, p_x)\Phi''_X(\delta x, \delta x) - p_x\Psi''(\boldsymbol{c}'(0_x)\delta n, \boldsymbol{c}'(0_x)\delta n)\right). \tag{5.83}$$

where

$$\boldsymbol{L}_{F,2}(\delta x, p_x) := \boldsymbol{f}_2(\delta x) + p_x\, A_2(y_+)^{-1}\boldsymbol{c}_{F,2}(\delta x) \tag{5.84}$$

$$\boldsymbol{r}_{F,2}(\delta x) := \boldsymbol{L}_{F,2}(\delta x, p_x) - \boldsymbol{L}(0_x, p_x) - \boldsymbol{L}'(0_x, p_x)\delta x - \frac{1}{2}\boldsymbol{L}''_2(0_x, p_x)(\delta x, \delta x) \tag{5.85}$$

$$\boldsymbol{s}_{F,2}(\delta x) := \boldsymbol{f}_2(\delta x + \delta s) - \boldsymbol{f}_2(\delta x) - \boldsymbol{f}'(0_x)\delta s. \tag{5.86}$$

We also have that:

$$-\delta s = \int_0^1 \boldsymbol{c}'_F(0_x)^- \left(\left(A_2(R^M_y(\sigma\delta y))^{-1}\boldsymbol{c}_{F,2}(\sigma\delta x)\right)' - (A_2(R^M_y(0_y))^{-1}\boldsymbol{c}_F(0_x))'\delta x\right) \tag{5.87}$$

Proof. We start by proving (5.87). Given that, $p_Y \circ c \circ R^X_x(\delta x) = y_+$ and $\delta y = (R^M_{y,2})^{-1}(y_+)$, we have that $A_2(y_+)^{-1} = (A_2(R^M_{y,2}(\delta y))^{-1}$, then given that $A(y) = Id$, and from (5.82), we have that:

$$\begin{aligned}
-\mathbf{c}'_F(0_x)\delta s &= A_2(y_+)^{-1}\mathbf{c}_{F,2}(\delta x) - A_2(y)^{-1}\mathbf{c}_F(0_x) - A_2(y)^{-1}\mathbf{c}'_F(0_x)\delta x \\
&= A_2(R^M_y(\delta y))^{-1}\mathbf{c}_{F,2}(\delta x) - A_2(R^M_y(0_y))^{-1}\mathbf{c}_F(0_x) - A_2(R^M_y(0_y))^{-1}\mathbf{c}'_F(0_x)\delta x \\
&= \int_0^1 \left(A_2(R^M_y(\sigma\delta y))^{-1}\mathbf{c}_{F,2}(\sigma\delta x)\right)'\delta x - A_2(R^M_y(0_y))^{-1}\mathbf{c}'_F(0_x))\delta x \; d\sigma
\end{aligned} \tag{5.88}$$

where, we implicitly used that $p_Y \circ c \circ R^X_x(\sigma\delta x) = R^M_y(\sigma\delta y)$, plus the fundamental theorem of calculus. In consequence, we get that:

$$-\delta s = \int_0^1 \mathbf{c}'_F(0_x)^- \left(\left(A_2(R^M_y(\sigma\delta y))^{-1}\mathbf{c}_{F,2}(\sigma\delta x)\right)' - \left(A_2(R^M_y(0_y))^{-1}\mathbf{c}_F(0_x)\right)'\delta x\right) d\sigma. \tag{5.89}$$

To proof (5.83), we observe that:

$$\begin{aligned}
\mathbf{r}_{F,2}(\delta x) + \mathbf{q}_1(\delta x) &= \mathbf{L}_{F,2}(\delta x, p_x) - \mathbf{L}(0_x, p_x) - \mathbf{L}'(0_x, p_x)\delta x - \frac{1}{2}\mathbf{L}''_2(0_x, p_x)(\delta x, \delta x) \\
&\quad + \mathbf{f}(0_x) + \mathbf{f}'(0_x)\delta x + \frac{1}{2}\mathbf{L}''_1(0_x, p_x)(\delta x, \delta x) \\
&= \mathbf{f}_2(\delta x) + p_x[A_2(y_+)^{-1}\mathbf{c}_{F,2}(\delta x) - \mathbf{c}_F(0_x) - \mathbf{c}'_F(0_x)\delta x] + \frac{1}{2}\left(\mathbf{L}''_1(0_x, p_x) - \mathbf{L}''_2(0_x, p_x)\right)(\delta x, \delta x) \\
&= \mathbf{f}_2(\delta x) - p_x\mathbf{c}'_F(0_x)\delta s - \frac{1}{2}\left(\mathbf{L}'(0_x, p_x)\Phi''_X(\delta x, \delta x) - p_x\Psi''(\mathbf{c}'_F(0_x)\delta x, \mathbf{c}'_F(0_x)\delta x)\right),
\end{aligned}$$

note that the formula (5.81) has been used. Again, just as in Lemma 5.2.1 given that $\mathbf{f}'(0_x)\delta s = -p_x\mathbf{c}'_F(0_x)\delta s$ and adding and subtracting $\mathbf{f}_2(\delta x + \delta s)$, we obtain (5.83). $\square$

Due to the previous considerations, we introduce the surrogate model $\tilde{\mathbf{q}}_F(\delta n)(\delta t)$ in order to get better consistency properties. We do it in a similar way as done in section 5.2.3. Taking into account the modifications for the current framework, we define $\tilde{\mathbf{q}}_F(\delta n)(\delta t)$ as:

$$\begin{aligned}\tilde{\mathbf{q}}_F(\delta n)(\delta t) &:= \mathbf{L}_{F,2}(\delta n, p_x) - (1-\nu)p_x\mathbf{c}_F(0_x) + (\mathbf{f}'(0_x) + \mathbf{L}_1''(0_x,p)\delta n)\delta t + \frac{1}{2}\mathbf{L}_1''(0_x,p)(\delta t,\delta t)\\ &= \mathbf{f}_2(\delta n) + p_x(A_2(y_+)^{-1}\mathbf{c}_{F,2}(\delta n) - (1-\nu)\mathbf{c}_F(0_x)) + (\mathbf{f}'(0_x) + \mathbf{L}_1''(0_x,p)\delta n)\delta t + \frac{1}{2}\mathbf{L}_1''(0_x,p)(\delta t,\delta t).\end{aligned} \tag{5.90}$$

Following the lines of the proof for Lemmas 5.2.2 and 5.2.3, it can be seen that:

$$\mathbf{f}_2(\delta x+\delta s) - \tilde{\mathbf{q}}_F(\delta n)(\delta t) = \mathbf{r}_{F,2}(\delta x) - \mathbf{r}_{F,2}(\delta n) + \mathbf{s}_{F,2}(\delta x) + \frac{1}{2}\mathbf{L}'(0_x,p_x)(\Phi_X''(\delta x,\delta x) - \Phi_X''(\delta n,\delta n)). \tag{5.91}$$

with $\mathbf{r}_{F,2}(v)$ and $\mathbf{s}_{F,2}(v)$ as defined in (5.85) and (5.86). Similarly as in Proposition 5.2.1, we have the following result.

Proposition 5.5.1. *Assume that there are constants $\omega_{\boldsymbol{c}_{2,F}}$, $\omega_{\boldsymbol{c}''_{2,F}}$ $\omega_{\boldsymbol{f}'_2}$ and $\omega_{\boldsymbol{f}''_2}$ such that*

$$\|\boldsymbol{c}'(0_x)^-\left((A_2(\tilde{y})^{-1}\boldsymbol{c}_{F,2}(v))' - (A_2(y)^{-1}\boldsymbol{c}(0_x))'\right)w\| \le \omega_{\boldsymbol{c}_{2,F}}\|v\|\|w\|, \tag{5.92}$$

$$|(\boldsymbol{f}_2''(v,p_x) - \boldsymbol{f}_2''(0_x,p_x))(v,w)| \le \omega_{\boldsymbol{f}_2''}\|v\|^2\|w\|, \tag{5.93}$$

$$|p_x\left((A_2(\tilde{y})^{-1}\boldsymbol{c}_{F,2}(v))'' - (A_2(y)^{-1}\boldsymbol{c}_{F,2}(0_x))''\right)(v,w)| \le \omega_{\boldsymbol{c}''_{2,F}}\|v\|^2\|w\|, \tag{5.94}$$

$$|(\boldsymbol{f}_2'(v) - \boldsymbol{f}'(0_x)))w| \le \omega_{\boldsymbol{f}_2'}\|v\|\|w\| \tag{5.95}$$

where $p_Y\circ c\circ R_x^X(v) = R_y^M(\tilde{v})$, $\tilde{y} := R_y^M(\tilde{v})$, and v and w are arbitrary. Then for arbitrary δx and simplified normal step δs as defined in (5.74) *we have the estimates:*

$$\|\delta s\| \le \frac{\omega_{\boldsymbol{c}_{2,F}}}{2}\|\delta x\|^2 \tag{5.96}$$

$$\begin{aligned}|\boldsymbol{f}_2(\delta x+\delta s) - \tilde{\mathbf{q}}_F(0_x,\delta n)(\delta t)| \le &\Big(\frac{\omega_{\boldsymbol{L}_2}}{3} + \frac{\omega_{\boldsymbol{f}_2'}\omega_{\boldsymbol{c}_{2,F}}}{2}(1+\frac{\omega_{\boldsymbol{c}_{2,F}}}{4}\|\delta x\|)\Big)\|\delta x\|^3\\ &+\frac{1}{2}|\boldsymbol{L}'(0_x,p_x)(\Phi_X''(\delta x^2) - \Phi_X''(\delta n^2))|\end{aligned} \tag{5.97}$$

with $\omega_{\boldsymbol{L}_2} := \omega_{\boldsymbol{f}_2''} + 2\omega_{\boldsymbol{c}''_{2,F}}$.

Proof. We proceed in a similar way as in the proof of Proposition 5.2.1. By (5.91), we have that:

$$|\mathbf{f}_2(\delta x+\delta s) - \tilde{\mathbf{q}}(\delta n)(\delta t)| \le |\mathbf{r}_{F,2}(\delta x)| + |\mathbf{r}_{F,2}(\delta n)| + |\mathbf{s}_{F,2}(\delta x)| + \frac{1}{2}|\mathbf{L}'(0_x,p_x)(\Phi_X''(\delta x)^2 - \Phi_X''(\delta n)^2)|. \tag{5.98}$$

We note the similarity of the expressions (5.91) and (5.27), therefore, we concentrate on the terms involving $\mathbf{r}_{F,2}$ and $\mathbf{s}_{F,2}$. For arbitrary v, we have that

$$\begin{aligned}\mathbf{r}_{F,2}(v) &:= \mathbf{L}_{F,2}(v,p_x) - \mathbf{L}(0_x,p_x) - \mathbf{L}'(0_x,p_x)v - \frac{1}{2}\mathbf{L}''_2(0_x,p_x)(v,v)\\ &= \mathbf{f}_2(v,p_x) - \mathbf{f}(0_x,p_x) - \mathbf{f}'(0_x,p_x)v - \frac{1}{2}\mathbf{f}''_2(0_x,p_x)(v,v)\\ &+ p_xA_2(y_+)^{-1}\mathbf{c}_{F,2}(v) - p_x\mathbf{c}(0_x) - p_x\mathbf{c}'(0_x)v - \frac{1}{2}p_x\mathbf{c}''_{F,2}(0_x)(v,v)\\ &:= \mathbf{r}^f_{F,2}(v) + \mathbf{r}^c_{F,2}(v)\end{aligned} \tag{5.99}$$

with

$$\mathbf{r}^f_{F,2}(v) = \mathbf{f}_2(v,p_x) - \mathbf{f}(0_x,p_x) - \mathbf{f}'(0_x,p_x)v - \frac{1}{2}\mathbf{f}''_2(0_x,p_x)(v,v) \tag{5.100}$$

and

$$\mathbf{r}^c_{F,2}(v) = p_xA_2(y_+)^{-1}\mathbf{c}_{F,2}(v) - p_x\mathbf{c}(0_x) - p_x\mathbf{c}'(0_x)v - \frac{1}{2}p_x\mathbf{c}''_{F,2}(0_x)(v,v). \tag{5.101}$$

Using (5.93), it can be seen that:

$$|\mathbf{r}^f_{F,2}(v)| \leq \frac{\omega_{\mathbf{f}''_2}}{6}\|v\|^3. \tag{5.102}$$

On the other hand, using $A_2(y)^{-1} = A_2(R^M_y(0_y))^{-1} = Id$, and $p_Y \circ c \circ R^X_x(v) = R^M_y(\tilde{v})$, we have

$$\begin{aligned}\mathbf{r}^c_{F,2}(v) =& p_xA_2(R^M_y(\tilde{v}))^{-1}\mathbf{c}_{F,2}(v) - p_xA_2(R^M_y(0_y))^{-1}\mathbf{c}(0_x) - p_xA_2(R_y(0_y))^{-1}\mathbf{c}'(0_x)v\\ &- \frac{1}{2}p_xA_2(R_y(0_y))^{-1}\mathbf{c}''_{F,2}(0_x)(v,v)\\ =& \int_0^1 p_x\left(A_2(R_y(\sigma\tilde{v}))^{-1}\mathbf{c}_{F,2}(\sigma v)\right)' v - p_x(A_2(R_y(0_y))^{-1}\mathbf{c}(0_x))'v d\sigma\\ &- \frac{1}{2}p_xA_2(R_y(0_y))^{-1}\mathbf{c}''_{F,2}(0_x)(v,v)\\ =& \int_0^1\int_0^1 p_x\left(A_2(R_y(\sigma\tau\tilde{v}))^{-1}\mathbf{c}_{F,2}(\sigma\tau v)\right)''\sigma v^2 - p_x(A_2(R_y(0_y))^{-1}\mathbf{c}_{F,2}(0_x))''\sigma v^2 d\tau d\sigma\\ =& \int_0^1\int_0^1 \frac{1}{\sigma\tau^2}p_x\Big(\left(A_2(R_y(\sigma\tau\tilde{v}))^{-1}\mathbf{c}_{F,2}(\sigma\tau v)\right)'' - (A_2(R_y(0_y))^{-1}\mathbf{c}_{F,2}(0_x))''\Big)(\sigma\tau v)^2 d\tau d\sigma\end{aligned} \tag{5.103}$$

therefore, using (5.94) and the previous expression, we get that

$$|\mathbf{r}^c_{F,2}(v)| \leq \frac{\omega_{\mathbf{c}''_{2,F}}}{6}\|v\|^3. \tag{5.104}$$

The latter is valid for any v, in particular for $v = \delta x$ and $v = \delta n$, therefore

$$|\mathbf{r}^c_{F,2}(\delta x)| + |\mathbf{r}^c_{F,2}(\delta n)| \leq \frac{\omega_{\mathbf{c}''_{2,F}}}{3}\|\delta x\|^3. \tag{5.105}$$

Using (5.87) and (5.92) we get (5.96). And similar as in Proposition 5.2.1 we also get

$$|\mathbf{s}_{F,2}(\delta x)| \leq \frac{\omega_{\mathbf{f}'}\omega_{\mathbf{c}_{2,F}}}{2}\|\delta x\|^2\left(\|\delta x\| + \frac{\omega_{\mathbf{c}_{2,F}}}{4}\|\delta x\|^2\right). \tag{5.106}$$

Finally, adding up all the expressions, we get (5.97). □

Given that the estimate (5.97) holds, we can combine the results of Theorem 5.4.1 and Proposition 5.4.2 to get superlinear convergence of the algorithm. In the following, we use the extended local result provided in section 5.4.1, applied to vector bundles. We assume that the composite step method is used to obtain a solution to the problem (5.57), and it generates a sequence x_k that converges to x_*, such that $\mathbf{c}_F(0_{x_*}) = 0$ and $\mathbf{c}_B(0_*) = 0_{y_*}$, i.e., $c \circ R^X_x(0_{x_*}) = R^M_{y_*}(0_{y_*}) = y_*$, for some $y_* \in M$. Therefore $\mathbf{c}_2(0_{x*})$ is unknown, just as in section 5.4.1.

Proposition 5.5.2. *Assume that the sequence x_k generated by the algorithm converges to a SSC point x_*, and assume that the conditions of Proposition 5.5.1 hold in a neighborhood of x_*. Then we have superlinear convergence.*

Proof. By the estimate (5.97), we have that Theorem 5.4.1 applies, and $\tau_k \to 1$. Then, the sequences $\delta x_k = \delta n_k + \delta t_k$ and $\delta x_k + \delta s_k$ approach asymptotically to the primal part Δx_k of the variant full-step defined in (5.45). Finally, by Proposition 5.4.2, the result follows. □

Chapter 6

Applications

This chapter presents applications to the theoretical considerations made in the previous sections. We start by considering a constrained eigenvalue problem as presented in [GGvM89]. There, the expression $x^T Ax$, for $x \in \mathbb{R}^{n+m}$ and A symmetric, is minimized. The problem is constrained to $x^T x = 1$, where additional linear constraints occur, namely, $Cx = t$, with C^T a full rank matrix and $t \in \mathbb{R}^m$. This problem is re-formulated, making the $(m+n)$-sphere as domain of both cost and constraint mappings, hence, landing in our framework. We continue with mechanical applications to flexible inextensible rods as treated in [GLT89]. There, the configuration space consist of elastic rods $y \in H^2([0,1];\mathbb{R}^3)$, that are inextensible, i.e., $\|y'(s)\| = 1$. First, we consider the forward problem in a mixed formulation. Next, in the discretized version, we solve the problem over the product space $(\mathbb{S}^2)^n$, for n being the number of nodes. Further instances are considered, namely, we continue with the case in which the inextensible rod can enter in contact with one of the planes delimiting the first octant in $\mathbb{R}^3$. The used approach is of that of interior point methods, where the inequalities are transformed into equalities with the introduction of slack variables that associates a barrier problem. We regard the space of slack variables, which belong to the positive cone, as a manifold with a Riemannian metric (see e.g., [NT$^+$02]). After that, we consider the optimal control problem of elastic inextensible rods. There, we minimize a tracking type functional, such that the configurations are constrained to be minimizers of the elastic potential energy. This setting leads us to consider a constrained optimization problem, where the constraint maps from a manifold to a vector bundle. In this case, vector bundle retractions based on vector transports are used. Finally, we close this chapter with some numerical simulations showing the impact of the nonlinear updates on the space of oriented tetrahedra applied to finite elasticity.

6.1 Constrained Eigenvalue Problem

Eigenvalue problems are of significant interest due to their wide range of applications. Problems in physics, relate eigenvalues to the study of vibrating structures, where the study of corresponding frequencies is done. In car manufacturing, it is of importance, to determine the acoustic eigenfrequencies and modes on the interior of a car, in order to find appropriate shape of the interior of the vehicle that reduces the buzzing noise of the motor. Further applications to quantum physics, relates to the solution of the Schrödinger equation, where the eigenvalues correspond to energy levels that a molecule can occupy. Examples of constrained eigenvalue problems arise, for instance, in cavity resonances in particle accelerators, where the time-harmonic Maxwell equations have to be solved, by considering only functions that are divergence free. These applications, and their theoretical and algorithmic treatment, can be seen with more detail in [AKZ12, GLT89, Par98, Cha11, DL86, GL86, Par98]. In this work, as the first application to our algorithm, we consider a constrained eigenvalue problem, as formulated in [GGvM89].

6.1.1 Problem formulation.

In this section we consider the problem:

$$\min_{x\in\mathbb{R}^{(n+m)}} x^T Ax \quad \text{s.t.} \quad \begin{aligned} Cx &= t, \\ x^T x &= 1, \end{aligned}$$

where

$$\begin{aligned}
&A \quad \text{is a (n+m) by (n+m) symmetric matrix, } n > 0,\\
&C^T \quad \text{is a (n+m) by m matrix with full rank,}\\
&t \quad \text{is a m dimensional vector with } \|C^+ t\| < 1.
\end{aligned}$$

We re-formulate it, as a constrained optimization problem on the $\mathbb{S}^{n+m}$ sphere:

$$\min_{x\in\mathbb{S}^{(n+m)}} f(x) \quad \text{s.t} \quad c(x) = 0. \tag{6.1}$$

where

$$f(x) = x^T Ax \tag{6.2}$$

and

$$c(x) = Cx - t. \tag{6.3}$$

As stated in [GGvM89], we consider the interesting case in which $\|C^+t\| < 1$, given that $\|C^+t\| = 1$ has the unique solution $x = (C^+)t$, and $\|C^+t\| > 1$ has no solution.

First order optimality conditions We derive the first order optimality conditions and the KKT-system for the problem (6.1). We first define the Lagrangian function:

$$L(x, \lambda) = x^T Ax + \lambda(Cx - t)$$

for the Lagrange multiplier $\lambda \in (\mathbb{R}^m)^* \cong \mathbb{R}^m$, we obtain:

$$\begin{aligned}
L_x(x,\lambda)\delta x &= (2x^T A + \lambda C)\delta x\\
L_\lambda(x,\lambda)\delta\lambda &= \delta\lambda(Cx - t)
\end{aligned}$$

yielding the KKT-system

$$(2x^T A + \lambda C)\delta x = 0 \quad \forall \delta x \in T_x\mathbb{S}^{n+m} \tag{6.4}$$

$$\delta\lambda(Cx - t) = 0 \quad \forall \delta\lambda \in \mathbb{R}^m. \tag{6.5}$$

6.1.2 The Pullbacked Problem

We pullback the mappings given in (6.2) and (6.3) using the parametrizations as defined in formula (3.27) for the sphere $\mathbb{S}^{(m+n)}$, obtaining:

$$\mathbf{f}(\vartheta) = \mu_x(\vartheta)^T A \mu_x(\vartheta) \tag{6.6}$$

and

$$\mathbf{c}(\vartheta) = C\mu_x(\vartheta) - t \tag{6.7}$$

for $\vartheta \in \mathbb{R}^{m+n}$, therefore we have that

$$\mathbf{f} : \mathbb{R}^{n+m} \to \mathbb{R}$$

and that

$$\mathbf{c} : \mathbb{R}^{n+m} \to \mathbb{R}^m.$$

Derivatives of the Pullback Quantities Using formulas (3.28) and (3.29), for first and second derivatives of the parametrizations, we get that:

$$\mathbf{f}'(\vartheta)\delta x = 2\mu_x(\vartheta)^T A D\mu_x(\vartheta)\delta x \tag{6.8}$$

for $\delta x \in \mathbb{R}^{m+n}$, and evaluating at $\vartheta = 0$, we get

$$\mathbf{f}'(0) = 2\mu_x(0)^T A D\mu_x(0)\delta x. \tag{6.9}$$

Taking second second derivative in direction $\delta\hat{x} \in \mathbb{R}^{m+n}$, we obtain:

$$\mathbf{f}''(\vartheta)(\delta\hat{x}, \delta x) = 2\mu_x(\vartheta)^T A D^2\mu_x(\vartheta)(\delta\hat{x}, \delta x) + 2(D\mu_x(\vartheta)\delta\hat{x})^T A D\mu_x(\vartheta)\delta x \tag{6.10}$$

evaluating at $\vartheta = 0$, the expression becomes

$$\mathbf{f}''(0)(\delta\hat{x}, \delta x) = 2\mu_x(0)^T A D^2\mu_x(0)(\delta\hat{x}, \delta x) + 2(D\mu_x(0)\delta\hat{x})^T A D\mu_x(0)\delta x \tag{6.11}$$

We now perform derivatives of the constraint map, in a similar fashion, for $\delta x, \delta\hat{x} \in \mathbb{R}^{n+m}$, we get that:

$$\mathbf{c}'(\vartheta)\delta x = CD\mu_x(\vartheta)\delta x \tag{6.12}$$

which at $\vartheta = 0$, becomes:

$$\mathbf{c}'(0)\delta x = CD\mu_x(0)\delta x. \tag{6.13}$$

The corresponding second derivative, is given by:

$$\mathbf{c}''(\vartheta)(\delta\hat{x}, \delta x) = CD^2\mu_x(\vartheta)(\delta\hat{x}, \delta x) \tag{6.14}$$

and evaluation at $\vartheta = 0$ yields

$$\mathbf{c}''(0)(\delta\hat{x}, \delta x) = CD^2\mu_x(0)(\delta\hat{x}, \delta x). \tag{6.15}$$

As already mentioned, we use the parametrization for the Sphere $\mathbb{S}^{n+m}$

$$\mu_{x,1}^{\mathbb{S}^{n+m}}(\zeta) = \frac{x + \Theta_{T_x\mathbb{S}^{n+m}}\,\zeta}{\|x + \Theta_{T_x\mathbb{S}^{n+m}}\,\zeta\|}$$

as defined in (3.27). And for the terms $D\mu_x$ and $D^2\mu_x$, we use the formulas (3.28) and (3.29), respectively.

Table 6.1: Numerical experiments for different values of n, m, where N=n+m.

N	n	m	cs-it	$\|C^+t\|$
10	6	4	6	0.0001
50	30	20	6	0.001
200	160	40	11	0.2
500	300	200	6	0.01
1000	600	400	11	0.1383

6.1.3 Numerical Results

In this section, we provide numerical simulations for the constrained eigenvalue problem. We remind the problem setting:

$$\min_{x \in \mathbb{S}^{n+m}} x^T A x \quad \text{s.t.} \quad Cx = t.$$

where A is a $(n+m)$ by $(n+m)$ symmetric matrix, with $n > 0$, C^T is a $n+m$ by m matrix with full rank, and $t \in \mathbb{R}^m$, is such that $\|C^+t\| < 1$. In our numerical simulations, we choose the symmetric matrix

$$A = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix} \in \mathbb{R}^{(n+m,n+m)}$$

and the vector

$$t = \alpha \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix},$$

with $0 < \alpha < 1$. Finally C is chosen to be a random matrix satisfying the condition $\|C^+t\| < 1$. We perform different experiments varying the dimensions of the problem.

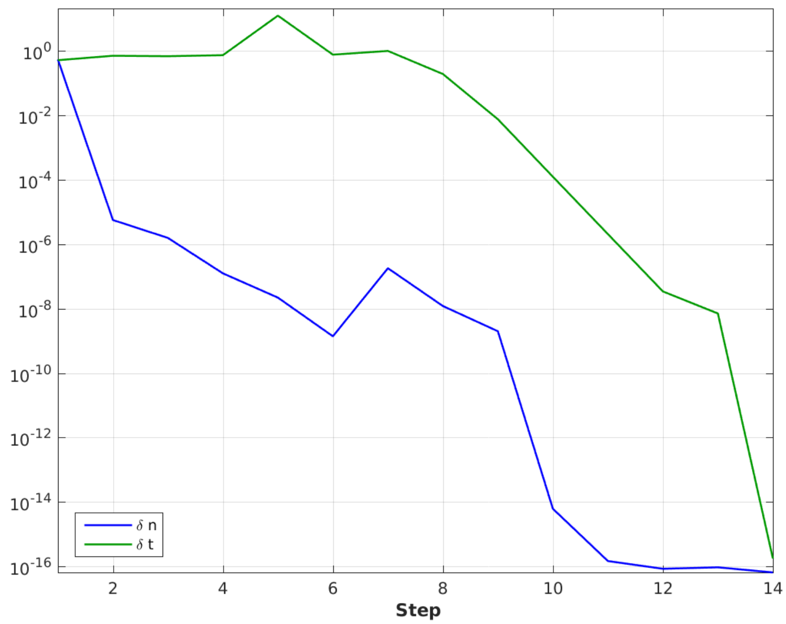


Figure 6.1: *Iteration history: Computed damping factors for normal and tangent steps for $n = 160$, $m = 40$*

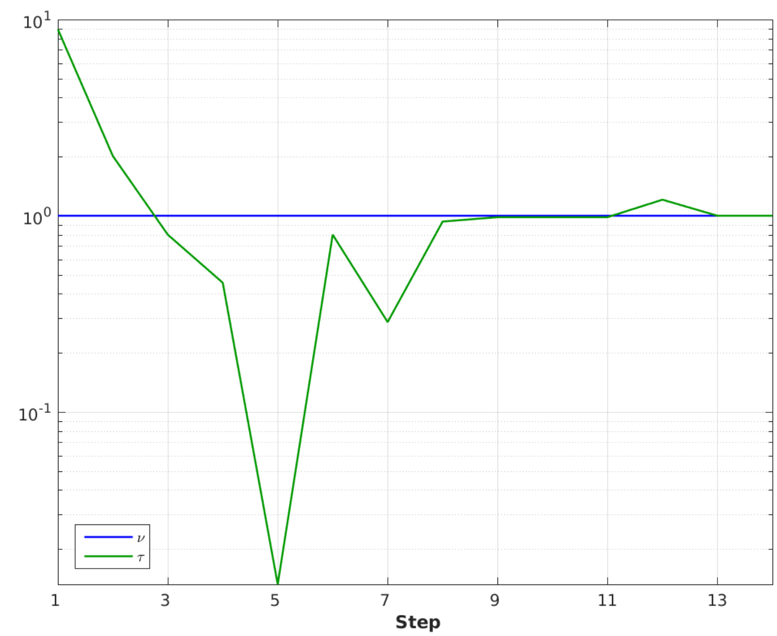


Figure 6.2: *Iteration history: Lengths of the steps, for $n = 160$ and $m = 40$*

6.2 Inextensible Rod

In this section, we test our method for the numerical simulation of flexible inextensible rods. Real-life problems include, for example, the study of the static and dynamic behavior of flexible pipelines used in off-shore oil production under the effects of streams, waves, and obstacles see e.g., [GLT89]. Further examples are found in protein structure comparison [LSZ11], where elastic curves are used to represent and compare protein structures. In this section, we consider the calculation of displacements of inextensible flexible rods. The mathematical setting of the problem and its analysis, which involves the Euler-Bernoulli bending energy, is an interesting problem due to its applications in several fields, making necessary, for its study, tools from differential geometry, nonlinear analysis and optimization. Some literature on the topic is available in [SSW19, GLT89, Bob15, Sin08, SKJJ10, Sim85, Bal76, MH94, TN04]. In particular, we consider the problem of finding a stable equilibrium position of an inextensible transversely isotropic elastic rod under dead load.
First, we provide the formulation and the mathematical analysis of the problem, followed by the discretization and the derivatives of the mappings over the manifold of kinematically admissible configurations. We finish with some numerical experiments.

6.2.1 Problem Formulation

Here, we provide the energetic formulation to the problem of finding the stable equilibrium position of an inextensible, transversely isotropic elastic rod under dead loading. For more details on the derivation of the model see [GLT89]. We consider the following minimization problem

$$\min_{y\in Y} J(y) \quad \text{s.t.} \quad y \in \tilde{V} \tag{6.16}$$

where the energy J and the manifold $\tilde{V}$, which describes the inextensibility condition are given by:

$$\begin{aligned} J(y) &= \frac{1}{2}\int_0^1 EI\left\langle y'', y''\right\rangle ds - \int_0^1 f.y\, ds, \\ \tilde{V} &= \{y \mid y \in H^2(0,1;\mathbb{R}^3), |y'(s)| = 1 \,\text{on}\, [0,1]\}. \end{aligned} \tag{6.17}$$

with boundary conditions

$$\begin{aligned} y(0) = y_a \in \mathbb{R}^3,\ \ y'(0) = y'_a \in \mathbb{S}^2 \\ y(1) = y_b \in \mathbb{R}^3,\ \ y'(1) = y'_b \in \mathbb{S}^2 \end{aligned} \tag{6.18}$$

Above, $EI(s) > 0$ is the flexural stiffness of the rod, f is the lineic density of external loads, y', y'' are the derivatives of y with respect to $s \in [0,1]$, and $\mathbb{S}^2$ is the 2-sphere.
We reformulate (6.17) as:

$$\min_{(y,v)\in Y\times V} J(y,v) \ \ s.t \ \ y' - v = 0. \tag{6.19}$$

with

$$J(y,v) = \frac{1}{2}\int_0^1 EI\left\langle v', v'\right\rangle ds - \int_0^1 f.y\, ds, \tag{6.20}$$

$$\begin{aligned} Y &= \{y \mid y \in H^2([0,1];\mathbb{R}^3) \text{ with } y(0) = y_a,\ y(1) = y_b\} \\ V &= \{v \mid v \in H^1([0,1];\mathbb{S}^2) \text{ with } v(0) = v_a,\ v(1) = v_b\} \end{aligned} \tag{6.21}$$

From the formulation given in (6.19), we get the constrained minimization problem:

$$\min_{(y,v)\in(Y\times V)} J(y,v) \;\; s.t \;\; C(y,v) = 0$$

where Y and V are given by:

$$\begin{aligned} Y &= H^2([0,1];\mathbb{R}^3), \\ V &= H^1([0,1];\mathbb{S}^2). \end{aligned}$$

6.2.2 Mathematical Analysis of the Problem

Concerning the study of existence and the uniqueness of solutions to the problem (6.17), we refer the reader to [GLT89, AR78, LS67, AR78, ET99, Fic73, MH94] for a detailed and complete mathematical analysis of these kind of problems. In the following, we assume that $(EI) \in L^\infty(0,1)$. Concerning to the existence properties of the problem (6.17), we have the following theorem.

Theorem 6.2.1. *Suppose that $|y_a - y_b| < L$ (with L the length of the Rod),* (6.18) *holds, and that the linear functional $w \longrightarrow \int_0^1 f \cdot w$ is continuous on $H^2([0,L];\mathbb{R}^3)$. Then the problem* (6.17) *has at least one solution.*

Proof. See [GLT89, VIII,§2]. □

First Order Optimality Conditions Here, we derive the first order optimality conditions and the corresponding KKT-system for the problem as formulated in (6.19), namely:

$$\begin{aligned} \min_{(y,v)\in Y\times V} & \frac{1}{2}\int_0^1 EI\left\langle v', v'\right\rangle ds - \int_0^1 f.y\, ds, \\ & s.t \qquad y' - v = 0, \\ & y(0) = y_a \in \mathbb{R}^3,\ y(1) = y_b \in \mathbb{R}^3 \\ & v(0) = v_a \in \mathbb{S}^2,\ v(1) = v_b \in \mathbb{S}^2. \end{aligned}$$

Then, we have that:

$$\begin{aligned} J_y(y,v)\delta y &= -\int_0^1 \langle f, \delta y\rangle\, ds, \qquad J_v(y,v)\delta v = \int_0^1 EI\left\langle v', \delta v'\right\rangle ds \\ c_y(y,v)\delta y &= \int_0^1 \left\langle \lambda, \delta y'\right\rangle ds \qquad c_v(y,v)\delta v = -\int_0^1 \langle \lambda, \delta v\rangle\, ds \\ c(y,v)\lambda &= \int_0^1 \left\langle y' - v, \lambda\right\rangle ds. \end{aligned}$$

yielding the KKT-system

$$\begin{aligned}
\int_0^1 \left\langle \lambda, \delta y' \right\rangle ds - \int_0^1 \langle f, \delta y \rangle \, ds = 0 \quad & \forall \delta y \in Y \\
\int_0^1 EI \left\langle v', \delta v' \right\rangle ds - \int_0^1 \langle \lambda, \delta v \rangle \, ds = 0 \quad & \forall \delta v \in T_v V \\
\int_0^1 \left\langle y' - v, \delta \lambda \right\rangle ds = 0 \quad & \forall \delta \lambda \in L_2([0,1], \mathbb{R}^3).
\end{aligned}$$

6.2.3 Finite Difference Approximation of the Problem

For discretization, we use the finite differences approach, see e.g.,[Tho13, QSS10]. We subdivide the interval $[0,1]$ uniformly

$$s_i = i \times h, \;\; i = 0, ..., n-1$$

where $h = \frac{1}{n-1}$. Evaluating at each nodal point, we denote

$$\begin{aligned}
y(s_i) = y_i \in \mathbb{R}^3, \;\; i = 0, ..., n-1 \\
v(s_i) = v_i \in \mathbb{S}^2, \;\; i = 0, ..., n-1.
\end{aligned} \tag{6.22}$$

with boundary conditions:

$$\begin{aligned}
y(0) = y_a \in \mathbb{R}^3, \qquad & y(1) = y_b \in \mathbb{R}^3 \\
v(0) = v_a \in \mathbb{S}^2, \qquad & v(1) = v_b \in \mathbb{S}^2.
\end{aligned}$$

Under this discretization scheme, the Riemann sum yields the approximation of the energy functional

$$J(y_i, v_i) = \frac{1}{2} \sum_{i=0}^{n-1} h \left\langle \frac{1}{h}(v_{i+1} - v_i), \frac{1}{h}(v_{i+1} - v_i) \right\rangle - \sum_{i=1}^{n} h \langle f_i, y_i \rangle . \tag{6.23}$$

Concerning to the constraint $C(y, v)$, performing forward finite differences to the equation

$$y' - v = 0$$

the discretized constraint mapping takes the form

$$\frac{y_{i+1} - y_i}{h} - v_i = 0 \quad i = 0, ..., n-1. \tag{6.24}$$

In the above discrete formulation, we denote the manifold $X = (\mathbf{R}^3 \times \mathbb{S}^2)^n$, with n the number of grid vertices. The elements of the manifold X are denoted by the Cartesian product

$$(y, v) = \prod_{i=0}^{n-1} (y_i, v_i), \qquad y_i \in \mathbb{R}^3, \, v_i \in \mathbb{S}^2.$$

The tangent space at $(y, v) \in X$ is given by the following direct sum of vector spaces

$$T_{(y,v)}X = \bigoplus_{i=0}^{n-1} \left(T_{y_i}\mathbb{R}^3 \oplus T_{v_i}\mathbb{S}^2\right).$$

Once the corrections

$$\delta n_y = \prod_{i=0}^{n-1} \delta n_{y_i}, \quad \delta t_y = \prod_{i=0}^{n-1} \delta t_{y_i}, \quad \delta n_v = \prod_{i=0}^{n-1} \delta n_{v_i}, \quad \delta t_v = \prod_{i=0}^{n-1} \delta t_{v_i}$$

are computed, we make:

$$\delta y = \prod_{i=0}^{n-1} (\delta n_{y_i} + \delta t_{y_i}) = \prod_{i=0}^{n-1} \delta y_i, \quad \delta v = \prod_{i=0}^{n-1} (\delta n_{v_i} + \delta t_{v_i}) = \prod_{i=0}^{n-1} \delta v_i$$

and the update, using the retraction map $R_{(y,v)}T_{(y,v)}X \longrightarrow X$, is done by:

$$(y^+, v^+) = R_{(y,v)}(\delta y, \delta v) = \prod_{i=0}^{n-1} (y_i + \delta y_i, R_{v_i}(\delta v_i)).$$

6.2.4 The Pullback of the Discretized Problem

We now pullback the energy functional J and the constraint mapping C using a local parametrizations at each v_i through μ_{v_i} as defined in (3.27) for the 2-sphere. From (6.23) the pullbacked energy functional takes the form:

$$\mathbf{J}(y, \vartheta) = \frac{EI}{2} \sum_{i=0}^{n-1} h \left\langle \frac{1}{h}(\mu_{v_{i+1}}(\vartheta_{i+1}) - \mu_{v_i}(\vartheta_i)), \frac{1}{h}(\mu_{v_{i+1}}(\vartheta_{i+1}) - \mu_{v_i}(\vartheta_i)) \right\rangle - \sum_{i=0}^{n-1} h \langle f_i, y_i \rangle. \tag{6.25}$$

and from (6.24), we get the corresponding discretized version of the constraint:

$$\mathbf{C}^i(y, \vartheta) = \frac{y_{i+1} - y_i}{h} - \mu_{v_i}(\vartheta_i) = 0 \tag{6.26}$$

for $i = 0, ..., n-1$, and where

$$\mu_{v_i}(\vartheta_i) : \mathbb{R}^2 \longrightarrow \mathbb{S}^2$$

is a local parametrization around v_i, with $\vartheta_i \in \mathbb{R}^2$.

Derivatives of the Pullbacked Maps From the discretized versions of the energy and constraint functionals (6.25) and (6.26), we proceed with the computation of the derivatives. First, derivatives are computed on the parametrization spaces and evaluated at the zero of each tangent space. Then, we can use the formulas given in (3.27) and (3.28), to get the desired expressions that are implemented in the computer.

Concerning the energy, we consider one summand in (6.25), namely:

$$\frac{EI}{2h}\left\langle(\mu_{v_{i+1}}(\vartheta_{i+1})-\mu_{v_i}(\vartheta_i)),(\mu_{v_{i+1}}(\vartheta_{i+1})-\mu_{v_i}(\vartheta_i))\right\rangle-\langle f_i,y_i\rangle \tag{6.27}$$

and taking derivative, we obtain:

$$\frac{EI}{h}\left\langle(D\mu_{v_{i+1}}(\vartheta_{i+1})\delta v_{i+1}-D\mu_{v_i}(\vartheta_i))\delta v_i,(\mu_{v_{i+1}}(\vartheta_{i+1})-\mu_{v_i}(\vartheta_i))\right\rangle-\langle f_i,\delta y_i\rangle \tag{6.28}$$

which at $\vartheta=0$, becomes

$$\frac{EI}{h}\left\langle D\mu_{v_{i+1}}(0_{i+1})\delta v_{i+1}-D\mu_{v_i}(0_i)\delta v_i,\mu_{v_{i+1}}(0_{i+1})-\mu_{v_i}(0_i)\right\rangle-\langle f_i,\delta y_i\rangle\,. \tag{6.29}$$

The second derivative of the summand (6.27) with perturbations δv and δw, is given by:

$$\frac{EI}{h}\left\langle D^2\mu_{v_{i+1}}(\vartheta_{i+1})\delta w_{i+1}\delta v_{i+1}-D^2\mu_{v_i}(\vartheta_i)\delta w_{i+1}\delta v_i,\mu_{v_{i+1}}(\vartheta_{i+1})-\mu_{v_i}(\vartheta_i)\right\rangle \tag{6.30}$$

$$+\frac{EI}{h}\left\langle D\mu_{v_{i+1}}(\vartheta_{i+1})\delta v_{i+1}-D\mu_{v_i}(\vartheta_i)\delta v_i,D\mu_{v_{i+1}}(\vartheta_{i+1})\delta w_{i+1}-D\mu_{v_i}(\vartheta_i)\delta w_i\right\rangle \tag{6.31}$$

and evaluation at $\vartheta=0$ yields:

$$\frac{EI}{h}\left\langle D^2\mu_{v_{i+1}}(0_{i+1})\delta w_{i+1}\delta v_{i+1}-D^2\mu_{v_i}(0_i)\delta w_{i+1}\delta v_i,\mu_{v_{i+1}}(0_{i+1})-\mu_{v_i}(0_i)\right\rangle \tag{6.32}$$

$$+\frac{EI}{h}\left\langle D\mu_{v_{i+1}}(0_{i+1})\delta v_{i+1}-D\mu_{v_i}(0_i)\delta v_i,D\mu_{v_{i+1}}(0_{i+1})\delta w_{i+1}-D\mu_{v_i}(0_i)\delta w_i\right\rangle \tag{6.33}$$

where formulas from Examples 3.2.3 can be used. Derivatives of the constraint map are taking by considering the formula (6.26). We take first derivative, obtaining:

$$\frac{1}{h}\delta y_{i+1}-\delta y_i-D\mu_{v_i}(\vartheta_i)\delta v_i \tag{6.34}$$

which, as usual, the value at the zero of the tangent space is obtained by making $\vartheta=0$, and we obtain:

$$\frac{1}{h}\delta y_{i+1}-\delta y_i-D\mu_{v_i}(0_i)\delta v_i. \tag{6.35}$$

Taking second derivative, we get:

$$-D^2\mu_{v_i}(\vartheta_i)\delta w_i\delta v_i \tag{6.36}$$

and evaluating at $\vartheta=0$ yields:

$$-D^2\mu_{v_i}(0_i)\delta w_i\delta v_i \tag{6.37}$$

where, again, formulas from 3.2.3 are used.

6.2.5 Numerical Results

We provide numerical simulations in order to illustrate the performance of the composite step method. We remind the problem setting:

$$\min_{(y,v)\in Y\times V} \frac{1}{2}\int_0^1 EI\left\langle v', v'\right\rangle\, ds - \int_0^1 \langle f, y\rangle\, ds \quad s.t. \quad y' - v = 0$$

where $EI > 0$ is the stiffness of the rod, and f describe the external loads. As initial configuration we consider a Rod of unit length which, in its unstressed state, is the helix with equation:

$$h(s) = [r\cos(\omega s), r\sin(\omega s), a^2\omega s]$$

with $s \in [0,1]$ $r > 0$, $a > 0$ and $\omega = \frac{1}{\sqrt{r^2+a^2}}$. This means that the rod is clamped at $y_A = [r,\ 0,\ 0]$ $y_B = [r,\ \cos(\omega),\ r\sin(\omega),\ a^2\omega]$. We perform numerical simulations for $r = 0.6$, $a = 0.5$ and consequently of ω, the stiffness of the rod will be constant and given by $EI = 1.0$, the external force that is applied to the rod is $1000e_3$ where $e_3 = [0,0,1]^T$.

Remark 6.2.1. *If $EI = 0$, $f = \rho g$ with $g = [0,0,-9.8]^T$ the gravity acceleration and the density of the rod is $\rho = cte$, with $v_a = v_b = 0$, then the unique solution to the problem is a catenoid curve. On the oder hand if $f = 0$, the solution reduces to Euler's elastica problem and there corresponds, to each solution of the problem, the solution obtained by symmetry with respect to the line joining the extremes of the Rod.*

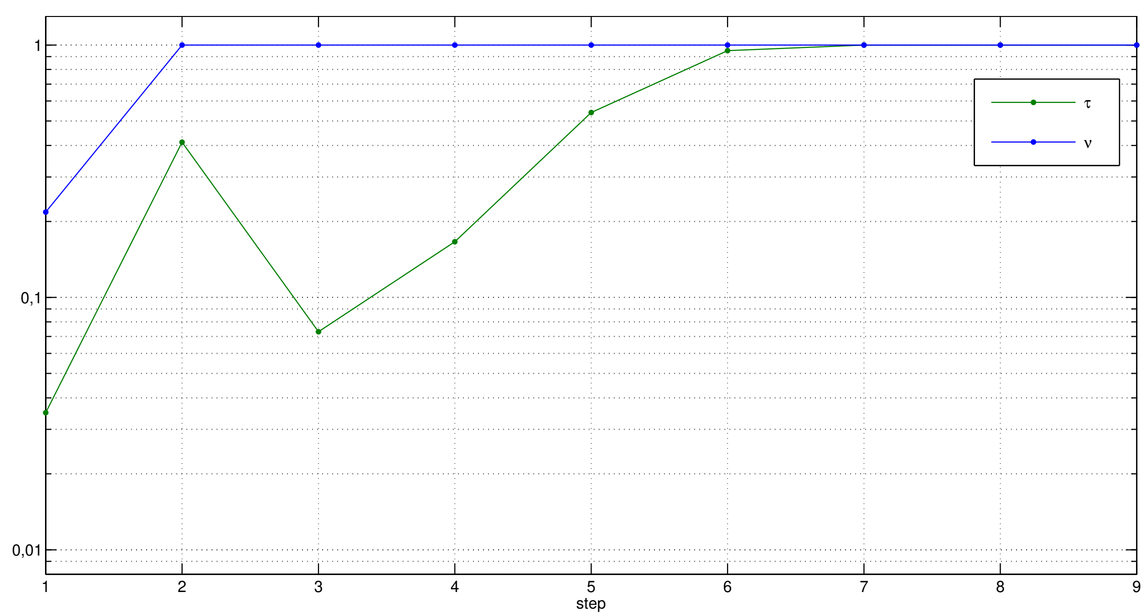


Figure 6.3: *Iteration history: computed damping factors for normal and tangent steps.*

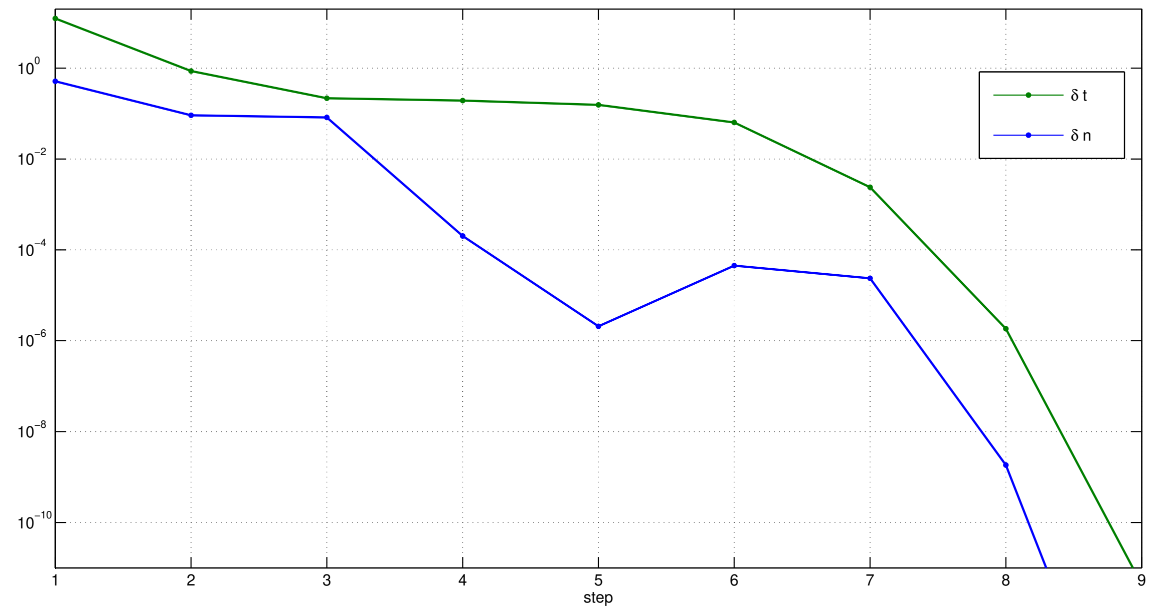


Figure 6.4: *Iteration history: Lengths of the steps.*

Table 6.2: Number of composite step iterations for different combinations of retraction. The pullback is done with the parametrization in the column and the update with the parametrization in the row. Here $\mu_{v,1}(\xi) = \frac{v+\xi}{\|v+\xi\|}$ and $\mu_{v,2}(\xi) = \exp(\xi)v$.

$R_1^X \setminus R_2^X$	$\mu_{v,1}$	$\mu_{v,2}$
$\mu_{v,1}$	9	9
$\mu_{v,2}$	10	10

Table 6.3: Number of composite step iterations for the problem with different number of nodes n. The pullback and updates are done with the parametrization $\mu_{v,2}(\xi) = \exp(\xi)v$. We observe that the problem is stable with respect to refinement of the mesh.

n	CS iter
120	9
240	12
480	8
960	10

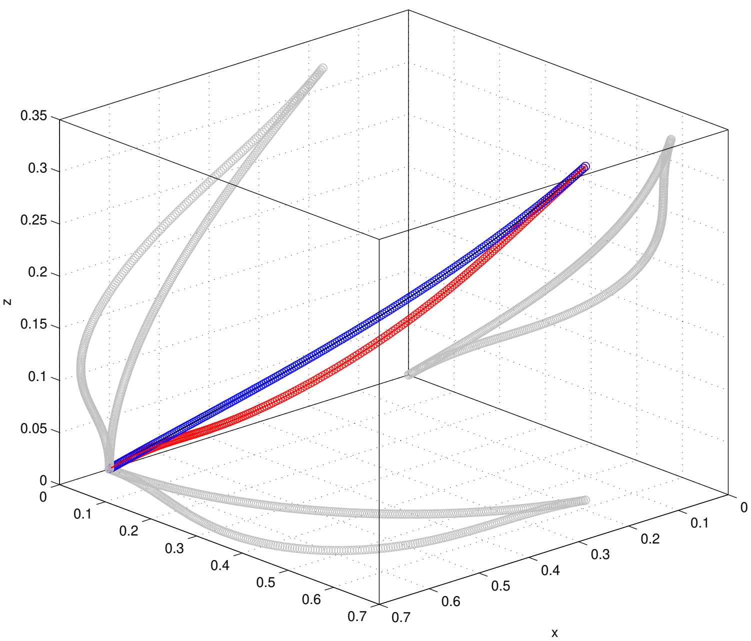


Figure 6.5: *Solutions of the rod problem. Perspective 1: Rod with external force* $1000\,e_3$, (*Blue initial configuration, red final configuration*).

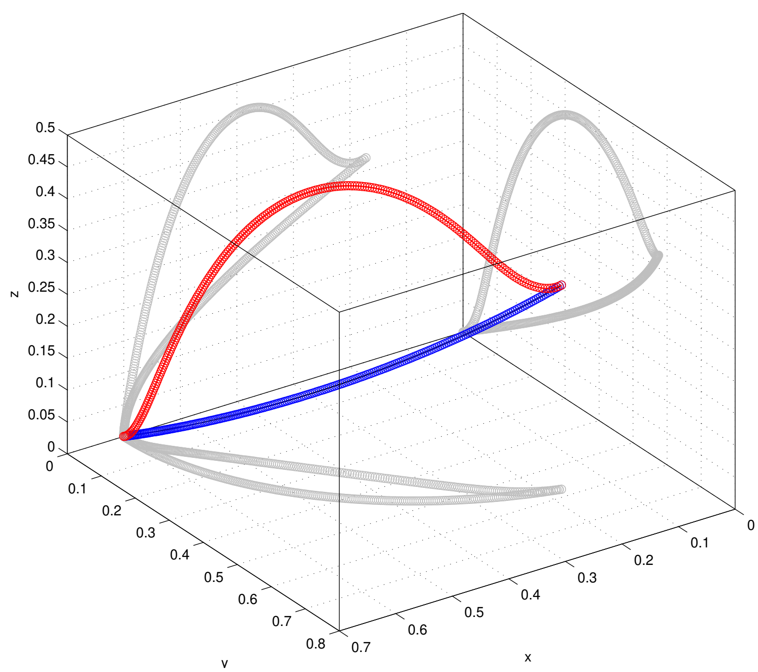


Figure 6.6: *Solutions of the rod problem. Perspective 2: Rod with external force* $1000\,e_3$, (*Blue initial configuration, red final configuration*).

6.3 Inextensible Rod, the Case with Contact

We now consider the case of an inextensible flexible rod as presented in the previous section, but with the additional requirement that it can enter in contact with one or various planes. In our concrete example, the rod $y = [y_1, y_2, y_3]$ is located over the first octant, this is:

$$\begin{aligned} y_1 &\geq 0, \\ y_2 &\geq 0, \\ y_3 &\geq 0. \end{aligned}$$

We suppose in addition, that the contact is frictionless. For the numerical solution of this problem, we use the interior point method techniques as presented in [NN94, NW06, FGW02, GOT05, Wri97, CGT00, SNW12, Nes13, Kar84, Wri92]. In our approach, we introduce the slack variable $\sigma \in K_+$, which belongs to the Riemannian manifold $(K_+, \langle \cdot, \cdot \rangle_\sigma)$ as defined in (2.5), which, together with the retraction defined in (3.6), allows us to apply our method.

6.3.1 Problem Formulation

For the contact case, we consider the following problem:

$$\min_{(y,v,\sigma) \in Y \times V \times \mathcal{K}_+} J_\mu(y, v, \sigma) \quad \text{s.t.} \quad c(y, v, \sigma) = 0 \tag{6.38}$$

where J_μ and c are given by:

$$J_\mu(y, v, \sigma) = \frac{1}{2} \int_0^1 \langle v', v' \rangle \, ds - \int_0^1 \langle f, y \rangle \, ds - \mu \int_0^1 \sum_{j=1}^{3} \log(\sigma_j) \, ds \qquad \text{s.t.} \qquad \begin{aligned} y' &= v \\ y &= \sigma \end{aligned} \tag{6.39}$$

and

$$\begin{aligned} Y &= \{y \in H^2(0, 1; \mathbb{R}^3)\} \\ V &= \{v \in H^1(0, 1; \mathbb{S}^2)\} \\ \mathcal{K}_+ &= \{\sigma \in H^2(0, 1; K_+)\} \end{aligned}$$

with $(K_+, \langle \cdot, \cdot \rangle_\sigma)$ as in (2.5). The barrier approach consists of finding approximate solutions of the problem (6.39), for a sequence of barrier parameters μ_k with $\mu_k \to 0$. The above formulation belongs to the class of interior point methods that are present in the literature [NW06, Meh92, NW06, SNW12]. As it is known, as long as μ tends to zero, the solution of the problem, approaches to the true solution. We choose a simple way to decrease μ, namely, we multiply by a constant $0 < \gamma < 1$.

6.3.2 Pullback of the Discretized Problem

In addition to the case without contact presented in the previous section, a new term in the cost functional appears, namely, the barrier function:

$$b(\mu,\sigma) = -\mu \int_0^1 \sum_{j=1}^{3} \log(\sigma_j)\, ds$$

where $\sigma = [\sigma_1, \sigma_2, \sigma_3]^T$. As before, we discretize by uniformly dividing the interval $[0,1]$

$$s_i = i \times h, \;\; i = 0, ..., n-1$$

where $h = \frac{1}{n-1}$. Evaluating at each nodal point we denote

$$\sigma(s_i) = \sigma_i \in K_+, \;\; i = 0, ..., n-1 \tag{6.40}$$

with boundary conditions:

$$\sigma(0) = \sigma_a \in K_+, \qquad \sigma(1) = \sigma_b \in K_+.$$

With that, the Riemann sum of the barrier functional reads:

$$b(\mu,\sigma_i) = -\mu \sum_{i=0}^{n-1} h \left(\log(\sigma_{1,i}) + \log(\sigma_{2,i}) + \log(\sigma_{3,i})\right)$$

with

$$\sigma_{j,i} = \sigma_j(s_i) \quad \text{for} \quad i = 0, ..., n-1 \;\; \text{and} \;\; j = 1, 2, 3.$$

Above, the index i counts the node, and the index j indicates the entry of the vector in the node i. We are now ready to perform the pullback of the discretized version of the barrier functional. Using the corresponding retraction for the space K_+ as defined in (3.6). Given that $T_\sigma K_+ \simeq \mathbb{R}^3$, the retraction and the parametrization can be taken equal, this is:

$$R_\sigma^{K_+}(\xi) = \begin{bmatrix} \sigma_1 \exp(\frac{1}{\sigma_1}\xi_1) \\ \sigma_2 \exp(\frac{1}{\sigma_2}\xi_2) \\ \sigma_3 \exp(\frac{1}{\sigma_3}\xi_3) \end{bmatrix},$$

with $\xi = [\xi_1, \xi_2, \xi_3]^T \in \mathbb{R}^3$. Performing the pullback, we get:

$$\mathbf{b}(\mu,\xi) = -\mu \sum_{i=0}^{n-1} \sum_{j=1}^{3} h \left(\log(\sigma_{j,i}) + \frac{1}{\sigma_{j,i}} \xi_{j,i} \right) \tag{6.41}$$

where $\xi_j \in T_{\sigma_j} K_+$ and $\xi_{j,i} = \xi_j(s_i)$, for $i = 0, ..., n-1$. The additional constraint $y = \sigma$, introduced in (6.39), in the discretized version, becomes $y_i = \sigma_i$ for $i = 0, ..., n-1$, therefore the pullback is given by:

$$\begin{bmatrix} y_{1,i} \\ y_{2,i} \\ y_{3,i} \end{bmatrix} = \begin{bmatrix} \sigma_{1,i} \exp(\frac{1}{\sigma_{1,i}}\xi_{1,i}) \\ \sigma_{2,i} \exp(\frac{1}{\sigma_{2,i}}\xi_{2,i}) \\ \sigma_{3,i} \exp(\frac{1}{\sigma_{3,i}}\xi_{3,i}) \end{bmatrix}. \tag{6.42}$$

where $\exp(\cdot)$ denotes the real exponential map, just as in (3.6), for $i = 0, ...n-1$.

Derivatives of the Pullbacked Maps The derivatives of the pullbacked barrier functional, and the additional constraint containing the slack variables are taken, in order to implement the composite step method. Concerning derivatives of the pullbacked barrier, we take one summand in equation (6.41)

$$-\mu h \left(\log(\sigma_{1,i}) + \frac{1}{\sigma_{1,i}}\xi_{1,i} + \log(\sigma_{2,i}) + \frac{1}{\sigma_{2,i}}\xi_{2,i} + \log(\sigma_{3,i}) + \frac{1}{\sigma_{3,i}}\xi_{3,i} \right)$$

and taking first derivative we obtain

$$-\mu h \left(\frac{1}{\sigma_{1,i}}\delta\xi_{1,i} + \frac{1}{\sigma_{2,i}}\delta\xi_{2,i} + \frac{1}{\sigma_{3,i}}\delta\xi_{3,i} \right)$$

with vanishing second derivative. Concerning derivatives of the pullbacked constraint mapping (6.42), we get that the first derivative ig given by:

$$\begin{bmatrix} \delta y_{1,i} \\ \delta y_{2,i} \\ \delta y_{3,i} \end{bmatrix} - \begin{bmatrix} \sigma_{1,i} \exp(\frac{1}{\sigma_{1,i}}\xi_{1,i})\frac{1}{\sigma_{1,i}}\delta\xi_{1,i} \\ \sigma_{2,i} \exp(\frac{1}{\sigma_{2,i}}\xi_{2,i})\frac{1}{\sigma_{2,i}}\delta\xi_{2,i} \\ \sigma_{3,i} \exp(\frac{1}{\sigma_{3,i}}\xi_{3,i})\frac{1}{\sigma_{3,i}}\delta\xi_{3,i} \end{bmatrix}_{|\xi=0}$$

which, evaluated at $\xi = 0$ becomes:

$$\begin{bmatrix} \delta y_{1,i} \\ \delta y_{2,i} \\ \delta y_{3,i} \end{bmatrix} - \begin{bmatrix} \delta\xi_{1,i} \\ \delta\xi_{2,i} \\ \delta\xi_{3,i} \end{bmatrix}.$$

Finally, the second derivative, now in direction $\delta\zeta$ takes the form:

$$-\begin{bmatrix} \sigma_{1,i} \exp(\frac{1}{\sigma_{1,i}}\xi_{1,i})\frac{1}{\sigma_{1,i}^2}\delta\zeta_{1,i}\delta\xi_{1,i} \\ \sigma_{2,i} \exp(\frac{1}{\sigma_{2,i}}\xi_{2,i})\frac{1}{\sigma_{2,i}^2}\delta\zeta_{2,i}\delta\xi_{2,i} \\ \sigma_{3,i} \exp(\frac{1}{\sigma_{3,i}}\xi_{3,i})\frac{1}{\sigma_{3,i}^2}\delta\zeta_{3,i}\delta\xi_{3,i} \end{bmatrix}_{|\xi=0}$$

and evaluating at $\xi = 0$, we obtain:

$$-\begin{bmatrix} \frac{1}{\sigma_{1,i}}\delta\zeta_{1,i}\delta\xi_{1,i} \\ \frac{1}{\sigma_{2,i}}\delta\zeta_{2,i}\delta\xi_{2,i} \\ \frac{1}{\sigma_{3,i}}\delta\zeta_{3,i}\delta\xi_{3,i} \end{bmatrix}.$$

Metric for the Normal Steps As we saw in (2.2), the set K_+ becomes a Riemannian manifold when the metric

$$\langle \xi, \xi \rangle_\sigma = \left\langle \frac{\mu}{\sigma^2}\xi, \xi \right\rangle$$

is used. For the computation of tangential steps, this metric is introduced as the second derivatives of the barrier function. Concerning the normal steps, in (5.18), we use the matrix whose diagonal is given by:

$$[\mathbf{M}_\sigma]_{ii} = \frac{\mu}{\sigma_i^2} \quad \text{for} \quad i = 1, ..., n-2,$$

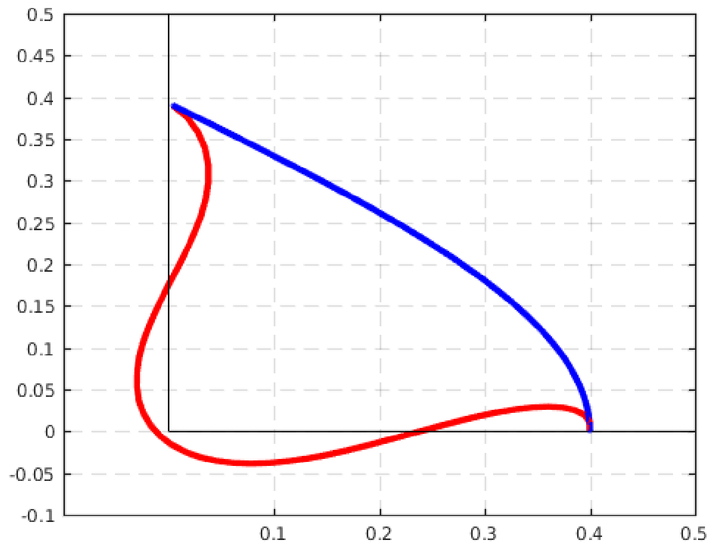


Figure 6.7: *Perspective plane xz: Final state of the rod without obstacles.*

this, for the block corresponding to the variable σ. Finally, once the corrections $\delta\xi$ are computed, we use the formula $\sigma_+ = R_\sigma^{K_+}(\delta\xi)$ to compute the updates, and the update rule assures us that σ_+ belongs to K_+.

6.3.3 Numerical results

Numerical simulations are now provided for the inextensible elastic rod which enters in contact with either one of the planes that delimit the first octant. We remind the continuous setting of the problem:

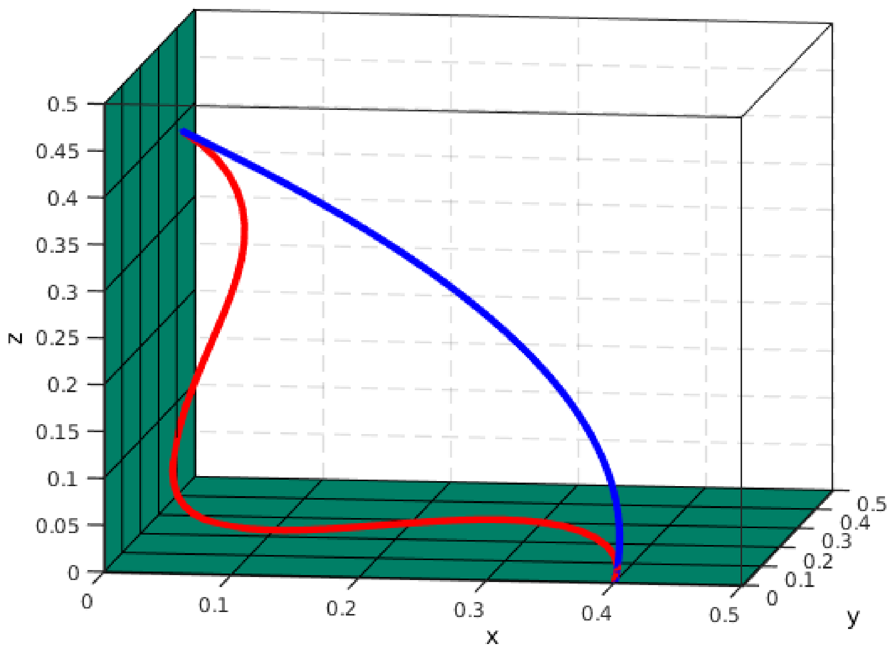
$$\min_{(y,v,\sigma,\mu_k)\in Y\times V\times\mathcal{K}_+} J(y,v,\sigma) = \frac{1}{2}\int_0^1 \langle v', v'\rangle\, ds - \int_0^1 \langle f, y\rangle\, ds - \mu_k \int_0^1 \sum_{j=1}^{3} \log(\sigma_j)\, ds \quad \text{s.t.} \quad y' = v$$

$$y = \sigma$$

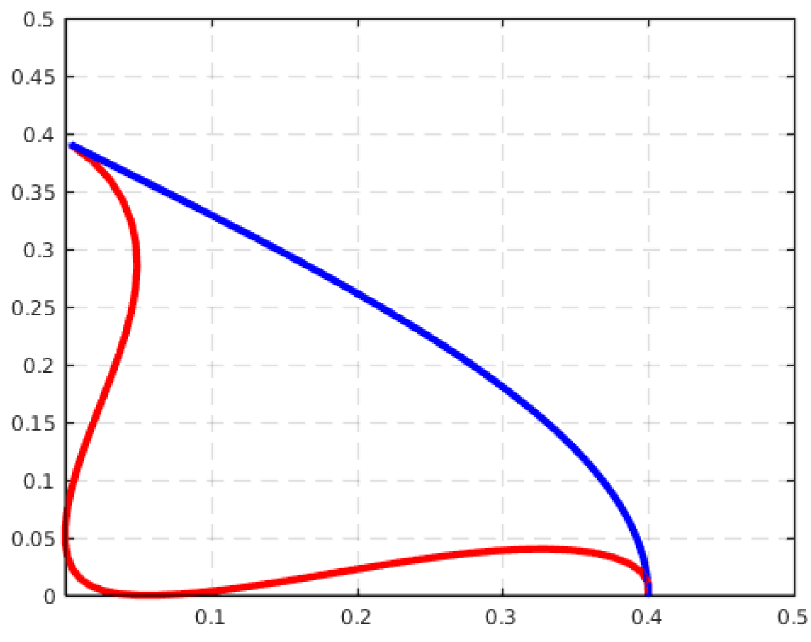
where, as the previous case, $EI > 0$ is the stiffness of the rod, and f describe external load. As initial configuration we consider the rod with equation:

$$h(s) = [r\cos(\omega s), r\sin(\omega s), a^2\omega s]$$

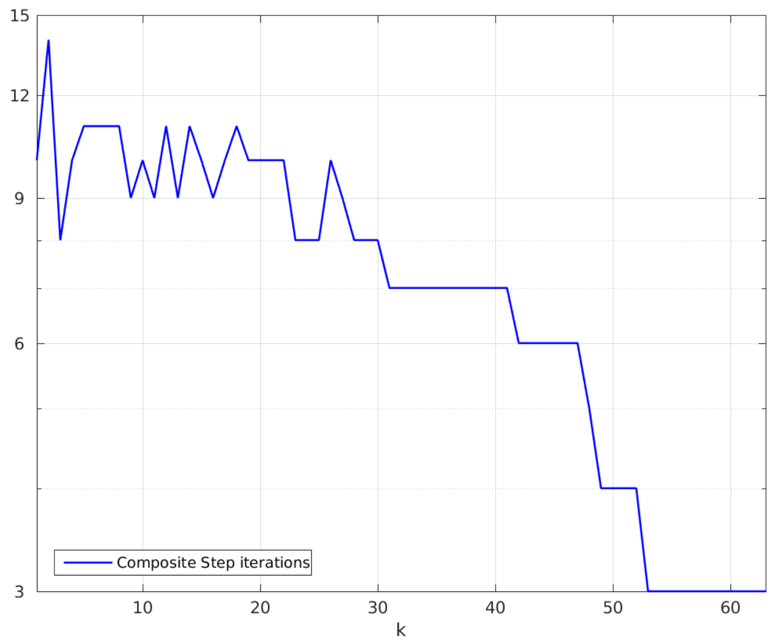
with $s \in [0,1]$ $r > 0$, $a > 0$ and $\omega = \frac{1}{\sqrt{r^2+a^2}}$. We perform numerical simulations for $r = 0.4$ and $a = 0.5$. The stiffness of the rod will be constant and given by $EI = 1.0$. The external force that is applied to the rod is $f = [-150, 10, -50]^T$. We use a simple path following method, in which for each k, we solve the problem for μ_k, letting $\mu_k \to 0$. We have chosen $\mu_k = 0.8 \cdot \mu_0$, with $\mu_0 = 10$, iterating until $\|\mu_k\| \leq 1.0e^{-5}$.



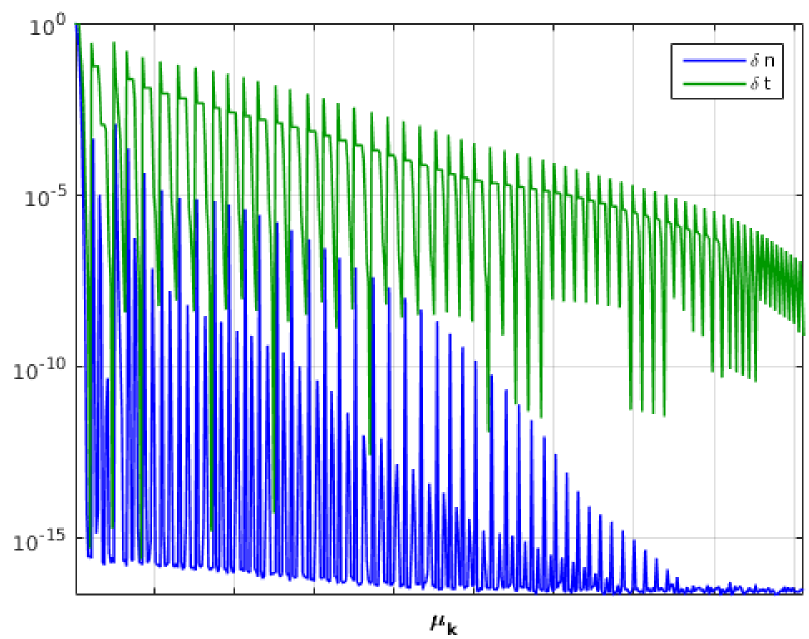
(a) *Perspective : Rod enter in contact with the planes xy and yz in green.*



(b) *Perspective plane xz: Rod enters in contact with the planes xy and yz.*



(a) *Number of composite steps iterations for each k in μ_k.*



(b) *Behaviour of the composite steps for each k in μ_k.*

6.4 Optimal Control of Inextensible Rods

Optimal control of partial differential equations constitute a widely studied topic. The problem consists of varying some input quantity that belongs to the space of controls so that an output state quantity reaches some desired configuration. For sake of the presentation, we do not go into details, and we refer the reader to [DlR15, HPUU08, Trö10] and [GH14, Kom06, LCC00] for the case of finite elasticity. In this section, we consider the problem of getting a specific desired configuration of a flexible inextensible rod. In our framework, the control acts on a cotangent bundle space, this is because the derivative of the energy functional belongs to the cotangent bundle of the configuration space. We start by following the considerations made in the abstract formulation given in sections 4.5 and 4.5.1, here, for the specific case of elastic inextensible rods. We continue with the corresponding discretization of the problem and the pullbacks of the involved mappings. In this section, vector bundle retractions and vector bundle connections are now needed for the space $(T\mathbb{S}^2)^*$, therefore we use the tools developed in sections 3.3.3 and 3.3.4. We finish by providing numerical simulations.

6.4.1 Optimal Control of Energy Minimizers: Elastic Inextensible Rods

We follow the considerations provided in section 4.5.1 in order to land in the framework of optimal control of energy minimizers for elastic inextensible rods. Here, the functional J is the elastic energy of an inextensible rod, with additional constraints, namely:

$$\min_{(y,v)\in Y\times V} J(y,v) \quad \text{s.t.} \quad C(y)=v$$

where the elastic energy $J : Y \times V \longrightarrow \mathbb{R}$ and the constraint $C : Y \to V$ are given by:

$$\begin{aligned} J(y,v) = \frac{1}{2}\int_0^1 EI\left\langle v', v'\right\rangle ds \quad \text{s.t.} \quad y' = v \\ y(0) = y_a \in \mathbb{R}^3,\ y(1) = y_b \in \mathbb{R}^3 \\ v(0) = v_a \in \mathbb{S}^2,\ v(1) = v_b \in \mathbb{S}^2. \end{aligned}$$

and

$$\begin{aligned} Y &= \{y \in H^2(0,1;\mathbb{R}^3)\} \\ V &= \{v \in H^1(0,1;\mathbb{S}^2)\}. \end{aligned}$$

In order to get first order optimality conditions as in (4.33), we consider retractions $R_y^Y : T_yY \longrightarrow Y$ and $R_v^V : T_vV \longrightarrow V$. We take variations of the map J, obtaining:

$$\begin{aligned} \frac{d}{d\varepsilon_v} J(R_v^V(\varepsilon_v \delta v))_{|\varepsilon_v=0} &= \int_0^1 EI\left\langle (DR_v^V(0_v)\delta v)', v'\right\rangle ds \\ &= \int_0^1 EI\left\langle v', \delta v'\right\rangle ds \end{aligned}$$

where the properties

$$\frac{d}{d\varepsilon_v} R_v^V(\varepsilon_v \delta v) = DR_v^V(\varepsilon_v \delta v)\delta v \quad \text{and} \quad DR_v^V(0) = id_{T_v V}$$

of the retraction R_v^V have been used. Concerning the constraint C, we consider:

$$\int_0^1 \left\langle (R_y(\varepsilon_y \delta y))' - R_v(\varepsilon_v \delta v)), \lambda \right\rangle ds = 0$$

where $\lambda \in \Lambda = L_2([0,1], \mathbb{R}^3)$, is the corresponding Lagrange multiplier. Taking variations with respect to y and v, we get that:

$$\begin{aligned} \int_0^1 \left\langle \lambda, \delta y' \right\rangle ds = 0 \\ -\int_0^1 \left\langle \lambda, \delta v \right\rangle ds = 0. \end{aligned}$$

Obtaining the corresponding first order optimality conditions:

$$\begin{aligned} \int_0^1 \left\langle \lambda, \delta y' \right\rangle \, ds = 0 \;\; \forall \delta y \in Y \\ \int_0^1 EI \left\langle v', \delta v' \right\rangle \, ds - \int_0^1 \left\langle \lambda, \delta v \right\rangle \, ds = 0 \;\; \forall \delta v \in T_v V \\ \int_0^1 \left\langle y' - v, \delta \lambda \right\rangle \, ds = 0 \;\; \forall \delta \lambda \in \Lambda. \end{aligned} \tag{6.43}$$

We now introduce the force field $Bu \in TY^*$, that acts on an element $\delta y \in T_y Y$ in the following way:

$$B(y)u := -\int_0^1 \left\langle u, \delta y \right\rangle, \tag{6.44}$$

with this, we are ready to write the optimal control problem.

6.4.2 Problem Formulation

Following the considerations of section 4.5.1, we consider the optimal control problem of a flexible inextensible rod by providing directly the constraints C and c_F, namely:

$$\min_{(y,v,\lambda,u) \in Y \times V \times \Lambda \times U} f(y, v, \lambda, u) \quad \text{s.t.} \quad \begin{aligned} c_F(y, v, \lambda, u) &= 0 \\ C(y, v, \lambda) &= 0 \end{aligned}$$

where f is given by the tracking type functional

$$f(y, v, \lambda, u) = \frac{1}{2}\|y - y_d\|^2_{L^2([0,1],\mathbb{R}^3)} + \frac{\alpha}{2}\|u\|^2_{L^2([0,1],\mathbb{R}^3)} + \frac{\gamma}{2}\|\lambda\|^2_{L^2([0,1],\mathbb{R}^3)}$$

and y_d is the desired state of the rod. If we insert the force field (6.44) into the formulation (6.43), then, the constraint mapping

$$c_F : Y \times V \times \Lambda \times U \longrightarrow Y^* \times TV^* \times \Lambda^*$$

in weak form, is given by:

$$\int_0^1 \left\langle \lambda, p_y' \right\rangle \, ds - \int_0^1 \left\langle u, p_y \right\rangle \, ds = 0 \;\; \forall p_y \in T_y Y \tag{6.45}$$

$$\int_0^1 EI \left\langle v', p_v' \right\rangle \, ds - \int_0^1 \left\langle \lambda, p_v \right\rangle \, ds = 0 \;\; \forall p_v \in T_v V \tag{6.46}$$

$$\int_0^1 \left\langle y' - v, p_\lambda \right\rangle \, ds = 0 \;\; p_\lambda \in \Lambda. \tag{6.47}$$

Where, $p_y \in Y$, $p_v \in T_v V$ and $p_\lambda \in \Lambda$ are the Lagrange multipliers, and

$$\Lambda = L^2([0,1], \mathbb{R}^3), \quad U = L^2([0,1], \mathbb{R}^3).$$

We provide the corresponding KKT-conditions of the problem:

$$\begin{aligned}
T_y f + pT_y c_F &:= \int_0^1 \left\langle y - y_d, \delta y \right\rangle \, ds + \int_0^1 \left\langle \delta y', p_\lambda \right\rangle \, ds = 0, \\
T_v f + pT_v c_F &:= \int_0^1 EI \left\langle \delta v', p_v' \right\rangle \, ds - \int_0^1 \left\langle \delta v, p_\lambda \right\rangle \, ds = 0, \\
T_\lambda f + pT_\lambda c_F &:= \int_0^1 \gamma \left\langle \lambda, \delta \lambda \right\rangle \, ds + \int_0^1 \left\langle \delta \lambda, p_y' \right\rangle \, ds - \int_0^1 \left\langle \delta \lambda, p_v \right\rangle \, ds = 0, \\
T_u f + pT_u c_F &:= \int_0^1 \alpha \left\langle u, \delta u \right\rangle \, ds - \int_0^1 \left\langle p_y, \delta u \right\rangle \, ds = 0, \\
p_y T c_F &:= \int_0^1 \left\langle \lambda, \delta p_y' \right\rangle \, ds - \int_0^1 \left\langle u, \delta p_y \right\rangle \, ds = 0, \\
p_v T c_F &:= \int_0^1 EI \left\langle v', \delta p_v' \right\rangle \, ds - \int_0^1 \left\langle \lambda, \delta p_v \right\rangle \, ds = 0, \\
p_\lambda T C &:= \int_0^1 \left\langle y' - v, \delta p_\lambda \right\rangle \, ds,
\end{aligned}$$

where

$$\begin{aligned}
T_y f + pT_y c_F &: Y \times \Lambda \longrightarrow Y^* \times \Lambda^*, & T_v f + pT_v c_F &: V \times T_v V \longrightarrow T_v V^* \times \Lambda^* \\
T_u f + pT_u c_F &: U \times Y \longrightarrow U^* \times Y^*, & p_y T c_F &: \Lambda \times U \longrightarrow Y^* \\
p_v T c_F &: V \times \Lambda \longrightarrow T_v V^*, & p_\lambda T C &: Y \times V \longrightarrow \Lambda^*
\end{aligned}$$

$$T_\lambda J + pT_\lambda c_F : Y \times \Lambda \times T_v V \longrightarrow Y^* \times \Lambda^* \times T_v V^*.$$

We remind that

$$Y = H^2([0,1], \mathbb{R}^3), \quad V = H^1([0,1], \mathbb{S}^2), \quad \Lambda = L^2([0,1], \mathbb{R}^3), \quad U = L^2([0,1], \mathbb{R}^3).$$

Additionally, we provide the involved variables with their respective spaces:

$$\begin{array}{llll} y \in Y, & \delta y \in Y, & p_y \in Y, & \delta p_y \in Y, \\ v \in V, & \delta v \in T_v V, & p_v \in T_v V, & \delta p_v \in T_v V, \\ \lambda \in \Lambda, & \delta\lambda \in \Lambda, & p_\lambda \in \Lambda, & \\ u \in U, & \delta u \in U. & & \end{array}$$

6.4.3 Finite Difference Approximation of the Problem

We discretize using finite differences. The interval $[0,1]$ is uniformly subdivided:

$$s_i = i \times h, \;\; i = 0, ..., n-1,$$

where $h = \frac{1}{n-1}$. Therefore, at each nodal point, we denote

$$\begin{aligned} y(s_i) &= y_i \in \mathbb{R}^3, \;\; i = 0, ..., n-1, \\ v(s_i) &= v_i \in \mathbb{S}^2, \;\; i = 0, ..., n-1, \\ \lambda(s_i) &= \lambda_i \in \mathbb{R}^3, \;\; i = 0, ..., n-1, \\ u(s_i) &= u_i \in \mathbb{R}^3, \;\; i = 0, ..., n-1, \end{aligned} \tag{6.48}$$

with boundary conditions:

$$\begin{array}{ll} y(0) = y_a \in \mathbb{R}^3, & y(1) = y_b \in \mathbb{R}^3 \\ v(0) = v_a \in \mathbb{S}^2, & v(1) = v_b \in \mathbb{S}^2. \\ \lambda(0) = \lambda_a \in \mathbb{R}^3, & \lambda(1) = \lambda_b \in \mathbb{R}^3 \\ u(0) = v_a \in \mathbb{R}^3, & u(1) = u_b \in \mathbb{R}^3. \end{array}$$

The approximation of the cost functional then reads:

$$f(y_i, v_i, \lambda_i, u_i) = \frac{1}{2} \sum_{i=0}^{n-1} h \left\langle y_i - y_{d_i}, y_i - y_{d_i} \right\rangle + \frac{\alpha}{2} \sum_{i=1}^{n} h \left\langle u_i, u_i \right\rangle + \frac{\lambda}{2} \sum_{i=1}^{n} h \left\langle \lambda_i, \lambda_i \right\rangle. \tag{6.49}$$

The corresponding discretized version of the constraint map c_F is given by:

$$\sum_{i=0}^{n-1} h \left\langle \lambda_i, \frac{1}{h}(p_{y_{i+1}} - p_{y_i}) \right\rangle - \sum_{i=0}^{n-1} h \left\langle u_i, p_{y_i} \right\rangle = 0 \tag{6.50}$$

$$\sum_{i=0}^{n-1} EI \left\langle -\frac{1}{h}(v_{i+1} - v_i) - h\lambda_i, p_{v_i} \right\rangle + \sum_{i=0}^{n-1} \left\langle \frac{1}{h}(v_{i+1} - v_i), p_{v_{i+1}} \right\rangle = 0 \tag{6.51}$$

$$\sum_{i=0}^{n-1} h \left\langle \frac{1}{h}(y_{i+1} - y_i) - v_i, p_{\lambda_i} \right\rangle = 0, \tag{6.52}$$

with $v_i \in \mathbb{S}^2$, $p_{y_i} \in T_{y_i}\mathbb{R}^3$, $p_{v_i} \in T_{v_i}\mathbb{S}^2$ and $p_{\lambda_i} \in T_{\lambda_i}\mathbb{R}^3$. The discretization of the map $C(y, v, \lambda) = 0$ is done as in section 6.2.3, therefore we omit it. From the discretized version of the constraint mapping c_F, we see that the terms $v_j \in \mathbb{S}^2$ and $p_{v_j} \in T_{v_j}\mathbb{S}^2$ for $j = 0, ..., n-1$, occur. In order to implement our method, suitable pullbacks on $\mathbb{S}^2$ and in $(T_v\mathbb{S}^2)^*$ are necessary.

6.4.4 Pullback of the Discretized Problem

We pullback the discretized objective and constrained mappings, and take their corresponding derivatives for implementation purposes. For this, we use the parametrizations for $\mathbb{S}^2$, $T\mathbb{S}^2$ and $(T\mathbb{S}^2)^*$ given in sections 3.3.3 and 3.3.4. The cost function involves terms on linear manifolds, therefore the retracted functional looks like:

$$\mathbf{f}(y_i, v_i, \lambda_i, u_i) = \frac{1}{2}\sum_{i=0}^{n-1} h\left\langle y_i - y_{d_i}, y_i - y_{d_i}\right\rangle + \frac{\alpha}{2}\sum_{i=1}^{n} h\left\langle u_i, u_i\right\rangle + \frac{\lambda}{2}\sum_{i=1}^{n} h\left\langle \lambda_i, \lambda_i\right\rangle. \tag{6.53}$$

On the other hand, observe in (6.51), that the terms $p_{v_i} \in T_{v_i}\mathbb{S}^2$ and $p_{v_{i+1}} \in T_{v_{i+1}}\mathbb{S}^2$ appear. Therefore, we use the connection provided in (2.49), and the expression for the pullback of c_F given in (4.44), obtaining:

$$\begin{aligned}&\sum_{i=0}^{n-1} EI\left\langle (A_{v_i}(\vartheta_i))^*\left(-\frac{1}{h}(\mu_{v_{i+1}}(\vartheta_{i+1}) - \mu_{v_i}(\vartheta_i)) - h\lambda_i\right), p_{v_i}\right\rangle + \\ &\left\langle (A_{v_{i+1}}(\vartheta_{i+1}))^*\left(\frac{1}{h}(\mu_{v_{i+1}}(\vartheta_{i+1}) - \mu_{v_i}(\vartheta_i))\right), p_{v_{i+1}}\right\rangle = 0\end{aligned}$$

where μ_{v_j} and A_{v_j} are parametrizations for $\mathbb{S}^2$ and $T\mathbb{S}^2$ as described in sections 3.3.3 and 3.3.4. Hence, the pullback of the discretized version of c_F, can be written as:

$$\sum_{i=0}^{n-1} h\left\langle \lambda_i, \frac{1}{h}(p_{y_{i+1}} - p_{y_i})\right\rangle - \sum_{i=0}^{n-1} h\left\langle u_i, p_{y_i}\right\rangle = 0 \tag{6.54}$$

$$\begin{aligned}&\sum_{i=0}^{n-1} EI\left\langle -\frac{1}{h}(\mu_{v_{i+1}}(\vartheta_{i+1}) - \mu_{v_i}(\vartheta_i)) - h\lambda_i, A_{v_i}(\vartheta_i)p_{v_i}\right\rangle + \\ &\left\langle \frac{1}{h}(\mu_{v_{i+1}}(\vartheta_{i+1}) - \mu_{v_i}(\vartheta_i)), A_{v_{i+1}}(\vartheta_{i+1})p_{v_{i+1}}\right\rangle = 0\end{aligned} \tag{6.55}$$

$$\sum_{i=0}^{n-1} h\left\langle \frac{1}{h}(y_{i+1} - y_i) - \mu_{v_i}(\vartheta_i), p_{\lambda_i}\right\rangle = 0, \tag{6.56}$$

with $p_{y_i} \in T_{y_i}\mathbb{R}^3$, $p_{v_i} \in T_{v_i}\mathbb{S}^2$, $p_{\lambda_i} \in T_{\lambda_i}\mathbb{R}^3$. Additionally, $\vartheta_i \in \mathbb{R}^2$ are the variables corresponding to the parametrization space for all $i = 1, .., n-1$.

Derivatives of the Pullback Quantities We take derivatives of the pullbacked discretized cost and constraint mappings. For the cost functional, derivatives are taken in the usual way, due to the linear nature of the spaces Y, U and Λ. On the other hand, for the constraint mapping, from the terms (6.55) and (6.56), we see that derivatives of the pullbacks μ_v and A_v are needed. We use the result provided in the Example 3.3.2, and the formulas given in Examples 3.2.3 and 3.3.4 for the specific parametrizations on the manifolds $\mathbb{S}^2$ and $T\mathbb{S}^2$, in order to properly differentiate over these spaces. We start by considering just one summand in (6.55):

$$\langle -\frac{1}{h}(\mu_{v_{i+1}}(\vartheta_{i+1}) - \mu_{v_i}(\vartheta_i)) - h\lambda_i, A_{v_i}(\vartheta_i)p_{v_i}\rangle + \langle \frac{1}{h}(\mu_{v_{i+1}}(\vartheta_{i+1}) - \mu_{v_i}(\vartheta_i)), A_{v_{i+1}}(\vartheta_{i+1})p_{v_{i+1}}\rangle$$

and by product rule, we get its first derivative:

$$\begin{aligned}
&\langle -\frac{1}{h}(D\mu_{v_{i+1}}(\vartheta_{i+1})\delta v_{i+1} - D\mu_{v_i}(\vartheta_i)\delta v_i) - h\delta\lambda_i, A_{v_i}(\vartheta_i)p_{v_i}\rangle \\
&+ \langle \frac{1}{h}(D\mu_{v_{i+1}}(\vartheta_{i+1})\delta v_{i+1} - D\mu_{v_i}(\vartheta_i)\delta v_i), A_{v_{i+1}}(\vartheta_{i+1})p_{v_{i+1}}\rangle \\
&+ \langle -\frac{1}{h}(\mu_{v_{i+1}}(\vartheta_{i+1}) - \mu_{v_i}(\vartheta_i)) - h\lambda_i, DA_{v_i}(\vartheta_i)\delta v_i p_{v_i}\rangle \\
&+ \langle \frac{1}{h}(\mu_{v_{i+1}}(\vartheta_{i+1}) - \mu_{v_i}(\vartheta_i)), DA_{v_{i+1}}(\vartheta_{i+1})\delta v_{i+1} p_{v_{i+1}}\rangle
\end{aligned}$$

which, evaluated at $\vartheta = 0$, becomes:

$$\begin{aligned}
&\langle -\frac{1}{h}(D\mu_{v_{i+1}}(0_{i+1})\delta v_{i+1} - D\mu_{v_i}(0_i)\delta v_i) - h\delta\lambda_i, p_{v_i}\rangle + \langle \frac{1}{h}(D\mu_{v_{i+1}}(0_{i+1})\delta v_{i+1} - D\mu_{v_i}(0_i)\delta v_i), p_{v_{i+1}}\rangle \\
&+ \langle -\frac{1}{h}(v_{i+1} - v_i) - h\lambda_i, DA_{v_i}(0_i)\delta v_i p_{v_i}\rangle + \langle \frac{1}{h}(v_{i+1} - v_i), DA_{v_{i+1}}(0_{i+1})\delta v_{i+1} p_{v_{i+1}}\rangle
\end{aligned}$$

and the formulas (3.28) and (3.93), for the terms $D\mu_{v_j}$ and DA_{v_j}, plus the properties $\mu_{v_j}(0_j) = v_i$ and $A_{v_j}(0_j)p_{v_j} = p_{v_j}$, for $j = 0, ..., n-1$, apply. We have used the connection provided in Example 3.3.2. We now take second derivative with perturbations δv and δw, as well as $\delta\lambda$ and $\delta\nu$, obtaining:

$$\begin{aligned}
&\langle -\frac{1}{h}(D^2\mu_{v_{i+1}}(\vartheta_{i+1})\delta w_{i+1}\delta v_{i+1} - D^2\mu_{v_i}(\vartheta_i)\delta w_i\delta v_i), p_{v_i}\rangle \\
&+ \langle \frac{1}{h}(D^2\mu_{v_{i+1}}(\vartheta_{i+1})\delta w_{i+1}, \delta v_{i+1} - D^2\mu_{v_i}(\vartheta_i)\delta w_i\delta v_i), p_{v_{i+1}}\rangle \\
&+ \langle -\frac{1}{h}(D\mu_{v_{i+1}}(\vartheta_{i+1})\delta v_{i+1} - D\mu_{v_i}(\vartheta_i)\delta v_i) - h\delta\lambda_i, DA_{v_i}(\vartheta_i)\delta w_i p_{v_i}\rangle \\
&+ \langle \frac{1}{h}(D\mu_{v_{i+1}}(\vartheta_{i+1})\delta v_{i+1} - D\mu_{v_i}(\vartheta_i)\delta v_i), DA_{v_{i+1}}(\vartheta_{i+1})\delta w_{i+1} p_{v_{i+1}}\rangle \\
&+ \langle -\frac{1}{h}(D\mu_{v_{i+1}}(\vartheta_{i+1})\delta w_{i+1} - D\mu_{v_i}(\vartheta_i)\delta w_i) - h\delta\nu_i, DA_{v_i}(\vartheta_i)\delta v_i p_{v_i}\rangle \\
&+ \langle \frac{1}{h}(D\mu_{v_{i+1}}(\vartheta_{i+1})\delta w_{i+1} - D\mu_{v_i}(\vartheta_i)\delta w_i), DA_{v_{i+1}}(\vartheta_{i+1})\delta v_{i+1} p_{v_{i+1}}\rangle \\
&+ \langle -\frac{1}{h}(\mu_{v_{i+1}}(\vartheta_{i+1}) - \mu_{v_i}(\vartheta_i)) - h\lambda_i, D^2A_{v_i}(\vartheta_i)(\delta v_i, \delta w_i)p_{v_i}\rangle \\
&+ \langle \frac{1}{h}(\mu_{v_{i+1}}(\vartheta_{i+1}) - \mu_{v_i}(\vartheta_i)), D^2A_{v_{i+1}}(\vartheta_{i+1})(\delta v_{i+1}, \delta w_{i+1})p_{v_{i+1}}\rangle
\end{aligned}$$

evaluating the latter at $\vartheta = 0$ and using the orthogonality relations

$$\left\langle D^2\mu_{v_j}(0_j)(\delta w_j, \delta v_j), p_{v_j}\right\rangle = 0, \quad \left\langle D\mu_{v_j}(0_j)\delta v_j, DA_{v_j}(0_j)(\delta w_j, p_{v_j})\right\rangle = 0,$$
$$\left\langle \mu_{v_j}(0_j)D^2A_{v_j}(\delta v_j, \delta w_j)p_{v_j}\right\rangle = 0,$$

we get:

$$
\begin{aligned}
=&\langle -\frac{1}{h}D^2\mu_{v_{i+1}}(0_{i+1})\delta w_{i+1}\delta v_{i+1}, p_{v_i}\rangle + \langle -\frac{1}{h}D^2\mu_{v_i}(0_i)\delta w_i\delta v_i, p_{v_{i+1}}\rangle \\
&+ \langle \frac{1}{h}D\mu_{v_{i+1}}(0_{i+1})\delta v_{i+1} + h\delta\lambda_i, -DA_{v_i}(0_i)\delta w_i p_{v_i}\rangle + \langle \frac{1}{h}D\mu_{v_i}(0_i)\delta v_i, -DA_{v_{i+1}}(0_{i+1})\delta w_{i+1}p_{v_{i+1}}\rangle \\
&+ \langle \frac{1}{h}D\mu_{v_{i+1}}(0_{i+1})\delta w_{i+1} + h\delta\nu_i, -DA_{v_i}(0_i)\delta v_i p_{v_i}\rangle + \langle \frac{1}{h}D\mu_{v_i}(0_i)\delta w_i, -DA_{v_{i+1}}(0_{i+1})\delta v_{i+1}p_{v_{i+1}}\rangle \\
&+ \langle \frac{1}{h}\mu_{v_{i+1}}(0_{i+1}) + h\lambda_i, -D^2A_{v_i}(0_{i+1})(\delta v_i, \delta w_i)p_{v_i}\rangle + \langle \frac{1}{h}\mu_{v_i}(0_i), -D^2A_{v_{i+1}}(0_{i+1})(\delta v_{i+1}, \delta w_{i+1})p_{v_{i+1}}\rangle
\end{aligned}
$$

where, as before, the formulas,(3.28), (3.29), (3.93) and (3.94), for the derivatives of the parametrizations can be used.
Now, we consider one summand in (6.56):

$$\langle y_{i+1} - y_i - h\mu_{v_i}(\vartheta_i), p_{\lambda_i}\rangle$$

and take its first derivative:

$$\langle \delta y_{i+1} - \delta y_i - hD\mu_{v_i}(\vartheta_i)\delta v_i, p_{\lambda_i}\rangle$$

which at $\vartheta = 0$ becomes

$$\langle \delta y_{i+1} - \delta y_i - hD\mu_{v_i}(0_i)\delta v_i, p_{\lambda_i}\rangle.$$

Consequently, the second derivative of this term is given by:

$$\langle -hD^2\mu_{v_i}(\vartheta_i)\delta w_i\delta v_i, p_{\lambda_i}\rangle$$

with its respective value at $\vartheta = 0$

$$\langle -hD^2\mu_{v_i}(0_i)\delta w_i\delta v_i, p_{\lambda_i}\rangle$$

where, again, the formulas (3.28) and (3.29) for $D\mu_{v_i}$ and $D^2\mu_{v_i}$ are used.

6.4.5 Numerical results

Numerical simulations are now presented for the optimal control problem of inextensible elastic rods. We remind the original continuous problem:

$$
\begin{aligned}
&\min \frac{1}{2}\|y - y_d\|^2_{L^2([0,1],\mathbb{R}^3)} + \frac{\alpha}{2}\|u\|^2_{L^2([0,1],\mathbb{R}^3)} \\
&\text{s.t.} \quad \min_{Y\times V} \frac{1}{2}\int_0^1 \langle v', v'\rangle\, ds - \int_0^1 \langle u, y\rangle\, ds \\
&\qquad\quad \text{s.t.} \quad y' - v = 0.
\end{aligned}
$$

and the corresponding reformulation via KKT-conditions with regularization of the Lagrange multiplier λ:

$$
\begin{aligned}
\min_{(y,v,\lambda,u)\in Y\times V\times\Lambda\times U} f(y,v,\lambda,u) \quad \text{s.t.} \quad c_F(y,v,\lambda,u) =& 0 \\
C(y,v) =& 0
\end{aligned}
$$

n	CS iter
50	21
100	21
150	23
200	20
250	20
350	22
400	27
500	25
600	36

Table 6.4: Number of composite step iterations for the problem with different number of nodes n.

with f, C and c_F given by:

$$f(y, v, \lambda, u) = \frac{1}{2}\|y - y_d\|^2_{L^2([0,1],\mathbb{R}^3)} + \frac{\alpha}{2}\|u\|^2_{L^2([0,1],\mathbb{R}^3)} + \frac{\gamma}{2}\|\lambda\|^2_{L^2([0,1],\mathbb{R}^3)}$$

$$C(y, v) = \int_0^1 \left\langle y' - v, \lambda \right\rangle \, ds = 0$$

and

$$c_F : Y \times V \times \Lambda \times U \longrightarrow Y^* \times TV^* \times \Lambda^*$$

$$\begin{aligned}
\int_0^1 \left\langle \lambda, p_y' \right\rangle \, ds - \int_0^1 \left\langle u, p_y \right\rangle \, ds = 0 \ \ \forall \delta y \in T_y Y \\
\int_0^1 EI \left\langle v', p_v' \right\rangle \, ds - \int_0^1 \left\langle \lambda, p_v \right\rangle \, ds = 0 \ \ \forall \delta v \in T_v V \\
\int_0^1 \left\langle y' - v, p_\lambda \right\rangle \, ds = 0 \ \ \delta \lambda \in \Lambda.
\end{aligned}$$

Where again, $EI > 0$ is the stiffness of the rod and, as initial configuration we consider a rod of unit length which, in its unstressed state, is the helix with equation:

$$h(s) = [r\cos(\omega s), r\sin(\omega s), a^2 \omega s]$$

with $s \in [0,1]$ $r > 0$, $a > 0$ and $\omega = \frac{1}{\sqrt{r^2+a^2}}$. We perform numerical simulations for $r = 0.6$, $a = 0.5$. The stiffness of the rod will be constant and given by $EI = 1$. Concerning the regularization parameters, we choose $\alpha = 2e^{-8}$ and $\gamma = 2e^{-7}$. The desired configuration is the single point $y_d = [0.4, 0.4, 0.12]^T \in \mathbb{R}^3$.

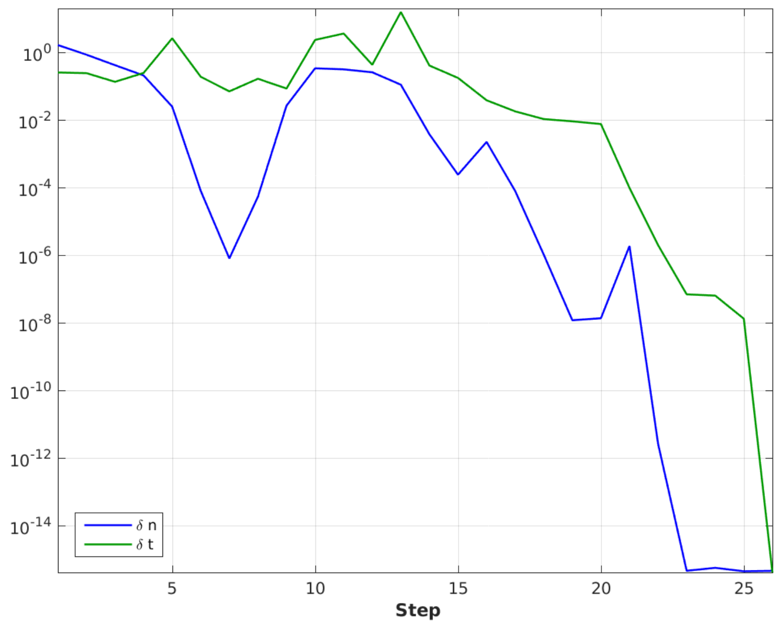


Figure 6.8: *Iteration history: Lengths of the steps*

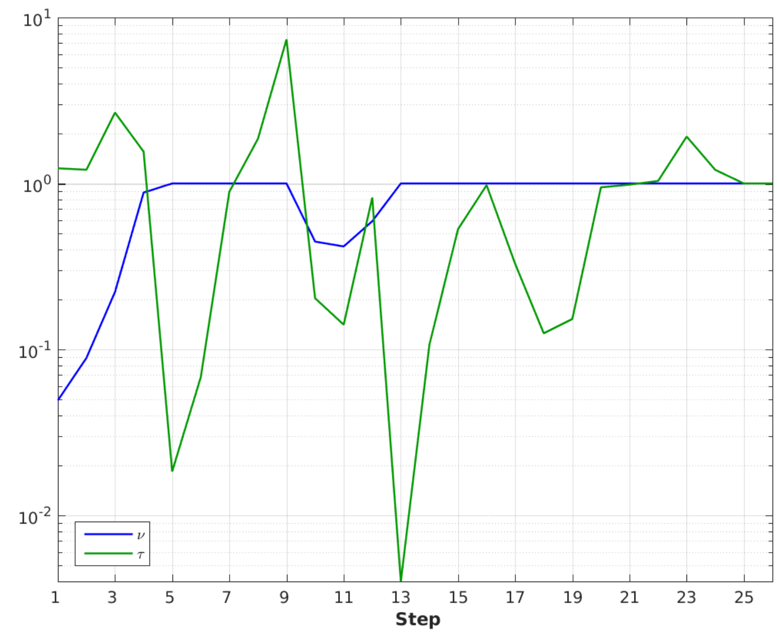


Figure 6.9: *Iteration history: Computed damping factors for normal and tangent steps*

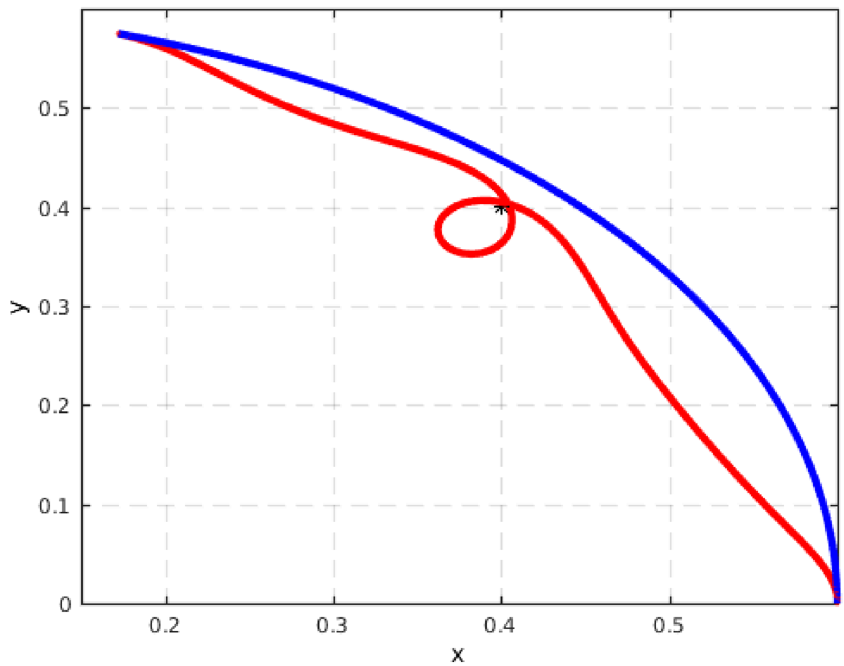


Figure 6.10: *Final configuration from xy perspective*

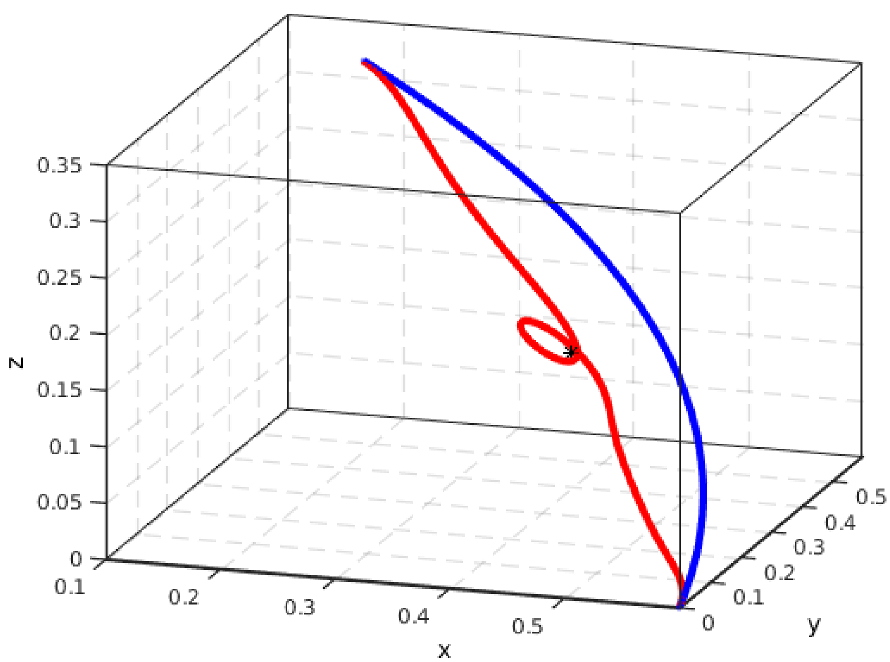


Figure 6.11: *Final configuration, another perspective*

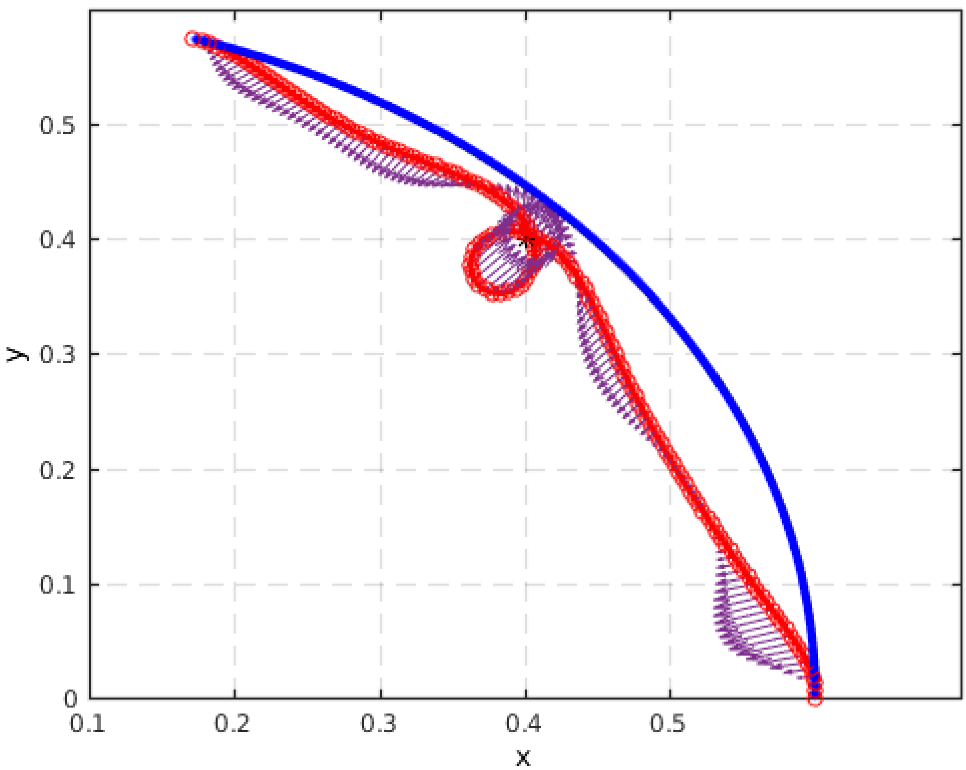


Figure 6.12: *Control field acting on the rod*

6.5 Perspectives: Non-linear Updates for Finite Elasticity

The present section aims to show the impact of the nonlinear updates applied to the space of orientation preserving tetrahedra as introduced in (3.9), in the context of finite elasticity. The discretization of an elastic body into tetrahedra is widely used to solve numerical problems in mechanics, see e.g., [Bra07, ZTNZ77, Red93, Wei16, Hug12]. Optimization algorithms for the solution of such numerical problems, find at each iteration a vector field of corrections that lie at each vertex of each tetrahedron. In order to get the updates, corrections are added to the nodes. One of the drawbacks of such approach, is that physical properties of the body can be lost, for instance, self penetration of the body can occur, and the updates have to be drastically damped, making the algorithms less efficient. Further phenomena such as rotations that might be present during the deformation are not exploited for the sake of efficiency. We introduce a new way to perform the updates. To do so, we use the retraction introduced in section 3.2.1 for the space of orientation preserving tetrahedra. Under this new approach, we observe that self penetration is avoided, and the rotations occurring during the deformation are taken into account, obtaining a better performance of the algorithm. In this work, we will consider only the forward problem, and for sake of the presentation, we skip most of the details on the theory of finite elasticity, therefore, the reader is referred to the available bibliography on the topic, see e.g., [GLT89, Cia88, Ped00, AR78, Bal02, BHK11, ACD+12, Gur82, SS+56, Bal76, Mar81, Arn13]. In the following, we assume that $\Omega \subset \mathbb{R}^3$ is an open, bounded, connected subset with a sufficiently smooth boundary, which can be thought of as the part of space occupied by a body before it is deformed. This is called the reference configuration, or simply the body. A deformation of the body is a mapping $\varphi : \Omega \to \mathbb{R}^3$ assumed to be smooth enough, injective, and orientation preserving.

Energetic Formulations. The problem consists of finding minimizers of the elastic energy functional representing the internal energy that is associated with a deformation of the body, namely:

$$J(\varphi) = \int_\Omega W(x, \nabla\varphi(x))\, dx - \int_\Omega g(x)\varphi(x)\, dx. \tag{6.57}$$

Equilibrium configurations are extremals of this total energy functional. The body Ω is subjected to body forces, which are represented by the vector field $g : \varphi(\Omega) \to \mathbb{R}^3$. The mapping g, represents the density of applied forces per unit volume in the deformed configuration. The search space, for the problem of minimizing J is:

$$X = \{\varphi \in W^{1,p}(\Omega) : \det(\nabla\varphi) > 0 \ a.e. \text{ in } \Omega \text{ and } \varphi = 0 \text{ a.e. on } \Gamma_d \subset \partial\Omega\}.$$

Thus, as we already mentioned, the body deformation is a smooth, one-to-one, orientation preserving vector field, defined on the reference configuration domain $\Omega \subset \mathbb{R}^3$. As we saw, the deformation must satisfy the orientation preserving condition:

$$\det(\nabla\varphi(x)) > 0. \tag{6.58}$$

The latter is the condition that we want to enforce in the discretized formulation when the body is decomposed into several tetrahedra. After that, updates, as defined in formula (3.9), can be performed. Now, the following minimization problem is considered:

$$\min_{\varphi \in X} J(\varphi).$$

In the discretized version, the body configuration Ω is decomposed as:

$$\Omega = \bigcup_{i\in I} T_i$$

where, each T_i is a tetrahedron with vertices $\{v_1^i, v_2^i, v_3^i, v_4^i\}$. We suppose that a correction vector field δv, is computed using the usual linear retraction $R_v^X(\delta v) = v + \delta v$. Then we get that, at each tetrahedron T_i, the correction δv^{T_i}, which is represented as $\{\delta v_1^i, \delta v_2^i, \delta v_3^i, \delta v_4^i\}$, is the corresponding vector field that will be updated in a nonlinear way.

6.5.1 Nonlinear Updates

We assume that the body Ω is decomposed into tetrahedron T_i and that a correction field has been computed. To update the iterates, we proceed in the following way: As done in (2.7), each tetrahedron T_i belonging to the subdivision, with vertices $\{v_1^i, v_2^i, v_3^i, v_4^i\}$, will be represented as:

$$T_i = \begin{bmatrix} | & | & | & | \\ v_1^i & v_2^i & v_3^i & v_4^i \\ | & | & | & | \\ 1 & 1 & 1 & 1 \end{bmatrix} \tag{6.59}$$

i.e., we have that $T_i \in \mathcal{T}_{pos}$ as defined in (2.8), in this case we have used T_i for naming the tetrahedra and for its representation in $\mathcal{T}_{pos}$. Following the structure given in (2.9), for the elements of the tangent space of $\mathcal{T}_{pos}$, we represent the corrections as:

$$\delta v_i = \begin{bmatrix} | & | & | & | \\ \delta v_1^i & \delta v_2^i & \delta v_3^i & \delta v_4^i \\ | & | & | & | \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{6.60}$$

where, for fixed i, the vector δv_j^i has its tail in the node v_j^i, for $j = 1, 2, 3, 4$. Making use of the formula (3.9), we get the updated tetrahedra T_i^+, namely:

$$R_{T_i}^{\mathcal{T}_{pos}}(\delta v_i) = \exp(\delta v_i T_i^{-1})T_i = T_i^+. \tag{6.61}$$

Therefore, we have that $T_i^+ = R_{T_i}^{\mathcal{T}_{pos}}(\delta v_i) \in \mathcal{T}_{pos}$

$$T_i^+ = \begin{bmatrix} | & | & | & | \\ (v_1^i)^+ & (v_2^i)^+ & (v_3^i)^+ & (v_4^i)^+ \\ | & | & | & | \\ 1 & 1 & 1 & 1 \end{bmatrix} \tag{6.62}$$

and the vertices of the updated tetrahedra T_i^+ are $\{(v_1^i)^+, (v_2^i)^+, (v_3^i)^+, (v_4^i)^+\}$. In particular, we have that $\det(T_i^+) > 0$ for all $i \in I$, thus, preserving the orientation. Given that the tetrahedrons will eventually separate, we re-join them by averaging. In figure 6.13, we depict the situation in

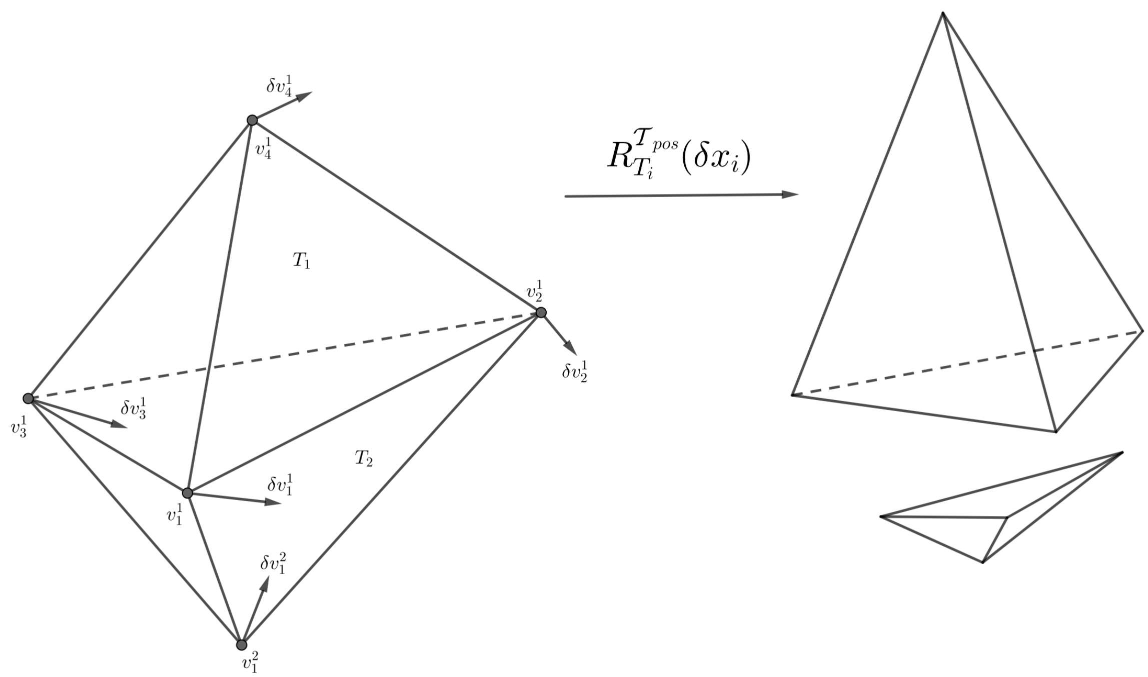


Figure 6.13: *Nonlinear update of tetrahedra T_1 and T_2*

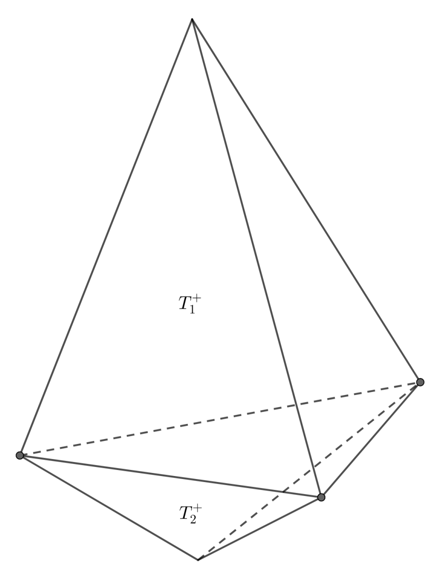


Figure 6.14: *Final tetrahedra after averaging*

which two tetrahedrons T_1 and T_2 joined together. The tetrahedron T_1 has nodes $\{v_1^1, v_2^1, v_3^1, v_4^1\}$, and the tetrahedron T_2 has nodes $\{v_1^2, v_2^2, v_3^2, v_4^2\}$. These objects are represented by T_1 and T_2 respectively in matrix notation as in (6.59), where, in particular, $v_1^1 = v_1^2$, $v_2^1 = v_2^2$ and $v_3^1 = v_3^2$. The correction fields $\{\delta v_1^1, \delta v_2^1, \delta v_3^1, \delta v_4^1\}$ and $\{\delta v_1^2, \delta v_2^2, \delta v_3^2, \delta v_4^2\}$, which are represented by the matrices δv_1 and δv_2 as in (6.60), are respectively updated using formula (6.61), obtaining:

$$T_1^+ = \exp(\delta v_1 T_1^{-1}) T_1 \quad \text{and} \quad T_2^+ = \exp(\delta v_2 T_2^{-1}) T_2.$$

When the nonlinear update is preformed, the tetrahedrons may separate, as sketched in the right-part of figure 6.13. We re-join the updated elements T_1^+ and T_2^+ by an averaging procedure, obtaining what is depicted in figure 6.14.

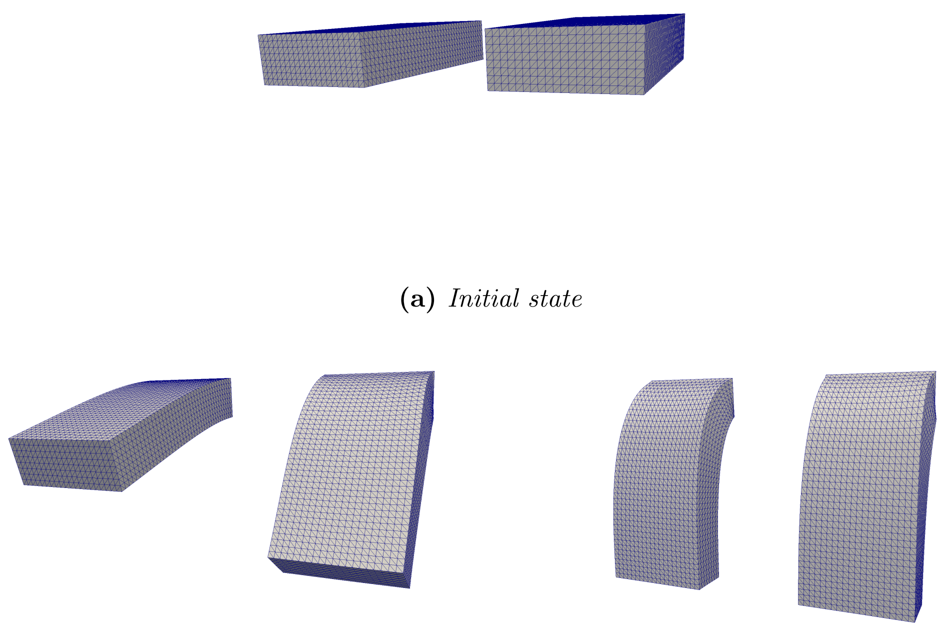
6.5.2 Numerical Experiments

The following numerical simulations were made by Matthias Stöcklein from the University of Bayreuth, whose help for this task we greatly appreciate. In this example, we use a compressible Mooney-Rivlin material law of the form:

$$W(x, \nabla\varphi) = a_0 \|\nabla\varphi\|^2 + a_1 \|\operatorname{cof}(\nabla\varphi)\|^2 + a_2 \det(\nabla\varphi)^2 - a_3 \log(\det(\nabla\varphi))$$

with

$$a_0 = 0.08625, \quad a_1 = 0.08625, \quad a_2 = 0.68875, \quad a_3 = 1.895.$$



(a) *Initial state*

(b) *First iteration* **(c)** *Final state*

Figure 6.15: *Iteration comparisons: Left, by linear updates. Right, by non-linear updates.*

In figure 6.15, we observe how the performance is improved by using the nonlinear updates. The object is clamped by one side to a wall, and a vertical force pointing downwards is applied to the body. We observe that the difference is high in comparison, where, in the left of each picture, the linear update is done, and in the right, the nonlinear update is performed. We also observe how the performance is better and visible already in the first iteration. In Figures 6.16 and 6.17, we observe that convergence is reached in 18 iterations with linear update, but using nonlinear update, the number reduces to 11, also the behavior of the functional suffers a dramatic decreased when nonlinear updates are used.

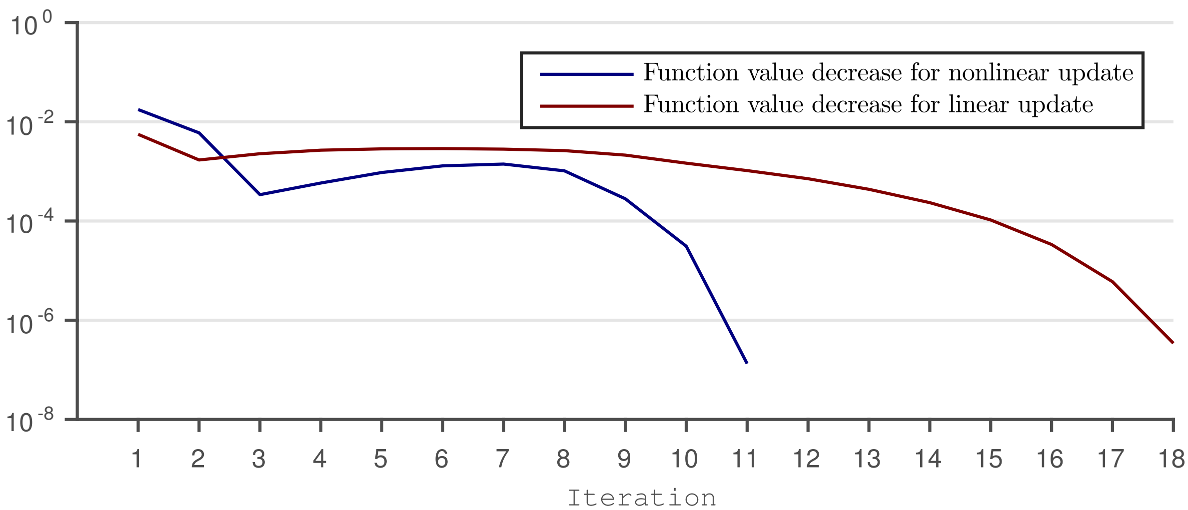


Figure 6.16: *Iteration history: Comparison of function value decrease. In blue nonlinear updates. In red linear updates.*

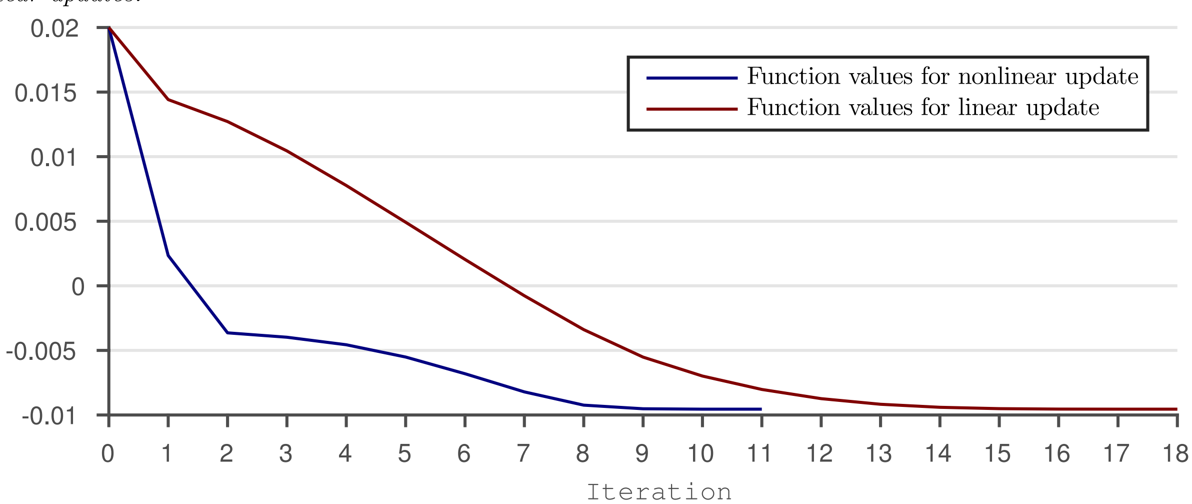


Figure 6.17: *Iteration history: Comparison of function values. In blue nonlinear updates. In red linear updates.*

Chapter 7

Conclusions and outlook

In this work, we have considered equality constrained optimization problems on differentiable manifolds. Thus, we have extended the unconstrained setting found in [AMS09], to the constrained one. Besides, for the solution of optimal control problems posed on differentiable manifolds, the formulation has been extended to the case in which the spaces are vector bundles. Specifically in our applications, we have considered the equality constrained formulation, where the target map of the constraint, maps into the co-tangent bundle, i.e., an special instance of a vector bundle. In [AMS09], the concept of retractions is introduced as a fundamental tool for the development of optimization algorithms on manifolds. We have extended the concept of retraction to the more general case where the manifold has the structure of a vector bundle. Through the concept of vector bundles connections [E$^+$67, Lan12a, Dom62, V$^+$67], we defined first and second order vector bundle retractions, as well as consistency properties for such maps.

In addition, once the equality constrained optimization problem is posed, first and second-order optimality conditions are derived. In particular, as a solution of a saddle point problem at each point on the manifold, a 1-form Lagrange multiplier $\hat{\lambda}$ arises. We showed that the existence of a potential function Λ, such that $d\hat{\lambda} = \Lambda$, depends on the integrability of the horizontal distribution $(\ker c'(x))^{\perp}$, in the sense of Frobenius.

Concerning the algorithmic part, we have extended the affine covariant composite step method presented in [LSW17], to the manifold case. This method was successfully used to solve optimal control problems involving finite strain elasticity [LSW14]. In the linear case [LSW17], the composite steps, δn and δt add up to a Lagrange-Newton step, and fast local convergence is obtained. The composite step method on manifolds uses a set of nonlinear retractions to pullback the cost and constraint mappings to linear spaces to compute the corrections, which are subsequently updated through a different set of retractions. The quality of the retractions plays a role in the performance of the algorithm, in particular, we proved that the algorithm converges super-linearly, even for first-order retractions, with the introduction of a surrogate model.

We applied our method to problems in linear algebra and finite elasticity. As a first application, we solved a constrained eigenvalue problem as proposed in [GGvM89], where minimization of a real functional having as a constraint a matrix of full rank is performed over the $\mathbb{S}^N$-sphere. We proceeded with examples of finite elasticity. More specifically, we considered the displacement calculations of flexible inextensible rods as in [GLT89]. The inextensibility condition led, in the discretized formulation, a problem on the product $(\mathbb{S}^2)^n$, where n is the number of nodes of the discretization. In the first simulation, we solved the forward problem of getting the final configuration of an elastic inextensible rod under dead load. Then, we considered the case, in which the rod enters in contact with one of the planes delimiting the positive cone $\mathcal{K}^+$. Using the approach given in [NT$^+$02], we regard the space $\mathcal{K}^+$ as a Riemannian manifold. We used interior point methods on this formulation, as found in the literature [NW06, Meh92, NW06, SNW12], where, thanks to the manifold structure, and the retractions defined on this space, our method was applicable. Finally, we considered the optimal control problem of elastic inextensible rods. We minimized a tracking type functional, constrained to be the minimizer of the elastic energy of the rod. Here, the differential of the elastic energy, maps into a cotangent bundle space. This structure arises, given that the differential of a real function on a manifold, is an element of the co-tangent bundle, which is an instance of a vector bundle. We implemented the newly introduced vector bundle retractions in this setting, in particular, tangent bundle retractions for the space $T\mathbb{S}^2$ are implemented, using the connection $\kappa_{T\mathbb{S}^2}$, given by the second fundamental form, regarding $\mathbb{S}^2$ as a submanifold of $\mathbb{R}^3$. We closed our applications, with an example of the introduced retractions on the space of orientation preserving tetrahedra $\mathcal{T}_{pos}$. In the context of finite elasticity, we considered the deformation calculation of a 3-dimensional body $\Omega \subset \mathbb{R}^3$. The body is discretized by subdividing it into tetrahedra. We showed the impact that the nonlinear updates defined as retractions on the space of orientation preserving tetrahedra $\mathcal{T}_{pos}$ have on the algorithm. We noticed that efficiency of the algorithm improved in a significant way, compared with the usual linear updates. In this final case, in contrast to the rod mechanics, the pullback of the discretized stored energy functional into the space $\mathcal{T}_{pos}$ through retractions was not performed, such pullback, would lead to a finite element discretization using the retraction $R^{\mathcal{T}_{pos}}$. In addition, thanks to the formulation over vector bundles, and the introduction of the retractions $R^{\mathcal{T}_{\rho}}$ for the space of volume preserving tetrahedra, the numerical solution of optimal control problems over the space of volume preserving diffeomorphims can be considered as a topic for future research.

Appendix A

This chapter aims to collect some basic definitions and results on linear topological spaces that support the nonlinear theory developed in this thesis.

A.1 Vector spaces

Definition A.1.1. *A topological vector space $\mathbb{E}$ over the real numbers $\mathbb{R}$, is a vector space with a topology such the operations of addition:*

$$\begin{aligned} &\mathbb{E} \times \mathbb{E} \to \mathbb{E} \\ &(v, w) \to v + w \end{aligned} \tag{A.1}$$

and scalar multiplication:

$$\begin{aligned} &\mathbb{R} \times \mathbb{E} \to \mathbb{E} \\ &(\alpha, w) \to \alpha w \end{aligned} \tag{A.2}$$

are continuous.

Definition A.1.2. *A norm on a topological vector space $\mathbb{E}$, is a non-negative function*

$$\|\cdot\|_{\mathbb{E}} : \mathbb{E} \to \mathbb{R} \tag{A.3}$$

such that for $t \in \mathbb{R}$, and for all $u, v \in \mathbb{E}$, it satisfies the following properties:

i) $\|u + v\|_{\mathbb{E}} \leq \|u\|_{\mathbb{E}} + \|v\|_{\mathbb{E}}$.

ii) $\|tu\|_{\mathbb{E}} = |t|\|u\|_{\mathbb{E}}$.

iii) If $\|v\|_{\mathbb{E}} = 0$ *then* $v = 0$.

Special cases of vector topological spaces are Banach and Hilbert spaces.

Definition A.1.3. *A Banach space $\mathbb{E}$, is a topological vector space, which is equipped with a norm $\|\cdot\|_{\mathbb{E}}$ and is complete with respect to the distant function induced by the norm. This means that every Cauchy sequence is convergent in $\mathbb{E}$.*

Definition A.1.4. *A Hilbert space $\mathbb{E}$, is a topological vector space, endowed with an inner product*

$$\begin{aligned}\mathbb{E}\times\mathbb{E} &\to \mathbb{R}\\ (v,w) &\to \langle v,w\rangle\end{aligned}$$

such that the norm on $\mathbb{E}$ defined by

$$\|v\|_{\mathbb{E}} := \sqrt{\langle v,v\rangle}$$

turns $\mathbb{E}$ into a complete space with respect to the distant function induced by this norm.

Definition A.1.5. *Let be $\mathbb{E}$ and $\mathbb{F}$ two topological vector spaces over $\mathbb{R}$. We say that a map $\tilde{\psi}:\mathbb{E}\to\mathbb{F}$ is a linear function if for any two elements $v,w\in\mathbb{E}$ and any scalar $\alpha\in\mathbb{R}$ the following two conditions are satisfied:*

$$\begin{aligned}\tilde{\psi}(v+w) &= \tilde{\psi}(v)+\tilde{\psi}(w)\\ \tilde{\psi}(\alpha v) &= \alpha\tilde{\psi}(v).\end{aligned}$$

The set of continuous linear maps of $\mathbb{E}$ into $\mathbb{F}$ is denoted by $L(\mathbb{E},\mathbb{F})$.

Definition A.1.6. *Let be $\mathbb{E}_1,\mathbb{E}_2,..,\mathbb{E}_r$ and $\mathbb{F}$ topological vector spaces over $\mathbb{R}$. We say that the map $\psi_r:\mathbb{E}_1\times...\times\mathbb{E}_r\to\mathbb{F}$ is a r-multilinear map if for all $j\in\{1,...,r\}$:*

$$\psi(v_1,..,v_{j-1},\alpha v_j+\beta w_j,v_{j+1},..,v_r)=\alpha\psi(v_1,..,v_{j-1},v_j,v_{j+1},..,v_r)+\beta\psi(v_1,..,v_{j-1},w_j,v_{j+1},..,v_r) \tag{A.4}$$

for all $v_i\in\mathbb{E}_i$ $i\in\{1,..,r\}$, $w_j\in\mathbb{E}_j$ and $\alpha,\beta\in\mathbb{R}$. We denote the continuous r-multilinear maps of the product $\mathbb{E}_1\times...\times\mathbb{E}_r$ into $\mathbb{F}$ by $L(\mathbb{E}_1,...,\mathbb{E}_r;\mathbb{F})$. If in addition $\mathbb{E}=\mathbb{E}_i$ for all $i\in\{1,...,r\}$ then we denote this space by $L^r(\mathbb{E},\mathbb{F})$.

Definition A.1.7. *Let be $\mathbb{E}$ and $\mathbb{F}$ topological vector spaces. We say that an r-multilinear map $\psi\in L^r(\mathbb{E},\mathbb{F})$ is symmetric if:*

$$\psi(v_1,...,v_i,...,v_j,...,v_r)=\psi(v_1,...,v_j,...,v_i,...,v_r),\quad v_1,...,v_r\in\mathbb{E}. \tag{A.5}$$

The r-multilinear symmetric maps are denoted by $L^r_{sym}(\mathbb{E},\mathbb{F})$.

Definition A.1.8. *Let be $\mathbb{E}$ and $\mathbb{F}$ topological vector spaces. We say that an r-multilinear map $\psi\in L^r(\mathbb{E},\mathbb{F})$ is alternating if:*

$$\psi(v_1,...,v_i,...,v_j,...,v_r)=0 \tag{A.6}$$

for all $v_1,...,v_r\in\mathbb{E}$ whenever $v_i=v_j$ for some $i\neq j$. The r-multilinear alternating maps are denoted by $L^r_a(\mathbb{E},\mathbb{F})$.

More details on multilinear functions can be found in [BW08, Bro12].

Remark A.1.1. *In particular, a continuous linear map into* $\lambda : \mathbb{E} \to \mathbb{R}$ *receives the name of functional.*

Definition A.1.9. *Let be* $\mathbb{E}$ *a normed topological space. We denote by* $\mathbb{E}^*$ *the set of all continuous linear functionals on* $\mathbb{E}$. *The dual norm on* $\mathbb{E}^*$ *is defined by:*

$$\|f\|_{\mathbb{E}^*} = \sup_{\|v\| \leq 1} |f(v)|, \quad v \in \mathbb{E}.$$

Given $f \in \mathbb{E}^*$ *and* $v \in \mathbb{E}$, *it is often written* $\langle f, v \rangle$ *instead of* $f(v)$, *and we say that* $\langle \cdot, \cdot \rangle$ *is the scalar product for the duality* $\mathbb{E}$, $\mathbb{E}^*$.

The Riesz Representation Theorem. Let be $\mathbb{E}$ a Hilbert space. Then for every $\lambda \in \mathbb{E}^*$ there exists an $v \in \mathbb{E}$ such that for every $w \in \mathbb{E}$, $\lambda(w) = \langle w, v \rangle$. Thus the Riesz representation theorem shows that $R : \mathbb{E} \to \mathbb{E}^*$, defined by $R(w)(v) = \lambda(v) = \langle w, v \rangle$ is an isomorphism. For more details on the proof see e.g., [Bre10, Eva10].

Definition A.1.10. *Let be* $\mathbb{E}$ *a Banach space and let be* $\mathbb{G}$ *a closed subspace. We consider an equivalence relation on* $\mathbb{E}$ *defined by* $v \sim w$ *if* $v - w \in \mathbb{G}$. *We denote:*

$$\mathbb{E}/\mathbb{G} \tag{A.7}$$

as the set of all equivalence classes, which is in turn a vector space. We call $\mathbb{E}/\mathbb{G}$ *the quotient space of* $\mathbb{E}$ *(mod* $\mathbb{G}$*). We have, in addition, that the canonical map* $\pi : \mathbb{E} \to \mathbb{E}/\mathbb{G}$, *which assigns to every* v *it equivalence class* $[v]$ *is linear and surjective.*

A.2 Derivatives of Maps

Definition A.2.1. *Let* $\mathbb{E}$, $\mathbb{F}$ *be two normed topological spaces. For* $U \subset$ *open in* $\mathbb{E}$, *we say that the continuous map* $f : U \to \mathbb{F}$ *is differentiable at a point* $x_0 \in U$ *if there exists a continuous linear map* $\Lambda : \mathbb{E} \to \mathbb{F}$ *such that:*

$$f(x_0 + v) = f(x_0) + \Lambda v + r(v) \tag{A.8}$$

where

$$\|r(v)\|_{\mathbb{F}} \|v\|_{\mathbb{E}}^{-1} \to 0 \quad \text{as} \quad \|v\|_{\mathbb{E}} \to 0. \tag{A.9}$$

In this way Λ *is uniquely determined, and we say that it is the derivative of* f *at* x_0. *It is an element of* $L(\mathbb{E}, \mathbb{F})$ *and it is denoted as* $Df(x_0)$ *or* $f'(x_0)$. *For more details, see e.g.,[AS67, Lan12a].*

Let be $\mathbb{E}$, $\mathbb{F}$ Banach spaces. Let be U open in $\mathbb{E}$ and let $f : U \to \mathbb{F}$ a differentiable function at each point of U. For $k \in \mathbb{N}$, we define the k-th derivative of f denoted by $D^k f$, inductively, as $D(D^{k-1} f)$. We have that

$$D^k f : U \to L(\mathbb{E}, L(\mathbb{E}, ..., L(\mathbb{E}, \mathbb{F})...))$$

where the latter space, can be identified with $L^k(\mathbb{E}, \mathbb{F})$ (see e.g.,[Lan12a]). We say that a map f is of class C^m if its m-th derivative D^m exists for $1 \leq m \leq k$, and is continuous.
We now mention indispensable Taylor formula.

Proposition A.2.1 (Taylor's Formula)**.** *Let $\mathbb{E}$ and $\mathbb{F}$ be Banach spaces. Let be be $U \subset \mathbb{E}$ an open subset of $\mathbb{E}$. Let be x, y two points of U such that the segment $x + ty$ lies in U for $0 \leq t \leq 1$. Let*

$$f : \mathbb{E} \to \mathbb{F}$$

be a C^p-function, and denote by $y^{(p)} := (y, ..., y)$ p-times. Then the function $D^p f(x + ty)y^{(p)}$ is continuous in t, and

$$f(x+y) = f(x) + \frac{Df(x)y}{1!} + \cdots + \frac{D^{p-1}f(x)y^{(p-1)}}{(p-1)!} + \int_0^1 \frac{(1-t)^{p-1}}{(p-1)!} D^p f(x+ty)y^{(p)}\, dt. \tag{A.10}$$

Proof. See [Lan12a, I,§3]. □

We observe that, for a differentiable function $f : U \subset \mathbb{E} \to \mathbb{R}$, the differential $f'(x_0) \in L(\mathbb{E}, \mathbb{R})$, i.e., $f'(x_0) \in \mathbb{E}^*$.

Definition A.2.2. *Let be $\mathbb{E}$ a Hilbert space with inner product $\langle \cdot, \cdot \rangle$. And let be $f : U \to \mathbb{R}$ differentiable at $x_0 \in U$. Then we define:*

$$\nabla f(x_0) = R^{-1}(Df(x_0)) \tag{A.11}$$

where, R is the Riesz isomorphism, and call $\nabla f(x_0) \in \mathbb{E}$ the gradient of f at x_0.

Proposition A.2.2. *If the function $f : U \to V$ is differentiable at x_0, and the function $g : V \to W$ is differentiable at $f(x_0)$, then $g \circ f$ is differentiable at x_0, and*

$$(g \circ f)'(x_0) = g'(f(x_0)) \circ f'(x_0). \tag{A.12}$$

Let us assume that U is open in $\mathbb{E}$, and let $f : U \to \mathbb{F}$ be differentiable at each point of U. If the mapping f' is continuous, we say that f is of class C^1. The k-th derivative $D^k f$ of f, is defined as $D(D^{k-1}f)$, with $D^k f \in L^k(\mathbb{E}, \mathbb{F})$. A map f is said to be of class C^k if its j-th derivative $D^j f$ exists for $1 \leq j \leq k$, and is continuous.

Theorem A.2.1 (The Inverse Function Theorem)**.** *Let be $\mathbb{E}$, $\mathbb{F}$ Banach spaces, and $U \in \mathbb{E}$ an open subset. Let be*

$$g : U \to \mathbb{F}$$

a smooth map such that for some $x \in U$ with $g(x) = y \in \mathbb{F}$, the derivative $Dg(x) : \mathbb{E} \to \mathbb{F}$ is an isomorphism. Then, there exists open neighborhoods $x \in \tilde{U} \subset U$ and $y \in \tilde{V} \subset \mathbb{F}$ such that, the map:

$$g_{|_{\tilde{U}}} : \tilde{U} \to \tilde{V} \tag{A.13}$$

is invertible. In addition, its inverse g^{-1} is also smooth and the following holds:

$$D(g^{-1})(y) = (Dg(x))^{-1} : \mathbb{F} \to \mathbb{E}. \tag{A.14}$$

Proof. See [Lan12b]. □

Theorem A.2.2 (The implicit Function Theorem). *Let be $\mathbb{E}_1, \mathbb{E}_2$ and $\mathbb{E}_3$ Banach spaces, and Let be U a neighborhood of a point (x_0, y_0) in the product $\mathbb{E}_1 \times \mathbb{E}_2$. Consider a C^1 map $F : U \to \mathbb{E}_3$, with $F(x_0, y_0) = 0$ and assume that the partial derivative $F_2(x_0, y_0) : \mathbb{E}_2 \to \mathbb{E}_3$ is a linear homeomorphism (i.e., F_2 bijective continuous and with continuous inverse). Then there exist open subsets $U_1 \subset \mathbb{E}_1$, $U_2 \subset \mathbb{E}_2$, and a mapping $y(x) : U_1 \to U_2$ such that, on $U_1 \times U_2$, we have:*

$$F(x, y(x)) = 0. \tag{A.15}$$

In addition, $y(x)$ is of class C^1, and for any $x \in U_1$

$$y'(x) = -\left(F_2(x, y(x))\right)^{-1} \circ F_1(x, y(x)). \tag{A.16}$$

Proof. See e.g.,[IT09, 0,§2]. □

A.3 Sobolev Spaces

For the variational formulations of the mechanical problems considered in this work, the use of Sobolev spaces is needed. In this section, we introduce these spaces and some properties, for a more detailed exposition see [AF03, Bre10, GLT89, ABM14, BP12, Eva10]. In this work, we assume the set Ω, which is in general defined as the interior of the continuous body under consideration in its reference configuration. The body Ω is supposed to be open, bounded, and connected in $\mathbb{R}^3$. The subsets $\Omega \subset \mathbb{R}^3$ are equipped with the classical Lebesgue measure of $\mathbb{R}^3$, denoted by dx.

Definition A.3.1. *Let $p \in \mathbb{R}$ with $1 < p < \infty$. We set*

$$L^p(\Omega) = \{f : \Omega \to \mathbb{R} \,|\, f \text{ is mesurable and } \int_\Omega |f|^p < \infty\}$$

with the norm

$$\|f\|_{L^p} = \|f\|_p = \left(\int_\Omega |f(x)|^p \, dx\right)^{1/p}.$$

If $p = \infty$, we set

$$L^\infty(\Omega) = \{f : \Omega \to \mathbb{R} \,|\, f \text{ is mesurable and there is } C \in \mathbb{R} \text{ s.t. } |f(x)| \leq C \text{ a.e on } \Omega\}$$

with the norm

$$\|f\|_{L^\infty} = \inf\{\, C \mid |f(x)| \leq C \text{ a.e on } \Omega\} \tag{A.17}$$

Theorem A.3.1 (Fischer-Riesz). *The space $L^p(\Omega)$ is a Banach space for any p, $1 \leq p \leq \infty$.*

Proof. See [Bre10, IV, §2] □

On the other hand, we define the space $\mathcal{D}(\Omega)$, as the space of real functions infinitely differentiable and with compact support in Ω. The topological dual $\mathcal{D}^*(\Omega)$ receive the name of space of distributions on Ω. In this way, any locally Lebesgue integrable real function $f : \Omega \to \mathbb{R}$ can be identified with a distribution by

$$\langle f, \phi \rangle = \int_\Omega f(x)\phi(x)\ dx \quad \text{ for all } \phi \in \mathcal{D}(\Omega)$$

with $\langle \cdot, \cdot \rangle$ denoting the duality pairing between $\mathcal{D}^*(\Omega)$ and $\mathcal{D}(\Omega)$. For $\alpha = \{\alpha_1, \alpha_2, \alpha_3\}$ in $\mathbb{N}^3$, and $|\alpha| = \alpha_1 + \alpha_2 + \alpha_3$, the α derivative of a distribution f is defined by

$$\langle \partial^\alpha f, \phi \rangle = (-1)^{|\alpha|} \left\langle f, \frac{\partial^{|\alpha|}\phi}{\partial x_1^{\alpha_1} \partial x_2^{\alpha_2} \partial x_3^{\alpha_3}} \right\rangle \quad \text{ for all } \phi \in \mathcal{D}(\Omega).$$

In particular, we have that a function f of class $C^{|\alpha|}$, this concept corresponds to the usual definition of the partial derivative $\partial^\alpha f$.
For $m \in \mathbb{N}$ and $p \in \mathbb{R}$, $1 \leq p \leq \infty$, we define the Sobolev space

$$W^{m,p}(\Omega) = \{g \in L^p(\Omega) \,|\, \partial^\alpha g \in L^p(\Omega) \text{ for all } \ |\alpha| < m\}, \tag{A.18}$$

with the norm

$$\|g\|_{m,p} = \left(\sum_{\alpha \leq m} \int_\Omega |\partial^\alpha g|^p\ dx \right)^{1/p} \qquad \text{if } p < \infty \tag{A.19}$$

$$\|g\|_{m,\infty} = \sup_{|\alpha| \leq m} \left(\sup_{x \in \Omega} \text{ess}\, |\partial^\alpha g(x)| \right) \qquad \text{if } p = \infty. \tag{A.20}$$

For $p = 2$, we denote $W^{m,2}(\Omega)$ by $H^m(\Omega)$, which is a Hilbert space for the scalar product.

$$\langle f, g \rangle = \sum_{|\alpha| \leq m} \int_\Omega \partial^\alpha f\ \partial^\alpha g\ dx. \tag{A.21}$$

We now state a couple of basic properties of such Sobolev spaces.

Theorem A.3.2. *For $1 < p < \infty$, $W^{m,p}$ is a Banach space.*

Proof. See [Bre10, AF03, GLT89, Con19]. □

An the important

Theorem A.3.3 (Sobolev Imbedding Theorem)**.** *Let p, with $1 \leq p \leq \infty$, be given and for $\Omega \subset \mathbb{R}^N$, we have that:*

i) for $0 \leq m < \frac{N}{p}$, $W^{m,p}(\Omega)$ is continuously imbedded in $L^q(\Omega)$ $\left(\frac{1}{q} = \frac{1}{p} - \frac{m}{N}\right)$;

ii) for $m = \frac{N}{p}$,$W^{m,p}(\Omega)$ is continuously imbedded in any $L^q(\Omega)$, $1 \leq q < \infty$;

iii) for $m > \frac{N}{p}$, $W^{m,p}(\Omega)$ is continuously imbedded in $C(\overline{\Omega})$. Where $\overline{\Omega}$ denotes the closure of Ω.

Proof. See [Bre10, AF03, Con19]. □

A.4 Matrices

Next, we introduce some formulas from matrix theory that are needed for the development of this work.

Definition A.4.1. *Let be $n, m \in \mathbb{N}$, with $n, m \geq 1$. A real matrix M of size $n \times m$, is a rectangular arrangement of real numbers, with n being the number of rows and m the number of columns of the arrangement. The representation is given by:*

$$M = \begin{bmatrix} m_{11} & \cdots & m_{1n} \\ \vdots & \ddots & \vdots \\ m_{n1} & \cdots & m_{nm} \end{bmatrix}, \tag{A.22}$$

which can also be written as

$$M = (m_{ij})_{1 \leq i \leq n,\, 1 \leq j \leq m.} \tag{A.23}$$

with $(m_{ij}) \in \mathbb{R}$, for all $i \in \{1, ..., n\}$ and $j \in \{1, ..., m\}$. The set of real matrices of size $n \times m$ is denoted by $\mathcal{M}_{n \times m}(\mathbb{R})$. The transpose of the matrix M, denoted by M^T, is defined as $M^T = (m_{ji})_{1 \leq i \leq m,\, 1 \leq j \leq n}$. In the case in which $n = m$, we say that the matrix is square. The set of square matrices of size n is denoted by $\mathcal{M}_n(\mathbb{R})$. The identity matrix $I_n \in \mathcal{M}_n(\mathbb{R})$ is defined by:

$$m_{ij} = \delta_i^j = \begin{cases} 1, & \text{if} \quad i = j \\ 0, & \text{if} \quad i \neq j \end{cases} \tag{A.24}$$

and its representation is given by

$$I_n = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 1 \end{bmatrix}. \tag{A.25}$$

We also say that a square matrix is symmetric if $M = M^T$, skew-symmetric if $M = -M^T$ and positive definite if $x^T M x > 0$ for every $x \neq 0$. Thus, we have the sets:

$$\mathrm{Sym}(n) = \{M \in \mathcal{M}_n(\mathbb{R}) |\, M = M^T\} \tag{A.26}$$

$$\mathrm{Skew}(n) = \{M \in \mathcal{M}_n(\mathbb{R}) |\, M = -M^T\} \tag{A.27}$$

$$\mathrm{Pos}(n) = \{M \in \mathcal{M}_n(\mathbb{R}) |\, x^T M x > 0 \text{ for all } x \in \mathbb{R}^n,\, x \neq 0\} \tag{A.28}$$

$$\mathrm{Met}(n) = \{M \in \mathcal{M}_n(\mathbb{R}) |\, M \in \mathrm{Pos}(n) \cap \mathrm{Sym}(n)\}. \tag{A.29}$$

Observe that, every matrix $M \in \mathcal{M}_n(\mathbb{R})$ can be written as:

$$M = \frac{1}{2}(M + M^T) + \frac{1}{2}(M - M^T) \tag{A.30}$$

where $\frac{1}{2}(M+M^T) \in \mathrm{Sym}(n)$ and $\frac{1}{2}(M-M^T) \in \mathrm{Skew}(n)$. Given that $\mathrm{Sym}(n) \cap \mathrm{Skew}(n) = 0$, then:

$$\mathcal{M}_n(\mathbb{R}) = \mathrm{Sym}(n) \oplus \mathrm{Skew}(n), \tag{A.31}$$

where, $\oplus$ denotes the direct sum.

Definition A.4.2. *Let be $n, m, p \in \mathbb{N}$ non-zero numbers. We define the product of two real matrices M and N as:*

$$\mathcal{M}_{n\times m}(\mathbb{R}) \times \mathcal{M}_{m\times p}(\mathbb{R}) \to \mathcal{M}_{n\times p}(\mathbb{R}) \tag{A.32}$$

$$(M, N) \to MN, \tag{A.33}$$

where the matrix $\tilde{M} = MN$ is given by the formula:

$$\tilde{m}_{ij} = \sum_{k=1}^{m} m_{ik}\, n_{kj}, \;\; 1 \le i \le n, \;\; 1 \le j \le p. \tag{A.34}$$

For $M \in \mathcal{M}_n(\mathbb{R})$, we have that $MI_n = I_nM = M$. The product is associative, but in general not commutative, i.e., in general $MN \neq NM$, for $M, N \in \mathcal{M}_n(\mathbb{R})$. For this reason, the commutator between the matrices M and N, given by $[M, N] = MN - NM$, is defined. In addition, for a given square matrix $M \in \mathcal{M}_n(\mathbb{R})$, we define by $M^2 = MM$, $M^3 = MM^2 = M^2M, \cdots,\; M^{k+1} = M^kM$, for $k \in \mathbb{N}$.

Definition A.4.3. *For a given $M \in \mathcal{M}_n(\mathbb{R})$. We say that the matrix M is invertible, if there exists $P \in \mathcal{M}_n(\mathbb{R})$, such that:*

$$MP = PM = I_n. \tag{A.35}$$

In such case, we say that P is the inverse of M, which is uniquely determined by M and is denoted by M^{-1}.

Definition A.4.4. *Let be $M = (m_{ij})_{1\le i,j\le n} \in \mathcal{M}_n(\mathbb{R})$ a square matrix. Denote by $\mathcal{S}_n$ the group of permutations over the set $\{1, 2, ..., n\}$. The determinant of M, denoted by $\det M$, is given by:*

$$\det M := \sum_{\sigma\in\mathbb{S}_n} \epsilon(\sigma) m_{1\sigma(1)} \cdots m_{n\sigma(n)}, \tag{A.36}$$

where $\epsilon(n) = \pm 1$ denotes the signature of ϵ, which is equal to $+1$ if σ is an even product of transpositions, and -1 otherwise.

Let be $M, N \in \mathcal{M}_n(\mathbb{R})$. We list some important properties of the determinant:

i) $\det I_n = 1$.

ii) $\det M^T = \det M$.

iii) If M is invertible then $\det M \neq 0$, and $\det M^{-1} = \frac{1}{\det M}$.

iv) $\det(MN) = \det M \, \det N$.

v) $\det(tM) = t^n \det M$, for $t \in \mathbb{R}$.

Definition A.4.5. *Let be $M \in \mathcal{M}_n(\mathbb{R})$. The i,j cofactor of the matrix M, is the real number c_{ij} given by:*

$$c_{ij} = (-1)^{i+j}\tilde{m}_{ij}$$

where $\tilde{m}_{ij}$ is the i,j minor of M, which is given by the determinant of the $(n-1)\times(n-1)$ matrix that results from deleting the i-th row and the j-th column of M. The matrix $C = (c_{ij})$ is the matrix of cofactors of M.

Definition A.4.6. *Let be $M \in \mathcal{M}_n(\mathbb{R})$ and C the corresponding matrix of cofactors. We define the adjugate matrix of M by:*

$$\operatorname{Adj}(M) = C^T. \tag{A.37}$$

Proposition A.4.1. *Let be $M \in \mathcal{M}_n(\mathbb{R})$. Then we have that:*

$$M \operatorname{Adj}(M) = \operatorname{Adj}(M)M = \det M I_n. \tag{A.38}$$

In particular, if M is invertible, $\det M \neq 0$ *and we have the identity:*

$$M^{-1} = \frac{1}{\det M}\operatorname{Adj}(M). \tag{A.39}$$

Proof. See e.g., [Ser01, II,§1]. □

We denote by $GL(n)$, the general linear group, to the set of all invertible elements of $\mathcal{M}_n(\mathbb{R})$. We have that $GL(n)$ is a multiplicative group. In addition, we call the special linear group $SL(n)$, to the set of matrices with determinant equals to one. $SL(n)$ is a subgroup of $GL(n)$. The orthogonal matrices are the matrices that satisfy the relation $M^{-1} = M^T$, and is denoted by $O(n)$. Furthermore, the orthogonal matrices with determinant equals to one, receive the name of special orthogonal group and the set is denoted by $SO(n)$.

Proposition A.4.2. *Let be $M \in \mathcal{M}_n(\mathbb{R})$. Then, the series*

$$\exp(M) := \sum_{k=0}^{\infty}\frac{1}{k!}M^k \tag{A.40}$$

is convergent, and the sum is called the exponential of M.

Proof. See e.g., [Ser01, VII,§2]. □

Proposition A.4.3. *Let be $M, N \in \mathcal{M}_n(\mathbb{R})$, such that $MN = NM$, then we have that*

$$\exp(M + N) = \exp(M)\exp(N). \tag{A.41}$$

Proof. See e.g., [Ser01, VII,§2]. □

As a consequence of the previous proposition and using the identities $\exp(0_n) = I_n$ and the identity $(M)(-M) = (-M)(M)$, we have

Proposition A.4.4. *For every $M \in \mathcal{M}_n(\mathbb{R})$, $\exp(M) \in GL(n)$, i.e., $\exp(M)$ is invertible and its inverse is given by $\exp(-M)$.*

Proof. We see that

$$I_n = \exp(0_n) = \exp(M - M) = \exp(M)\exp(-M) \tag{A.42}$$

then the result follows. □

Moreover, we have the following result:

Proposition A.4.5. *If $M \in \mathrm{Sym}(n)$ then $\exp(M) \in \mathrm{Met}(n)$, and if $M \in \mathrm{Skew}(n)$ then we get that $\exp(M) \in O(n)$. Furthermore, The exponential map:*

$$\exp(\cdot) : \mathrm{Sym}(n) \to \mathrm{Met}(n) \tag{A.43}$$

is an isomorphism.

Proof. See e.g., [Lan12a, XII,§1]. □

If we introduce a parameter $t \in \mathbb{R}$, and define $g(t) = \exp(tM)$ for $M \in \mathcal{M}_n(\mathbb{R})$. In particular we see that, for $s \in \mathbb{R}$, $g(s+t) = g(s)g(t)$, and g is differentiable, in particular, we see that:

$$g'(t) = \lim_{s \to 0} \frac{g(t)g(s) - g(t)}{s} = g(t)M \quad \text{and} \quad g'(t) = \lim_{s \to 0} \frac{g(s)g(t) - g(t)}{s} = Mg(t) \tag{A.44}$$

therefore, we have the formula:

$$\frac{d}{dt}\exp(tM) = M(\exp(tM)) = (\exp(tM))M. \tag{A.45}$$

The trace operator is defined as:

$$\mathrm{tr} : \mathcal{M}_n(\mathbb{R}) \to \mathbb{R} \tag{A.46}$$

$$M \to \mathrm{tr}(M) = \sum_{i=1}^{n} m_{ii}. \tag{A.47}$$

Let be $M, N \in \mathcal{M}_n(\mathbb{R})$, some properties of the trace operator are:

i) $\mathrm{tr}(M + N) = \mathrm{tr}(M) + \mathrm{tr}(N)$.

ii) $\mathrm{tr}(tM) = t\,\mathrm{tr}(M)$, $t \in \mathbb{R}$.

iii) $\mathrm{tr}(M) = \mathrm{tr}(M^T)$.

iv) $\mathrm{tr}(MN) = \mathrm{tr}(NM)$.

v) If $M \in \mathrm{Sym}(n)$ and $N \in \mathrm{Skew}(n)$, then $\mathrm{tr}(MN) = 0$.

Finally, we list some useful formulas involving the derivative of the determinant and the Jacobi's identity.

Proposition A.4.6. *Let be $h(t) : \mathbb{R} \to GL(n)$, given by $h(t) = M(t)$, a differentiable function and $N \in \mathcal{M}_n(\mathbb{R})$. Then we have the following identities:*

i) $\frac{d}{dt}\det(I_n + tN) = \operatorname{tr} N$.

ii) $\frac{d}{dt}\det M(t) = \det M(t) \operatorname{tr}\left(M(t)^{-1}\frac{d}{dt}M(t)\right)$.

iii) $\det(\exp(N)) = \exp\operatorname{tr}(N)$.

Proof. For a complete proof see e.g., [Ser01, Ber09]. The identity *ii)* is the well known Jacobi's formula. □

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Publications

[OS19] Julian Ortiz and Anton Schiela. A composite step method for equality constrained optimization on manifolds. *https://epub.uni-bayreuth.de/4258/*, 2019.

[SO19] Anton Schiela and Julian Ortiz. Second order directional shape derivatives. *https://epub.uni-bayreuth.de/4227/*, 2019.

Some parts of this work are contained in [OS19]. Specifically, sections 5.1-5.4 from Chapter 5, in which the composite step method on manifolds is presented. Basic properties of retractions from chapter 3 involving their consistency, and the content of section 4.2.1, where the pullbacked Lagrange function is defined. Concerning applications, the setting, and corresponding numerical simulations for elastic inextensible rods under dead load of section 6.2, are also contained in the cited paper.

Eidesstattliche Versicherung

Hiermit versichere ich an Eides statt, dass ich die vorliegende Arbeit selbstständig verfasst und keine anderen als die von mir angegebenen Quellen und Hilfsmittel verwendet habe.

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Julián Ortiz