Extended retraction maps: a seed of geometric integrators

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Abstract

The classical notion of retraction map used to approximate geodesics is extended and rigorously defined to become a powerful tool to construct geometric integrators. Using the geometry of the tangent and cotangent bundles, we are able to tangently and cotangent lift such a map so that these lifts inherit the same properties as the original one and they continue to be extended retraction maps. In particular, the cotangent lift of this new notion of retraction map is a natural symplectomorphism, what plays a key role for constructing geometric integrators and symplectic methods. As a result, a wide range of numerical methods are recovered and canonically constructed by using different extended retraction maps, as well as some operations with Lagrangian submanifolds.

Keywords: retraction maps, symplectic methods, discrete variational calculus, canonical transformations of the tangent and cotangent bundles.

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1 Introduction

The notion of retraction map is an essential tool in different research areas like optimization theory, numerical analysis, interpolation (see [Absil, Mahony, and Sepulchre 2008] and references therein). For instance, in optimization theory, the goal is to find a value $x$ in a differentiable manifold $M$ such that $f(x)$ is the minimum of a function $f : M \rightarrow \mathbb{R}$. In the case that $M$ is a linear space as $\mathbb{R}^n$ equipped with the standard inner product, the notions of gradient or Hessian of the function $f$ are properly defined and give us useful local information to localize the possible candidates to minimize $f$. Moreover, gradient descent or Newton’s method can also be used to search for a solution.

Riemannian geometry allows us to introduce similar concepts to gradient and Hessian in a differentiable manifold paving the way for optimization. But we need another important ingredient: how to move on a manifold. In Riemannian geometry this notion is given by the exponential map. On a Riemannian manifold $(M, g)$ (or more generally a semi-Riemannian manifold) remember that any geodesic $\sigma : I \subset \mathbb{R} \rightarrow M$ with initial velocity $\dot{\sigma}(0) = \xi$ in the tangent space of $M$ at $x$, $T_x M$, is locally obtained using the exponential map $\exp_x : U \subset T_x M \rightarrow M$ by $\exp_x(t\xi) = \sigma(t)$ (see for instance [do Carmo 1992]). However, only in simple examples it is possible to explicitly compute the exponential map of a Riemannian manifold. Therefore, efficient approximations of geodesics are crucial for designing algorithms on manifolds. Here is where retraction maps play an important role (see [Absil and Malick 2012, Absil, Mahony, and Sepulchre 2008] and references therein).

Roughly speaking, retraction maps provide a way to select a smooth curve on a differentiable manifold given an initial position and velocity. Such a curve is an approximation of the Riemannian exponential map. More specifically, a retraction is typically defined as a local $C^1$-map $R_x : U_x \subset T_x M \rightarrow M$ such that $R_x(0) = x$ and $\frac{d}{dt}|_{t=0} R_x(t\xi) = T_0_x R_x(\xi) = \xi$ for all $\xi \in T_x M$, where we...
use the identification $T_{U_0}T_x M \equiv T_x M$. Observe that, since we are using first order approximations, this definition is independent of the initial Riemannian metric (see [Abraham and Marsden 1978]). However, for second or higher order retractions the particular Riemannian metric does play a role. The property $\frac{d}{dt}|_{t=0} R_g(t \xi) = \xi$ implies that $d_g(R_g(t \xi), \sigma(t)) = O(t^2)$, where $d_g$ denotes the Riemannian distance (see [Shub 1986]).

For our purposes we will need a more general definition of a retraction map. We construct an extended retraction map $R_d : U \subset TM \to M \times M$ in Definition 2.2, where the image of $\xi \in U$ is now two “nearby” points of $M$. As an example, if we have a Riemannian manifold $(M, g)$, with associated exponential map $exp$, then an extended retraction map is $R_d(\xi) = (exp_{\tau_M(\xi)}(-\frac{1}{2} \xi), exp_{\tau_M(\xi)}(\frac{1}{2} \xi))$, where $\tau_M : TM \to M$ is the canonical projection. We precisely discuss the properties of these extended retraction maps in Section 2. We understand such maps as discretizations of the tangent bundle because they take values in two copies of the configuration manifold. That is why they are denoted by $R_d$.

In numerical analysis, if we have a vector field $X$ on $M$ and we want to find a numerical approximation of the integral curves, a natural idea is to use an extended retraction map and consider the following first order discrete equation:

$$hX(\tau_M(R_d^{-1}(x_k, x_{k+1}))) = R_d^{-1}(x_k, x_{k+1}). \quad (1.1)$$

Given an initial condition $x_0$ we can solve the implicit system (1.1) to find a sequence $\{x_k\}$ which is an approximation of $\{x(kt)\}$, where $x(t)$ is the integral curve of $X$ with initial condition $x_0$ and $h$ is the time step. For instance, if $M$ is the vector space $\mathbb{R}^n$ and $R_d(x, v) = (x - \frac{h}{2} v, x + \frac{h}{2} v)$, then Equation (1.1) becomes

$$\frac{x_{k+1} - x_k}{h} = X\left(\frac{x_k + x_{k+1}}{2}\right).$$

Our main interest in this article consists of designing numerical methods for second order differential equations (SODEs) and mainly for Hamilton’s equations. For instance, a second order differential equation $\ddot{x} = f(x, \dot{x})$ is geometrically represented by a special vector field

$$\Gamma(x, \dot{x}) = \dot{x} \frac{\partial}{\partial x} + f(x, \dot{x}) \frac{\partial}{\partial \dot{x}},$$

which is now defined on the tangent bundle $TM$ of $M$ [Abraham and Marsden 1978]. These vector fields are called SODEs.

On the other hand, it is well-known that the classical Hamiltonian equations are defined on the cotangent bundle $T^* M$ of the manifold $M$. Therefore, we face the problem of how, given a retraction map on $M$, we can lift it to the tangent and cotangent bundles.

In Section 3.1, we lift an extended retraction map on a manifold to the tangent bundle using the canonical involution. This tangent lift makes possible to define geometric discretizations of SODEs in Section 4.

In Section 3.2 we lift an extended retraction map on a manifold to the cotangent bundle using well-known constructions from symplectic geometry. We show in Section 3.3 that this cotangent lift is nothing else than the dual construction of the above-mentioned tangent lift. Moreover, it is essential to prove that the cotangent lift of an extended retraction map is always a symplectomorphism because that makes possible to construct symplectic integrators for Hamilton’s equations and Euler-Lagrange equations in Section 5.
In Section 3.4 we carefully work out a few examples of the extended retraction maps on different manifolds.

In Section 5.3 we compare the geometric integrators from Section 5.1 with the theory of discrete variational calculus [Marsden and West 2001].

Our definitions of cotangent lift of extended retraction maps combined with composition of Lagrangian submanifolds lead to the construction of general symplectic methods for Hamilton’s equation in Section 6.

Along the paper we show how well-known geometric methods (Newmark, Störmer-Verlet, etc) are obtained using the new tools described here. Hence, the work developed in this paper opens the path to define geometric integrators for more complex mechanical systems that may include forced systems, system with constraints, optimal control problems, Dirac systems, etc. We have briefly described future research lines in Section 7. Appendix A summarizes the most important notions from symplectic geometry and composition of Lagrangian submanifolds used in the paper.

# 2 Retraction maps

A retraction map plays the role of generalizing the linear-search methods in Euclidean spaces to general manifolds. On a manifold with nonzero curvature to move along the tangent line does not guarantee that the motion stays on the manifold. The retraction map provides the tool to define the notion of moving in a direction of a tangent vector while staying on the manifold. That is why retraction maps have been widely used to construct numerical integrators of ordinary differential equations, since it allows us to move from a point and a velocity to one nearby point and then discretize the differential equation.

The first definition of retraction map found in the literature is the following one.

**Definition 2.1.** [Absil, Mahony, and Sepulchre 2008, Chapter 4] A retraction map on a manifold $\mathcal{M}$ is a smooth mapping $R$ from the tangent bundle $\mathcal{T}\mathcal{M}$ onto $\mathcal{M}$. Let $R_x$ denote the restriction of $R$ to $T_x\mathcal{M}$, the following properties are satisfied:

1. $R_x(0_x) = x$ where $0_x$ denotes the zero element of the vector space $T_x\mathcal{M}$.
2. With the canonical identification $T_0_x\mathcal{T}\mathcal{M} \cong T_x\mathcal{M}$, $R_x$ satisfies
   \[ DR_x(0_x) = T_0_xR_x = \text{Id}_{T_x\mathcal{M}}, \]
   (2.1)
   where $\text{Id}_{T_x\mathcal{M}}$ denotes the identity mapping on $T_x\mathcal{M}$.

The condition (2.1) is known as local rigidity condition since, given $\xi \in T_x\mathcal{M}$, the curve $\gamma_{\xi}(t) = R_x(t\xi)$ has $\xi$ as tangent vector at $x$, i.e.

$\dot{\gamma}_\xi(t) = \langle DR_x(t\xi), \xi \rangle$ and, in consequence, $\dot{\gamma}_\xi(0) = \text{Id}_{T_x\mathcal{M}}(\xi) = \xi$.

This notion connects with the geometric interpretation of the exponential map $\exp$ on Riemannian manifolds given in [do Carmo 1992, Chapter 3.2]. Therefore the image of $\xi$ through the exponential map is a point on the Riemannian manifold obtained by moving along a geodesic a length equal to the norm of $\xi$ starting with the velocity $\xi/\|\xi\|$, that is,

$\exp_x(\xi) = \sigma(\|\xi\|)$,
where \( \sigma \) is the unit speed geodesic such that \( \sigma(0) = x \) and \( \dot{\sigma}(0) = \xi/\|\xi\| \).

Remember that the exponential map is a typical example of a retraction map. With all that in mind we are able to generalize the property of local rigidity in Definition 2.1 that allows a discretization of the tangent bundle of the configuration manifold opening a new path to construct numerical integrators.

After studying the contribution studied in [Cuell and Patrick 2009, Marrero, Martín de Diego, and Martínez 2016] we define a generalization of the retraction map in Definition 2.1. Given a point and a velocity, we obtain two nearby points that are not necessarily equal to the initial base point. As discussed in the sequel, numerical methods will be recovered from this new notion of retraction map.

**Definition 2.2.** A map \( R_d: U \subset TM \to M \times M \) given by

\[
R_d(x, v) = (R^1(x, v), R^2(x, v)),
\]

where \( U \) is an open neighborhood of the zero section of \( TM \), defines an extended retraction map on \( M \) if it satisfies

1. \( R_d(x, 0) = (x, x) \),
2. \( T_0 R^2_x - T_0 R^1_x: T_0 T_x M \simeq T_x M \to T_x M \) is equal to the identity map on \( T_x M \) for any \( x \) in \( M \), where \( R^i_x \) denotes the restrictions of \( R^i \), \( i = 1, 2 \), to \( T_x M \).

If \( R^1(x, v) = x \), the two properties in Definition 2.2 guarantee that the both properties in Definition 2.1 are satisfied. Thus, as mentioned, Definition 2.2 generalizes Definition 2.1.

**Proposition 2.3.** Let \( R_d \) be an extended retraction map on \( M \), \( R_d \) is a local diffeomorphism from some neighborhood of the zero section of \( TM \).

**Proof.** Let \( (x^i) \) be local coordinates for \( M \) centered at \( x \), and \( (x^i, v^i) \) be the corresponding induced coordinates on \( TM \). By the definition of the extended retraction map, the Jacobian matrix of \( R_d \) at \( (x^i, 0) \) is locally written as

\[
\begin{pmatrix}
\text{Id} & \frac{\partial R^1}{\partial v}(x, 0) \\
\text{Id} & \frac{\partial R^2}{\partial v}(x, 0)
\end{pmatrix},
\]

where \( \text{Id} \) denotes the identity matrix. Note that the regularity of that Jacobian matrix is equivalent to the invertibility of the following matrix

\[
\begin{pmatrix}
\text{Id} & \frac{\partial R^1}{\partial v}(x, 0) \\
0 & \frac{\partial R^2}{\partial v}(x, 0) - \frac{\partial R^1}{\partial v}(x, 0)
\end{pmatrix} = \begin{pmatrix}
\text{Id} & \frac{\partial R^1}{\partial v}(x, 0) \\
0 & \text{Id}
\end{pmatrix},
\]

due to the property 2 in Definition 2.2. Therefore, the inverse function theorem guarantees that \( R_d \) is a local diffeomorphism from some neighborhood of the identity section to its image.

There is a general and interesting way to obtain extended retraction maps from the usual retraction maps. The following result is very useful for the Examples 2.6 and 2.7.
Proposition 2.4. Let $R: TM \to M$ be a retraction map as in Definition 2.1. For any $\theta \in [0, 1]$ the map $R_\theta: TM \to M \times M$ given by

$$R_\theta(x, v) = (R(x, -\theta v), R(x, (1 - \theta)v))$$

is an extended retraction map on $M$.

Proof. From the definition of retraction map it is immediate that $R_\theta(x, 0) = (R(x, 0), R(x, 0)) = (x, x)$ and $T_0R^2_x - T_0R^1_x = (1 - \theta)T_0R_x + \theta T_0R_x \equiv \text{Id}_{T_xM}$.

The extended retraction map can be associated with known numerical methods constructed from a retraction map. For step size $h$ and retraction map $R^h(x, v) = x + hv$ on the Euclidean space, one possible extended retraction map is $R^h_\theta(x, v) = (x, x + hv)$ that corresponds with a first order integrator method as described, for instance, in [McLachlan and Perlmutter 2006]. However, other extended retraction maps may be defined from the same retraction map to construct different integrators. For example, for step size $h$ and the above retraction map $R^h$ we define:

$$R^h_\theta(x, v) = (R^{-h/2}(x, v), R^{h/2}(x, v)),$$

that corresponds with a second order method as described in [McLachlan and Perlmutter 2006].

Example 2.5. Let us provide some examples of retractions typically used in the literature for the construction of numerical methods, see [Iserles 2009], that can be associated with extended retractions maps satisfying the properties in Definition 2.2.

1. The explicit Euler method: $R_\theta(x, v) = (x, x + v)$.
2. The midpoint rule: $R_\theta(x, v) = \left( x - \frac{v}{2}, x + \frac{v}{2} \right)$.
3. The \(\theta\)-method: $R_\theta(x, v) = (x - \theta v, x + (1 - \theta)v)$ where $\theta \in [0, 1]$.

As known, for $\theta \in \{0, 1/2\}$, we recover the first two maps from the third one. All these methods are defined on the Euclidean vector space $\mathbb{R}^n$.

Example 2.6. Given a Riemannian manifold $(M, g)$ and the associated exponential map $\exp_x: T_xM \to M$ we can define the following map

$$R_\theta(x, \xi) = (\exp_x(-\xi/2), \exp_x(\xi/2)),$$  \hspace{1cm} (2.2)

that satisfies the properties in Definition 2.2. Let us give some specific examples of extended retraction maps that can be associated with the exponential map.

For instance, on the sphere $S^2$ with the Riemannian metric induced by the restriction of the standard metric on $\mathbb{R}^3$ we have that

$$\exp_x(\xi) = \cos(\|\xi\|) x + \sin(\|\xi\|) \frac{\xi}{\|\xi\|}, \quad \xi \in T_xS^2.$$

Thus we move along the greatest circle that are the geodesics on the sphere. Remember that $\exp_x(0_x) = x$ and the exponential map is a continuous map. Hence, we can define the following extended retraction map on $M$:

$$R_\theta(x, \xi) = \left( \cos \left( \frac{\|\xi\|}{2} \right) x - \sin \left( \frac{\|\xi\|}{2} \right) \frac{\xi}{\|\xi\|}, \cos \left( \frac{\|\xi\|}{2} \right) x + \sin \left( \frac{\|\xi\|}{2} \right) \frac{\xi}{\|\xi\|} \right).$$  \hspace{1cm} (2.3)
Another option is to use as a retraction map on the sphere the projection
\[ R_\theta(\xi) = \frac{x + \xi}{\|x + \xi\|} \]
that leads to the following extended retraction map:
\[ R_d(x, \xi) = \left( \frac{x - \xi/2}{\|x - \xi/2\|}, \frac{x + \xi/2}{\|x + \xi/2\|} \right). \]

Proposition 2.4 for \( \theta = 1/2 \) guarantees that both maps are extended retraction maps.

Example 2.7. Consider a Lie group \( G \) and denote by \( \mathfrak{g} \) its Lie algebra. It is a fact that any element \( \xi \) in the Lie algebra is in one-to-one correspondence with a left-invariant vector field on \( G \), \( X_\xi = T_eL_g(\xi) \), where \( e \) is the identity element of \( G \) and \( L_g : G \to G \) denotes the left-translation map. If \( \gamma_\xi : \mathbb{R} \to G \) is an integral curve of \( X_\xi \) with initial condition \( \gamma_\xi(0) = e \), then we can generate a map between the Lie algebra and the Lie group called the exponential map:
\[ \exp(\xi) = \gamma_\xi(1). \]
It is possible to check that the map \( R : TG \to G \) given by
\[ (g, X) \mapsto g \exp(T_gL_g^{-1}(X)) \]
is a retraction map where \( X(g) \in T_gG \). Then, we define an extended retraction map on the Lie group \( G \), \( R_d : TG \to G \times G \), as follows
\[ R_d(g, X) = \left( g \exp\left(-\frac{1}{2}T_gL_g^{-1}(X)\right), g \exp\left(\frac{1}{2}T_gL_g^{-1}(X)\right) \right). \]
The properties in Definitions 2.1 and 2.2 are satisfied because the tangent map \( T_e \exp \) is the identity map.

In the case of \( SO(3) = \{ A \in GL(3, \mathbb{R}) \mid AA^T = A^TA = \text{Id}_3, \det A = 1 \} \), we have that an element \( (A, X) \in TSO(3) \) is given by a pair of matrices such that \( A \in SO(3) \) and \( XA^T + AX^T = 0 \). Therefore, the Lie algebra \( \mathfrak{so}(3) \) is the set of skew-symmetric matrices: \( \xi = A^TX \in \mathfrak{so}(3) \). The above retraction map for \( SO(3) \) becomes:
\[ R(A, X) = A \exp(A^TX). \]
The exponential map could be replaced by the Cayley transformation:
\[ \text{cay} : \mathfrak{so}(3) \to SO(3), \quad \xi \mapsto \text{cay}(\xi) = (\text{Id}_3 - \xi/2)^{-1}(\text{Id}_3 + \xi/2), \]
where \( \text{Id}_3 \) stands for the identity matrix. Then we define the following retraction map \( R_{\text{cay}} : TSO(3) \to SO(3) \):
\[ R_{\text{cay}}(A, X) = A \text{cay}(A^TX) = A(\text{Id}_3 - A^TX/2)^{-1}(\text{Id}_3 + A^TX/2). \]
As shown in Proposition 2.4, we obtain the following extended retraction map \( R_{d,\text{cay}} : TSO(3) \to SO(3) \times SO(3) \):
\[ R_{d,\text{cay}}(A, X) = (R_{\text{cay}}(A, -X/2), R_{\text{cay}}(A, X/2)) = (A(\text{Id}_3 + A^TX/4)^{-1}(\text{Id}_3 - A^TX/4), A(\text{Id}_3 - A^TX/4)^{-1}(\text{Id}_3 + A^TX/4)). \]

3 Lift of extended retraction maps
We can construct extended retraction maps, as described in Definition 2.2, on any manifold. When studying mechanical systems, it may be useful to define
extended retraction maps on the tangent bundle for the Lagrangian framework or on the cotangent bundle for the Hamiltonian framework. As extended retraction maps can be defined on different manifolds, we introduce the notation $R_d^{T,M}$ so that the superscript tells us the domain of such a map. Thus, the map $R_d^{T,M} : TM \to M \times M$ is called an extended retraction map on $M$. The name of the map emphasizes where the image takes values. Note that $M$ could be equal to the tangent bundle $TQ$ or to the cotangent bundle $T^*Q$ depending on the dynamics under study.

Here, we are interested in constructing specific extended retraction maps on the tangent and cotangent bundle obtained from an extended retraction map on the base manifold. The objective is to generate geometric integrators on the tangent and cotangent bundle obtained from an extended retraction maps

Proposition 3.2. Let $F : M_1 \to M_2$ be a diffeomorphism. The cotangent lift $\hat{F} : T^*M_1 \to T^*M_2$ of $F$ is defined by

$$\hat{F}(\alpha_1) = T^*_F(\alpha_1)$$

and $T^*_F$ is the tangent map of $F$ whose matrix is the Jacobian matrix of $F$ at $x \in M_1$ in a local chart.

As the tangent map $T_xF$ is linear, the dual map $T^*_F : T^*_F M_2 \to T^*_F M_1$ is defined as follows:

$$\langle (T^*_F(\alpha_2), v_x) \rangle = \langle \alpha_2, T_xF(v_x) \rangle$$

for every $v_x \in T_x M_1$.

Note that $(T^*_F(\alpha_2)) \in T^*_F M_1$.

To define the cotangent lift in Section 3.2, we need the cotangent lift of the inverse of the extended retraction map. So, we fix the notation for such a cotangent lift.

Definition 3.1. Let $F : M_1 \to M_2$ be a diffeomorphism. The vector bundle morphism $\hat{F} : T^*M_1 \to T^*M_2$ defined by

$$\hat{F} = T^*F^{-1}$$

is called the cotangent lift of $F^{-1}$.

In other words, $\hat{F}(\alpha_x) = T^*_F(\alpha_x)$ where $\alpha_x \in T^*_x M_1$. Obviously, $(T^*F^{-1}) \circ (T^*_F) = \text{Id}_{T^*M_2}$.

We quickly review here some notions from symplectic geometry, see Appendix A for more details. Denote by $\pi_M : T^*M \to M$ the canonical projection of the cotangent bundle and define the Liouville 1-form $\theta_M \in \Omega^1(T^*M)$ by $\langle \theta_M(\alpha_x), X_{\alpha_x} \rangle = \langle \alpha_x, T_{\alpha_x} \pi_M(X_{\alpha_x}) \rangle$ where $X_{\alpha_x} \in T_{\alpha_x}T^*M$ and denote by $\omega_M = -d\theta_M$ the canonical symplectic 2-form on $T^*M$. Thus $(T^*M, \omega_M)$ is a symplectic manifold. For a diffeomorphism $F : M_1 \to M_2$, we recall the well-known proposition for symplectic manifolds in [Libermann and Marle 1987].

Proposition 3.2. Let $F : M_1 \to M_2$ be a diffeomorphism. The cotangent lift $\hat{F} : T^*M_1 \to T^*M_2$ of $F^{-1}$ is a symplectomorphism for the symplectic manifolds $(T^*M_1, \omega_{M_1})$ and $(T^*M_2, \omega_{M_2})$. In other words, the symplectic 2-form is preserved by the pull-back of $\hat{F}$:

$$\hat{F}^* \omega_{M_2} = \omega_{M_1} \text{ where } \hat{F}^* : \Omega^2(T^*M_2) \to \Omega^2(T^*M_1).$$
3.1 Tangent lift of retraction maps

Equivalently, the inverse of the cotangent lift $\hat{F}^{-1} : T^*M_2 \to T^*M_1$ is also a symplectomorphism.

Some expressions in coordinates will be useful in the sequel. Take local coordinates $q = (q^1, \ldots, q^n)$ on $M_1$ and $x = (x^1, \ldots, x^n)$ on $M_2$ and induced coordinates $(q, v)$ on $TM_1$ and $(x, u)$ on $TM_2$, respectively. If $F : M_1 \to M_2$ is written in local coordinates as $(q^1, \ldots, q^n) \to (F^1(q), \ldots, F^n(q))$ Then

$$TF(q, v) = \left( F^i(q); \frac{\partial F^i}{\partial q^j}(q)v^j \right).$$

Taking now induced coordinates $(q, p)$ on $T^*M_1$ and $(x, r)$ on $T^*M_2$ we have that

$$\hat{F}(q, p) = \left( F^i(q); p_j \frac{\partial (F^{-1})^j}{\partial x^i}(F(q)) \right).$$

If we consider the matrices,

$$D_q F = \left( \frac{\partial F^i}{\partial q^j}(q) \right)_{1 \leq i, j \leq \dim M_1} \quad \text{and} \quad D_{F(q)} F^{-1} = \left( \frac{\partial (F^{-1})^i}{\partial x^j}(F(q)) \right)_{1 \leq i, j \leq \dim M_2}.$$

Note that

$$D_{F(q)} F^{-1} = [D_q F]^{-1}.\]$$

When we restrict the previous maps $TF$ and $\hat{F}$ to a fiber we induce the maps

$$T_q F : T_q M_1 \to T_{F(q)} M_2 \quad v \mapsto D_q F v^T$$

and

$$\hat{T}_q : T^*_q M_1 \to T^*_{F(q)} M_2 \quad p \mapsto ((D_q F)^{-1})^T p^T = p (D_q F)^{-1}.\]$$

Consequently,

$$\hat{F}^{-1}_{F(q)} : T^*_{F(q)} M_2 \to T^*_q M_1 \quad r \mapsto r D_q F. \quad (3.1)$$

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We prove that if we suitably lift the extended retraction map $R_d : TQ \to Q \times Q$ on $Q$ in Definition 2.2, we obtain a new extended retraction on the tangent bundle $TQ$. These constructions are able to provide a geometric framework to obtain numerical integrators for second-order differential equations (SODEs), see Section 4, and for the dynamics of mechanical systems as shown in Sections 5 and 6.

Remember that the notation $R_d^{TTQ}$ for an extended retraction map on $TQ$ makes clear the manifold to be discretized, that is, $R_d^{TTQ} : TTQ \to TQ \times TQ$. To define it from an extended retraction map $R_d : TQ \to Q \times Q$ on $Q$ is necessary to use the canonical involution map $\kappa_Q$ that shows the double vector bundle structure of the vector bundle $TTQ$ and defines a vector bundle isomorphism, as described for instance in [Tulczyjew 1976a, Tulczyjew and Urbański 1999].

Let us recall here the definition of the canonical involution. Let $Q$ be a smooth manifold of dimension $n$, $\tau_Q : TQ \to Q$ be the canonical tangent
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bundle projection and $TTQ$ the double tangent bundle of $Q$. The manifold $TTQ$ naturally admits two vector bundle structures. The first vector bundle structure is the canonical one with vector bundle projection $\tau_{TTQ} : TTQ \rightarrow TQ$. For the second vector bundle structure of $TTQ$, the vector bundle projection is given by $T\tau_{Q} : TTQ \rightarrow TQ$. The canonical involution $\kappa_{Q} : TTQ \rightarrow TTQ$ is a vector bundle isomorphism (over the identity of $TQ$) between the two previous vector bundles. In fact, $\kappa_{Q}$ is characterized by the following condition: let $\Phi : U \subseteq \mathbb{R}^2 \rightarrow Q$ be a smooth map on an open subset $U$ of $\mathbb{R}^2$ defined by

$$(t, s) \mapsto \Phi(t, s) \in Q,$$

then

$$\kappa_{Q} \left( \frac{\partial}{\partial t} \frac{\partial}{\partial s} \Phi(t, s) \right) = \frac{\partial}{\partial s} \frac{\partial}{\partial t} \Phi(t, s).$$

Note that $\kappa_{Q}$ is an involution of $TTQ$, that is, $\kappa_{Q}^{2} = \text{Id}_{TTQ}$. If $(q, v)$ are canonical fibered coordinates of $TQ$ and $(q, v, \dot{q}, \dot{v})$ are the corresponding local fibered coordinates of $TTQ$, then

$$\kappa_{Q}(q, v, \dot{q}, \dot{v}) = (q, \dot{q}, v, \dot{v}).$$

Having all this in mind, remember that the tangent lift of a vector field $X$ on $Q$ does not define a vector field on $TQ$. It is necessary to consider the composition $\kappa_{Q} \circ TX$ to obtain a vector field on $TQ$ that is called complete lift $X^{c}$ of the vector field $X$. A similar trick must be used to lift an extended retraction map from $TQ$ to $TTQ$ as shown in the following diagram.

$$
\begin{array}{ccc}
TTQ & \xrightarrow{\kappa_{Q}} & TQ \times TQ \\
\downarrow{\kappa_{Q}} & & \downarrow{\kappa_{Q}} \\
TTQ & \xrightarrow{T\tau_{d}} & T(Q \times Q) \\
\downarrow{T\tau_{Q}} & & \downarrow{T\tau_{Q} \times Q} \\
TQ & \xrightarrow{\tau_{d}} & Q \times Q
\end{array}
$$

The following proposition shows that $T\tau_{d} \circ \kappa_{Q}$ is an extended retraction map on $TQ$. Note that $T(Q \times Q)$ and $TQ \times TQ$ are trivially identified. From now on, such a map is denoted by $R_{d}^{T}$ to emphasize it is obtained by tangentially lifting $\tau_{d}$.

**Proposition 3.3.** If $\tau_{d}$ is an extended retraction map on $Q$, then $R_{d}^{T} = T\tau_{d} \circ \kappa_{Q}$ is an extended retraction map on $TQ$.

**Proof.** In local coordinates $(q, v, \dot{q}, \dot{v})$ of $TTQ$ we have that $T\tau_{d}(q, v, \dot{q}, \dot{v}) = (\tau_{d}(q, v), D_{(q, v)}\tau_{d}(q, v)(\dot{q}, \dot{v})^{T})$ and

$$R_{d}^{T}(q, \dot{q}, v, \dot{v}) = (\tau_{d}(q, v), D_{(q, v)}\tau_{d}(q, v)(\dot{q}, \dot{v})^{T}).$$

Remember the abuse of notation because $T(Q \times Q)$ and $TQ \times TQ$ are trivially identified.

Let us prove that the properties in Definition 2.2 are satisfied.
1. As $R_d$ is an extended retraction map on $Q$ such that $R_d(v_q) = (R^1(v_q), R^2(v_q))$ for $v_q \in T_qQ$. We know that $R_d(q, 0) = (q, q)$ for all $q \in Q$. Consequently, $D_{\partial_q}R^i = Id_{n \times n}$ for all $i = 1, 2$. Thus,

$$R_d^T(q, \dot{q}, 0, 0) = (R_d(q, 0), D_{\partial_q}R_d(\dot{q}, 0))^T = (q, q, \dot{q}, \dot{q}) = (q, \dot{q}; q, \dot{q}),$$

where we use the natural identification between $T(Q \times Q)$ and $TQ \times TQ$.

2. For the second property, knowing that $R_d(q, v) = (R^1(q, v), R^2(q, v))$ we write

$$R_d^T(q, \dot{q}, v, \dot{v}) = ((TR^1)(q, v; \dot{q}, \dot{v}), (TR^2)(q, v; \dot{q}, \dot{v})).$$

We need to compute

$$T_{(0,0)\langle q, q \rangle} (TR^i)_{\langle q, q \rangle} : T_{(0,0)\langle q, q \rangle} T_{\langle q, q \rangle} TQ \equiv T_{\langle q, q \rangle} TQ \rightarrow T_{\langle q, q \rangle} TQ,$$

for $i = 1, 2$, to prove that the map $T_{(0,0)\langle q, q \rangle} (TR^2)_{\langle q, q \rangle} - T_{(0,0)\langle q, q \rangle} (TR^1)_{\langle q, q \rangle}$ is the identity map understood as an application from $T_{\langle q, q \rangle} TQ$ to itself. At $(q, \dot{q}, 0, 0)$, the linear map $T_{(0,0)\langle q, q \rangle} (TR^i)_{\langle q, q \rangle}$ is given by the following matrix

$$\begin{pmatrix}
\partial_v R^i(q, 0) & 0 \\
\partial_q \partial_v R^i(q, 0) & \partial_v R^i(q, 0)
\end{pmatrix}.$$

Using again the properties of the extended retraction map $R_d$, the Jacobian matrix of $T_{(0,0)\langle q, q \rangle} (TR^2)_{\langle q, q \rangle} - T_{(0,0)\langle q, q \rangle} (TR^1)_{\langle q, q \rangle}$ is:

$$\begin{pmatrix}
\partial_v R^2(q, 0) - \partial_v R^1(q, 0) & 0 \\
\partial_q (\partial_v R^2(q, 0) - \partial_v R^1(q, 0)) & \partial_v R^2(q, 0) - \partial_v R^1(q, 0)
\end{pmatrix} = Id_{2n \times 2n},$$

as needed. Note that $\partial_q \partial_v (R^2 - R^1)(q, 0) = 0$ because $\partial_v (R^2 - R^1)(q, 0) = Id_{n \times n}$.

\[\Box\]

**Remark 3.4.** If we use the retraction map obtained from the exponential map of a Riemannian metric $g$ as in Equation (2.2), then the tangent lift of this specific retraction map is associated with the complete lift of $g$, denoted by $g^C$, which is a semi-riemannian metric on $TQ$ (see details in [Yano and Ishihara 1973, Anahory Simoes, Marrero, and Martín de Diego 2020]).

### 3.2 Cotangent lift of retraction maps

To encompass the Lagrangian and Hamiltonian dynamics together to build numerical integrators, we are interested in defining a very particular notion of extended retraction map on the cotangent bundle.

Given an extended retraction map $R_d : TQ \rightarrow Q \times Q$ we know that the cotangent lift $\tilde{R}_d : T^*TQ \rightarrow T^*(Q \times Q)$ is a symplectomorphism between the symplectic manifolds $(T^*TQ, \omega_{TQ})$ and $(T^*(Q \times Q), \omega_{Q \times Q})$ as mentioned in Proposition 3.2.

According to Definition 3.1, in local coordinates $(q, v, p_q, p_v)$ for $T^*TQ$ the cotangent lift of $R_d$ is given by:

$$\tilde{R}_d : T^*TQ \rightarrow T^*(Q \times Q)$$

$$(q, v, p_q, p_v) \mapsto (R_d(q, v), (p_q, p_v) (D_{(q,v)}R_d)^{-1})$$
where \((D_{(q,v)}R_d)^{-1}\) is the inverse of the Jacobian matrix of \(R_d\).

We use the cotangent lift \(\tilde{R}_d\) of the extended retraction map on \(Q\) to define an extended retraction map on \(T^*Q\) that must be a map from \(TT^*Q\) to \(T^*Q \times T^*Q\).

For this purpose it is necessary to use the canonical symplectomorphism \(\alpha_Q : TT^*Q \to T^*TQ\) between double vector bundles (see [Tulczyjew 1976b, Tulczyjew and Urbański 1999]). Locally,

\[
\alpha_Q : TT^*Q \longrightarrow T^*TQ \\
(q, p, \dot{q}, \dot{p}) \longrightarrow (q, \dot{q}, p, \dot{p}).
\]

As described in [Tulczyjew 1976b], the symplectomorphism \(\alpha_Q\) is between the symplectic manifold \((TT^*Q, d\tau \omega_Q)\) and the natural symplectic manifold \((T^*TQ, \omega_{TQ})\). Recall that in local coordinates \((q, p, \dot{q}, \dot{p})\) for \(TT^*Q\), the symplectic form \(d\tau \omega_Q\) has the following expression: \(d\tau \omega_Q = dq \wedge d\dot{p} + d\dot{q} \wedge dp\). Moreover, we need the diffeomorphism

\[
\Phi : T^*Q \times T^*Q \longrightarrow T^*(Q \times Q) \\
(q_0, p_0; q_1, p_1) \longrightarrow (q_0, q_1, p_0, p_1)
\]

which is also a symplectomorphism between \((T^*(Q \times Q), \omega_{Q \times Q})\) and \((T^*Q \times T^*Q, \Omega_{12} = pr_2^*\omega_Q - pr_1^*\omega_Q)\), where \(pr_i : T^*(Q \times Q) \to T^*Q \times T^*Q\) denotes the projection into the \(i\)-th factor of the cartesian product in the image.

The following diagram shows how to define the extended retraction map on \(T^*Q\) from the one on \(Q\).

\[
\begin{array}{ccc}
TT^*Q & \xrightarrow{R^T_d} & T^*Q \times T^*Q \\
\alpha_Q \downarrow & & \Phi^{-1} \downarrow \\
T^*TQ & \xrightarrow{\tilde{R}_d} & T^*(Q \times Q) \\
\pi_{TQ} \downarrow & & \pi_{Q \times Q} \downarrow \\
TQ & \xrightarrow{R_d} & Q \times Q
\end{array}
\]

Now we prove that \(R^T_d\) is an extended retraction map on \(T^*Q\) according to Definition 2.2. From now on, it will be called the cotangent lift of \(R_d\).

**Proposition 3.5.** Let \(R_d : TQ \to Q \times Q\) be an extended retraction map on \(Q\) as in Definition 2.2. Then \(R^T_d = \Phi^{-1} \circ \tilde{R}_d \circ \alpha_Q : TT^*Q \to T^*Q \times T^*Q\) is an extended retraction map on \(T^*Q\).

**Proof.** Let us compute the cotangent lift of the tangent map of \(R_d\) for local coordinates \((q, v, p_q, p_v)\) of \(T^*TQ\):

\[
\tilde{R}_d(q, v, p_q, p_v) = (R_d(q, v), (p_q, p_v)\{(D_{(q,v)}R_d)^{-1}\}).
\]

Expressing the inverse of \((DR_d)^{-1}\) as a matrix with two blocks \((DR_d)^{-1} \in M_{2n \times n}, i = 1, 2\), that is

\[
(D_{(q,v)}R_d)^{-1} = ((D_{(q,v)}R_d)_1^{-1} (D_{(q,v)}R_d)_2^{-1})
\]

and

\[
(D_{(q,v)}R_d)^{-1} = \begin{pmatrix}
\partial_q R_1(q, v) & \partial_v R_1(q, v) \\
\partial_q R_2(q, v) & \partial_v R_2(q, v)
\end{pmatrix}^{-1}.
\]
We can write
\[ R_d^{T^*}(q, p, \dot{q}, \dot{p}) = (R^1(q, \dot{q}), -(\dot{p}, p)(D_{(q, \dot{q})} R_d)^{-1}; R^2(q, \dot{q}), (\dot{p}, p)(D_{(q, \dot{q})} R_d)^{-1}) \, . \]
Let us check if it satisfies the properties in Definition 2.2:
1. Note that the Jacobian matrix of \( R_T^* \) at \((q, 0)\) is
\[ D_{(q, 0)} R_d = \begin{pmatrix} \text{Id} & \partial_v R^1(q, 0) \\ \text{Id} & \partial_v R^2(q, 0) \end{pmatrix} \, . \]
As \( \partial_v R^2(q, 0) - \partial_v R^1(q, 0) = \text{Id} \), the inverse is
\[ (D_{(q, 0)} R_d)^{-1} = \begin{pmatrix} \text{Id} + \partial_v R^2(q, 0) & -\partial_v R^1(q, 0) \\ -\text{Id} & \text{Id} \end{pmatrix} \, . \]
Thus,
\[ R_d^{T^*}(q, p, 0, 0) = (R^1(q, 0), -(0, p)(D_{(q, \dot{q})} R_d)^{-1}; R^2(q, 0), (0, p)(D_{(q, \dot{q})} R_d)^{-1}) \, , \]
and it is straightforward that \( R_d^{T^*}(q, p, 0, 0) = (q, p; q, p) \).
2. We must prove that \( T_{(q, p, 0, 0)} (R_d^{T^*})^2 = T_{(q, p, 0, 0)} (R_d^{T^*}) \) is the identity map from \( T_{(q, p, 0, 0)} T^* Q \simeq T_{(q, p)} T^* Q \) to itself.
Let us compute the following derivatives for \( i = 1, 2 \):
\[
\frac{d}{dt} \bigg|_{t=0} \left( R_d^{T^*} \right)^i (q, p, t\dot{q}, t\dot{p}) .
\]
For instance, for \( i = 1 \) we have
\[
\frac{d}{dt} \bigg|_{t=0} \left( R_d^{T^*} \right)^1 (q, p, t\dot{q}, t\dot{p}) = \frac{d}{dt} \bigg|_{t=0} \left[ R^1(q, \dot{t}\dot{q}), -(t\dot{p}, p)(D_{(q, t\dot{q})} R_d)^{-1}\right] .
\]
Using the expression for the derivative of an inverse matrix, we have that
\[
\frac{d}{dt} \bigg|_{t=0} (D_{(q, t\dot{q})} R_d)^{-1} \text{ is equal to }
\]
\[
- \begin{pmatrix} \text{Id} + A & -A \\ -A & \text{Id} \end{pmatrix} \begin{pmatrix} \partial_v \partial_v R^1(q, 0) & \partial_v \partial_v R^1(q, 0) \\ \partial_v \partial_v R^2(q, 0) & \partial_v \partial_v R^2(q, 0) \end{pmatrix} \begin{pmatrix} \text{Id} + A & -A \\ -A & \text{Id} \end{pmatrix} = \begin{pmatrix} \partial_v \partial_v R^1(q, 0) - \partial_v \partial_v R^2(q, 0) & \partial_v \partial_v R^2(q, 0) - \partial_v \partial_v R^1(q, 0) \end{pmatrix}
\]
where \( A = \partial_v R^1(q, 0) \) and \((*)\) denotes terms that are not explicitly needed in the computations. We have used that \( \partial_v \partial_v (R^2 - R^1)(q, 0) = 0 \) since \( \partial_v (R^2 - R^1)(q, 0) = \text{Id}_{n \times n} \). Thus,
\[
\frac{d}{dt} \bigg|_{t=0} \left[ R^1(q, \dot{t}\dot{q}), -(t\dot{p}, p)(D_{(q, t\dot{q})} R_d)^{-1}\right] = \begin{pmatrix} \partial_v R^1(q, 0) \\ p(\partial_v \partial_v R^1(q, 0) - \partial_v \partial_v R^2(q, 0)) - \text{Id} - (\partial_v R^1(q, 0))^T \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}
\]
Analogously,
\[
\frac{d}{dt} \bigg|_{t=0} \left[ R^2(q, t\dot{q}), (t\dot{p}, p)(D_{(q, t\dot{q})} R_d)^{-1}\right] = \begin{pmatrix} \partial_v R^2(q, 0) \\ p(\partial_v \partial_v R^1(q, 0) - \partial_v \partial_v R^2(q, 0)) - (\partial_v R^1(q, 0))^T \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}
\]
As a result,
\[
\left( \begin{array}{cc} \partial_v R^2(q,0) & 0 \\ C & -\partial_v R^1(q,0) \end{array} \right) - \left( \begin{array}{cc} \partial_v R^1(q,0) & 0 \\ C & -\partial_v R^2(q,0) \end{array} \right) = \left( \begin{array}{cc} \text{Id} & 0 \\ 0 & \text{Id} \end{array} \right)
\]

where \( C = p(\partial_v \partial_v R^1(q,0) - \partial_v \partial_v R^2(q,0)) \).

As the composition of symplectomorphisms is a symplectomorphism [Liber- mann and Marle 1987], the following result is straightforward.

**Proposition 3.6.** Let \( R_d : TQ \to Q \times Q \) be a retraction map on \( Q \), then \( R^*_d = \Phi^{-1} \circ \hat{R}_d \circ \alpha_Q : T^{*}Q \to T^{*}Q \times T^{*}Q \) is a symplectomorphism between \((T(T^{*}Q), d_{T^{*}Q})\) and \((T^{*}Q \times T^{*}Q, \Omega_{12})\).

As a consequence,
\[
(R^*_d)^{-1}(\Omega_{12}) = d_{T^{*}Q}.
\]

The above result is essential to obtain symplectic methods in the following sections.

When constructing numerical integrators in Section 5 for Hamiltonian systems, the inverse map of \( R^*_d : TT^{*}Q \to T^{*}Q \times T^{*}Q \) is useful. Using Proposition 3.5 we specifically write the inverse map
\[
(R^*_d)^{-1} = \alpha^{-1}_Q \circ \hat{R}^{-1}_d \circ \Phi : T^{*}Q \times T^{*}Q \to TT^{*}Q.
\]

In local coordinates \((q_0, p_0; q_1, p_1)\) for \( T^{*}Q \times T^{*}Q \) and using (3.1), it is quite simple to compute the inverse map
\[
(R^*_d)^{-1} = \alpha^{-1}_Q \left( R^{-1}_d(q_0, q_1), (-p_0, p_1) \right) (3.2)
\]

Remember that \( \alpha^{-1}_Q(q, v, p_q, p_v) = (q, p_v, v, p_q) \).

### 3.3 Duality between the cotangent and the tangent lift of extended retraction maps

After introducing both the tangent and cotangent lift of extended retraction maps, we show here the existing duality between the two maps.

For an extended retraction map on \( Q \), we consider the tangent lift \( R^T_d : TTQ \to TQ \times TQ \) defined by \( R^T_d = TR_d \circ \kappa_Q \) and the corresponding cotangent lift \( R^*_d = \Phi^{-1} \circ \hat{R}_d \circ \alpha_Q : TT^{*}Q \to T^{*}Q \times T^{*}Q \). As mentioned earlier, \( TT^{*}Q \) is a symplectic manifold with the 2-form \( d_{TT^{*}Q} \) that induces a natural pairing as follows. Let \( v \in TT^{*}Q \) and let \( w \in TTQ \) such that \( \tau_{TTQ}(w) = T\pi_Q(v) \), the pairing \( \langle \cdot, \cdot \rangle \) induced by the symplectic structure of \( TT^{*}Q \) is given by
\[
\langle v, \kappa_Q(w) \rangle = \frac{d}{dt} \langle \sigma_v(t), \gamma_{\hat{w}}(t) \rangle(0) = \langle \alpha_Q(v), w \rangle,
\]
where \( \alpha_Q : TT^{*}Q \to T^{*}TQ, \sigma_v : I \to T^{*}Q \) and \( \gamma_{\hat{w}} : I \to TQ \) satisfy \( \dot{\sigma}_v(0) = v \) and \( \dot{\gamma}_{\hat{w}}(0) = \hat{w} \) with \( \kappa_Q(w) \) and \( \pi_Q \circ \sigma_v \circ \tau_Q \circ \gamma_{\hat{w}} \).
3.4 Examples

Proposition 3.7. The tangent lift and the cotangent lift of an extended retraction map on $Q$ satisfy the following equality:

$$\langle \Phi(\alpha_{q_0}, \alpha_{q_1}), R^T_d(w) \rangle = \left\langle \left( R^T_d \right)^{-1}(\alpha_{q_0}, \alpha_{q_1}), w \right\rangle^T,$$

where $w \in TTQ$, $(R_d)^{-1}(q_0, q_1) = T\tau_Q(w)$ and the pairing $\langle \cdot, \cdot \rangle^T$ is induced by the symplectic structure of $TT^*Q$.

Proof. Observe that

$$\langle \Phi(\alpha_{q_0}, \alpha_{q_1}), R^T_d(w) \rangle = \left\langle (\hat{R}_d \circ \Phi)^{-1}(\alpha_{q_0}, \alpha_{q_1}), \kappa_Q(w) \right\rangle$$

$$= \left\langle (\alpha_Q)^{-1}(\hat{R}_d \circ \Phi)(\alpha_{q_0}, \alpha_{q_1}), w \right\rangle^T$$

$$= \left\langle (R^T_d)^{-1}(\alpha_{q_0}, \alpha_{q_1}), w \right\rangle^T.$$ 

3.4 Examples

We resume Examples 2.5, 2.6, 2.7 to construct the lifts of extended retraction maps described in the previous sections. In other words, we define extended retraction maps on $TQ$ and $T^*Q$ starting from an extended retraction map on $Q$.

Example 3.8. We focus now on the mid-point rule described in Example 2.5 to define the tangent and cotangent lift of that extended retraction map. Assume that $Q$ is a vector space and let $R_d: TQ \to Q \times Q$ be the extended retraction map induced by the mid-point rule as follows $R_d(q, v) = (q - \frac{1}{2}v, q + \frac{1}{2}v)$. If we compute the inverse map $R^{-1}_d(q_0, q_1) = \left( \frac{q_0 + q_1}{2}, q_1 - q_0 \right)$, we construct the sequence of points that will be used either for optimization or numerical integration as the discrete flow

$$\phi_d: Q \times Q \to Q$$

$$(q_0, q_1) \mapsto (\tau_Q \circ R^{-1}_d)(q_0, q_1) = \tau_Q \left( \frac{q_0 + q_1}{2}, q_1 - q_0 \right) = \frac{q_0 + q_1}{2}.$$ 

Thus, the mid-point rule is recovered.

To define the tangent lift of the extended retraction map $R^T_d: TTQ \to TQ \times TQ$ on $TQ$ we first need to compute the tangent map whose matrix is

$$DR_d = \begin{pmatrix}
\text{Id} & -\frac{1}{2} \text{Id} \\
\frac{1}{2} \text{Id} & \text{Id}
\end{pmatrix}.$$ 

The tangent lift of $R_d$ is given by:

$$R^T_d(q, \dot{q}, v, \dot{v}) = (TR_d \circ \kappa_Q)(q, q, v, \dot{v}) = TR_d(q, v; \dot{q}, \dot{v})$$

$$= \left( q - \frac{1}{2} v, q + \frac{1}{2} v; \dot{q} - \frac{1}{2} \dot{v}, \dot{q} + \frac{1}{2} \dot{v}, \right)$$

$$= \left( q - \frac{1}{2} v, \dot{q} - \frac{1}{2} \dot{v}; q + \frac{1}{2} v, \dot{q} + \frac{1}{2} \dot{v}, \right).$$
where we naturally identify elements of $T(Q \times Q)$ with elements of $TQ \times TQ$.

We can also compute the inverse map:

$$\left( R_T^T \right)^{-1}(q_0, v_0; q_1, v_1) = \left( \frac{q_0 + q_1}{2}, \frac{v_0 + v_1}{2}; q_1 - q_0, v_1 - v_0 \right).$$

To compute the cotangent lift of $R_d$, that is, $R_T^T : TT^*Q \to T^*Q \times T^*Q$, we first need the tangent map of the inverse map $R_T^{-1}(q_0, q_1) = \left( \frac{q_0 + q_1}{2}, q_1 - q_0 \right):$

$$DR_T^{-1} = \begin{pmatrix} \frac{1}{2} \text{Id} & \frac{1}{2} \text{Id} \\ -\text{Id} & \text{Id} \end{pmatrix}.$$

Thus the cotangent lift of $R_T^{-1}$ is given by:

$$\widetilde{R_d}(q, v, p_0, p_0) = \left( R_d(q, v), (p_0, p_0)(D(q,v)R_T^{-1}) \right) = \left( q - \frac{1}{2}v, q + \frac{1}{2}v; \frac{p_0}{2} - p_0, \frac{p_0}{2} + p_0 \right).$$

Finally, the cotangent lift of $R_d$ is the following extended retraction map on $T^*Q$:

$$R_T^T(q, p, \dot{q}, \dot{p}) = \left( \Phi^{-1} \circ \widetilde{R_d} \circ \alpha_Q \right)(q, p, \dot{q}, \dot{p}) = \left( \Phi^{-1} \circ \widetilde{R_d} \right)(q, \dot{q}, \dot{p}, p)$$

$$= \Phi^{-1} \left( q - \frac{1}{2} \dot{q}, q + \frac{1}{2} \dot{q}; \frac{\dot{p}}{2} - p, \frac{\dot{p}}{2} + p \right) = \left( q - \frac{1}{2} \dot{q}, q + \frac{1}{2} \dot{q}; \frac{\dot{p}}{2} + p \right).$$

The inverse map $\left( R_T^T \right)^{-1} : T^*Q \times T^*Q \to TT^*Q$ is given by:

$$\left( R_T^T \right)^{-1}(q_0, p_0; q_1, p_1) = \left( \frac{q_0 + q_1}{2}, \frac{p_0 + p_1}{2}; q_1 - q_0, p_1 - p_0 \right).$$

**Example 3.9.** Let us lift the extended retraction map in Example 2.6. To simplify the computations we consider the retraction map that fixes the first point (compared with (2.3)) as follows

$$R_d(x, \xi) = \left( x, \cos(\|\xi\|)x + \sin(\|\xi\|)\frac{\xi}{\|\xi\|} \right).$$

Remember that $x \cdot x^T = 1$ and $x \cdot \xi^T = 0$ because the manifold $Q$ is the sphere $S^2$.

The tangent map of $R_d$ is given by the matrix

$$D(x, \xi)R_d = \begin{pmatrix} \text{Id} & 0 \\ \cos(\|\xi\|) \text{Id} & N(x, \xi) \end{pmatrix},$$

where

$$N_{ij} = -\sin(\|\xi\|)\frac{\xi_jx_i}{\|\xi\|} + \cos(\|\xi\|)\frac{\xi_i \xi_j}{\|\xi\|} + \sin(\|\xi\|) \begin{cases} \frac{\|\xi\|^2 - \xi_i \xi_i}{\|\xi\|^3}, & \text{for } i = j, \\ \frac{-\xi_i \xi_j}{\|\xi\|^3}, & \text{for } i \neq j, \end{cases}$$
are the entries of the invertible matrix \(N(x, \xi)\). Thus, the tangent lift of \(R_d\) is the following extended retraction map on \(TQ\):

\[
R_d^T(x, \dot{x}, \xi, \dot{\xi}) = (TR_d \circ \kappa_Q)(x, \dot{x}, \xi, \dot{\xi}) = TR_d(x, \xi; \dot{x}, \dot{\xi})
\]

\[
= \left(x, \cos \left(||\xi||\right) x + \sin \left(||\xi||\right) \frac{\xi}{||\xi||}, \dot{x}, \cos(||\xi||) \frac{\xi}{||\xi||}, \cos(||\xi||) \frac{\xi}{||\xi||} \right). 
\]

To compute the cotangent lift of \(R_d\), \(R_d^{-1} : T^*Q \to T^*Q \times T^*Q\), we first need the tangent map of the inverse map \(R_d^{-1}\) or, equivalently, the inverse of the tangent map:

\[
DR_d^{-1} = (DR_d)^{-1} = \begin{pmatrix} \text{Id} & 0 \\ -\cos(||\xi||) N^{-1} & N^{-1} \end{pmatrix}.
\]

Thus the cotangent lift of \(R_d^{-1}\) is given by:

\[
\tilde{R}_d(x, \xi, p_x, p_d) = \left(R_d(x, \xi), (p_x, p_d) (D(x, \xi) R_d)^{-1}\right).
\]

Finally, the extended retraction map on \(T^*Q\) is obtained as follows:

\[
R_d^T(x, p, \dot{x}, \dot{p}) = \left(\Phi^{-1} \circ \tilde{R}_d \circ \alpha_Q\right)(x, p, \dot{x}, \dot{p}) = \left(\Phi^{-1} \circ \tilde{R}_d\right)(x, \dot{x}, \dot{p}, p)
\]

\[
= \Phi^{-1}(x, \cos(||\dot{x}||) x + \sin(||\dot{x}||) \frac{\dot{x}}{||\dot{x}||}; \dot{p} - \cos(||\dot{x}||) p N^{-1}, p N^{-1})
\]

\[
\equiv \left(x, -\dot{p} + \cos(||\dot{x}||) p N^{-1}; \cos(||\dot{x}||) x + \sin(||\dot{x}||) \frac{\dot{x}}{||\dot{x}||}, p N^{-1}\right).
\]

**Example 3.10.** Let us lift the extended retraction map in Example 2.7. As in the previous example, to simplify the computations we consider the extended retraction map \(R_{d,cay} : TSO(3) \to SO(3) \times SO(3)\) that fixes the first point (compared with (2.4)) as follows:

\[
R_{d,cay}(A, X) = (A, A \cay(A^T X)) = \left(A, A (\text{Id}_3 - A^T X/2)^{-1} (\text{Id}_3 + A^T X/2)\right).
\]

The tangent map of \(R_{d,cay}\) is given by the matrix

\[
D_{(A,X)}R_{d,cay} = \begin{pmatrix} \text{Id} & 0 \\ \frac{d}{dA} \cay(A^T X) A^T & \frac{d}{dX} \cay(A^T X) A^T \end{pmatrix}
\]

\[
= \begin{pmatrix} \text{Id} & 0 \\ 0 & 0 \end{pmatrix}.
\]

Thus,

\[
R_{d,cay}^T(A, \dot{A}, X, \dot{X}) = (TR_{d,cay} \circ \kappa_Q)(A, \dot{A}, X, \dot{X}) = TR_d(A, X, \dot{A}, \dot{X})
\]

\[
= \left(A, A \cay(A^T X), \dot{A}, M \dot{A} + N \dot{X}\right)
\]

\[
\equiv \left(A, \dot{A}; A \cay(A^T X), M \dot{A} + N \dot{X}\right),
\]
where $N$ is an invertible matrix. To compute the extended retraction map $R_{d,cay}^*: T^*Q \to T^*Q \times T^*Q$ on $T^*Q$ as the cotangent lift of $R_d$, we first need the tangent map of the inverse map $R_{d,cay}^{-1}$ or, equivalently, the inverse of the tangent map:

$$DR_{d,cay}^{-1} = (DR_{d,cay})^{-1} = \begin{pmatrix} \text{Id} & 0 \\ -N^{-1}M & N^{-1} \end{pmatrix}.$$ 

Thus the cotangent lift of $R_{d,cay}^{-1}$ is given by:

$$\hat{R}_{d,cay}(A, X, p_A, p_X) = \left( R_{d,cay}(A, X), (p_A, p_X) (DR_{d,cay})^{-1} (A, X) \right).$$

Finally, the extended retraction map on $T^*Q$ is obtained as follows:

$$R_{d,cay}^*(A, p, \dot{A}, \dot{p}) = (\Phi^{-1} \circ \hat{R}_{d,cay} \circ \alpha_Q) (A, p, \dot{A}, \dot{p}) = (\Phi^{-1} \circ \hat{R}_{d,cay}) (A, \dot{A}, \dot{p}, p)$$

$$= \Phi^{-1} (A, A\text{cay}(A^T \dot{A}), \dot{p} - pN^{-1}M, pN^{-1})$$

$$= (A, pN^{-1}M - \dot{p}; A\text{cay}(A^T \dot{A}), pN^{-1}).$$

4 Retractions associated to SODEs

The tangent lift of extended retraction maps defined in Section 3 appears naturally when geometrically designing discretizations of second order differential equations (SODEs). Remember that a second order differential equation is a vector field $\Gamma$ such that $\tau_{TQ}(\Gamma) = T\tau_Q(\Gamma)$. This implies that the vector field $\Gamma$ is a section of the second order tangent bundle $T^{(2)}Q$, as described in [de León and Rodrigues 1985]. Locally, if we take coordinates $(q^i)$ on $Q$ and induced coordinates $(q^i, \dot{q}^i)$ on $TQ$, then

$$\Gamma = \dot{q}^i \frac{\partial}{\partial q^i} + \Gamma^i(q, \dot{q}) \frac{\partial}{\partial \dot{q}^i}.$$

To find the integral curves of $\Gamma$ is equivalent to solve the following system of second order differential equations:

$$\frac{d^2 q^i}{dt^2} = \Gamma^i \left( q, \frac{dq}{dt} \right).$$

Now, we want to discretize these equations using the notion of extended retraction map defined on $TQ$ as in Definition 2.2. Here we have two options: we could directly define an extended retraction map on $TQ$ denoted by $R_{d,TQ}^*: TTQ \to TQ \times TQ$ or we could tangently lift an extended retraction map on $Q$ to obtain $R_{d,cay}^*: TTQ \to TQ \times TQ$ as defined in Proposition 3.3.

Let us consider in general that we have an extended retraction map on $TQ$, $R_{d,TQ}^*: TTQ \to TQ \times TQ$,

given by $R_{d,TQ}^*(q, v, \dot{q}, \dot{v}) = \left( (R_{d,TQ})^1 (q, v, \dot{q}, \dot{v}), (R_{d,TQ})^2 (q, v, \dot{q}, \dot{v}) \right)$. Note that $(R_{d,TQ})^i (q, v, \dot{q}, \dot{v}) \in TQ$ for $i = 1, 2$. 
4.1 Newmark method from an extended retraction map

A first option for discretizing a SODE $\Gamma$ consists of the following implicit discrete equation:

$$\left( (R^{TTQ})^2 \circ h \Gamma \right)(q_k, v_k) = \left( (R^{TTQ})^1 \circ h \Gamma \right)(q_{k+1}, v_{k+1}), \quad (4.1)$$

where $h$ is a positive small real number that determines the step size. The numerical method starts from the initial data $(q_k, v_k) \in T_q Q$, then the Equation (4.1) is solved implicitly to obtain $(q_{k+1}, v_{k+1}) \in T_{q_{k+1}} Q$. Section 4.1 shows that an extended retraction map on $T Q$, not coming from a tangent lift, recovers Newmark method using the discretization method in (4.1). Geometrically, these methods given in (4.1) are based on the structure of groupoid of an implicit difference equation, in this case $T Q \times T Q \Rightarrow T Q$ (see [Iglesias-Ponte, Marrero, Martín de Diego, and Padrón 2013] for more details).

A second option for discretizing a SODE consists of the following numerical scheme:

$$h \Gamma \left( \tau_{TQ} \circ (R^{TTQ}_d)^{-1} \right)(q_k, v_k; q_{k+1}, v_{k+1}) = \left( R^{TTQ}_d \right)^{-1}(q_k, v_k; q_{k+1}, v_{k+1}). \quad (4.2)$$

As in (4.1), the numerical method is usually implicit. We will focus on this discretization process in Sections 4.2 and 5 when constructing geometric integrators for mechanical systems.

Let us do a simple example to show that the numerical schemes in (4.1) and (4.2) are usually different.

**Example 4.1.** Consider the extended retraction map on $T Q$ obtained from a tangent lift in Example 3.8 and the inverse map:

$$R_d^T(q, \dot{q}, v, \dot{v}) = \left( q - \frac{1}{2} v, \dot{q} - \frac{1}{2} \dot{v}; q + \frac{1}{2} v, \dot{q} + \frac{1}{2} \dot{v} \right),$$

$$(R_d^T)^{-1}(q_0, v_0; q_1, v_1) = \left( \frac{q_0 + q_1}{2}, \frac{v_0 + v_1}{2}; q_1 - q_0, v_1 - v_0 \right).$$

The method in Equation (4.1) becomes:

$$\frac{q_{k+1} - q_k}{h} = \frac{v_k + v_{k+1}}{2},$$

$$\frac{v_{k+1} - v_k}{h} = \frac{1}{2} (\Gamma(q_k, v_k) + \Gamma(q_{k+1}, v_{k+1})).$$

However, for the same extended retraction map on $T Q$ the method in (4.2) is given by the following equations:

$$\frac{q_{k+1} - q_k}{h} = \frac{v_k + v_{k+1}}{2},$$

$$\frac{v_{k+1} - v_k}{h} = \Gamma \left( \frac{q_k + q_{k+1}}{2}, \frac{v_k + v_{k+1}}{2} \right).$$

### 4.1 Newmark method from an extended retraction map

An example of discretization using Equation (4.1) is the Newmark method [Newmark 1959], a classical time-stepping method very common in structural mechanical codes. For simplicity, we consider a typical mechanical Lagrangian $L : T \mathbb{R}^n \to \mathbb{R}$:

$$L(q, \dot{q}) = \frac{1}{2} \dot{q} M \dot{q}^T - V(q),$$
where \((q, \dot{q}) \in T\mathbb{R}^n\), \(M\) is a positive definite constant matrix and \(V\) is a potential function. The corresponding Euler-Lagrange equations are:

\[
\ddot{q} = -M^{-1}\nabla V(q),
\]

where \(\nabla\) denotes the gradient of the potential function.

The Newmark methods are widely used in simulations of such mechanical systems, including even external forces [Kane, Marsden, Ortiz, and West 2000]. To construct the method two real parameters \(\alpha\) and \(\beta\) are selected so that the algorithm determines \((q_{k+1}, \dot{q}_{k+1})\) in terms of \((q_k, \dot{q}_k)\) as follows:

\[
\begin{align*}
q_{k+1} &= q_k + h\dot{q}_k + \frac{h^2}{2}((1-2\beta)a_k + 2\beta a_{k+1}) \\
\dot{q}_{k+1} &= \dot{q}_k + h((1-\gamma)a_k + \gamma a_{k+1}),
\end{align*}
\]

where \(a_k = -M^{-1}\nabla V(q_k)\) and \(a_{k+1} = -M^{-1}\nabla V(q_{k+1})\).

We show here that the family of Newmark methods can be obtained from an extended retraction map on the tangent bundle \(TQ\). Let us define \(R_{d}^{TTQ} : T\mathbb{R}^n \rightarrow T\mathbb{R}^n \times T\mathbb{R}^n \equiv \mathbb{R}^{2n} \times \mathbb{R}^{2n}\) by

\[
\begin{align*}
(R_{d}^{TTQ})^1(q, v, \dot{q}, \dot{v}) &= \left(q - \frac{1}{2}h^2 \dot{q} + \frac{1}{2}(\gamma - 2\beta)\dot{v}, v - \gamma\dot{v}\right), \\
(R_{d}^{TTQ})^2(q, v, \dot{q}, \dot{v}) &= \left(q + \frac{1}{2}h^2 \dot{q} + \frac{1}{2}(\gamma - 2\beta)\dot{v}, v + (1-\gamma)\dot{v}\right),
\end{align*}
\]

The Jacobian matrix of \(R_{d}^{TTQ}\) is

\[
\begin{pmatrix}
\text{Id} & 0 & -\frac{1}{2} \text{Id} & \frac{1}{2}(\gamma - 2\beta) \text{Id} \\
0 & \text{Id} & 0 & -\gamma \text{Id} \\
\text{Id} & 0 & \frac{1}{2} \text{Id} & \frac{1}{2}(\gamma - 2\beta) \text{Id} \\
0 & \text{Id} & 0 & (1-\gamma) \text{Id}
\end{pmatrix}.
\]

It is straightforward that \(R_{d}^{TTQ}\) satisfies both properties in Definition 2.2. Hence, \(R_{d}^{TTQ}\) is an extended retraction map on \(TQ\).

The Euler-Lagrange equations (4.3) can be rewritten as the submanifold \(S\) of \(T^{(2)}Q \subset TTQ\),

\[
S = \{(q, \dot{q}, a) \mid a = -M^{-1}\nabla V(q)\},
\]

with the natural inclusion \(i : T^{(2)}Q \hookrightarrow TTQ, i(q, \dot{q}, a) = (q, \dot{q}, \dot{q}, a)\).

Hence, the dynamics induced by the Newmark method is equivalent to the following algorithm:

1. Take an initial position and velocity \((q_k, \dot{q}_k)\).
2. Evaluate \(a_k = -M^{-1}\nabla V(q_k)\).
3. Solve the system obtained from (4.1):

\[
(R_{d}^{TTQ})^2(q_k, \dot{q}_k; h\dot{q}_k, ha_k) = (R_{d}^{TTQ})^1(q_{k+1}, \dot{q}_{k+1}; h\dot{q}_{k+1}, ha_{k+1}),
\]

where \(a_{k+1} = -M^{-1}\nabla V(q_{k+1})\).
Observe that Equation (4.5) is equal to

\[ q_k + \frac{h}{2} \dot{q}_k + \frac{h^2}{2}(\gamma - 2\beta) a_k = \ q_{k+1} - \frac{h}{2} \dot{q}_{k+1} - \frac{h^2}{2}(\gamma - 2\beta) a_{k+1}, \]

\[ \dot{q}_k + h(1-\gamma) a_k = \ \dot{q}_{k+1} - h\gamma a_{k+1}. \]

After algebraic manipulation, they are equivalent to the well-known Newmark method in Equation (4.4).

Note that if \( \gamma = 1/2 \) and \( \beta = 1/4 \), then \( R_{TTQ}^T \) is precisely the tangent lift of the extended retraction map on \( Q \) coming from the mid-point rule as described in Example 3.8.

### 4.2 Retraction maps associated with discrete second order equations

In this section we briefly discuss the possibility to find a discrete version of a second order differential equation (SODE) using a second order discrete equation (SOdE).

According to [Marsden and West 2001], a SOdE is given by a map \( \Gamma_d : Q \times Q \to Q \times Q \times Q \times Q \) such that

\[ \Gamma_d(q_0, q_1) = (q_0, q_1, \tilde{\Gamma}_d(q_0, q_1)). \]

Given an extended retraction map on \( Q \) and a second order vector field \( \Gamma \), we wonder if, under any assumption, the tangent lift of the extended retraction map, \( R_{TQ}^T \), could define a discrete second order equation \( \Gamma_d \). The specific question is: When does an extended retraction map \( R_d \) make Diagram (4.6) commutative?

![Diagram](4.6)

**Proposition 4.2.** Let \( Q \) be a vector space and \( \Gamma \) be a SODE. If \( R_d : TQ \to Q \times Q \) is the extended retraction map on \( Q \) defined from the \( \theta \)-method:

\[ R_d(q, v) = (q - \theta v, q + (1-\theta)v), \]  

then Diagram (4.6) is commutative, that is,

\[ (R_d, R_d) \circ R_{TQ}^T \circ \Gamma \circ R_d^{-1} : Q \times Q \to Q \times Q \times Q \times Q \]

defines a second order discrete equation (SOdE).

**Proof.** Let \( (q, v) \) local coordinates for \( TQ \). Let \( R_d(q, v) = (R_d^1(q, v), R_d^2(q, v)) \), we compute

\[ (R_d^T \circ \Gamma) (q, v) = (T(q,v)R_d^1(\Gamma(q,v)), T(q,v)R_d^2(\Gamma(q,v))). \]
If we apply now \((R_d, R_d): TQ \times TQ \rightarrow Q \times Q \times Q \times Q\), the resulting expression defines a SODE if and only if the second and third component are equal, that is,

\[
R_d^2(T(q,v)R_d^1(\Gamma(q,v))) = R_d^1(T(q,v)R_d^2(\Gamma(q,v))). \tag{4.8}
\]

It is a straightforward computation to verify that the extended retraction maps defined from the \(\theta\)-method in (4.7) satisfy Equation (4.8).

In fact, the above proposition could be stated more generally. Any extended retraction map that satisfies Equation (4.8) defines a SODE by the tangent lift of that map.

Equation (4.8) is equivalent to the commutativity of the following diagram:

\[
\begin{array}{c}
T^{(2)}Q \subset TTTQ \xrightarrow{T R_2^d} TQ \\
\downarrow r \quad \quad \downarrow r' \\
TQ \quad \quad \quad Q \\
\downarrow r \quad \quad \downarrow r' \\
T^{(2)}Q \subset TTTQ \xrightarrow{T R_1^d} TQ
\end{array}
\]  

(4.9)

In particular, if the extended retraction map \(R_d: TQ \rightarrow Q \times Q\) is defined from a standard retraction map as in Definition 2.1, that is, \(R_d^1 = \tau_Q\), then Diagram (4.9) becomes

\[
\begin{array}{c}
T^{(2)}Q \subset TTTQ \xrightarrow{T R_2^d} TQ \\
\downarrow \tau_Q \quad \downarrow r' \\
TQ \quad Q \\
\downarrow r \quad \downarrow r' \\
T^{(2)}Q \subset TTTQ \xrightarrow{T R_1^d} TQ
\end{array}
\]  

since \((\tau_Q \circ T R_2^d)(\Gamma) = (R_d^2 \circ T \tau_Q)(\Gamma)\). Therefore any standard retraction map defines a SODE \(\Gamma_{\theta}\).

## 5 Construction of geometric integrators from retraction maps

In this section we describe how geometric integrators are obtained for both Hamiltonian and Euler-Lagrange equations by discretizing their equations using extended retraction maps. In Section 5.3, we establish the relation with discrete variational calculus where the variational principles are discretized to obtain the discrete flow (see [Marsden and West 2001]).

In Section 5.1 we look at the Hamiltonian framework [Abraham and Marsden 1978]. Hamiltonian systems have the property that the associated flow is a symplectic transformation. As described in [Sanz-Serna and Calvo 1994, Hairer, Lubich, and Wanner 2010, Blanes and Casas 2016], it is important to define numerical methods that also preserve that property. Remember that a
5.1 Geometric integrators in Hamiltonian framework

Let \( H : T^*Q \to \mathbb{R} \) be a Hamiltonian function with corresponding Hamiltonian vector field \( X_H \) derived from Hamilton’s equations:

\[
i_{X_H} \omega_Q = dH.
\]

The triple \((T^*Q, \omega_Q, H)\) defines a Hamiltonian system. Equivalently, an integral curve of \( X_H \) is solution to Hamilton’s equations:

\[
\frac{dq^i}{dt} = \frac{\partial H}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q^i},
\]

where \((q^i, p_i)\) are canonical coordinates on \( T^*Q \) (see [Abraham and Marsden 1978]). In other words, a solution \( \gamma : I \to T^*Q \) of Hamilton’s equations must satisfy

\[
\omega^*_Q (\dot{\gamma}(t)) = dH(\gamma(t)), \text{ equivalently } \dot{\gamma}(t) = \omega^*(dH(\gamma(t))).
\]

An extended retraction map on \( T^*Q \), that is, \( R^{TT^*Q}_d : T(T^*Q) \to T^*Q \times T^*Q \) defines the following numerical integrator for step size \( h \):

\[
\left( R^{TT^*Q}_d \right)^{-1}(q_0, p_0; q_1, p_1) = \omega^*(h dH \left( \left( \pi_{T^*Q} \circ \left( R^{TT^*Q}_d \right)^{-1} \right) (q_0, p_0; q_1, p_1) \right)). \tag{5.1}
\]

Equivalently, similar to Equation (4.2), we have

\[
h X_H \left( \left( \pi_{T^*Q} \circ \left( R^{TT^*Q}_d \right)^{-1} \right) (q_0, p_0; q_1, p_1) \right) = \left( R^{TT^*Q}_d \right)^{-1}(q_0, p_0; q_1, p_1). \tag{5.2}
\]

This numerical integrator may be defined for any extended retraction map on \( T^*Q \). However, if such a map is the cotangent lift of an extended retraction map of \( Q \) (see Section 3.2), then the numerical integrator is symplectic as stated in the following proposition.

**Proposition 5.1.** Let \( R_d : TQ \to Q \times Q \) be an extended retraction map on \( Q \) and \( H : T^*Q \to \mathbb{R} \) be a Hamiltonian function. Equation (5.1) written for the cotangent lift of \( R_d \), that is, \( R^*_{d^*} \), defines a symplectic integrator of the Hamiltonian system \((T^*Q, \omega_Q, H)\).

**Proof.** Lagrangian submanifolds are defined in Appendix A. As the submanifold \( dH \left( \left( \pi_{T^*Q} \circ \left( R^{TT^*Q}_d \right)^{-1} \right) (q_0, p_0; q_1, p_1) \right) \) in Equation (5.1) is Lagrangian on
5.1 Geometric integrators in Hamiltonian framework

Proposition 3.6 guarantees that Equation (5.1) determines a Lagrangian submanifold of \((T^*Q \times T^*Q, \Omega_{12})\). Locally, such a manifold can be expressed as the graph of a local symplectomorphism \(\varphi: T^*Q \to T^*Q\), see [Libermann and Marle 1987] for more details. Consequently, the geometric method obtained from Equation (5.1) is symplectic.

Let us use the above result to obtain some of the symplectic numerical methods known in the literature.

**Example 5.2.** Let \(H: T^*Q \to \mathbb{R}\) be a Hamiltonian function, the cotangent lift (3.3), (3.4) of the extended retraction map associated to the mid-point rule in Example 3.8 used in Equation (5.1) leads to the following equations:

\[
\begin{align*}
\left(\frac{q_0 + q_1}{2}, \frac{p_0 + p_1}{2}, q_1 - q_0, p_1 - p_0\right) &= \left(\frac{q_0 + q_1}{2}, \frac{p_0 + p_1}{2},
\left.\frac{1}{2} \frac{\partial H}{\partial p}\right|_{q_0 + q_1, p_0 + p_1}, -\left.\frac{1}{2} \frac{\partial H}{\partial q}\right|_{q_0 + q_1, p_0 + p_1}\right) = \left(\frac{q_0 + q_1}{2}, \frac{p_0 + p_1}{2}, q_1 - q_0, p_1 - p_0\right)
\end{align*}
\]

Equivalently, the equations describe the following symplectic integrator:

\[
\frac{q_1 - q_0}{h} = \left.\frac{\partial H}{\partial p}\right|_{\frac{q_0 + q_1}{2}, \frac{p_0 + p_1}{2}} ,
\frac{p_1 - p_0}{h} = -\left.\frac{\partial H}{\partial q}\right|_{\frac{q_0 + q_1}{2}, \frac{p_0 + p_1}{2}} .
\]

The above integrator corresponds with an implicit second-order symplectic method with initial condition \((q_0, p_0)\).

**Example 5.3.** The extended retraction map on \(Q, R_d(q, v) = (q - v, q)\), is lifted to the cotangent bundle as follows

\[
R_d^T: \quad TT^*Q \to T^*Q \times T^*Q \quad (q, p, \dot{q}, \dot{p}) \mapsto (q - \dot{q}, p, q, \dot{p}) .
\]

As \((R_d^T)^{-1}(q_0, p_0, q_1, p_1) = (q_1, p_0, q_1 - q_0, p_1 - p_0)\), Equation (5.1) leads to the following symplectic method:

\[
\frac{q_1 - q_0}{h} = \frac{1}{2} \frac{\partial H}{\partial p}(q_1, p_0) ,
\frac{p_1 - p_0}{h} = -\frac{1}{2} \frac{\partial H}{\partial q}(q_1, p_0) .
\]

For a Hamiltonian \(H(p, q) = \frac{1}{2} p M p + V(q)\), with \(M\) a constant positive definite matrix, the integrator is an explicit symplectic method.

**Example 5.4.** Now consider a Hamiltonian function \(H: T^*S^2 \to \mathbb{R}\) on \(T^*S^2\) that we identify with the tangent bundle \(TS^2\):

\[
T^*S^2 \equiv \{(x, p) \in \mathbb{R}^3 \times \mathbb{R}^3 \mid \|x\| = 1, \ x \cdot p = 0\} .
\]

For the discretization of the corresponding Hamiltonian equations we will use the retraction map \(R_d: TS^2 \to S^2 \times S^2\) given by

\[
R_d(x, \xi) = \left(x, \frac{x + \xi}{\|x + \xi\|}\right) ,
\]
whose inverse is precisely:
\[ R_d^{-1}(x_0, x_1) = \left( x_0, \frac{x_1}{x_0 \cdot x_1} - x_0 \right), \]
whenever it is well defined. Now, we will compute the inverse of the cotangent lift of the extended retraction map given in Equation (3.2), that is,
\[ \left( R_d^T \right)^{-1}(x_0, p_0; x_1, p_1) = \alpha_Q^{-1} \left( R_d^{-1}(x_0, x_1), (-p_0, p_1) D_{R_d^{-1}(x_0, x_1)} R_d \right). \]
Having in mind the definition of $T^*S^2$, it can be computed that the matrix $D_{R_d^{-1}(x,y)}R_d$ is equal to:
\[ D_{R_d^{-1}(x,y)}R_d = \begin{pmatrix} \text{Id}_{3 \times 3} & 0 \\ (x \cdot y) \text{Id}_{3 \times 3} & C \end{pmatrix}, \]
where $C$ is the matrix with entries
\[ c_{ij} = \begin{cases} (x \cdot y) \left[ 1 + (x \cdot y)y_i x_i - y_i^2 \right] & \text{if } i = j, \\ (x \cdot y) \left[ (x \cdot y)y_i x_j - y_i y_j \right] & \text{if } i \neq j. \end{cases} \]
Therefore,
\[ \left( R_d^T \right)^{-1}(x_0, p_0; x_1, p_1) = \left( x_0, p_1 C; \frac{1}{x_0 \cdot x_1} x_1 - x_0, -p_0 + (x_0 \cdot x_1)p_1 \right). \]
As a result, we obtain the following symplectic integrator for Hamilton’s equations:
\[ \frac{1}{x_k \cdot x_{k+1}} x_{k+1} - x_k = \frac{h}{2} \left( \frac{\partial H}{\partial p}(x_k, p_k C) \right), \]
\[ -p_k + (x_k \cdot x_{k+1})p_{k+1} = -h \frac{\partial H}{\partial q}(x_k, p_k C). \]

**Remark 5.5.** Another option to construct geometric integrators is to use an expression similar to (4.1) but now adapted for Hamiltonian vector fields, that is,
\[ \left( R_d^{TT^*Q} \right)^2 \circ hX_H(q_k, p_k) = \left( R_d^{TT^*Q} \right)^1 \circ hX_H(q_{k+1}, p_{k+1}). \]
Note that here the extended retraction map on $T^*Q$ does not have to be the cotangent lift of one on $Q$. However, even if the cotangent lift is considered, the method is not necessarily symplectic. For instance, for the extended retraction map coming from the mid-point rule in Examples 2.5 and 3.8, we obtain the symmetric second-order method:
\[ \frac{q_{k+1} - q_k}{h} = \frac{1}{2} \left( \frac{\partial H}{\partial p}(q_k, p_k) + \frac{\partial H}{\partial p}(q_{k+1}, p_{k+1}) \right), \]
\[ \frac{p_{k+1} - p_k}{h} = \frac{1}{2} \left( \frac{\partial H}{\partial q}(q_k, p_k) + \frac{\partial H}{\partial q}(q_{k+1}, p_{k+1}) \right). \]
However, this method is not symplectic because, in general, $dq_{k+1} \wedge dp_{k+1} - dq_k \wedge dp_k \neq 0$ when restricted to the numerical scheme.
Remark 5.6. Observe that our method gives us a constructive way to derive symplectic integrators for Hamiltonian systems. It will be interesting to compare our methods with other previous approaches ([Leok and Zhang 2011]), specially when the configuration space is a Lie group and we can use well-known retraction maps such as exponential maps and other approximations. See [Iserles, Munthe-Kaas, Nørsett, and Zanna 2000, Bou-Rabee and Marsden 2009, Celledoni, Marthinsen, and Owren 2014, Bogfjellmo and Marthinsen 2016].

5.2 Geometric integrators in Lagrangian framework

Let us consider a regular Lagrangian function $L : TQ \to \mathbb{R}$ so that there exists a second-order vector field $\Gamma_L$ on $TQ$ and Euler-Lagrange equations are given by

$$i_{\Gamma_L} \Omega_L = dE_L,$$

where $E_L$ is the energy function and $\Omega_L$ is the symplectic Lagrange 2-form obtained by the pull-back of the Legendre map $FL : TQ \to T^*Q$ of the natural symplectic form on $T^*Q$, that is, $\Omega_L = (FL)^*\omega_Q$ (see [Abraham and Marsden 1978] for more details).

As in (4.2), an extended retraction map on $TQ$, that is, $R_d^{TTQ} : TTQ \to TQ \times TQ$, defines the following numerical integrator:

$$R_d^{TTQ} \left( h \Gamma_L \left( \left( \tau_{TQ} \circ \left( R_d^{TTQ} \right)^{-1} \right)(q_0, v_0; q_1, v_1) \right) \right) = (q_0, v_0; q_1, v_1). \quad (5.3)$$

Equivalently,

$$h \Gamma_L \left( \left( \tau_{TQ} \circ \left( R_d^{TTQ} \right)^{-1} \right)(q_0, v_0; q_1, v_1) \right) = \left( R_d^{TTQ} \right)^{-1} (q_0, v_0; q_1, v_1).$$

As the Lagrangian function is regular, we could move to the Hamiltonian framework and construct a symplectic numerical integrator using the cotangent lift of a retraction map on $Q$ as in Proposition 5.1. It remains to prove if the obtained numerical integrator is an extended retraction map on $TQ$ as described in Definition 2.2.

Remember that the manifold $(TQ \times TQ, \Omega^1_{L} - \Omega^0_{L})$ is symplectic. Locally, the symplectic 2-form is given by $\Omega^1_{L} - \Omega^0_{L} = (FL^{-1}, FL^{-1})^*(dq^1 \wedge dp^1 - dq^0 \wedge dp^0)$.

Proposition 5.7. Let $R_d : TQ \to Q \times Q$ be an extended retraction map on $Q$ and $L : TQ \to \mathbb{R}$ be a regular Lagrangian function. The two following facts are satisfied:

(a) the map $R_d^L = (FL^{-1}, FL^{-1}) \circ R_d^{TTQ} \circ TFL : TTQ \to TQ \times TQ$ defines a symplectic numerical integrator of the Euler-Lagrange equations for $L$;

(b) the above-mentioned map $R_d^L$ is an extended retraction map on $TTQ$.

Proof. First, we prove property (a). As the Lagrangian function is regular, the Legendre map is a local diffeomorphism. Propositions 3.2 and 5.1 guarantee that $R_d^L$ is a symplectomorphism because it is a composition of symplectomorphisms. Hence, $R_d^L$ defines a symplectic numerical integrator in Equation (5.3).

The diagram below shows the constructive process for $R_d^L$: 

\[
\begin{array}{ccc}
TQ & \xrightarrow{TFL} & T^*Q \\
\downarrow \tau_{TQ} & & \downarrow (FL)^*\omega_Q \\
TQ & \xrightarrow{TFL^{-1}} & TQ \\
\end{array}
\]
In other words, the Lagrangian submanifold \( \text{Im} \Gamma_L \) of \((TTQ, (TFL)^\ast (dt \omega_Q))\) is preserved by \( R_d^L \) and the numerical method in Equation (5.3) is symplectic.

For (b), we must prove the properties in Definition 2.2 for the map \( R_d^L : TTQ \to TQ \times TQ \).

1. Note that \( R_d^L(v_q, 0_{v_q}) = (v_q, v_q) \) because

\[
R_d^L(v_q, 0_{v_q}) = \left( (FL^{-1}, FL^{-1}) \circ R_d^{T^\ast} \right) (FL(v_q); 0_{FL(v_q)}) = (FL^{-1}, FL^{-1})(FL(v_q); FL(v_q)) = (v_q, v_q).
\]

The second equality is true because \( R_d^{T^\ast} \) is an extended retraction map on \( T^\ast Q \) as shown in Proposition 3.5.

2. We must prove that \( T_{(q,v,0,0)} (R_d^L(q,v,0_{v_q})^2 - R_d^L(q,v,0_{v_q}) (R_d^L(q,v,0_{v_q}) \right) is the identity map from \( T_{(q,v,0,0)} TTQ \simeq T_{(q,v)} TQ \) to itself.

Let us first compute it for \( i = 1, 2 \):

\[
\left. \frac{d}{dt} \right|_{t=0} FL^{-1} \left( (R_d^{T^\ast})^i (TFL)(q,v,t \dot{q}, t \dot{v}) \right) = DFL^{-1}(q,v,0_{v_q}) D_{3,4} (TFL)(q,v,0_{v_q}).
\]

Note that \( D_{3,4} (TFL)(q,v,0_{v_q}) \) is the fiber derivative of the tangent map \( TFL \). Knowing that the tangent map is linear on the fiber, together with the fact that \( R_d^{T^\ast} \) is an extended retraction map on \( T^\ast Q \) and it satisfies the second property in Definition 2.2, we can conclude that the map \( R_d^L \) satisfies the second property for being an extended retraction map on \( TQ \).

It can be proved that only for a very specific extended retraction map \( R_d \) on \( Q \) and Lagrangian function, the retraction map \( R_d^L \) of \( TTQ \) is the tangent lift of \( R_d \).

**Corollary 5.8.** Let \( L(q,v) = \frac{1}{2} v^T M v - V(q) \) be the Lagrangian function, being \( M \) a positive-definite symmetric constant mass matrix and \( V \) the potential function. If \( R_d : TQ \to Q \times Q \) is the extended retraction map on \( Q \) given by the mid-point rule in Example 2.5, then \( R_d^L \) is the tangent lift of \( R_d \).

**Proof.** The Legendre transformation for \( L \) in the corollary is \( FL(q,v) = (q, Mv) \) and the inverse map is \( FL^{-1}(q,p) = (q, M^{-1}p) \). Thus,

\[
R_d^L(q,v,\dot{q}, \dot{v}) = (R_d^L(q,\dot{q}), -(\dot{v},v)) DR_d^{-1}(q,\dot{q}, \dot{v})_{\ast,1}; R_d^L(q,\dot{q}, \dot{v}) DR_d^{-1}(q,\dot{q}, \dot{v})_{\ast,2}
\]
where \( A_{i,s} \) denotes the \( i \)th column of the matrix \( A \). This expression is equal to the tangent lift \( R_d^T \) if
\[
-(\dot{v}, v)D\Gamma_{R}^{-1}(q, \dot{q}), 1 = D_{(q,s)}R^1_d(q, v)(\dot{q}, \dot{v})^T
\]
\[
(\dot{v}, v)D\Gamma_{R}^{-1}(q, \dot{q}), 2 = D_{(q,s)}R^2_d(q, v)(\dot{q}, \dot{v})^T
\]
Both equalities are satisfied if the extended retraction map \( R_d \) is given by the mid-point rule, see Example 2.5.

**Example 5.9.** Let us consider a Lagrangian second-order vector field given by \( \ddot{q} = -M^{-1} \nabla V(q) \). The numerical method in Equation (5.3) for the mid-point rule described in Example 3.8 becomes:
\[
R_d^T \left( h \Gamma_L \left( \frac{q_0 + q_1}{2}, \frac{v_0 + v_1}{2} \right) \right) = (q_0, v_0, q_1, v_1)
\]
\[
R_d^T \left( \frac{q_0 + q_1}{2}, \frac{v_0 + v_1}{2}, h(q_1 - q_0), -hM^{-1} \nabla \left( \frac{q_0 + q_1}{2} \right) \right) = (q_0, v_0, q_1, v_1).
\]
Given \((q_0, v_0)\), the numerical integrator is defined implicitly by
\[
\frac{v_0 + v_1}{2} = \frac{q_1 - q_0}{h},
\]
\[
\frac{v_1 - v_0}{h} = -M^{-1} \nabla \left( \frac{q_0 + q_1}{2} \right).
\]
After some straightforward computations, we obtain that this discrete method is rewritten as an implicit second order discrete equation given by:
\[
\frac{q_2 - 2q_1 + q_0}{h^2} = -\frac{1}{2}M^{-1} \left( \nabla V \left( \frac{q_0 + q_1}{2} \right) + V \left( \frac{q_1 + q_2}{2} \right) \right)
\]
In the next subsection we will explore the relation of these methods with discrete variational calculus.

### 5.3 Discrete variational calculus

As mentioned in [Marsden and West 2001], a usual way to design symplectic integrators from a Lagrangian system consists of discretizing the variational principle using a discrete Lagrangian map. Many of these discrete maps are obtained from a continuous Lagrangian map and a retraction map on \( Q \) by discretizing the continuous action as follows
\[
\mathcal{S}(q_0, q_1) = \int_0^h L(q(t), \dot{q}(t)) \, dt \approx hL \left( \frac{1}{h}R_d^{-1}(q_0, q_1) \right) = L^h_d(q_0, q_1),
\]
where \( q(t) \) is the unique solution of the Euler-Lagrange equations such that \( q(0) = q_0 \) and \( q(h) = q_1 \) with \( h \) enough small. Observe that if \( R_d^{-1}(q_0, q_1) = v_q \in T_qQ \) then \( \frac{1}{h}R_d^{-1}(q_0, q_1) = \frac{1}{h}v_q \in T_qQ \). Therefore, the discrete Lagrangian \( L^h_d : Q \times Q \rightarrow \mathbb{R} \) is defined by \( L^h_d = h \circ \frac{1}{h}R_d^{-1} \).

If we consider the Hamiltonian function \( \hat{H}(p, q) = \langle p, \dot{q} \rangle - L(q, \dot{q}) \) then we can simultaneously consider the discretization of both the Lagrangian and Hamiltonian framework. The following diagram is commutative by construction (see
Example 5.10. Given a regular Lagrangian $L : TQ \to \mathbb{R}$, where $Q$ is a vector space and consider as discrete Lagrangian $L^h_d(q_0, q_1) = hL\left(\frac{q_0 + q_1}{2}, \frac{q_0 - q_1}{h}\right)$. Using Example 3.8, the left-hand side of Equation (5.4) and the right-hand side of (5.5), we obtain the following integrator:

\[
\frac{p_{k+1} - p_k}{h} = \partial_L \left(\frac{q_k + q_{k+1}}{2}, \frac{q_{k+1} - q_k}{h}\right),
\]

\[
\frac{p_k + p_{k+1}}{2} = \partial\tilde{L} \left(\frac{q_k + q_{k+1}}{2}, \frac{q_{k+1} - q_k}{h}\right).
\]

6 Composition of geometric integrators

The construction of symplectic integrators based on extended retraction maps is closely related to the notion of Lagrangian submanifolds, as already appears in Section 5. For instance, Equation (5.2) defines the following Lagrangian $\mathcal{L}^h$ of the symplectic manifold $(T^*Q \times T^*Q, \Omega_{12})$:

\[
\mathcal{L}^h = \left\{(\alpha_q, \beta_q) \in T^*Q \times T^*Q \mid (\alpha_q, \beta_q) = R^T_d \left(hX_H\left(\gamma_{q''}\right)\right)\right\}
\]
where $\gamma_{q'} = (\tau_{T^*Q} \circ (R^*_Q)^{-1})(\alpha_q, \beta_{q'}) \in T^*Q$.

Now, we will use some well-known properties of Lagrangian submanifolds as the composition of Lagrangian submanifolds (see Appendix A and [Guillemin and Sternberg 1990] for more details) to describe a particularly elegant method to construct high-order methods from a given low-order integrator (see Hairer, Lubich, and Wanner [2010]). To be more precise, we are going to geometrically describe the composition of two (or more) geometric integrators defined by different extended retraction maps. As a particular example, we will recover the well-known Störmer-Verlet method, a second-order symplectic method.

Let $R_{d,1}$ and $R_{d,2}: TQ \to Q \times Q$ be two extended retraction maps on $Q$ and $H: T^*Q \to \mathbb{R}$ be a Hamiltonian function, using Equation (5.2) we define two Lagrangian submanifolds of $(T^*Q \times T^*Q, \Omega_{12})$ as follows:

$$
\mathcal{L}^{h/2}_1 = \left\{ (q_k, p_k; q_{k+1/2}, p_{k+1/2}) \in T^*Q \times T^*Q \mid \exists \gamma_{k,k+1/2} \in T^*Q \text{ s. t.} \gamma_{k,k+1/2} = \left( \tau_{T^*Q} \circ (R^*_{d,1})^{-1} \right)(q_k, p_k; q_{k+1/2}, p_{k+1/2}) \right\},
$$

$$
\mathcal{L}^{h/2}_2 = \left\{ (q_{k+1/2}, p_{k+1/2}; q_{k+1}, p_{k+1}) \in T^*Q \times T^*Q \mid \exists \gamma_{k+1/2,k+1} \in T^*Q \text{ s. t.} \gamma_{k+1/2,k+1} = \left( \tau_{T^*Q} \circ (R^*_{d,2})^{-1} \right)(q_{k+1/2}, p_{k+1/2}; q_{k+1}, p_{k+1}) \right\},
$$

where

$$
\gamma_{k,k+1/2} = \left( \tau_{T^*Q} \circ (R^*_{d,1})^{-1} \right)(q_k, p_k; q_{k+1/2}, p_{k+1/2}) \in T^*Q,
$$

$$
\gamma_{k+1/2,k+1} = \left( \tau_{T^*Q} \circ (R^*_{d,2})^{-1} \right)(q_{k+1/2}, p_{k+1/2}; q_{k+1}, p_{k+1}) \in T^*Q.
$$

After some technical conditions of clean intersection (see [Guillemin and Sternberg 2013]) we compose the above two Lagrangian submanifolds,

$$
\mathcal{L}^{h/2}_2 \circ \mathcal{L}^{h/2}_1 = \left\{ (\alpha_q, \beta_{q'}) \in T^*Q \times T^*Q \mid \exists \gamma_{q'} \in T^*Q \text{ with } (\alpha_q, \gamma_{q'}) \in \mathcal{L}^{h/2}_1, (\gamma_{q'}, \beta_{q'}) \in \mathcal{L}^{h/2}_2 \right\},
$$

obtaining an immersed Lagrangian submanifold. Thus, it generates a new symplectic integrator. Moreover, it is possible to compose more than two Lagrangian submanifolds to generate more involved methods where the intermediate points $\gamma_{q'}$ play the role of micro-nodes (see [Marsden and West 2001, Leok and Shingel 2012, Campos 2014]).

**Example 6.1.** Let $Q = \mathbb{R}^n$, we consider the two extended retraction maps $R_{d,1}(q,v) = (q, q + v)$ and $R_{d,2}(q,v) = (q - v, q)$. Then, we compute their corresponding cotangent lifts, $R^*_{d,1}$ and $R^*_{d,2}$ as described in Section 3.2, and obtain

$$
\mathcal{L}^{h/2}_1 = \left\{ (q_k, p_k; q_{k+1/2}, p_{k+1/2}) \mid p_{k+1/2} = p_k - \frac{h}{2} \nabla_q H(q_k, p_{k+1/2}), q_{k+1/2} = q_k + \frac{h}{2} \nabla_p H(q_k, p_{k+1/2}) \right\},
$$

$$
\mathcal{L}^{h/2}_2 = \left\{ (q_{k+1/2}, p_{k+1/2}; q_{k+1}, p_{k+1}) \mid p_{k+1} = p_{k+1/2} - \frac{h}{2} \nabla_q H(q_{k+1}, p_{k+1/2}), q_{k+1} = q_{k+1/2} + \frac{h}{2} \nabla_p H(q_{k+1}, p_{k+1/2}) \right\}.
$$
The composition $L_2^{h/2} \circ L_1^{h/2}$ gives a new symplectic integrator that corresponds with the Störmer-Verlet method [Hairer, Lubich, and Wanner 2010]:

\[
\begin{align*}
p_{k+1/2} &= p_k - \frac{h}{2} \nabla_q H(q_k, p_{k+1/2}), \\
q_{k+1} - \frac{h}{2} \nabla_p H(q_{k+1}, p_{k+1/2}) &= q_k + \frac{h}{2} \nabla_p H(q_k, p_{k+1/2}), \\
p_{k+1} &= p_{k+1/2} - \frac{h}{2} \nabla_q H(q_{k+1}, p_{k+1/2}).
\end{align*}
\]

When discrete Lagrangian functions are given as in Section 5.3, Equations (5.2) and (5.5) can be expressed as Lagrangian submanifolds of $(\mathcal{T}Q \times \mathcal{T}Q, \Omega_{12})$ and many of the methods described in [Marsden and West 2001, Leok and Shingel 2012] are recovered.

For instance, for a small positive step size $h$, we consider the following two extended retraction maps on $Q$, $R_{d,i} : \mathcal{T}Q \to \mathcal{T}Q$:

\[
R_{d,1} \left( q, \frac{h}{2} v \right) = \left( q, q + \frac{h}{2} v \right), \quad \text{with inverse} \quad R_{d,1}^{-1}(q_0, q_1) = \left( q_0, q_1 - q_0 \frac{h}{2} \right),
\]

\[
R_{d,2} \left( q, \frac{h}{2} v \right) = \left( q - \frac{h}{2} v, q \right), \quad \text{with inverse} \quad R_{d,2}^{-1}(q_0, q_1) = \left( q_1, q_1 - q_0 \frac{h}{2} \right).
\]

We define the discrete Lagrangian functions $L_{d,i} = \left( h \circ (R_{d,i})^{-1} \right) : \mathcal{T}Q \times \mathcal{T}Q \to \mathbb{R}$ such that the image of $(\Phi^{-1} \circ dL_{d,i})$ define the Lagrangian submanifolds $L_i$ of the symplectic manifold $(\mathcal{T}Q \times \mathcal{T}Q, \Omega_{12})$. The submanifolds $L_i$ define a discrete dynamical system whose equations are locally described by

\[
L_i = \{(q_0, p_0; q_1, p_1) \in \mathcal{T}Q \times \mathcal{T}Q \mid p_0 = -D_1L_{d,i}^1(q_0, q_1), \quad p_1 = D_2L_{d,i}^2(q_0, q_1)\}.
\]

The composition

\[
L_2 \circ L_1 = \{(\alpha_1, \alpha_2) \mid \exists \alpha_{1/2} \in \mathcal{T}Q \text{ s. t. } (\alpha_1, \alpha_{1/2}) \in L_1, \ (\alpha_{1/2}, \alpha_2) \in L_2\}
\]

has associated the dynamics given by the discrete Lagrangian $L_2^3(q_0, q_2) = L_2^1(q_0, q_1) + L_2^2(q_1, q_2)$, that plays the role of generating function (see also [de León, Jiménez, and Martín de Diego 2012]). The discrete equations are

\[
\begin{align*}
p_0 &= -D_1L_{d}^1(q_0, q_1), \\
0 &= D_2L_{d}^1(q_0, q_1) + D_1L_{d}^2(q_1, q_2), \\
p_2 &= D_2L_{d}^2(q_1, q_2).
\end{align*}
\]

### 6.1 Symplectic symmetric methods

If we have a Lagrangian submanifold $\mathcal{L}$ of $(\mathcal{T}Q \times \mathcal{T}Q, \Omega_{12})$, then the transpose $\mathcal{L}^\dagger$ defined by

\[
\mathcal{L}^\dagger = \{(\alpha_q, \beta_q') \in \mathcal{T}Q \times \mathcal{T}Q \mid (\beta_q', \alpha_q) \in \mathcal{L}\}
\]

is also a Lagrangian submanifold of $(\mathcal{T}Q \times \mathcal{T}Q, \Omega_{12})$.

For a Hamiltonian function and an extended retraction map on $\mathcal{T}Q$, we consider the following Lagrangian submanifold used in the previous section:

\[
\mathcal{L}^h = \left\{ (\alpha_q, \beta_q') \in \mathcal{T}Q \times \mathcal{T}Q \mid \exists \beta_q'' \in \mathcal{T}Q \text{ s. t. } (\alpha_q; \beta_q') = R_d^{\dagger h} (h \circ X_H (\gamma_{q''})) \right\}.
\]
As described in [Hairer, Lubich, and Wanner 2010, Marsden and West 2001], the composition of symplectic methods (seen here as Lagrangian submanifolds) gives rise to new symplectic methods. For instance, the Lagrangian submanifold \((L^{h/2} \circ L^{h/2})^\dagger\) is another way to interpret the Störmer-Verlet method considered in the previous section.

**Definition 6.2.** A symplectic method defined by \(L^h\) is symmetric if \((L^h)^\dagger = L^{-h}\).

**Proposition 6.3.** Let \(\iota : Q \times Q \to Q \times Q\) be the inversion map defined by \(\iota(q, q') = (q', q)\). If \(R_d(v_q) = \iota(R_d(-v_q))\) for all \(v_q \in T_qQ\), then \(L^h\) is symmetric.

**Proof.** Observe that \((L^h)^\dagger \subseteq \{(\beta_{q'}, \alpha_q) \in T^*Q \times T^*Q \mid \exists \gamma_{q''} \in T^*Q\ s.t. (\alpha_q, \beta_{q'}) = R_d^T(h X_H(\gamma_{q''}))\}\).

As \(R_d^T = \Phi^{-1} \circ R_d \circ \alpha_Q : TT^*Q \to T^*Q \times T^*Q\) is the cotangent lift of \(R_d\), we have
\[
R_d^T (X_H(\gamma_{q''})) = (\Phi^{-1} \circ \iota \circ R_d \circ \alpha_Q) (-X_H(\gamma_{q''})) = \iota_{T^*Q} (R_d^T (-X_H(\gamma_{q''})))
\]

where \(\iota_{T^*Q} : T^*Q \times T^*Q \to T^*Q \times T^*Q\) is the corresponding inversion on \(T^*Q\). Thus, we immediately deduce that \((L^h)^\dagger = L^{-h}\).

**7 Conclusions and future work**

In this paper we have introduced the lift of a new notion of retraction maps to tangent and cotangent bundles which are the phase spaces of mechanical systems. These lifts allow us to derive geometric integrators for systems defined by a Lagrangian or Hamiltonian function. Standard constructions in symplectic geometry, as well as properties of Lagrangian submanifolds, create a geometric framework to obtain several well-known symplectic integrators. Our geometric point of view opens the door for new types of applications of retraction maps, as well as, for the construction of geometric (symplectic) integrators following simple rules (lifting of retractions, composition and generating functions for Lagrangian submanifolds, etc). Now, we will mention some promising future research lines.

**7.1 Reduced systems and systems with holonomic constraints**

The notion of lift of retraction maps can be easily extended to the Lie algebroid setting using the Lie algebroid prolongation [de León, Marrero, and Martínez 2005]. This theory covers all the examples of reduced systems by symmetry groups. Therefore, combining both constructions we can directly apply our...
results to the construction of geometric integrators for Lagrangian or Hamiltonian functions invariant under the action of a symmetry Lie group [Weinstein 1996, Márero, Martín de Diego, and Martínez 2006]. It is also well-known how to produce geometric integrators for systems subject to holonomic constraints. Thus, it will be interesting to produce constrained geometric integrators using our approach and compare them with [Leimkuhler and Reich 2004, McLachlan, Modin, Verdier, and Wilkins 2014].

7.2 Discrete gradient methods

In general for ordinary differential equations in \( \mathbb{R}^n \) in skew-gradient form, i.e. \( \dot{x} = \Pi(x) \nabla H(x) \) where \( x \in \mathbb{R}^n \) and \( \Pi(x) \) is a skew-symmetric matrix, it is clear that \( H \) is a first integral. Using discretizations of the gradient \( \nabla H(x) \) it is possible to define a class of integrators that preserve exactly the first integral \( H \) (see [Gonzalez 2000, McLachlan, Quispel, and Robidoux 1999]). They are defined as follows: let \( H: \mathbb{R}^n \rightarrow \mathbb{R} \) be a differentiable function, then \( \nabla H : \mathbb{R}^2 \rightarrow \mathbb{R}^N \) is a discrete gradient of \( H \) if it is continuous and satisfies

\[
\nabla H(x, x')^T (x' - x) = H(x') - H(x), \quad \text{for all } x, x' \in \mathbb{R}^n,
\]

\[
\nabla H(x, x) = \nabla H(x), \quad \text{for all } x \in \mathbb{R}^n. \quad (7.1)
\]

For a Hamiltonian system \( H: T^*Q \rightarrow \mathbb{R} \), we can generalize the previous construction by using an extended retraction map \( R_d^{TT^*Q} \) on a general differentiable manifold \( T^*Q \). We define a discrete gradient as a map \( dH: T^*Q \times T^*Q \rightarrow T^*T^*Q \) that makes the following diagram commutative

\[
\begin{array}{ccc}
T^*Q \times T^*Q & \xrightarrow{\pi H} & T^*T^*Q \\
\downarrow (R_d^{TT^*Q})^{-1} & & \downarrow \pi_{T^*Q} \\
TT^*Q & \xrightarrow{\tau_{T^*Q}} & T^*Q 
\end{array}
\]

Similar to (7.1), \( \overline{dH} \) must verify the following properties:

\[
\langle \overline{dH}(x, x'), (R_d^{TT^*Q})^{-1}(x, x') \rangle = H(x') - H(x), \quad \text{for all } x, x' \in T^*Q,
\]

\[
\overline{dH}(x, x) = dH(x), \quad \text{for all } x \in T^*Q.
\]

In this case, an energy preserving integrator would be

\[
(R_d^{TT^*Q})^{-1}(x, x') = \omega^*(x'')(\overline{dH}(x, x'))
\]

where \( x'' = \tau_{T^*Q}((R_d^{TT^*Q})^{-1}(x, x')) \). We will explore this possibility in a future paper (see also [Celledoni, Mørkholm, and Owren 2014, Celledoni, Eidsnes, Owren, and Ringholm 2020], for the case of extension to manifolds, in special, Riemannian manifolds).

7.3 Higher-order retractions and higher order lagrangian systems

Another topic to explore is the use of higher-order retraction maps since in this paper we have only focused on first-order retraction maps. Remember that,
for instance, a second-order retraction map $R_{x}: TM \rightarrow M$ on a Riemannian manifold $M$ is a retraction map such that, for all $x \in M$ and all $\xi \in T_{x}M$, the curve $c(t) = R_{x}(t\xi)$ has zero acceleration at $t = 0$, that is, $\frac{d^{2}c}{dt^{2}}(0) = 0$, mimicking the case of Riemannian geodesics [Absil, Mahony, and Sepulchre 2008, Absil and Malick 2012, Boumal, Absil, and Cartis 2019]. It would be interesting to study the relation of higher-order retractions with the order of the obtained numerical methods.

Another topic of interest is related with the discretization of higher-order Lagrangian systems $L : T^{(k)}Q \rightarrow \mathbb{R}$ using appropriate higher-order lifts of retraction maps. These constructions will be useful for interpolation problems on manifolds and for optimal control problems (see [Crouch and Silva Leite 1995, Gay-Balmaz, Holm, Meier, Ratiu, and Vialard 2012, Colombo, Ferraro, and Martín de Diego 2016]).

### 7.4 Geometric integration of Dirac systems

Dirac structures were introduced in [Courant and Weinstein 1988, Courant 1990] as a way to unify presymplectic and Poisson geometries giving a way to collect in the same geometric framework many situations of interest in mechanics and mathematical physics. As an example we can think of the Dirac structure $D \subset TT^{*}Q \oplus T^{*}T^{*}Q$ induced by the canonical symplectic structure $\omega_{Q}$, that is

$$D = \{(X_{\alpha q}, \lambda_{\alpha q}) \in TT^{*}Q \oplus T^{*}T^{*}Q \mid i_{X_{\alpha q}} \omega_{Q} = \lambda_{\alpha q}\}.$$  

For a Hamiltonian system $H : T^{*}Q \rightarrow \mathbb{R}$, we can write Hamilton’s equations as

$$X_{\alpha q} \oplus \frac{dH}{d\alpha q} \in D_{\alpha q},$$  

with $\alpha q \in T^{*}Q$. As studied in the literature, Dirac structures are more general than the above example. They can be given by a Poisson tensor, for instance, or could not satisfy the integrability condition admitting new generalizations as in the case of nonholonomic constraints (see [Barbero Liñán, Cendra, García Toraño, and Martín de Diego 2019]). Moreover, it is also interesting to study the case of Dirac systems where the dynamics is not induced by a function on the cotangent bundle (as in the case of standard Hamiltonian dynamics), but for a general Lagrangian submanifold $S$ of $(T^{*}T^{*}Q, \omega_{T^{*}Q})$ (as in the case of singular Lagrangians, optimal control theory, etc). Now, Equation (7.2) must be replaced by

$$X_{\alpha q} \oplus S_{\alpha q} \in D_{\alpha q}.$$  

Extended retraction maps could also be used here to deduce geometric integrators. Let $R_{d} : TQ \rightarrow Q \times Q$ be an extended retraction map on $Q$, the cotangent lift of $R_{d}$ defines the following geometric integrator

$$\left(R_{d}^{\tau}ight)^{-1}(q_{k}, p_{k}; q_{k+1}, p_{k+1}) \oplus S_{\gamma_{k,k+1}} \in D_{\gamma_{k,k+1}}$$

where $\tau_{T^{*}Q} \left(\left(R_{d}^{\tau}ight)^{-1}(q_{k}, p_{k}; q_{k+1}, p_{k+1})\right) = \gamma_{k,k+1}$. We will study in a forthcoming paper the design of Dirac integrators using the lift of the retraction maps, their geometrical properties (preservation of the associated presymplectic foliation, etc.) and compare them with other approaches on this topic ([Leok and Ohsawa 2011, Leok and Shingel 2012]).
7.5 Morse families for Lagrangian submanifolds and symplectic integration

In this paper it is clear the close relationship between the design of different symplectic methods and the construction of Lagrangian submanifolds. The notion of a Morse family or phase function was introduced in [Hörmander 1971] (see also [Weinstein 1979]) and it is possible to prove that locally any Lagrangian submanifold is the image of a Lagrangian immersion generated by a Morse family. In a recent paper [Barbero Liñán, Cendra, García Torano, and Martín de Diego 2019], we have combined Dirac structures and Morse families to obtain a geometric formalism that unifies most of the scenarios in mechanics (constrained calculus, nonholonomic systems, optimal control theory, higher-order mechanics, etc.), as the examples in the paper show. Employing the techniques introduced here we aim to study the construction of geometric integrators for all the above-mentioned cases, as well as, the notion of Morse family to construct new geometric integrators.

A Lagrangian submanifolds

We review here the main properties of Lagrangian submanifolds needed in the paper. More details can be found in [Libermann and Marle 1987, Weinstein 1971, Guillemin and Sternberg 2013].

A symplectic manifold \((M, \omega)\) is a differentiable manifold \(M\) with a non-degenerate closed 2-form \(\omega\) on \(M\). Therefore, for each \(x \in M\), \((T_x M, \omega_x)\) is a symplectic vector space and, in particular, \(M\) is even dimensional. The vector bundle isomorphisms \(\Omega^\flat = \flat \omega : T M \rightarrow T^* M\) and \(\Omega^\sharp = (\flat \Omega)^{-1} : T^* M \rightarrow TM\) are defined fiberwise.

Let \((M, \omega)\) be a symplectic manifold. An immersed submanifold, or immersion, \(f : N \rightarrow M\) is Lagrangian if so is the space \(T f(T_x N)\) as a subspace of \(T f(x) M\), for each point \(x \in N\). Note that an immersion \(f : N \rightarrow M\) is Lagrangian if only if \(f^* \omega = 0\) and the dimension of \(N\) is half the dimension of \(M\).

A fundamental example of a symplectic manifold is the cotangent bundle \(T^* Q\) of an arbitrary manifold \(Q\). It is equipped with a canonical exact symplectic structure \(\omega_Q = -d\theta_Q\) where \(\theta_Q\) is the canonical 1-form on \(T^* Q\), defined as follows. Denote by \(\pi_Q : T^* Q \rightarrow Q\) the canonical projection, then

\[
(\theta_Q)_{\alpha_q} (X_{\alpha_q}) = \langle \alpha_q, T_{\alpha_q} \pi_Q(X_{\alpha_q}) \rangle,
\]

where \(X_{\alpha_q} \in T_{\alpha_q}T^* Q\), \(\alpha_q \in T^* Q\) and \(q \in Q\). In canonical bundle coordinates \((q^i, p_i)\) on \(T^* Q\) the projection reads \(\pi_Q(q^i, p_i) = q^i\), and one finds easily that \(\theta_Q\) has coordinate expression \(\theta_Q = p_i dq^i\). The 2-form \(\omega_Q = -d\theta_Q\) is a symplectic form on \(T^* Q\) whose local expression is

\[
\omega_Q = dq^i \wedge dp_i .
\]

Darboux’s theorem states that for an arbitrary symplectic manifold \((M, \omega)\), there exist local coordinates \((q^i, p_i)\) in a neighbourhood of each point in \(M\) such that \(\omega = dq^i \wedge dp_i\). It follows that all symplectic manifolds are locally isomorphic.

As described in [Śniatycki and Tulczyjew 1972/73, Guillemin and Sternberg 2013] two symplectic manifolds can be composed to construct a Lagrangian
submanifold in the product of symplectic manifolds. Let \((M_i, \omega_i)\) be symplectic manifolds. A Lagrangian submanifold \(L\) of \(M_1^- \times M_2\) is called a canonical relation, where \(M_1^-\) denotes the manifold \(M_1\) with the symplectic form \(-\omega\). Thus \(L\) is a subset of \(M_1 \times M_2\) and is a Lagrangian submanifold for the symplectic form \(\omega_2 - \omega_1\). Any symplectomorphism \(f: M_1 \to M_2\) defines a canonical relation with the graph of \(f\), \(L_f\).

If \(L_1 \subset M_1 \times M_2\) and \(L_2 \subset M_2 \times M_3\), the composition \(L_2 \circ L_1\) is a subset of \(M_1 \times M_3\) such that for any \((\alpha_1, \alpha_3) \in L_2 \circ L_1\) there exists \(\alpha_2 \in M_2\) such that \((\alpha_1, \alpha_2) \in L_1\) and \((\alpha_2, \alpha_3) \in L_2\). Let \(pr_2^i: L_i \to M_2\) be the projection of \(L_i\) onto \(M_2\). Let \(F \subset M_1 \times M_2 \times M_2 \times M_3\) be given by the inverse image of the diagonal set \(\Delta_{M_2} = \{ (\alpha_2, \alpha_2) \}\) through \((pr_1^1 \times pr_2^2)^{-1}\), that is,

\[
F = (pr_1^1 \times pr_2^2)^{-1}(\Delta_{M_2}).
\]

This set is not guaranteed to be a submanifold and the restriction of \(\pi_{13}: M_1 \times M_2 \times M_2 \times M_3 \to M_1 \times M_3\) to \(F\) is not necessarily an embedding. As a set it is true that \(L_2 \circ L_1 = \pi_{13}(F)\).

**Theorem A.1.** [Guillemin and Sternberg 2013, Chapter 4.1, Theorem 8] If the canonical relations \(L_1\) and \(L_2\) intersect cleanly, then their composition \(L_2 \circ L_1\) is an immersed Lagrangian submanifold of \(M_1^- \times M_2\).

**Theorem A.2.** [Guillemin and Sternberg 2013, Chapter 4.2, Theorem 10] If the canonical relations \(L_1\) and \(L_2\) intersect cleanly and the projection \(\pi_{13}\) restricted to \(F\) onto \(M_1 \times M_3\), denoted by \(\kappa\), is proper and the inverse image of every point in \(L_2 \circ L_1\) by \(\kappa\) is connected, then \(L_2 \circ L_1\) is a canonical relation and \(\kappa\) is a smooth fibration with compact connected fibers.

When the hypotheses of the previous theorem are satisfied, it is said that \(L_2\) and \(L_1\) are composable.

Consequently, two Lagrangian submanifolds of the original two symplectic manifolds can be composed to obtain a Lagrangian submanifold in the new space.

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