HIGHER-ORDER DISCRETE VARIATIONAL PROBLEMS WITH CONSTRAINTS

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Abstract. An interesting family of geometric integrators for Lagrangian systems can be defined using discretizations of the Hamilton’s principle of critical action. This family of geometric integrators is called variational integrators.

In this paper, we derive new variational integrators for higher-order lagrangian mechanical system subjected to higher-order constraints. From the discretization of the variational principles, we show that our methods are automatically symplectic and, in consequence, with a very good energy behavior. Additionally, the symmetries of the discrete Lagrangian imply that momenta is conserved by the integrator. Moreover, we extend our construction to variational integrators where the lagrangian is explicitly time-dependent. Finally, some motivating applications of higher-order problems are considered; in particular, optimal control problems for explicitly time-dependent underactuated systems and an interpolation problem on Riemannian manifolds.

1. Introduction

1.1. General background and motivation. Recently, higher-order variational problems have been studied for their important applications in aeronautics, robotics, computer-aided design... where are necessary variational principles that depend on higher-order derivatives (see [10, 11, 12, 14, 15, 17, 23]). The dynamics of these systems are governed by variational principles on higher-order tangent bundles. Therefore, it is quite interesting to develop structure-preserving numerical integration schemes for this kind of systems.

Discrete mechanics has become a field of intensive research activity in the last decades [26, 27, 28, 32]. Many of the geometric properties of a mechanical system in the continuous case admit an appropriate counterpart in the discrete setting. In this sense, variational integrators preserve some invariants of the mechanical system, in particular, momentum and symplecticity (see [19, 21, 22, 27]).

In this paper, we construct a geometric integrator determined by a discretization of a variational principle derived by a higher-order Lagrangian. Such type of discrete mechanical systems have been recently studied in [4, 6, 13] (without the presence of constraints) for applications in optimal control, trajectory planning and theoretical physics.

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For time stepping algorithms with fixed time steps, the theorem proved by Ge and Marsden [18] divides the set of geometric algorithms into those that are energy-momentum preserving and those that are symplectic-momentum preserving. The construction of energy-momentum-symplectic integrators is indeed possible if one allows time step adaptation [21]. One purpose of this paper is to extend the results previously obtained for conservative mechanical systems with constraints to the case of time-dependent higher-order lagrangian systems subjected to time-dependent higher-order constraints following the approach given in [24] and also study time-dependent higher-order Lagrangian mechanics with either fixed or adaptive time-stepping.

Some of the possible applications are the following. The first involves an important class of controlled mechanical systems, underactuated mechanical systems [7], [31] which include spacecraft, underwater vehicles, mobile robots, helicopters, wheeled vehicles, mobile robots, underactuated manipulators, etc. The purpose is find a discrete path which solve the discrete controlled equations obtained by a variational procedure and minimize a discrete cost function subject to initial and final boundary conditions.

Another interesting application of higher-order variational principle will be Riemannian cubic splines (see [6, 15, 16, 29]) which generalizes the typical Euclidean cubic splines. The problem consists of minimizing the mean-square of the covariant acceleration on a Riemannian manifold, with given initial and final conditions, and also some interpolation constraints. Many authors call this type of problems, dynamic interpolation problems, since the trajectories interpolating the points are obtained through solutions of dynamical systems, rather than being given a priori by polynomials. In our paper, we will propose a discrete variational method for interpolating cubic splines on a Riemannian manifold. As an example, we consider the discretization of cubics splines on the sphere adding holonomic constraint. The restriction from $\mathbb{R}^3$ to the sphere will give a second-order lagrangian system subjected to a holonomic constraints, which is one of the cases studied are in our paper.

To be self-contained, we first introduce a short background on variational integration, discrete mechanics and discrete variational systems with constraints.

1.2. Discrete Mechanics and variational integrators. Let $Q$ be a $n$-dimensional differentiable manifold defining the configuration space of a lagrangian system. If we denote by $(q^i)$ with $1 \leq i \leq n$ a local coordinate system on $Q$, then $(q^i, \dot{q}^i)$ is the associated local coordinate system on the tangent bundle $TQ$.

Given a Lagrangian function $L : TQ \rightarrow \mathbb{R}$ that describe the dynamic of the system, their trajectories are the solutions of the Euler-Lagrange equations given by

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} = 0, \quad 1 \leq i \leq n. \quad (1.1)$$

It is well known that the origin of these equations is variational (see [11], [25] and references therein) and they are a system of implicit system of second order differential equations.
In the following, we will assume that the Lagrangian is regular; that is, the matrix \( \frac{\partial^2 L}{\partial q \partial \dot{q}} \) is non-singular. Under this regularity hypothesis, the existence and uniqueness of the solution of the equations is guaranteed.

In order to numerically simulate these equations, one possibility consists of defining (see for example [27]) variational integrators which are derived from a discrete variational principle. These integrators preserve the symplectic structure and have a good behavior of the energy of the system (see [19]). In addition, if a symmetry of a Lie group is considered, they preserve the corresponding momentum.

For discretizing a Lagrangian system, first, it is necessary to replace the velocity by the cartesian product \( \mathbb{R} \times Q \mathbb{R} \), where \( q \) are given by the extremals of the discrete action given fixed points \( q \).

The discrete Hamilton’s principle establishes that the solutions of this system are local extrema of the discrete action \( A_d : \mathbb{R}^{N+1} \to \mathbb{R} \) given by

\[
A_d(q_{0,N}) := A_d(q_0, q_1, ..., q_N) := \sum_{k=1}^{N} L_d(q_{k-1}, q_k)
\]

where \( q_k \in Q \) with \( 0 \leq k \leq N \).

The discrete Hamilton’s principle establishes that the solutions of this system are given by the extremals of the discrete action given fixed points \( q_0 \) and \( q_N \).

Extremizing \( A_d \) over the space of discrete paths, \( q_{0,N} \), with fixed initial and final conditions, we obtain the discrete Euler-Lagrange equations

\[
D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) = 0, \quad 1 \leq k \leq N - 1,
\]

where \( D_1 L_d \) and \( D_2 L_d \) denotes the derivatives of the discrete lagrangian \( L_d \) respect to the first and the second argument, respectively.

It is well known that, under some regularity conditions (the matrix \( D_{12} L_d(q_k, q_{k+1}) \) is non-singular), it is possible to define the discrete flow \( \Upsilon_d : Q \times Q \to Q \times Q \) given by

\[
\Upsilon_d(q_{k-1}, q_k) := (q_k, q_{k+1})
\]

where \( q_{k+1} \) is the unique solution of the discrete Euler-Lagrange equations with initial values \( (q_{k-1}, q_k) \).

We introduce now two discrete Legendre transformations associated to \( L_d \):

\[
\mathcal{F}^- L_d : Q \times Q \to T^* Q \quad \mathcal{F}^+ L_d : Q \times Q \to T^* Q
\]

\[
(q_0, q_1) \mapsto (q_0, -D_1 L_d(q_0, q_1)), \quad (q_0, q_1) \mapsto (q_1, D_2 L_d(q_0, q_1)),
\]

(1.2)

and the discrete Poincaré-Cartan 2-form \( \omega_d := (\mathcal{F}^+ L_d)^* \omega_Q = (\mathcal{F}^- L_d)^* \omega_Q \), where \( \omega_Q \) is the canonical symplectic form on \( T^* Q \). If the discrete Lagrangian \( L_d \) is regular, that is, the matrix \( \frac{\partial^2 L_d}{\partial q \partial \dot{q}} \) is non-degenerate then \( \omega_d \) is a symplectic form. These conditions are also equivalent to that \( \mathcal{F}^- L_d \) or \( \mathcal{F}^+ L_d \) are local diffeomorphisms.

The discrete algorithm determined by \( \Upsilon_d \) preserves the symplectic structure on \( (T^* Q \times Q, \omega_d) \), i.e., \( \Upsilon_d^* \omega_d = \omega_d \). Moreover, if \( G \) acts on \( Q \) and the discrete
Lagrangian is invariant under the diagonal action associated on $Q \times Q$, then the discrete momentum map $J_d: Q \times Q \to \mathfrak{g}^*$ defined by
\[
\langle J_d(q_k, q_{k+1}), \xi \rangle := \langle D_2 L_d(q_k, q_{k+1}), \xi Q(q_{k+1}) \rangle
\]
is preserved by the discrete flow. Here, $\xi Q$ denotes the fundamental vector field determined by $\xi \in \mathfrak{g}$, where $\mathfrak{g}$ is the Lie algebra of $G$,
\[
\xi Q(q) = \frac{d}{dt} \bigg|_{t=0} (\exp(t\xi) \cdot q)
\]
for $q \in Q$ (see [27] for more details). Therefore, these integrators are symplectic-momentum preserving.

Now, consider a lagrangian system with constraints determined by a constraint submanifold $M$ of $TQ$ given by the vanishing of $m$ (independent) differential functions $\phi^\alpha: TQ \to \mathbb{R}$. If we discretize this system, the submanifold $M$ is replaced by a discrete constraint submanifold $M_d \subset Q \times Q$ determined by the vanishing of $m$ independent constraints functions $\phi^\alpha_d: Q \times Q \to \mathbb{R}$.

In order to find the trajectories of this discrete lagrangian system with constraints from a variational point of view, we compute the critical point of a discrete action subjected to the constraint equations; that is,
\[
\begin{aligned}
\min_{\Phi^\alpha_d(q_k, q_{k+1}) = 0} A_d(q(0,N)) & \quad \text{with } q_0 \text{ and } q_N \text{ fixed} \\
\text{subject to } & \quad \lambda^\alpha \in \mathbb{R}^m \quad 1 \leq \alpha \leq m \quad \text{and} \quad 0 \leq k \leq N - 1.
\end{aligned}
\tag{1.3}
\]

We define the augmented Lagrangian $\tilde{L}_d: Q \times Q \times \mathbb{R}^m \to \mathbb{R}$ by
\[
\tilde{L}_d(q_0, q_1, \lambda) := L_d(q_0, q_1) + \lambda^\alpha \Phi^\alpha_d(q_0, q_1).
\]
This Lagrangian gives rise the following unconstrained discrete variational problem,
\[
\begin{aligned}
\min_{q_k \in Q} A_d (q(0,N), \lambda^{(0,N-1)}) & \quad \text{with } q_0 \text{ and } q_N \text{ fixed} \\
q_k \in Q & \quad \lambda_k \in \mathbb{R}^m \quad k = 0, \ldots, N - 1, \quad q_N \in Q
\end{aligned}
\tag{1.4}
\]
where
\[
A_d (q(0,N), \lambda^{(0,N-1)}) := \sum_{k=0}^{N-1} \tilde{L}_d(q_k, q_{k+1}, \lambda^k)
\]
and $\lambda^k$ is a $m$-vector with components $\lambda^k_\alpha$, $1 \leq \alpha \leq m$, which plays the role of the lagrangian multipliers.

From the classical lagrangian multiplier lemma and under some regularity conditions, its well know that the solutions of Problem (1.3) are the same that the ones in Problem (1.4). Therefore, applying standard discrete variational calculus we deduce that the solutions of problem (1.3) verify the following set of difference equations
\[
\begin{aligned}
D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) + \\
\lambda_\alpha^k D_1 \Phi^\alpha_d(q_k, q_{k+1}) + \lambda_{\alpha-1}^k D_2 \Phi^\alpha_d(q_{k-1}, q_k) = 0 & \quad 1 \leq k \leq N - 1, \\
\Phi^\alpha_d(q_k, q_{k+1}) = 0 & \quad 1 \leq \alpha \leq m \quad \text{and} \quad 0 \leq k \leq N - 1.
\end{aligned}
\tag{1.5}
\]
If the matrix
\[
\begin{pmatrix}
D_1 L_d + \lambda_\alpha D_1 \Phi^\alpha_d & D_2 \Phi^\alpha_d \\
(D_1 \Phi^\alpha_d)^T & 0_{m \times m}
\end{pmatrix}
\]
is non-singular, by a direct application of the implicit function theorem, we deduce that there exists an application

$$
\tilde{\Upsilon}_d : \mathcal{M}_d \times \mathbb{R}^m \rightarrow \mathcal{M}_d \times \mathbb{R}^m,
$$
given by

$$
\tilde{\Upsilon}_d(q_{k-1}, q_k, \lambda^{k-1}) := (q_k, q_{k+1}, \lambda^k)
$$
where \((q_{k+1}, \lambda^k)\) is the unique solution of equation (1.5) given \((q_{k-1}, q_k, \lambda^{k-1})\).

In [4], it is shown that the discrete flow \(\tilde{\Upsilon}_d\) preserves a symplectic form naturally defined on \(\mathcal{M}_d \times \mathbb{R}^m\). Moreover, if \(L_d\) and the constraint \(\Phi^\alpha_d\) are invariant under the action of a symmetry Lie group, \(\tilde{\Upsilon}_d\) preserves the associated momentum.

1.3. Organization of the paper. The paper is structured as follows. In Section 2 we present some variational problems with constraints which will be later analyzed using the techniques developed in Section 3. The first one is an optimal control problem for underactuated mechanical systems and the second one is an interpolation problem on a Riemannian manifold.

In Section 3 we develop a discrete variational calculus for higher-order lagrangian mechanical systems with higher-order constraints and next, in Section 4 we apply these techniques to higher-order discrete time-dependent Lagrangian systems. Moreover, we construct the theory of discrete time-dependent second-order constrained systems with fixed time-stepping.

Finally, we solve an optimal control problem for an underactuated time-dependent mechanical systems and an interpolation problem on Riemannian manifolds using the integrator proposed in Section 3. In this application, cubic splines are restricted to the sphere introducing holonomic constraints.

2. Some higher-order variational problems with constraints

In this section we will introduce some notions about higher-order tangent bundle geometry.

Given the manifold \(Q\), it is possible to introduce an equivalence relation in the set \(C^k(\mathbb{R}, Q)\) of \(k\)-differentiable curves from \(\mathbb{R}\) to \(Q\). By definition, two curves \(\gamma_1(t)\) and \(\gamma_2(t)\) in \(Q\) where \(t \in (-a, a)\) with \(a \in \mathbb{R}\), have contact of order \(k\) at \(q_0 = \gamma_1(0) = \gamma_2(0)\) if there is a local chart \((\varphi, U)\) of \(Q\) such that \(q_0 \in U\) and

$$
\left. \frac{d^s}{dt^s} (\varphi \circ \gamma_1(t)) \right|_{t=0} = \left. \frac{d^s}{dt^s} (\varphi \circ \gamma_2(t)) \right|_{t=0},
$$
for all \(s = 0, ..., k\).

The equivalence class of a curve \(\gamma\) will be denoted by \([\gamma]_0^{(k)}\). The set of equivalence classes will be denoted by \(T^{(k)}Q\) and one can see that it has a natural structure of differentiable manifold. Moreover, \(\tau_Q^{(k)} : T^{(k)}Q \rightarrow Q\) given by \(\tau_Q^{(k)}([\gamma]_0^{(k)}) = \gamma(0)\) is a fiber bundle called the tangent bundle of order \(k\) of \(Q\).

Given a differentiable function \(f : Q \rightarrow \mathbb{R}\) and \(l \in \{0, ..., k\}\), its \(l\)-lift \(f^{(l,k)}\) to \(T^{(k)}Q\), \(0 \leq l \leq k\), is the differentiable function defined as

$$
\left. \frac{d^l}{dt^l} (f \circ \gamma(t)) \right|_{t=0} = f^{(l,k)}([\gamma]_0^{(k)}).
$$

Of course, these definitions can be applied to functions defined on open sets of \(Q\).
From a local chart \((q^i)\) on a neighborhood \(U\) of \(Q\), it is possible to induce local coordinates \((q^{(0)i}, q^{(1)i}, \ldots, q^{(k)i})\) on \(T^{(k)}U = (\tau_Q^k)^{-1}(U)\), where \(q^{(s)i} = (q^i)^{(s,k)}\) if \(0 \leq s \leq k\). Sometimes, we will use the standard conventions, \(q^{(0)i} \equiv q^i, q^{(1)i} \equiv \dot{q}^i\) and \(q^{(2)i} \equiv \ddot{q}^i\).

In this section we present two interesting higher-order variational problems that we will be study in this paper: an underactuated optimal control problem and an interpolation problem on Riemannian manifolds.

2.1. Optimal control for underactuated mechanical systems. Consider an underactuated Lagrangian control systems; that is, a Lagrangian control system such that the number of the control inputs is less than the dimension of the configuration space (superarticulated mechanical system following the nomenclature introduced in [2]) \(Q\) which is the cartesian product of two differentiable manifolds \(Q = Q_1 \times Q_2\). Denote by \((q^A) = (q^a, q^\alpha)\) with \(1 \leq A \leq n\) a coordinate local system on \(Q\), where \((q^a)\) \((1 \leq a \leq r)\) and \((q^\alpha)\) \((r + 1 \leq \alpha \leq n)\) are local coordinates on \(Q_1\) and \(Q_2\) respectively. In what follows we assume that all control systems are controllable; that is, for any two points \(x_0\) and \(x_f\) in the configuration space, there exits and admissible control \(u(t)\) defined on some interval \([0,T]\) such that the system with initial condition \(x_0\) reaches the point \(x_f\) at time \(T\) (see for more details [5, 7]).

Adding the control subset \(U \subset \mathbb{R}^r\) where \(u(t) \in U\) is the control parameter. We assume that the controlled external forces \((u^a)\) can be applied only on \(Q_1\).

Thus, given the Lagrangian \(L : TQ = TQ_1 \times TQ_2 \to \mathbb{R}\), the motion equations of the system are written as

\[
\begin{align*}
\frac{d}{dt} \left( \frac{\partial L}{\partial q^a} \right) - \frac{\partial L}{\partial q^a} &= u^a \\
\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^\alpha} \right) - \frac{\partial L}{\partial \dot{q}^\alpha} &= 0
\end{align*}
\]

where \(a = 1, \ldots, r\) and \(\alpha = r + 1, \ldots, n\).

Given a cost function \(C : TQ_1 \times TQ_2 \times U \to \mathbb{R}\), the optimal control problem consists on finding a trajectory \((q^a(t), \dot{q}^a(t), u^a(t))\) of state variables and control inputs satisfying equations (2.1) from given initial and final conditions \((q^a(t_0), \dot{q}^a(t_0), \ddot{q}^a(t_0)), (q^a(t_f), \dot{q}^a(t_f), \ddot{q}^a(t_f))\) respectively, minimizing the cost functional

\[
\mathcal{A}(q(\cdot)) := \int_{t_0}^{t_f} C(q^a, \dot{q}^a, \ddot{q}^a, u^a) \, dt.
\]

It is well know (see [3]) that this optimal control problem is equivalent to the following second-order variational problem with second-order constraints:

Extremize

\[
\overline{\mathcal{A}}(q(\cdot)) := \int_{t_0}^{t_f} \overline{L}(q^a(t), \dot{q}^a(t), \ddot{q}^a(t), \dddot{q}^a(t)) \, dt
\]

subject to the second order constraints given by

\[
\Phi^\alpha(q^a, \dot{q}^a, \ddot{q}^a, \dddot{q}^a) := \frac{d}{dt} \left( \frac{\partial L}{\partial \dddot{q}^\alpha} \right) - \frac{\partial L}{\partial \dddot{q}^\alpha} = 0 \quad \text{with} \quad \alpha = r + 1, \ldots, n
\]
where $L : T^{(2)}Q \to \mathbb{R}$ is defined as

$$L(q^a, q^\alpha, \dot{q}^a, \dot{q}^\alpha, \ddot{q}^a, \ddot{q}^\alpha) := C \left( q^a, q^\alpha, \dot{q}^a, \dot{q}^\alpha, \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^a} \right) - \frac{\partial L}{\partial q^a} \right).$$

Thus, a second order variational problem can be used for reformulate this type of underactuated optimal control problem. For more details about this problem see [12] and [14] for the case when the configuration space is a Lie group.

2.2. Interpolation problem on Riemannian manifolds. The construction of interpolating splines on manifolds is useful in many applications (see [15, 16, 20, 29]). Consider a Riemannian manifold $(Q, G)$ where $G$ is the metric and $\frac{D}{Dt}$ is the covariant derivative associated to the Levi-Civita connection $\nabla$. If $(q_i)$ is a local coordinate system on $Q$, the covariant derivative of the velocity $\dot{q}$ is locally given by

$$\frac{D}{Dt} \dot{q} = \ddot{q}^k + \Gamma_{ij}^k(q) \dot{q}^i \dot{q}^j$$

where $\Gamma_{ij}^k(q)$ are the Christoffel symbols of the metric $G$ at point $q$.

Then, one can consider the Lagrangian $L : T^{(2)}Q \to \mathbb{R}$ defined as

$$L(q, \dot{q}, \ddot{q}) := \frac{1}{2} G_q \left( \frac{D}{Dt} \dot{q}, \frac{D}{Dt} \ddot{q} \right).$$

(2.2)

Given $N + 1$ points $q_i \in Q$ with $i = 0, \ldots, N$ and tangent vectors $v_0 \in T_{q_0}Q$ and $v_N \in T_{q_N}Q$, the interpolation problem consists of finding a curve which minimize the action

$$A(q(\cdot)) = \int_{t_0}^{t_N} L(q, \dot{q}, \ddot{q}) dt = \frac{1}{2} \int_{t_0}^{t_N} G_{q(t)} \left( \frac{D}{Dt}(\dot{q}(t)), \frac{D}{Dt}(\ddot{q}(t)) \right) dt,$$

(2.3)

among all the continuous curves defined on $[t_0, t_N]$, smooth on $[t_i, t_{i+1}]$, for $t_0 \leq t_1 \leq \ldots \leq t_N$, subject to the interpolating constraints

$q(t_i) = q_i$ for all $i \in \{2, \ldots, N - 2\}$

and the boundary conditions

$q(t_0) = q_0, \quad q(t_N) = q_N,$

$$\frac{Dq}{dt}(t_0) = v_0, \quad \frac{Dq}{dt}(t_N) = v_N.$$
\[ \mathcal{A}(q(\cdot)) := \int_{t_0}^{t_N} L_k(q, \dot{q}, \ldots, q^{(k)}) dt = \frac{1}{2} \int_{t_0}^{t_N} \mathcal{G} \left( \frac{D^{k-1} \dot{q}}{Dt^{k-1}}, \frac{D^{k-1} \ddot{q}}{Dt^{k-1}} \right) dt, \]

where the curves \( q(t) \in Q \), are continuous in \([t_0, t_N]\) and \( k - 1 \) piecewise smooths on \([t_i, t_{i+1}]\), for \( t_0 \leq t_1 \leq \ldots \leq t_N \) subjected to the interpolation constraints

\[ q(t_i) = q_i \quad \text{for all } i \in \{2, \ldots, N - 2\} \]

and the \( 2k \) boundary conditions

\[ q(t_0) = q_0, \quad q(t_N) = q_N, \]

\[ \frac{D^{(i)} q}{dt^l}(t_0) = v_0^{(i)}, \quad \frac{D^{(i)} q}{dt^l}(t_N) = v_N^{(i)}. \]

for all \( 1 \leq l \leq k - 1 \).

Thus, the Euler-Lagrange equations for the higher-order Lagrangians \( L_k \) are given by

\[ \frac{D^{2k-1}}{Dt^{2k-1}} \dot{q}(t) + \sum_{j=2}^{k} (-1)^j R \left( \frac{D^{2k-j-1}}{Dt^{2k-j-1}} \dot{q}(t), \frac{D^{j-2}}{Dt^{j-2}} \ddot{q}(t) \right) \ddot{q}(t) = 0, \]

where \( R \) denotes the curvature tensor associated to \( \nabla \) (see [8, 9, 29]).

3. Higher-order algorithm for variational calculus with higher-order constraints

In this section an integrator for higher-order mechanics with higher-order constraints is derived from a discrete variational principle by considering some regularity condition. We show that this algorithm preserves the discrete symplectic structure and the momentum associated to a Lie group of symmetries.

3.1. Higher-order discrete variational calculus. The natural space substituting the higher-order tangent bundle \( T^{(k)}Q \) is \( Q^{k+1} \) (the cartesian product of \( k + 1 \)-copies of \( Q \)) and therefore a higher-order discrete Lagrangian is an application \( L_d : Q^{k+1} \to \mathbb{R} \). For simplicity, we use the notation as in [4]: if \((i, j) \in (\mathbb{N}^*)^2 \) with \( i < j \), \( q_{(i,j)} \) denotes the \((j - i) + 1\)-upla \((q_i, q_{i+1}, \ldots, q_{j-1}, q_j)\).

Fixed initial and final conditions \((q_{(0,k-1)}, q_{(N-k+1,N)}) \in Q^{2k} \) with \( N > 2k \), we define the set of admissible curves with boundary conditions \( q_{(0,k-1)} \) and \( q_{(N-k+1,N)} \)

\[ C^N(q_{(0,k-1)}, q_{(N-k+1,N)}) := \{ \overline{q}_{(0,N)} \mid \overline{q}_{(0,k-1)} = q_{(0,k-1)}, \overline{q}_{(N-k+1,N)} = q_{(N-k+1,N)} \}. \]

Let us define the discrete action over an admissible sequence discrete path as \( \mathcal{A}_d : C^N(q_{(0,k-1)}, q_{(N-k+1,N)}) \to \mathbb{R} \) given by

\[ \mathcal{A}_d(q_{(0,N)}) := \sum_{i=0}^{N-k} L_d(q_{(i,i+k)}). \]

The discrete variational principle states that the solutions of the discrete system determined by \( L_d \) must extremize the action on the curves with given fixed points.
Thus, we obtain the following system of \((N - 2k + 1)n\) difference equations.

\[
D_{k+1}L_d(q_{(0,k)}) + \ldots + D_1L_d(q_{(k,2k)}) = 0,
D_{k+1}L_d(q_{(1,k+1)}) + \ldots + D_1L_d(q_{(k+1,2k+1)}) = 0,
\vdots
D_{k+1}L_d(q_{(N-2k,N-k)}) + \ldots + D_1L_d(q_{(N-k,N)}) = 0.
\] (3.1)

Here, given a smooth function \(F : Q^{k+1} \to \mathbb{R}\), \(D_jF\) denotes the derivative on the \(j\)-factor of \(F\).

These equations are called higher-order discrete Euler-Lagrange equations. Under some regularity hypotheses it is possible to define a discrete flow \(\Upsilon_d : Q^{2k} \to Q^{2k}\) by

\[
\Upsilon_d(q_{(i,2k+i-1)}) := q_{(i+1,2k+i)}
\]

from equations (3.1). In [4] the authors proof that this flow is symplectic-momentum preserving.

### 3.2. Higher-order algorithm for variational calculus with higher-order constraints.

In this subsection we consider a higher-order Lagrangian systems with higher-order constraints given by \(m\) smooth (independent) functions \(\Phi^\alpha_d : Q^{k+1} \to \mathbb{R}\) with \(1 \leq \alpha \leq m\).

We denote by \(\tilde{M}_d\) the constraints submanifold of \(Q^{2k}\) locally determined by the vanishing of these \(m\) functions. Then,

\[
\tilde{M}_d := \{q_{(i,i+k)} \mid \Phi^\alpha_d(q_{(i,i+k)}) = 0 \text{ where } 1 \leq \alpha \leq m \text{ and } 0 \leq i \leq N - k\}.
\]

Therefore, we can consider the following problem called higher-order discrete variational calculus with constraints

\[
\begin{aligned}
\min & \mathcal{A}_d(q_{(0,N)}) \text{ with } (q_{(0,k-1)},q_{(N-k+1,N)}) \text{ fixed} \\
\text{subject to } & \Phi^\alpha_d(q_{(i,i+k)}) = 0 \text{ with } 1 \leq \alpha \leq m \text{ and } 0 \leq i \leq N - k.
\end{aligned}
\]

It is well know that this classical optimization problem with higher-order constraints is equivalent to the following unconstrained higher-order variational problem (which results singular) for \(\tilde{L}_d(q_{(i,i+k)},\lambda^i_\alpha) := L_d(q_{(i,i+k)}) + \lambda^i_\alpha \Phi^\alpha_d(q_{(i,i+k)})\) defined on \(Q^{k+1} \times \mathbb{R}^m\) with \(q_{(i,i+k)} \in Q^{k+1}\), \((\lambda_\alpha) = (\lambda_1,\ldots,\lambda_m) \in \mathbb{R}^m\), \(0 \leq i \leq N - k\) :

\[
\begin{aligned}
\min & \tilde{\mathcal{A}}_d(q_{(0,N)},\lambda^{(0,N-k)}) \text{ with } (q_{(0,k-1)},q_{(N-k+1,N)}) \text{ fixed} \\
& q_{(i,i+k)} \in Q^{k+1} \text{ and } \lambda^i \in \mathbb{R}^m \text{ with } 0 \leq i \leq N - k
\end{aligned}
\]

where

\[
\tilde{\mathcal{A}}_d(q_{(0,N)},\lambda^{(0,N-k)}) := \sum_{i=0}^{N-k} \tilde{L}_d(q_{(i,i+k)},\lambda^i_\alpha),
\] (3.2)

\(\lambda^{(0,N-k)} := (\lambda^0,\ldots,\lambda^{N-k})\) and \(\lambda^i\) is a vector with components \(\lambda^i_\alpha, 1 \leq \alpha \leq m\).

In the next, we do not impose the boundary conditions \((q_{(0,k-1)},q_{(N-k+1,N)})\).

Thus, we consider as space of admissible paths

\[
C^{(N,N-k)} := \{(q_0,q_1,\ldots,q_N,\lambda^0,\lambda^1,\ldots,\lambda^{N-k}) \in Q^{N+1} \times \mathbb{R}^{(N-k)m}\},
\]
and computing the differential of the action
\[
d\tilde{A}_d(q_{(0,N)}, \lambda^{(0,N-k)}) : (\delta q_{(0,N)}, \delta \lambda^{(0,N-k)}) = \\
\sum_{i=0}^{k-1} \left( \sum_{j=1}^{i+1} D_j L_d(q_{(i-j+1,i-j)+1+k}) + \lambda^{i-j+1}_\alpha D_j \Phi^\alpha_d(q_{(i-j+1,i-j)+1+k}) \right) \delta q_i + \\
\sum_{i=k}^{N-k} \left( \sum_{j=1}^{i+1} D_j L_d(q_{(i-j+1,i-j)+1+k}) + \lambda^{i-j+1}_\alpha D_j \Phi^\alpha_d(q_{(i-j+1,i-j)+1+k}) \right) \delta q_i + \\
\sum_{i=N-k+1}^{N} \left( \sum_{j=i-N+k+1}^{k+1} D_j L_d(q_{(i-j+1,i-j)+1+k}) \right) \delta q_i \\
+ \lambda^{i-j+1}_\alpha D_j \Phi^\alpha_d(q_{(i-j+1,i-j)+1+k}) \right) \delta q_i + \sum_{i=0}^{N-k} \Phi^\alpha_d(q_{(i,i+k)}) \delta \lambda^\alpha_i.
\]

The two expressions corresponding to the boundary terms are called the Discrete Poincaré-Cartan 1-forms on $Q^{2k} \times \mathbb{R}^{km}$ and they are given by
\[
\Theta^-_{L_d}(q_{(0,2k-1)}, \lambda^{(0,k-1)}) := \\
- \sum_{i=0}^{k-1} \left( \sum_{j=1}^{i+1} D_j L_d(q_{(i-j+1,i-j)+1+k}) + \lambda^{i-j+1}_\alpha D_j \Phi^\alpha_d(q_{(i-j+1,i-j)+1+k}) \right) dq_i
\]
and
\[
\Theta^+_{L_d}(q_{(0,2k-1)}, \lambda^{(0,k-1)}) := \\
\sum_{i=N-k+1}^{N} \left( \sum_{j=i-N+k+1}^{k+1} D_j L_d(q_{(i-j+1,i-j)+1+k}) \right) dq_i.
\]

In order to write the higher-order discrete Euler-Lagrange equations in an analogous way to discrete Euler-Lagrange equations according to [27] we may define the discrete higher-order Euler-Lagrange operator $\mathcal{E}\tilde{L}_d : Q^{2k+1} \times \mathbb{R}^{(N-k)m} \to T^*Q^k$ given by
\[
\mathcal{E}\tilde{L}_d(q_{(i,2k+i)}, \lambda^{(i,N-k+i-1)}) := \\
\sum_{j=1}^{k+1} \left[ D_j L_d(q_{(i-j+1+k,i-j+1+2k)}) + \lambda^{i-j+k+1}_\alpha D_j \Phi^\alpha_d(q_{(i-j+k+1,i-j+2k+1)}) \right] dq_{i+k}.
\]

Summarizing, we have the following result

**Theorem 3.1.** If $L_d : Q^{k+1} \to \mathbb{R}$ is a discrete Lagrangian and $\Phi^\alpha_d : Q^{k+1} \to \mathbb{R}$ with $1 \leq \alpha \leq m$ (independent) smooth functions, there exists a unique differential mapping $\mathcal{E}\tilde{L}_d : Q^{2k+1} \times \mathbb{R}^{(N-k)m} \to T^*Q^k$ and there exist two 1-forms $\Theta^+_{L_d}$ and $\Theta^-_{L_d}$ on $Q^{2k} \times \mathbb{R}^{km}$, such that for all variations $(\delta q_0, ..., \delta q_N)$ and $(\delta \lambda^\alpha_0, ..., \delta \lambda^\alpha_{N-k})$ the
differential of the discrete action $\tilde{A}_d$ defined in (3.2) verifies the following equality

$$
d\tilde{A}_d(q_{0,N}), \lambda^{(0,N-k)}((\delta q_{0,N}), \delta \lambda^{(0,N-k)}) = \sum_{i=0}^{N-2k} \epsilon \tilde{L}_d(q_{1,2k+i}), \lambda^{(i,k+i)} \delta q_{k+i} + \Theta_\tilde{L}_d^+(q_{N-2k+1,N}) \delta q_{N-2k+1,N} - \Theta_\tilde{L}_d^-(q_{0,2k-1}) \delta q_{0,2k-1} + \sum_{i=0}^{N-k} \Phi_\tilde{L}_d^\alpha(q_{i,i+k}) \delta \lambda^\alpha_i.
$$

If we consider variations at the fixed initial and final conditions $(q_{0,k-1}, q_{N-k+1,N})$, the critical trajectories of the unconstrained problem are given by the curves that annihilate $\partial \tilde{A}_d/\partial q_i$ and the constraints equations $\partial \tilde{A}_d/\partial \lambda^\alpha_i$.

Thus, the higher-order discrete Euler-Lagrange equations with constraints are

$$
\begin{align*}
0 &= \epsilon \tilde{L}_d(q_{i,2k+i}), \lambda^{(i,N-k+i-1)}) \quad 0 \leq i \leq N - 2k \\
0 &= \Phi_\tilde{L}_d^\alpha(q_{i,i+k}) \quad 0 \leq i \leq N - k. 
\end{align*}
$$

Therefore, using the implicit function theorem, we can establish the following regularity condition (see [3] for a similar proof)

**Proposition 3.2.** If the matrix

$$
\begin{pmatrix}
D_{(1,k+1)} L_d(q_{1,k+1}) + \lambda_\alpha D_{(1,k+1)} \Phi_\tilde{L}_d^\alpha(q_{1,k+1}) & D_{k+1} \Phi_\tilde{L}_d^\alpha(q_{1,k+1}) \\
(D_{(1,k+1)} \Phi_\tilde{L}_d^\alpha(q_{1,k+1}))^T & 0
\end{pmatrix}
$$

is non-singular, there exists an application $\tilde{\gamma}_d : \tilde{M}_d \times \mathbb{R}^{km} \to \tilde{M}_d \times \mathbb{R}^{km}$ given by

$$
\tilde{\gamma}_d(q_{i,i+2k-1}), \lambda^{(i,i+k-1)} := (q_{i+1,i+2k}), \lambda^{(i+1,i+k)}
$$

where $q_{2k+i}$ and $\lambda^{i+k}$ with $1 \leq \alpha \leq m$ is the unique solution of the equation (3.4) with initial conditions $(q_{0,i+2k-1}, \lambda^{(i,i+k-1)})$ with $0 \leq i \leq N - k$.

Here, if $F$ is a smooth function on $Q^{k+1}$, $D_{(1,k+1)}F$ denotes the partial derivative of $F$ with respect to first and the last variables.

**Remark 3.3.** Discrete Poincaré-Cartan 2-form: It is easy to shown that

$$
\sum_{i=0}^{k-1} d\tilde{L}_d(q_{i,i+k}), \lambda^i = \Theta_\tilde{L}_d^+(q_{0,2k-1}), \lambda^{(0,k-1)}) + \Theta_\tilde{L}_d^-(q_{0,2k-1}), \lambda^{(0,k-1)}).
$$

Therefore, using $d^2 = 0$, it follows that $d\Theta_\tilde{L}_d^- = d\Theta_\tilde{L}_d^+$. Thus, there exists a unique 2-form $\Omega_\tilde{L}_d := -d\Theta_\tilde{L}_d^- = -d\Theta_\tilde{L}_d^+$, which will be called the Discrete Poincaré-Cartan 2-form.

**Remark 3.4.** Symplectic behavior: By considering the canonical inclusion $j : \tilde{M}_d \times \mathbb{R}^{km} \to Q^{k+1} \times \mathbb{R}^{km}$ we derive a 2-form $\Omega_M := j^* \Omega_\tilde{L}_d$ on $\tilde{M}_d \times \mathbb{R}^{km}$ where $\Omega_\tilde{L}_d$ is 2-form defined on Remark 3.3. Therefore it is a natural question to ask about conditions that ensure the symplectic character of the 2-form $\Omega_M$. By
using similar techniques that in [3] one could establish conditions that guarantee
that the 2-form \( \Omega_{\tilde{M}_d} \) is symplectic and moreover

\[
(\Upsilon_{|\tilde{M}_d \times \mathbb{R}^{km}})^* \Omega_{\tilde{M}_d} = \Omega_{\tilde{M}_d}.
\]

More specifically, if the matrix \( (D_{(1,k+1)}L_d + \lambda_\alpha D_{(1,k+1)}\Phi^\alpha_d) \) is non-singular, the
discrete 2-form \( \Omega_{\tilde{M}_d} \) is symplectic if and only if the matrix

\[
\begin{pmatrix}
(D_{(1,k+1)}L_d + \lambda_\alpha D_{(1,k+1)}\Phi^\alpha_d) & D_{k+1}\Phi^\alpha_d \\
(D_1\Phi^\alpha_d)^T & 0
\end{pmatrix}
\]

is nondegenerate.

\[\Box\]

**Remark 3.5. Momentum preservation:** Given an action of a Lie group \( G \) on \( Q \), we can consider the associated \( G \)-action on \( Q^{k+1} \) defined as

\[
g \cdot q(i,k+i) = (g \cdot q_i, g \cdot q_{i+1}, \ldots, g \cdot q_{i+k})
\]

and its trivial extension on \( Q^{2k} \times \mathbb{R}^{km} \) for \( g \in G \).

As this last action results symplectic, denoting by \( g \) the Lie algebra associated
with the Lie group \( G \), we can define two higher-order discrete momentum maps

\[
J_d^\pm : Q^{2k} \times \mathbb{R}^{km} \to g^*
\]
given by

\[
J_d^\pm(q(i,2k+i-1), \lambda^{(i,i+k-1)}) : g \to \mathbb{R}
\]

\[
\xi \mapsto \langle \Theta_d^\pm L_d(q(i,i+2k-1), \lambda^{(i,i+k-1)}), \xi_{Q^{2k}}(q(i,i+2k-1)) \rangle,
\]

for \( \xi \in g \).

Is easy see that if the discrete Lagrangian \( L_d \) and the discrete constraints \( \Phi^\alpha_d \)
are \( G \)-invariant, the higher-order discrete momentum maps coincides and then, we
can define the higher-order discrete momentum map that results conserved by
the discrete flow \( \Upsilon_d \). That is,

\[
J_d := J_d^+ = J_d^-, \quad \text{and} \quad J_d \circ \Upsilon_d = J_d.
\]

\[\Box\]

4. **Theoretical Examples and Applications**

4.1. **Higher-order discrete time-dependent Lagrangian systems.** In this
subsection we consider higher-order discrete time-dependent lagrangian system
with higher-order constraints. The configuration space for this type of systems
is \( \tilde{Q} = \mathbb{R} \times Q \) where \( Q \) is a \( n \)-dimensional manifold. The algorithm ([3,5]) can be
adapted for obtain a variational integrator for this kind of systems. In this case,
the discrete action \( A_d : \tilde{Q}^{N+1} \to \mathbb{R} \) is defined as

\[
A_d(t(0,N), q(0,N)) := \sum_{i=0}^{N-k} (t_{i+k} - t_i)L_d(t(i,i+k), q(i,i+k)).
\] 4.1
As it is well known (see [21], [24] and references therein) the evolution of the energy is given by the discrete Euler-Lagrange equations corresponding to the temporal variable. The equations involving derivatives on \( t_i \) are

\[
0 = \sum_{j=1}^{k+1} D_j L_d(t_{i-j+1}, t_i, h_i, q_{(i,j-k+1)})(t_{i-j+k+1} - t_{i-j+1}) \tag{4.2}
\]

By considering \( h_k = t_{k+1} - t_k \), we can define the new Lagrangian \( \overline{L}_d \) given by

\[
\overline{L}_d(t_i, h(i,i+k-1), q(i,i+k)) = L_d(t_{i+k}, h(i,i+k)) = L_d(t_i, t_i + h_i, t_i + h_i + h_{i+1}, \ldots, t_i + h_i + h_{i+1} + \ldots + h_{i+k-1}, q(i,i+k))
\]

Then we have the following relation between the derivatives of \( L_d \) and \( \overline{L}_d \)

\[
\frac{\partial L_d}{\partial t_j} = \frac{\partial \overline{L}_d}{\partial t_j} \quad \text{for} \quad 1 \leq j \leq k
\]

\[
D_j L_d = D_j \overline{L}_d - D_{j+1} \overline{L}_d \quad \text{for} \quad 1 \leq j \leq k
\]

\[
D_j L_d = D_j \overline{L}_d \quad \text{for} \quad j = k + 1,
\]

Substituting these expressions in (4.2) we obtain the following equation

\[
\sum_{i=1}^{k} D_j \overline{L}_d(t_{i-j+1}, h(i,j-1,i-j+k), q(i,j+1,i-j+k+1))(h_{i-j+1} + \ldots + h_{i-j+k})
\]

\[-D_{j+1} \overline{L}_d(t_{i-j+1}, h(i,j-1,i-j+k), q(i,j+1,i-j+k+1))(h_{i-j+1} + \ldots + h_{i-j+k})
\]

\[+D_{k+1} \overline{L}_d(t_{i-k}, h(i-k,i-1), q(i-k,i))(h_{i-j+1} + \ldots + h_{i-1}) - \overline{L}_d(t_i, h(i,k-1), q(i,k))
\]

\[+ \overline{L}_d(t_{i-k}, h(i,k-1), q(i,k)) = 0.
\]

The higher-order discrete energy is defined as

\[
E_d = -\frac{\partial}{\partial t_i} \left( \sum_{j=1}^{k} \overline{L}_d(t_{i-j+1}, h(i,j-1,i-j+k), q(i,j+1,i-j+k+1))(h_{i-j+1} + \ldots + h_{i-j+k}) \right)
\]

\[= - \sum_{j=1}^{k} D_j \overline{L}_d(t_{i-j+1}, h(i,j-1,i-j+k), q(i,j+1,i-j+k+1))(h_{i-j+1} + \ldots + h_{i-j+k})
\]

\[- \sum_{j=1}^{k} \overline{L}_d(t_{i-j+1}, h(i,j-1,i-j+k), q(i,j+1,i-j+k+1)).
\]

A direct computation shows that

\[
E_d(t_{i-k+1}, h_{i-k+1}, \ldots, h_{i-1}, q(i-k+1,i-1)) - E_d(t_{i-k}, h_{i-k}, \ldots, h_{i+k-2}, q(i-k,i+k-2)) =
\]

\[-D_1 \overline{L}_d(t_i, h(i,i+k), q(i,i+k))(h_i + \ldots + h_{i+k}).
\]

That is,

\[
D_1 \overline{L}_d(t_i, h(i,i+k), q(i,i+k)) = \frac{1}{h_i + \ldots + h_{i+k}} (E_d(t_{i-k+1}, h_{i-k+1}, \ldots, h_{i-1}, q(i-k+1,i-1))
\]

\[-E_d(t_{i-k}, h_{i-k}, \ldots, h_{i+k-2}, q(i-k,i+k-2))).
\]
If the discrete Lagrangian is autonomous then we obtain the preservation of the discrete energy $E_d$ and the derived variational method will be a symplectic energy-momentum preserving method (see [21] [24] for first order systems).

4.2. Time-dependent higher-order Lagrangians with fixed time-step size.
In the following, we consider a time-dependent Lagrangian systems given by a lagrangian $L : \mathbb{R} \times T^{(2)}Q \to \mathbb{R}$ with local coordinates $(t, q^A, \dot{q}^A, \ddot{q}^A); 1 \leq A \leq n = \dim Q$. Assume for simplicity that $Q$ is a vector space This kind of systems are unconstrained, but with fixed time step size $t_{k+1} - t_k = h$ for $k = 0, \ldots, N - 1$, and $h > 0$.

We may construct a discrete Lagrangian $L_d : 3\mathbb{R} \times 3Q \to \mathbb{R}$ as

$$L_d(t_k, t_{k+1}, t_{k+2}, q_k, q_{k+1}, q_{k+2}) = L \left( \frac{t_{k+2} + t_{k+1} + t_k}{3}, \frac{q_k + q_{k+1} + q_{k+2}}{3}, \frac{q_{k+2} - q_k}{t_{k+2} - t_k}, \frac{q_{k+1} - q_k}{(t_{k+2} - t_{k+1})} \right),$$

where $3\mathbb{R} \times 3Q = \mathbb{R} \times \mathbb{R} \times \mathbb{R} \times Q \times Q \times Q$.

Define the constraint submanifold

$$\mathcal{N}_d = \{(t_0, t_1, t_2, q_0, q_1, q_2) \in 3\mathbb{R} \times 3Q \mid t_1 = t_0 + h \text{ and } t_2 = t_1 + h\}$$

for some constant $h > 0$. This submanifold corresponds to the vanishing of the constraints

$$\Phi_d^{(1)}(t_0, t_1, t_2, q_0, q_1, q_2) = t_1 - t_0 - h;$$
$$\Phi_d^{(2)}(t_0, t_1, t_2, q_0, q_1, q_2) = t_2 - t_1 - h;$$

and now take the augmented Lagrangian

$$\tilde{L}_d(t_k, t_{k+1}, t_{k+2}, q_k, q_{k+1}, q_{k+2}, \lambda) = L_d(t_k, t_{k+1}, t_{k+2}, q_k, q_{k+1}, q_{k+2}) + \lambda \Phi_d^\alpha(t_k, t_{k+1}, t_{k+2}, q_k, q_{k+1}, q_{k+2}),$$

with $\alpha = 1, 2$.

This lagrangian gives rise to the following equations of motion

$$0 = (t_{k+2} - t_k)D_1 L_d(t_k, t_{k+1}, t_{k+2}, q_k, q_{k+1}, q_{k+2}) + (t_{k+1} - t_{k-1})D_5 L_d(t_{k-1}, t_k, t_{k+1}, q_{k-1}, q_k, q_{k+1}) + (t_k - t_{k-2})D_6 L_d(t_{k-2}, t_{k-1}, t_k, q_{k-2}, q_{k-1}, q_k)$$
$$0 = (t_{k+2} - t_k)D_1 L_d(t_k, t_{k+1}, t_{k+2}, q_k, q_{k+1}, q_{k+2}) + L_d(t_{k-2}, t_{k-1}, t_k, q_{k-2}, q_{k-1}, q_k) + \lambda_1^{k-1} - \lambda_2^{k-1} + \lambda_2^{k-2} - \lambda_1^k$$
$$0 = (t_k - t_{k-2})D_3 L_d(t_{k-2}, t_{k-1}, t_k, q_{k-2}, q_{k-1}, q_k) - L_d(t_k, t_{k+1}, t_{k+2}, q_k, q_{k+1}, q_{k+2})$$
$$0 = t_{k+1} - t_k - h;$$
$$0 = t_k - t_{k-1} - h, \text{ where } 2 \leq k \leq N - 2.$$


Finally, observe that these equations are completely decoupled, so we can choose the first equation. Therefore, we obtain

$$0 = D_4 L_d(t_k, t_k + h, t_k + 2h, q_k, q_{k+1}, q_{k+2})$$
$$+ D_5 L_d(t_k - h, t_k, t_k + h, q_{k-1}, q_k, q_{k+1})$$
$$+ D_6 L_d(t_k - 2h, t_k - h, t_k, q_{k-2}, q_{k-1}, q_k),$$

with $k = 2, \ldots, N - 2$ and $t_0, q_0, q_1, q_{N-q}, q_N$ fixed points and time.

Observe that this equation has precisely the same form as the discrete Euler-Lagrange equations in the time-independent case.

Finally, we remark that an extension of this setup can be used for more sophisticated step size control, by taking the constraint function to be (for example),

$$\Phi_1(t_k, t_{k+1}, t_{k+2}, q_k, q_{k+1}, q_{k+2}) = t_{k+1} - t_k - h(q_k, q_{k+1}, q_{k+2})$$
and

$$\Phi_2(t_k, t_{k+1}, t_{k+2}, q_k, q_{k+1}, q_{k+2}) = t_{k+2} - t_{k+1} - h(q_k, q_{k+1}, q_{k+2}),$$

where $h : Q^3 \to \mathbb{R}, h > 0$ is some step size function. In this case,

$$D_j \Phi_d(t_k, t_{k+1}, t_{k+2}, q_k, q_{k+1}, q_{k+2}) = -D_{j-3}h(q_k, q_{k+1}, q_{k+2}), \quad j = 4, 5, 6.$$ This differs considerably from the constant $h$.

**Example 4.1.** As an illustrative example of discrete time-dependent higher-order mechanical system we consider a deformed elastic cylindrical beam with both ends fixed. This example is not time-dependent system, but it can be modeled using a configuration bundle over a compact subset of $\mathbb{R}$, where the coordinates in the base configuration represents every transversal section of the beam. We take, instead of a compact subset, the whole real line as the base manifold. This example has been also study in [30] in the continuous setting. The second-order Lagrangian is given by

$$L(t, q, \dot{q}, \ddot{q}) = \frac{1}{2} \mu(t) \ddot{q}^2 + \rho(t)q$$ (4.3)

where $\mu, \rho$ are differentiable functions that only depend on the coordinate $t$ and represent physical parameters of the beam. If the beam is homogeneous, $\rho$ and $\mu$ are constants (with $\mu \neq 0$), and thus the Lagrangian density is autonomous, that is, it does not depend explicitly on the coordinate of the base manifold (see [30] and references therein).

The discrete lagrangian associated to (4.3) defined on $3(\mathbb{R} \times Q)$ is given by

$$L_d = \frac{1}{2} \mu \left( \frac{t_{k+2} + t_{k+1} + t_k}{3} \right) \left( \frac{q_{k+2} - q_{k+1}}{(t_{k+2} - t_{k+1})^2} - \frac{q_{k+1} - q_k}{(t_{k+1} - t_k)(t_{k+2} - t_{k+1})} \right)^2$$
$$+ \rho \left( \frac{t_{k+2} + t_{k+1} + t_k}{3} \right) \frac{q_{k+2} + q_{k+1} + q_k}{3},$$
and the associated implicit discrete algorithm is given by

\[
0 = \frac{1}{3} \left[ \rho \left( \Delta [t_{k+1}] \right) (h_{k+1} + h_k) + \rho \left( \Delta [t_k] \right) (h_k + h_{k-1}) + \rho \left( \Delta [t_{k-1}] (h_{k-1} + h_{k-2}) \right) \right]
\]

\[
+ \mu \left( \Delta [t_{k+1}] \right) \left( \frac{q_{k+2} - q_{k+1}}{h_{k+1}^2} - \frac{q_{k+1} - q_k}{h_k h_{k+1}} \right) \frac{h_{k+1} + h_k}{h_{k+1} h_k}
\]

\[
- \mu \left( \Delta [t_k] \right) \left( \frac{q_{k+1} - q_k}{h_k^2} - \frac{q_k - q_{k-1}}{h_{k-1} h_k} \right) \left( \frac{h_k + h_{k-1}}{h_k^2} + \frac{h_k + h_{k-1}}{h_{k-1} h_k} \right)
\]

\[
+ \mu \left( \Delta [t_{k-1}] \right) \left( \frac{q_k - q_{k-1}}{h_{k-1}^2} - \frac{q_{k-1} - q_{k-2}}{h_{k-2} h_{k-1}} \right) \frac{h_{k-1} + h_{k-2}}{h_{k-1}^2 - h_{k-2} h_{k-1}}
\]

\[
0 = \frac{h_{k+1} + h_k}{3} \partial_t \rho(\partial \Delta [t_{k-1}]) \Delta [q_{k-1}] - \rho(\Delta [t_{k+1}]) \Delta [q_{k+1}]
\]

\[
+ \mu(\Delta [t_{k-1}]) \left( \frac{q_{k-1} - q_{k-2}}{h_{k-1}^2} - \frac{q_k - q_{k-1}}{h_{k-2} h_{k-1}} \right) \frac{h_{k-1} + h_k}{h_{k-1} h_k}
\]

\[
+ \frac{h_k + h_{k-1}}{6} \partial_t \mu(\Delta [t_{k-1}]) \left( \frac{q_{k+2} - q_{k+1}}{h_{k+1}^2} - \frac{q_{k+1} - q_k}{h_k h_{k+1}} \right)^2
\]

\[
- \frac{1}{2} \mu(\Delta [t_{k-1}]) \left( \frac{q_{k-1} - q_k}{h_{k-1}^2} - \frac{q_k - q_{k-1}}{h_{k-2} h_{k-1}} \right)^2 + \frac{h_k + h_{k-1}}{3} \partial_{t_k} \mu(\Delta [t_{k+1}]) \Delta [q_k]
\]

\[
- \frac{(q_{k+1} - q_k)(h_{k+1} + h_k)}{h_{k+1}^2} \partial_t \mu(\Delta [t_{k-1}]) \left( \frac{q_{k+2} - q_{k+1}}{h_{k+1}^2} - \frac{q_{k+1} - q_k}{h_k h_{k+1}} \right)^2
\]

\[
+ \frac{h_k + h_{k-1}}{6} \partial_{t_k} \mu(\Delta [t_{k-1}]) \left( \frac{q_{k+1} - q_k}{h_{k}^2} - \frac{q_k - q_{k-1}}{h_{k-1} h_k} \right)^2
\]

\[
+ \frac{h_{k-1} + h_{k-2}}{3} \partial_{t_k} \rho(\Delta [t_{k-1}]) \Delta [q_{k-1}]
\]

\[
+ h_k \mu(\Delta [t_{k+1}]) \left( \frac{q_{k+1} - q_k}{h_{k}^2} - \frac{q_k - q_{k-1}}{h_{k-1} h_k} \right) \left( \frac{2(q_{k+1} - q_k)}{h_{k}^3} - \frac{(q_{k+1} - q_k)(h_{k} - h_{k+1})}{h_{k}^2 - h_{k+1}^2} \right)
\]

\[
+ \frac{h_{k-1} + h_{k-2}}{6} \partial_{t_k} \mu(\Delta [t_{k-1}]) \left( \frac{q_k - q_{k-1}}{h_{k-1}^2} - \frac{q_{k-1} - q_{k-2}}{h_{k-2} h_{k-1}} \right)^2
\]

\[
- \mu(\Delta [t_{k-1}]) \left( \frac{q_k - q_{k-1}}{h_{k-1}^2} - \frac{q_{k-1} - q_{k-2}}{h_{k-2} h_{k-1}} \right) \left( \frac{2(q_k - q_{k-1})}{h_{k-1}^3} - \frac{(q_k - q_{k-1})(h_{k-1} - h_{k})}{h_{k-1}^2 - h_{k}^2} \right),
\]

for \(2 \leq k \leq N - 2\) where \(h_k = t_{k+1} - t_k\), \(\Delta [t_k] = \frac{t_{k+1} + t_k + t_{k-1}}{3}\), \(\Delta [q_k] = \frac{q_{k+1} + q_k + q_{k-1}}{3}\) and \(\partial_{t_k}\) denotes the partial derivative of a function with respect to the variable \(t_k\).

### 4.3. Optimal control of underactuated time-dependent mechanical systems.

In this subsection, we will construct a variational integrator for the time-dependent underactuated optimal control problem that we have introduced in Subsection 2.1.

Consider a discrete second-order time-dependent Lagrangian system given by the function \(L_d : (\mathbb{R} \times Q)^2 \rightarrow \mathbb{R}\) where \(Q = Q_1 \times Q_2\). An element \((t_0, q_0^0, t_1, q_1^0) \in (\mathbb{R} \times Q)^2\) admits a global decomposition of the form \((t_0, q_0^{a_0}, q_0^a, t_1, q_1^a, q_1^0)\) with \(1 \leq a \leq m\), \(m + 1 \leq \alpha \leq n\) and the discrete second-order constraints are given by \(\Phi^0_d : (\mathbb{R} \times Q)^2 \rightarrow \mathbb{R}\), determining the submanifold \(M_d\).
Consider the following discrete time-dependent underactuated mechanical system,

\[
(t_i - t_{i-1})D^a_d L_d(t_{i-1}, q^A_{i-1}, t_i, q^A_i) + (t_{i+1} - t_i)D^a_d L_d(t_i, q^A_i, t_i, q^A_{i+1}) = u^a_i \\
(t_i - t_{i-1})D^a_d L_d(t_{i-1}, q^A_{i-1}, t_i, q^A_i) + (t_{i+1} - t_i)D^a_d L_d(t_i, q^A_i, t_i, q^A_{i+1}) = 0
\]

with \(1 \leq i \leq n\), \(1 \leq a \leq m\) and \(m + 1 \leq \alpha \leq n\). Denote by \(D^a_d\) and \(D^a_i\) the partial derivatives with respect to coordinates \(a\) and \(\alpha\), respectively.

The optimal control problem is determined prescribing the discrete cost functional

\[
\mathcal{A}_d(t(0,N), q^A_{(0,N)}, u^a_{(0,N-1)}) = \sum_{i=0}^{N-1} C(t_i, q^A_i, t_{i+1}, q^A_{i+1}, u^a_i)
\]

with initial and final conditions \(t_0, q_0, t_1, q_1\) and \(t_{N-1}, q_{N-1}, t_N, q_N\) respectively.

Since the control variables appear explicitly the previous optimal control problem is equivalent to the second-order variational problem with constraints determined by

\[
\min \widetilde{\mathcal{A}}_d(t(0,N), q^A_{(0,N)}, u^a_{(0,N-1)}) = \sum_{i=0}^{N-2} \widetilde{L}_d(t_i, q^A_i, t_{i+1}, q^A_{i+1}, t_{i+2}, q^A_{i+2})
\]

and the constraints

\[
\Phi^a_d(t_i, q^A_i, t_{i+1}, q^A_{i+1}, t_{i+2}, q^A_{i+2}) = (t_{i+1} - t_i)D^a_d L_d(t_i, q^A_i, t_{i+1}, q^A_{i+1}) + (t_{i+2} - t_{i+1})D^a_d L_d(t_{i+1}, q^A_{i+1}, t_{i+2}, q^A_{i+2}) = 0
\]

where,

\[
\widetilde{L}_d(t_i, q^A_i, t_{i+1}, q^A_{i+1}, t_{i+2}, q^A_{i+2}) = C(t_i, q^A_i, t_{i+1}, q^A_{i+1}, (t_{i+1} - t_i)D^a_d L_d(t_i, q^A_i, t_{i+1}, q^A_{i+1}),
\]

\[
\quad + (t_{i+2} - t_{i+1})D^a_d L_d(t_{i+1}, q^A_{i+1}, t_{i+2}, q^A_{i+2})\).
\]

Now, define \(\mathcal{T}_d : (\mathbb{R} \times Q)^3 \times \mathbb{R}^m \rightarrow \mathbb{R}\) by \(\mathcal{T}_d = \widetilde{L} + \lambda_\alpha \Phi^a_d\) and our problem is related to the discrete variational problem

\[
\min \overline{\mathcal{A}}_d(t(0,N), q^a_{(0,N)}, q^\alpha_{(0,N)}, \lambda^{(0,N-2)}_\alpha)
\]

where

\[
\overline{\mathcal{A}}_d(t(0,N), q^a_{(0,N)}, q^\alpha_{(0,N)}, \lambda^{(0,N-2)}_\alpha) = \sum_{i=0}^{N-2} \overline{L}_d(t_i, q^a_i, q^\alpha_i, t_{i+1}, q^a_{i+1}, q^\alpha_{i+1}, t_{i+2}, q^a_{i+2}, q^\alpha_{i+2}, \lambda^i_\alpha).
\]

In order to apply the techniques developed in the previous section (where the configuration space is \(\mathbb{R} \times Q\)) we assume the regularity condition given in Theorem 3.2.

Thus, for all point in \(\mathcal{M}_d = \{(r, x, y, t, z) \in (\mathbb{R} \times Q)^3 \mid \Phi^a_d(r, x, y, t, z) = 0\}\) and \(\lambda^\alpha \in \mathbb{R}^m\) with \(1 \leq \alpha \leq m\), the discrete flow

\[
\mathcal{Y}_d : \mathcal{M}_d \times \mathbb{R}^{2m} \rightarrow \mathcal{M}_d \times \mathbb{R}^{2m}
\]

where

\[
(t_0, q_0, t_1, q_1, t_2, q_2, t_3, q_3, \lambda^0_\alpha, \lambda^1_\alpha) \mapsto (t_1, q_1, t_2, q_2, t_3, q_3, t_4, q_4, \lambda^1_\alpha, \lambda^2_\alpha)
\]

is given by \(t_4, q_4\) and \(\lambda_2, \lambda_2\), determined from the initial conditions \(t_0, q_0, t_1, q_1, t_2, q_2, t_3, q_3, \lambda^1_\alpha, \lambda^2_\alpha\).
Here, $\mathcal{M}_d$ denotes the submanifold of $(\mathbb{R} \times Q)^4$ given by
$$
\mathcal{M}_d = \{(t_0, q_0, t_1, q_1, t_2, q_2, t_3, q_3) \mid \Phi^\alpha_d(t_0, q_0, t_1, q_1, t_2, q_2) = 0, \Phi^\alpha_d(t_1, q_1, t_2, q_2, t_3, q_3) = 0\}
$$
with $1 \leq \alpha \leq m$.

Using similar techniques than in Section 3 it is possible to show that, under the regularity assumptions, this discrete flow is symplectic.

### 4.4. Interpolation problem on Riemannian manifolds.

In what follows, we will obtain a geometric integrator for the interpolation problem considered in Section 2.2, but, in this case, we will add a holonomic constraint given by the restriction to the sphere $S^2$ on $\mathbb{R}^3$. More concretely, the configuration manifold is $Q = \mathbb{R}^3$ with the Euclidean metric and subject to the holonomic constraint
$$
\Phi(q) = q \cdot q - r^2 = 0, \quad q \in \mathbb{R}^3
$$
where $r > 0$ is the radius of the sphere on $\mathbb{R}^3$ centering in the origin and $\cdot$ denotes the Euclidean inner product on $Q$. This constraint determines the submanifold of $Q$ given by
$$
\mathcal{M} = \{q \in \mathbb{R}^3 \mid q \cdot q = r^2\}.
$$

The discrete Lagrangian $L_d : 3\mathbb{R}^3 \to \mathbb{R}$ is given by
$$
L_d(q_0, q_1, q_2) = \frac{h}{2} \left( \frac{q_2 - 2q_1 + q_0}{h^2} \right)^2
$$
with $h > 0$ the time step.

Fix a subset $I$ where $I \subset \{2, \ldots, N-2\}$ representing the indices corresponding to the interpolating constraints.

Therefore, the discrete interpolating problem consists on finding a path $q(0,N)$ minimizing the cost functional
$$
A_d(q(0,N)) = \sum_{k=0}^{N-2} L_d(q_k, q_{k+1}, q_{k+2})
$$
subject the constraint
$$
\Phi_d(q_k) = q_k \cdot q_k - r^2 = 0,
$$
and fixed the interpolating points $q_i \in S^2$ for all $i \in I$ and $q_0, q_1, q_{N-1}, q_N \in S^2$ given initial and final conditions. That is, to find a path $(q_0, q_1, \ldots, q_N)$ which solves the equations
$$
0 = D_1 L_d(q_k, q_{k+1}, q_{k+2}) + \lambda^k D \Phi_d(q_k) + D_2 L_d(q_{k-1}, q_k, q_{k+1}) + D_3 L_d(q_{k-2}, q_{k-1}, q_k)
$$
for $k \in \{2, \ldots, N-2\} \setminus I$ (that is, except on points of $I$) and the interpolating constraints and the initial and final conditions.

In other words, the solution of the interpolation problem is the path which solves the equations
$$
0 = \frac{1}{h^3} (q_{k+2} - 4q_{k+1} + 6q_k - 4q_{k-1} + q_{k-2}) + 2\lambda^k q_k \text{ for } k \notin I
$$
$$
0 = q_{k+2} - r^2
$$
$$
q_i = q(t_i), \text{ for } i \in I
$$
with \( k = 2, \ldots, N - 2 \) for paths \((q_0, q_1, q_2, \ldots, q_N)\) such that \(q_j \in S^2\) with \( j = 0, \ldots, N \) and \(q_0, q_1, q_{N-1}, q_N\) are given boundary conditions.

From these equations, we obtain the following systems of equations

\[
\lambda^k = -\frac{1}{2r^2h^3}(q_{k+2}q_k - 4q_{k+1}q_k + q_{k-2}q_k - 4q_{k-1}q_k + 6r^2)
\]

\[
0 = \frac{1}{h^3}(q_{k+2} - 4q_{k+1} + 6q_k - 4q_{k-1} + q_{k-2})
\]

\[
-\frac{q_k}{r^2h^3}(q_{k+2}q_k - 4q_{k+1}q_k + q_{k-2}q_k - 4q_{k-1}q_k + 6r^2)
\]

4.5. **Conclusions.** In this paper we have developed a variational integrator for higher-order Lagrangian systems with constraints. We have considered the case of time-dependent Lagrangian systems, and we have analyzed the behavior of the energy evolution associated with this type of systems. Moreover, we have also studied time-dependent second order constrained mechanics with fixed time-stepping.

We have derived variational integrators for higher-order Lagrangian mechanics with constraints in some interesting cases, for instance, an optimal control problem for an underactuated time-dependent mechanical systems and an interpolation problem for Riemannian manifolds.

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