Geometric integrators and nonholonomic mechanics

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Abstract

A geometric derivation of nonholonomic integrators is developed. It is based in the classical technique of generating functions adapted to the special features of nonholonomic systems. The theoretical methodology and the integrators obtained are different from the obtained in [12]. In the case of mechanical systems with linear constraints a family of geometric integrators preserving the nonholonomic constraints is given.

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1 Introduction

1.1 Introduction to nonholonomic mechanics

The theory of systems with nonholonomic constrains goes back to the XIX century. D’Alembert’s or Lagrange-D’Alembert’s principle of virtual work and Gauss principle of least constraint can be considered to be the first solutions to the analysis of systems with constraints, holonomic or not. After a period of decay, recently many authors show a new interest in that theory and also in its relation to the new developments in control theory, subriemannian geometry, robotics, etc (see, for instance,[44]). The main characteristic of this period was that Geometry was used in a systematic way (see L.D. Fadeev and A.M. Vershik [48] as an advanced and fundamental reference and, also, [3, 4, 7, 10, 13, 23, 24, 27, 28, 29, 37])

As is well known, in most problems of particle mechanics, the motion of the particles is constrained in some way; this is the term used to denote the condition that some motions or configurations are not allowed. First, we will start with a configuration space \( Q \), which is a \( n \)-dimensional differentiable manifold, with local coordinates \( q^i \). General two-side or equality constraints are functions of the form \( \phi^a(q^i, \dot{q}^i) = 0, 1 \leq a \leq m \), depending, in general, on configuration coordinates and their velocities. The various kinds of constraints we are concerned with will roughly come in two types:
holonomic and nonholonomic, depending whether the constraint is derived from a constraint in the configuration space or not. Therefore, the dimension of the space of configurations is reduced by holonomic constraints but not by nonholonomic constraints. Thus, holonomic constraints permit a reduction in the number of coordinates of the configuration space needed to formulate a given problem (see [44]).

We will restrict ourselves to the case of nonholonomic constraints, since the case of holonomic constraints, and, in particular, the construction of holonomic integrators, is well established in the existing literature. Geometrically, nonholonomic constraints are globally described by a submanifold $\tilde{M}$ of the velocity phase space $TQ$, the tangent bundle of the configuration space $Q$. In case $\tilde{M}$ is a vector subbundle of $TQ$, we are dealing with linear constraints. We will usually refer to $\tilde{M}$ as $D$ and, in such case, the constraints are alternatively defined by a distribution $D$ on the configuration space $Q$. If this distribution is integrable, we are precisely in the case of holonomic constraints. In case $\tilde{M}$ is an affine subbundle modeled on a vector bundle $D$, we are in the case of affine constraints. In the sequel, we will denote by $D$ the constraint submanifold on the velocity phase space, no matter if they are determined by linear or nonlinear constraints.

Given the constraints, we need to specify the dynamical evolution of the system. The central concepts permitting the extension of mechanics from the Newtonian point of view to the Lagrangian one are the notions of virtual displacements and virtual work; these concepts were formulated in the developments of mechanics, in their application to statics. In nonholonomic dynamics, the procedure is given by Lagrange-D’Alembert’s principle. We usually consider nonholonomic constraints of linear type, which are the constraints that we will regard as natural in a mechanical sense (although the extension for general nonholonomic constraint will be straightforward). We now come to the description of the constraint forces; for constraints of that type, Lagrange-D’Alembert’s principle allows us to determine the set of possible values of the constraint forces only from the set of admissible kinematic states, that is, from the constraint manifold $D$ determined by the vanishing of the nonholonomic constraints. Therefore, assuming that the dynamical properties of the system are mathematically described by a configuration space $Q$, by a Lagrangian function $L$ and by a distribution determining the linear constraints $D$, the equations of motion, following Lagrange-D’Alembert’s principle, are

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} = 0,$$

where $\delta q^i$ denotes the virtual displacements verifying

$$\mu^a \delta q^i = 0$$

and $D^a = \text{span}\{\mu^a = \mu^a dq^i\}$ (for the sake of simplicity, we will assume that the system is not subject to non-conservative forces). By using the Lagrange multiplier rule we obtain that

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} = \bar{\lambda}_a \mu^a_i.$$
The term on the right represents the constraint force or reaction force induced by the constraints. The functions $\bar{\lambda}_a$ are Lagrange multipliers to be determined in order to obtain a set of second order differential equations. These Lagrangian multipliers are computed using the constraint equations. An interesting remark, that will be used in the sequel, is that whenever the Lagrange multipliers $\bar{\lambda}_a = \bar{\lambda}_a(q^i, \dot{q}^i)$ have been determined, then the system of equations (3) can be considered a Lagrangian system subject to external conservative forces given by the right-hand side term, taking, obviously, an initial condition on the constraint submanifold $D$. Automatically, the choice of the Lagrange multipliers $\bar{\lambda}_a$ implies that the solution integral curves also verifies the constraint equations.

1.2 Introduction to Geometric Integration and Discrete Mechanics

Standard methods for simulating the motion of a dynamical system, generically called numerical integrators, usually take an initial condition and move it in the direction specified by the equation of motion or an appropriate discretization. But these standard methods ignore all the geometric features of many dynamical systems, as for instance, for Hamiltonian systems we have preservation of the symplectic form, energy (in the autonomous case) and symmetries, if any. However, new methods have been recently developed, called geometric integrators, which are concerned with some of the extra features of geometric nature of the dynamical systems. Usually, these integrators, in simulations, can run for long times with lower spurious effects (for instance, bad energy behavior for conservative systems) than the traditional ones. As is well known, the typical test example is the simulation of the solar system. Therefore, there is presently a great interest in geometric integration of differential equations as, for instance, symplectic integrators of Hamiltonian systems [16, 47].

Discrete variational integrators appear as a special kind of geometric integrators. These integrators have their roots in the optimal control literature in the 1960’s and 1970’s (Jordan and Polack [19], Cadzow [8], Maeda [35, 36]) and in 1980’s by Lee [25, 26], Veselov [43, 49]. In these papers, there appear the discrete action sum, discrete Euler-Lagrange equations, discrete Noether theorem...

Although this kind of symplectic integrators have been considered for conservative systems [17, 20, 38, 42, 50, 51], it has been recently shown how discrete variational mechanics can include forced or dissipative systems [21, 42], holonomic constraints [15, 42], time-dependent systems [30, 42], frictional contact [46] and nonholonomic constraints (see [10, 12]). Moreover, it has been also discussed reduction theory [5, 6, 40, 41], extension to field theories [18, 39] and quantum mechanics [45]. All these integrators have demonstrated exceptionally good longtime behavior and the research of this topic is interesting for numerical and geometric considerations.

Now, we will describe the discrete variational calculus, following the approach in [50] (see also [2, 14]). A discrete Lagrangian is a map $L_d : Q \times Q \rightarrow \mathbb{R}$ (this discrete Lagrangian may be considered as an approximation of the continuous Lagrangian $L : TQ \rightarrow \mathbb{R}$). Define the action sum

3
The discrete variational principle or Cadzow’s principle states that the solutions of the discrete system determined by $L_d$ must extremize the action sum given fixed points $q_0$ and $q_N$. Extremizing $S_d$ over $q_k$, $1 \leq k \leq N - 1$, we obtain the following system of difference equations

$$D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) = 0.$$ 

These equations are usually called the discrete Euler-Lagrange equations. Under some regularity hypothesis (the matrix $(D_{12} L_d(q_k, q_{k+1}))$ is regular) this implicit system of difference equations defines a discrete flow $\Upsilon : Q \times Q \rightarrow Q \times Q$, by $\Upsilon(q_{k-1}, q_k) = (q_k, q_{k+1})$.

The geometrical properties corresponding to this numerical method are obtained defining the discrete Legendre transformation associated to $L_d$ by

$$F L_d : \quad Q \times Q \quad \rightarrow \quad T^*Q$$

$$(q_0, q_1) \quad \mapsto \quad (q_0, -D_1 L_d(q_0, q_1)),$$

and the 2-form $\omega_d = F L_d^* \omega_Q$, where $\omega_Q$ is the canonical symplectic form on $T^*Q$. The discrete algorithm determined by $\Upsilon$ preserves the symplectic form $\omega_d$, i.e., $\Upsilon^* \omega_d = \omega_d$. Moreover, if the discrete Lagrangian is invariant under the diagonal action of a Lie group $G$, then the discrete momentum map $J_d : Q \times Q \rightarrow g^*$ defined by $(J_d(q_k, q_{k+1}), \xi) = (D_2 L_d(q_k, q_{k+1}), \xi(q_{k+1}))$ is preserved by the discrete flow. Therefore, these integrators are symplectic-momentum preserving integrators. Here, $\xi_Q$ is the fundamental vector field determined by $\xi \in g$.

Another alternative approach to discrete variational calculus comes from the classical theory of generating functions (see, for instance, [1]). Since $(T^*Q, \omega_Q)$ is an exact symplectic manifold, where $\omega_Q$ is the canonical symplectic form of $T^*Q$ and $\omega_Q = -d\theta_Q$, the symplectic flow $F_h : T^*Q \rightarrow T^*Q$ of a Hamiltonian vector field $X_H$ is a canonical transformation, and then Graph($F_h$), the graph of $F_h$, is a Lagrangian submanifold of the symplectic manifold $(T^*Q \times T^*Q, \Omega)$ where $\Omega = \pi_2^* \omega_Q - \pi_1^* \omega_Q$. Here, we denote by $\pi_i : T^*Q \times T^*Q \rightarrow T^*Q$, $i = 1, 2$ the canonical projections. Therefore, denoting $\Theta = \pi_2^* \theta_Q - \pi_1^* \theta_Q$ we have that

$$i_{F_h}^* \Omega = -d i_{F_h}^* \Theta = 0,$$

where $i_{F_h} : \text{Graph}(F_h) \hookrightarrow T^*Q \times T^*Q$ is the canonical inclusion. Then, at least locally, there exists a function $S^h : \text{Graph}(F_h) \rightarrow \mathbb{R}$ such that $i_{F_h}^* \Theta = dS^h$. Taking $(q^i, p_i)$ as natural coordinates in
Graph($F_h$) and $(q^i, p_i, q^i, p_i)$ the coordinates in $T^*Q \times T^*Q$, then, locally $\mathcal{S}^h$ is a function of $(q, p)$ coordinates. Hence, along Graph($F_h$), we have $q^i = q^i(q, p)$ and $p^i = p^i(q, p)$ and moreover
\[
p_i \, dq^i - p_i \, dq^i = d\mathcal{S}^h(q, p) .
\]
Assume that in a neighborhood of some point $x \in$ Graph($F_h$), we can change this system of coordinates by new independent coordinates $(q^i, q^i)$ (the local condition is that $\det (\partial q / \partial p) \neq 0$). In such a case, the function $\mathcal{S}^h$ can be locally expressed as $\mathcal{S}^h = \mathcal{S}^h(q, p) = \mathcal{S}^h(q, q)$. The function $\mathcal{S}^h(q, q)$ will be called a generating function of the first kind of the canonical transformation $F_h$. Moreover,
\[
\begin{aligned}
p_i &= -\frac{\partial \mathcal{S}^h}{\partial q^i} , \\
p_i &= \frac{\partial \mathcal{S}^h}{\partial q^i} .
\end{aligned}
\]
A nice and useful interpretation of the discrete Euler-Lagrange equations is the following theorem [22, 32].

**Theorem 1.1** Let the function $S^{Nh}$ be defined by
\[
S^{Nh}(q_0, q_N) = \sum_{k=0}^{N-1} S^h(q_k, q_{k+1}) ,
\]
where $q_k, 1 \leq k \leq N - 1$, are stationary points of the right-hand side, that is
\[
0 = D_2 S^h(q_{k-1}, q_k) + D_1 S^h(q_k, q_{k+1}) , \quad 1 \leq k \leq N - 1 ,
\] then $S^{Nh}$ is a generating function of first class for $F_{Nh} : T^*Q \to T^*Q$, for $h$ sufficiently small and where $F_{Nh}$ denotes the flow of $X_H$ over time $Nh$.

Moreover, if we start with a regular Lagrangian function $L : TQ \to \mathbb{R}$, and $H : T^*Q \to \mathbb{R}$ is the locally associated Hamiltonian, then we also have the following result (for example, see [32]).

**Proposition 1.2** A generating function of the first kind for $F_h$ is given by
\[
S^h(q_0, q_1) = \int_0^h L(q(t), \dot{q}(t)) \, dt ,
\]
where $q(t)$ is a solution of the Euler-Lagrange equations such that $q(0) = q_0$ and $q(h) = q_1$.

The conclusion is that the discrete variational calculus consists in taking an approximation of the generating function $S^h$. From this approximation we obtain a new Lagrangian submanifold of $T^*Q \times T^*Q$ and the relation between subsequent steps is given by [1] for the new generating function, which are precisely the discrete Euler-Lagrange equations. The symplecticity and preservation of momentum are now direct consequences of this description.
1.3 Introduction to nonholonomic integrators

In a recent paper, J. Cortés and S. Martínez [12] have proposed a construction of nonholonomic integrators which is useful for numerical considerations. Their construction is based on the discrete Lagrange-D’Alembert’s principle. Assuming that the constraints are given by a distribution $D$, this principle states that

$$
(D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k))_i \delta q^i_k = 0, \quad 1 \leq i \leq N - 1,
$$

where $\delta q_k \in D_{q_k}$ and, in addition $(q_k, q_{k+1}) \in D_d$. Here $D_d$ denotes a discrete constraint space $D_d \subset Q \times Q$. This integrator has a good performance and naturally inherits some geometric properties of the continuous problem. Observe that the method is based on the discretization of the Lagrangian and a coherent discretization of the constraints, and both determine the discrete constraint forces.

Alternatively, we propose a nonholonomic integrator also based on the discretization of the Lagrangian function (in a more precise sense, we discretize the action function) but now we take a coherent discretization of the constraint forces and both determine the discrete constraint submanifold. This method gives us, in general, different integrators from those in [12]. The last considerations of the previous section will be our starting point to study nonholonomic integrators, and our equations will be conceptually equivalent to the proposed for systems with external forces (see [12]). In the particular case of mechanical systems with linear constraint in the velocities, we study a subclass of our family of nonholonomic integrators with the property of preservation of the original nonholonomic constraints.

2 Geometrical formulation of nonholonomic systems

Let $Q$ be a $n$-dimensional differentiable manifold, with local coordinates $(q^i)$. The tangent bundle $TQ$, with induced coordinates $(q^i, \dot{q}^i)$, is equipped with two fundamental geometrical objects [33]: the Liouville vector field $\Delta$ and the vertical endomorphism $S$. In natural bundle coordinates we have

$$
\Delta = \dot{q}^i \frac{\partial}{\partial \dot{q}^i}, \quad S = dq^i \otimes \frac{\partial}{\partial \dot{q}^i}.
$$

Consider a Lagrangian system, with Lagrangian $L : TQ \rightarrow \mathbb{R}$, subject to nonholonomic constraints, defined by a submanifold $D$ of the velocity phase space $TQ$. We will assume that $\dim D = 2n - m$ and that $D$ is locally described by the vanishing of $m$ independent functions $\phi^a$ (the “constraint functions”).

In geometrical terms, D’Alembert’s principle (or Chetaev’s principle for nonlinear constraints) implies that the constraint forces, regarded as 1-forms on $TQ$ along $D$, take their values in the subbundle $S^*(TD^o)$ of $T^*TQ$, where $TD^o$ denotes the annihilator of $TD$ in $T^*TQ$. In an intrinsic
way, the equations of motion can be written as (see [27, 29])

\[(i_X \omega_L - dE_L)|_D \in S^*(TD^o),
X|_D \in TD,
\]

where \(\omega_L\) is the Poincaré-Cartan 2-form defined by \(\omega_L = -d(S^*(dL))\) and \(E_L = \Delta(L) - L\) is the energy function.

In the sequel we will also assume that the following admissibility condition holds

\[\dim TD^o = \dim S^*(TD^o).\]

This essentially means that the matrix \((\partial \phi^a / \partial \dot{q}^j)\) has rank \(m\) everywhere.

We now turn to the Hamiltonian description of the nonholonomic system on the cotangent bundle \(T^*Q\) of \(Q\) [3, 24, 37]. The canonical coordinates on \(T^*Q\) are denoted by \((q^i, p_i)\), and the cotangent bundle projection will be \(\pi_Q : T^*Q \rightarrow Q\). Assuming the regularity of the Lagrangian, we have that the Lagrangian and Hamiltonian formulations are locally equivalent. If we suppose, in addition, that the Lagrangian \(L\) is hyperregular, then the Legendre transformation \(\text{Leg} : TQ \rightarrow T^*Q, (q^i, \dot{q}^i) \mapsto (q^i, p_i = \partial L/\partial \dot{q}^i)\), is a global diffeomorphism. The constraint functions on \(T^*Q\) become \(\Psi^a = \phi^a \circ \text{Leg}^{-1}\), i.e.

\[\Psi^a(q^i, p_i) = \phi^a(q^i, \partial H/\partial p_i),\]

where the Hamiltonian \(H : T^*Q \rightarrow \mathbb{R}\) is defined by \(H = E_L \circ \text{Leg}^{-1}\). Since locally \(\text{Leg}^{-1}(q^i, p_i) = (q^i, \partial H/\partial p_i)\), then

\[H = p_i \dot{q}^i - L(q^i, \dot{q}^i),\]

where \(\dot{q}^i\) is expressed in terms of \(q^i\) and \(p_i\) using \(\text{Leg}^{-1}\).

The equations of motion for the nonholonomic system on \(T^*Q\) can now be written as follows

\[
\begin{align*}
\dot{q}^i &= \frac{\partial H}{\partial p_i} - \lambda^a \frac{\partial \Psi^a}{\partial q^i} \mathcal{H}_{ji}, \\
\dot{p}_i &= -\lambda^a \frac{\partial \Psi^a}{\partial q^i},
\end{align*}
\]

(5)

together with the constraint equations \(\Psi^a(q, p) = 0\), where \(\mathcal{H}_{ij}\) are the components of the inverse of the matrix \((\mathcal{H}^{ij}) = (\partial^2 H/\partial p_i \partial p_j)\). Note that

\[
(\frac{\partial \Psi^a}{\partial p_j} \mathcal{H}_{ji})(q, p) = (\frac{\partial \phi^a}{\partial q^i} \circ \text{Leg}^{-1})(q, p).
\]

The symplectic 2-form \(\omega_L\) is related, via the Legendre map, with the canonical symplectic form \(\omega_Q\) on \(T^*Q\). Let \(M\) denote the image of the constraint submanifold \(D\) under the Legendre transformation, and let \(F\) be the distribution on \(T^*Q\) along \(M\), whose annihilator is given by

\[F^o = \text{Leg}_*(S^*(TD^o)).\]
Observe that \( F^o \) is locally generated by the \( m \) independent 1-forms
\[
\mu^a = \frac{\partial \Psi^a}{\partial p_i} H_{ij} dq^j, \quad 1 \leq a \leq m.
\]

The “Hamilton equations” for the nonholonomic system can be then rewritten in intrinsic form as
\[
(i_X \omega_Q - dH)|_M \in F^o \\
X|_M \in TM.
\]

Suppose in addition that the following compatibility condition \( F^\perp \cap TM = \{0\} \) holds, where \( \perp \) denotes the symplectic orthogonal with respect to \( \omega_Q \). Observe that, locally, this condition means that the matrix
\[
(C^{ab}) = \begin{pmatrix}
\frac{\partial \Psi^a}{\partial p_i} H_{ij} \\
\frac{\partial \Psi^b}{\partial p_j}
\end{pmatrix}
\]
(7)
is regular. On the Lagrangian side, the compatibility condition is locally written as
\[
\det(C^{ab}) = \det \left( \frac{\partial \phi^a}{\partial \dot{q}^i} W_{ij} \frac{\partial \phi^b}{\partial \dot{q}^j} \right) \neq 0,
\]
(8)
where \( W_{ij} \) are the entries of the Hessian matrix \( \left( \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} \right)_{1 \leq i,j \leq n} \). The compatibility condition is not too restrictive, since, taking into account the admissibility assumption, it is trivially verified by the usual systems of mechanical type (i.e. with a Lagrangian of the form kinetic minus potential energy), where the \( H_{ij} \) represent the components of a positive definite Riemannian metric. The compatibility condition guarantees in particular the existence of a unique solution of the constrained equations of motion (6) which, henceforth, will be denoted by \( X_{H,M} \) on the Hamiltonian side and \( \xi_{L,D} \) on the Lagrangian side.

Moreover, if we denote by \( X_H \) the Hamiltonian vector field of \( H \), i.e., \( i_X \omega_Q = dH \) then, using the constraint functions, we may explicitly determine the Lagrange multipliers \( \lambda_a \) as
\[
\lambda_a = -C_{ab} X_H(\Psi^b).
\]

Next, writing the 1-form
\[
\Lambda = -C_{ab} X_H(\Psi^b) \frac{\partial \Psi^a}{\partial p_j} H_{ji} dq^i,
\]
the nonholonomic equations are equivalently rewritten as
\[
\begin{cases}
\dot{q}^i = \frac{\partial H}{\partial p_j}, \\
\dot{p}_i = -\frac{\partial H}{\partial q^i} - \Lambda_i,
\end{cases}
\]
(9)
for initial conditions \((q_0, p_0) \in M\) and \( \Lambda = \Lambda_i dq^i \). We also denote by \( \Lambda = Leg^*(\Lambda) \) the 1-form on \( TQ \) which represents the constraint force once the Lagrange multipliers have been determined.

Now, consider the flow \( F_t : M \to M, \ t \in I \subseteq \mathbb{R} \) of the vector field \( X_{H,M} \), solution of the nonholonomic problem.
Since (9) is geometrically rewritten as
\[ i_{X_{H,M}}\omega = dH + \Lambda , \]
\[ (i_{\xi_{L,D}}\omega_L = dE_L + \Lambda, \text{ with } \Lambda = Leg^*\Lambda, \text{ on the Lagrangian side}) \text{ then} \]
\[ L_{X_{H,M}}\theta_Q = d(i_{X_{H,M}}\theta_Q - H) - \Lambda , \]
or, equivalently,
\[ L_{X_{H,M}}\theta_Q = d(L \circ Leg^{-1}) - \Lambda . \]
Now, from the dynamical definition of the Lie derivative, we have
\[ F_t^*(L_{X_{H,M}}\theta_Q) = \frac{d}{dt}(F_t^*\theta_Q) , \]
and integrating, we obtain the following expression, with some abuse of notation,
\[ F_t^*\theta_Q - \theta_Q = d \left( \int_0^h L \circ \tilde{F}_t \, dt \right) - \int_0^h F_t^*\Lambda , \quad (10) \]
where \( \tilde{F}_t \) is the flow of the vector field \( \xi_{L,D} \). In next sections, we will study geometric integrators which verify a discrete version of equation (10).

3 “Generating functions” and nonholonomic mechanics

Next, we will follow similar arguments for the construction of generating functions for symplectic or canonical maps [1]. However, because of equation (10), we have that the nonholonomic flow is not a canonical transformation; i.e.,
\[ F_t^*\omega_Q - \omega_Q = d \left( \int_0^h F_t^*\Lambda \right) . \quad (11) \]
This description will allow us to construct a new family of nonholonomic integrators for equations (3). Denote by \( \pi_i : T^*Q \times T^*Q \to T^*Q, i = 1, 2, \) the canonical projections. Consider the following forms
\[ \Theta = \pi_2^*\theta_Q - \pi_1^*\theta_Q , \]
\[ \Omega = \pi_2^*\omega_Q - \pi_1^*\omega_Q = -d\Theta . \]
Denote by \( i_{F_h} : \text{Graph}(F_h) \hookrightarrow T^*Q \times T^*Q \) the inclusion map and observe that \( \text{Graph}(F_h) \subset M \times M \). Then, from (11)
\[ i_{F_h}^*\Omega = (\pi_1|\text{Graph}(F_h))^*(F_h^*\omega - \omega_Q) \]
\[ = (\pi_1|\text{Graph}(F_h))^* \left( d \left( \int_0^h F_t^*\Lambda \right) \right) , \]
Let \((q_0, p_0, q_1, p_1)\) be coordinates in \(T^*Q \times T^*Q\) in a neighborhood of some point in \(\text{Graph}(F_h)\). If \((q_0, p_0, q_1, p_1) \in \text{Graph}(F_h)\) then \(\Psi^a(q_0, p_0) = 0\) and \(\Psi^a(q_1, p_1) = 0\). Moreover, along \(\text{Graph}(F_h)\), \(q_1 = q_1(q_0, p_0)\) and \(p_1 = p_1(q_0, p_0)\),

\[
p_1 dq_1 - p_0 dq_0 = d \left( \int_0^h L(q(t), \dot{q}(t)) \, dt \right) - \int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) \, dt,
\]

where \((q(t), \dot{q}(t)) = \bar{F}_t(q_0, q_0)\) with \(\text{Leg}(q_0, \dot{q}_0) = (q_0, p_0)\). Here, \(\bar{F}_t\) denotes the flow of \(\xi_{L,D}\). Equation \((12)\) is satisfied along \(\text{Graph}(F_h)\).

Assume that, in a neighborhood of some point \(x \in \text{Graph}(F_h)\), we can change this system of coordinates to a new coordinates \((q_0, q_1)\). Denote by

\[
S^h(q_0, q_1) = \int_0^h L(q(t), \dot{q}(t)) \, dt,
\]

where \(q(t)\) is a solution curve of the nonholonomic problem with \(q(0) = q\) and \(q(h) = q_1\). This solution always exists for adequate values of \(q_0\) and \(q_1\). In fact, observe that

\[
q_1 = q_0 + h \frac{\partial H}{\partial p}(q_0, p_0) + o(h^2),
\]

hence, since \(\det \left( \frac{\partial^2 H}{\partial p \partial p} \right) \neq 0\), we locally have that \(p_0 = p_0(q_0, q_1, h)\). But, in addition, \((q_0, p_0) \in M\); therefore \(\varphi^a(q_0, q_1, h) = \Psi^a(q_0, p_0(q_0, q_1, h)) = 0\). Then, the curve

\[
(q(t), \dot{q}(t)) = \text{Leg}^{-1}(F_t(q_0, p_0(q_0, q_1, h)))
\]

verifies the required assumptions if \(\varphi^a(q_0, q_1, h) = 0\).

Thus, we deduce that\(^1\)

\[
\begin{align*}
p_0 &= - \frac{\partial S^h}{\partial q_0} + \int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_0}, \\
p_1 &= \frac{\partial S^h}{\partial q_1} - \int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_1},
\end{align*}
\]

where \((q_0, q_1)\) verifies the constraint functions \(\varphi^a(q_0, q_1, h) = 0\), now explicitely defined by

\[
\varphi^a(q_0, q_1, h) = \Psi^a(q_0, - \frac{\partial S^h}{\partial q_0}(q_0, q_1) + \int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_0}), \quad 1 \leq a \leq m,
\]

with \(q(t)\) solution of the nonholonomic problem with \(q(0) = q_0\) and \(q(h) = q_h\).

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\(^1\)For a function \(f(x, y)\) with \(x, y \in \mathbb{R}^n\) we use the notation \(\partial f/\partial x\) (respectively, \(\partial f/\partial y\)) to write the partial derivative with respect the first \(n\)-variables (resp., the second \(n\)-variables).
Next, we will show how the group composite law of the flow $F_h$

$$F_{Nh} = F_h \circ \ldots \circ F_h$$

is expressed in terms of the corresponding “generating functions” $S^h$. Moreover, the following theorem will result in a new construction of numerical integrators for nonholonomic mechanics when we change the “generating function” and the constraint forces by appropriate approximations.

As a generalization of Theorem 1.1 we have the following theorem.

**Theorem 3.1** The function $S^{Nh}$, the “generating function” for $F_{Nh}$, is given by

$$S^{Nh}(q_0, q_N) = \sum_{k=0}^{N-1} S^h(q_k, q_{k+1}) ,$$

where $q_k$, $1 \leq k \leq N - 1$, are points verifying

$$D_2 S^h(q_{k-1}, q_k) + D_1 S^h(q_k, q_{k+1}) = \int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_0} + \int_h^{2h} \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_0} ,$$

and $q(t)$ is a solution curve of the nonholonomic problem with $q(0) = q_{k-1}$ and $q(h) = q_k$ (respectively, $q(h) = q_k$ and $q(2h) = q_{k+1}$) for the first integral (resp., second integral) of the right-hand side.

**Proof:** It is suffices to prove the result for $N = 2$; that is,

$$S^{2h}(q_0, q_2) = S^h(q_0, q_1) + S^h(q_1, q_2) ,$$

where $q_1$ verifies condition (15).

Since

$$p_1 \, dq_1 - p_0 \, dq_0 = dS^h(q_0, q_1) - \int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) ,$$

$$p_2 \, dq_2 - p_1 \, dq_1 = dS^h(q_1, q_2) - \int_h^{2h} \tilde{\Lambda}(q(t), \dot{q}(t)) ,$$

then

$$p_2 \, dq_2 - p_0 \, dq_0 = d \left( S^h(q_0, q_1) + S^h(q_1, q_2) \right) - \int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) - \int_h^{2h} \tilde{\Lambda}(q(t), \dot{q}(t)) .$$

Since the variables $q_1$ do not appear on the left-hand side term, it follows that

$$0 = D_2 S^h_1(q_0, q_1) + D_1 S^h_2(q_1, q_2) - \int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_0} - \int_h^{2h} \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_0} ,$$

and for a choice of $q_1$ verifying (16) then

$$S^{2h}(q_0, q_2) = S^h(q_0, q_1) + S^h(q_1, q_2) .$$
is a “generating function of the first kind” of $F_{2h}$ because

$$p_2 dq_2 - p_0 dq_0 = dS^{2h}(q_0, q_2) - \int_0^{2h} \tilde{\Lambda}(q(t), \dot{q}(t)) \, dq.$$  

Equations (15) determine a implicit system of difference equations which permit us to obtain $q_2$ from the initial data $q_0$ and $q_1$. An interesting consequence is that these equations preserve the constraint submanifold determined by the constraints $\varphi^a = 0$, $1 \leq a \leq m$. In fact, if $\varphi^a(q_0, q_1, h) = 0$ (that is $\Psi^a(q_0, p_0) = 0$) then

$$\varphi^a(q_1, q_2, h) = \Psi^a(q_1, \frac{\partial S^h}{\partial q_1}(q_0, q_1) - \int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_1} ),$$

and now applying (13) we obtain that

$$\varphi^a(q_1, q_2, h) = \Psi^a(q_1, p_1) = 0,$$

since $F_h(q_0, p_0) = (q_1, p_1)$ and the flow preserves the constraints.

The next remark will be a key result for the construction of nonholonomic integrators.

**Remark 3.2** Replace equation (13) by

$$\begin{cases} p_0 = -\frac{\partial \tilde{S}^h}{\partial q_0} + \alpha^h_0(q_0, q_1), \\ p_1 = \frac{\partial \tilde{S}^h}{\partial q_1} - \alpha^h_1(q_0, q_1), \end{cases}$$  

(17)

where $\tilde{S}^h$ is a function of $(q_0, q_1)$ coordinates and $\alpha^h = \alpha^h_0 \, dq_0 + \alpha^h_1 \, dq_1$ and replace the constraints functions by

$$\varphi^a(q_0, q_1, h) = \Psi^a(q_0, -\frac{\partial \tilde{S}^h}{\partial q_0} + \alpha^h_0(q_0, q_1) ),$$

(18)

that is,

$$p_1 dq_1 - p_0 dq_0 = d\tilde{S}^h - \alpha^h,$$

along $\tilde{\varphi}^a = 0$.

Assume that

$$\det \left( \frac{\partial^2 \tilde{S}^h}{\partial q_0 \partial q_1} - \frac{\partial \alpha^h_0}{\partial q_1} \right) \neq 0,$$

(19)

then, applying the implicit function theorem we have that, locally, $q_1 = q_1(q_0, p_0)$, and then the mapping

$$G_h(q_0, p_0) = (q_1, p_1)$$

is well-defined.

Consider the mapping $G_{Nh}$ defined by

$$G_{Nh} = G_h \circ \ldots \circ G_h.$$.  


Following a similar argument to Theorem 3.1, $\text{Graph}(G_{Nh})$ is described by

$$
\begin{cases}
    p_0 = -\frac{\partial \tilde{S}^{Nh}}{\partial q_0}(q_0, q_N) + \alpha_0^{Nh}(q_0, q_N), \\
    p_N = \frac{\partial \tilde{S}^{Nh}}{\partial q_N}(q_0, q_N) - \alpha_1^{Nh}(q_0, q_N),
\end{cases}
$$

where $\tilde{S}^{Nh}(q_0, q_N) = \sum_{k=0}^{N-1} \tilde{S}^h(q_k, q_{k+1})$ and $\alpha^{Nh}(q_0, q_N) = \sum_{k=0}^{N-1} \alpha^h(q_k, q_{k+1})$. Here, the $q_k$'s, $1 \leq k \leq N - 1$, verify

$$
D_2 \tilde{S}^h(q_{k-1}, q_k) + D_1 \tilde{S}^h(q_k, q_{k+1}) = \alpha_1^h(q_{k-1}, q_k) + \alpha_0^h(q_k, q_{k+1}), \quad 1 \leq k \leq N - 1.
$$

### 3.1 Constraint error analysis

As we have seen, if our “generating function” is $S^h$, then we have exact preservation of the constraints $\varphi^a$. We now investigate what happens when the “generating function” is an approximation. We follow similar arguments to those in subsection 2.3.1 in [12].

Assume that $Q$, and also $TQ$ and $T^*Q$, are finite-dimensional vector spaces with inner product $\langle ., . \rangle$ and corresponding norm $\| . \|$.

Consider an “approximated generating function” $\tilde{S}^h$ and an approximated discrete constraint force $\alpha^h = \alpha_i^h dq^i$ for the nonholonomic problem both of order $r$; hence, there exists an open set $U \subset D$ with compact closure and constants $c, d_i > 0$, $1 \leq i \leq n$, and $H > 0$ such that

$$
\tilde{S}^h(q_0, q_1) = S^h(q_0, q_1) + C(q_0, q_1, h)h^{r+1}
$$

$$
\alpha_i^h = \int_0^h \dot{\Lambda}_i(q(t), \dot{q}(t)) dt + D_i(q_0, q_1, h)h^{r+1}
$$

for all solution $q(t)$ of the nonholonomic problem with $q(0) = q_0$, $q(h) = q_1$ and initial condition belonging to $U$ and $h \leq H$. Here $C$ and $D_i$, $1 \leq i \leq n$, are functions such that $\|C(q_0, q_1, h)\| \leq c$ and $\|D_i(q_0, q_1, h)\| \leq d_i$ on $U$.

Taking derivatives we have that

$$
\frac{\partial \tilde{S}^h}{\partial q_0}(q_0, q_1) = \frac{\partial S^h}{\partial q_0}(q_0, q_1) + \frac{\partial C}{\partial q_0}(q_0, q_1, h)h^{r+1}
$$

and also

$$
\alpha_0^h(q_0, q_1) = (\alpha_0^h)\frac{\partial q^i}{\partial q_0} = \int_0^h \dot{\Lambda}_i(q(t), \dot{q}(t)) \frac{\partial q^i}{\partial q_0} dt + \sum_{i=1}^n \frac{\partial D_i}{\partial q_0}(q_0, q_1, h)h^{r+1}
$$

where now $\alpha^h = \alpha_0^h dq_0 + \alpha_1^h dq_1$.

Therefore, we deduce that

$$
\tilde{\varphi}^a(q_0, q_1, h) = \Psi^a(q_0, -\frac{\partial \tilde{S}}{\partial q_0} + \alpha_0(q_0, q_1))
$$

$$
= \Psi^a(q_0, -\frac{\partial S^h}{\partial q_0} + \int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_0} dt + E^a(q_0, q_1, h)h^{r+1}
$$

$$
= \Psi^a(q_0, p_0) + E^a(q_0, q_1, h)h^{r+1} = E^a(q_0, q_1, h)h^{r+1}
$$
where $E^a$ are bounded functions. Then, the discrete algorithm preserves the constraints up to order $r$.

### 3.2 Local error analysis

Assuming that

$$\det \left( \frac{\partial^2 \tilde{S}^h}{\partial q_0 \partial q_1} - \frac{\partial \alpha h}{\partial q_0} \right) \neq 0,$$

we obtain a discrete flow $G^h : V \subseteq M \rightarrow M$. It is easy to show, from conditions (22) and (23), that $G^h$ is an integrator of $X_{H,M}$ of order $r$, following similar arguments to those used in the subsection above (see also Theorem 2.3.1., in [42]).

### 4 Nonholonomic integrators

In the sequel and for simplicity assume that $Q$ is a vector space. Since $S^h(q_0, q_1) = \int_0^h L(q(t), \dot{q}(t)) \, dt$, where $q(t)$ is a nonholonomic solution with $q(0) = q_0$ and $q(h) = q_1$, using Remark 3.2 we can obtain nonholonomic integrators by taking adequate approximations of the “generating function” $S^h$ and the extra-term $\int_0^h \tilde{\Lambda}(q(t), \dot{q}(t))$.

Consider, for instance, the approximation

$$S^h_\alpha(q_0, q_1) = hL((1 - \alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h}),$$

for some parameter $\alpha \in [0, 1]$. (In general, we will write $S^h_\alpha(q_0, q_1) \approx S^h(q_0, q_1)$.)

A natural approximation of the constraint forces adapted to our choice of approximation for $S^h$ are

$$\int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_0} \approx (1 - \alpha)h\tilde{\Lambda}((1 - \alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h}),$$

$$\int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_1} \approx \alpha h\tilde{\Lambda}((1 - \alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h}).$$

Consequently, equations (21) give us the following numerical method for nonholonomic systems

$$D_2S^h_\alpha(q_{k-1}, q_k) + D_1S^h_\alpha(q_k, q_{k+1}) = \alpha h\tilde{\Lambda}((1 - \alpha)q_{k-1} + \alpha q_k, \frac{q_k - q_{k-1}}{h})$$

$$+ (1 - \alpha)h\tilde{\Lambda}((1 - \alpha)q_k + \alpha q_{k+1}, \frac{q_{k+1} - q_k}{h}), \quad 1 \leq k \leq N - 1,$$

with initial condition satisfying

$$\tilde{\varphi}^a(q_0, q_1, h) = \Psi^a(q_0, -\frac{\partial S^h_\alpha}{\partial q_0}(q_0, q_1) + (1 - \alpha)h\tilde{\Lambda}((1 - \alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h})) = 0.$$
Remark 4.1 Obviously, it is possible to produce a wider variety of discrete methods. For example,

\[ S^{h}_{\text{sym}, \alpha} = \frac{1}{2} S^{h}_\alpha + \frac{1}{2} S^{h}_{1-\alpha}, \]

gives a second-order method for any \( \alpha \in [0, 1] \). Also, higher-order approximations of the function \( S^{h} \) may be considered.

Example 4.2 Nonholonomic particle.

Consider the Lagrangian \( L : T\mathbb{R}^3 \to \mathbb{R} \)

\[ L = \frac{1}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - (x^2 + y^2), \]

subject to the constraint

\[ \phi = \dot{z} - y\dot{x} = 0. \]

It is easy to compute the nonholonomic differential equations

\[
\begin{align*}
\ddot{x} &= -\frac{2x + y\dot{x}\dot{y}}{1 + y^2} \\
\ddot{y} &= -2y \\
\ddot{z} &= -\frac{2xy + \dot{x}\dot{y}}{1 + y^2},
\end{align*}
\]

where now the constraint 1-form is

\[ \check{\Lambda} = \frac{2xy - \dot{x}\dot{y}}{1 + y^2}(dz - ydx). \]

Taking

\[ S^{h}_{1/2}(x_0, y_0, z_0, x_1, y_1, z_1) = \frac{h}{2} \left[ \left( \frac{x_1 - x_0}{h} \right)^2 + \left( \frac{y_1 - y_0}{h} \right)^2 + \left( \frac{z_1 - z_0}{h} \right)^2 \right] - \left( \frac{x_0 + x_1}{2} \right)^2 - \left( \frac{y_0 + y_1}{2} \right)^2, \]

we obtain the nonholonomic integrator

\[
\begin{align*}
\frac{x_1 - x_0}{h} - \frac{h^2}{2} \frac{(x_1+x_0)(y_1+y_0) - (x_1-x_0)(y_1-y_0)}{h^2} &- \frac{h^2}{2} \cdot \frac{y_1 + y_0}{2} + \frac{h^2}{2} \cdot \frac{y_2 + y_1}{2} \\
\frac{y_1 - y_0}{h} - \frac{h^2}{2} \cdot \frac{y_2 - y_1}{h} - \frac{h^2}{2} \cdot \frac{y_2 + y_1}{2} &= 0, \\
\frac{z_1 - z_0}{h} - \frac{h^2}{2} \cdot \frac{z_2 - z_1}{h} &- \frac{h^2}{2} \cdot \frac{z_2 + z_1}{2} \\
&= \frac{h}{2} \left[ \left( \frac{x_1+x_0}{2} \right)^2 + \left( \frac{y_1+y_0}{2} \right)^2 \right] + \frac{h}{2} \left[ \left( \frac{x_2-x_1}{2} \right)^2 + \left( \frac{y_2+y_1}{2} \right)^2 \right].
\end{align*}
\]
The constraint function on $\mathbb{R}^3 \times \mathbb{R}^3$ is

$$\tilde{\varphi}(x_0, y_0, z_0, x_1, y_1, z_1, h) = -\frac{z_1 - z_0}{h} - \frac{h}{2} \frac{\frac{(x_1 + x_0)(y_1 + y_0)}{2} - \frac{(x_1 - x_0)(y_1 - y_0)}{h^2}}{1 + \left(\frac{y_1 + y_0}{2}\right)^2} + y_0 \left[ \frac{x_1 - x_0}{h} + h \frac{x_1 + x_0}{2} - \frac{h}{2} \frac{\frac{(x_1 + x_0)(y_1 + y_0)}{2} - \frac{(x_1 - x_0)(y_1 - y_0)}{h^2}}{1 + \left(\frac{y_1 + y_0}{2}\right)^2} \cdot y_1 + y_0 \right].$$

The following two figures show the preservation of energy as a key point of comparison of computational implementations of the method exposed above to other methods.

The first figure compares the method introduced here to the traditional Runge-Kutta method of fourth order, showing an improvement in several orders of magnitude. Observe that, in this scale, the value of the energy in each step of our algorithm is practically undistinguishable from the initial value of the energy.

![Graph showing energy comparison between proposed method and Runge-Kutta method.](image)

The second figure is a comparison between our method and the one appeared in [10, 12]. A similar behaviour is observed. Nevertheless, a slightly better behaviour can also be appreciated, where the proposed algorithm shows on average a better preservation of the original energy.
For the same initial conditions and data, the following graph shows a very good behaviour of the constraint function evolution with time (notice the small scale).

5 Mechanical systems with linear constraints. Geometric numerical methods preserving constraints

Suppose that the mechanical system, given by the Lagrangian $L : TQ \to \mathbb{R}$

$$L(v_q) = \frac{1}{2}g(v_q, v_q) - V(q)$$
is subjected to nonholonomic constraints $\phi^a : TQ \to \mathbb{R}$, $1 \leq a \leq m$. Since the nonholonomic constraints usually found in mechanics are linear in the velocities we will assume that

$$\phi^a(q, \dot{q}) = \mu^a_i(q)q^i, \ 1 \leq a \leq m.$$  

From a geometric point of view, these linear constraints are determined by prescribing a distribution $\mathcal{D}$ on $Q$ of dimension $n - m$ such that the annihilator of $\mathcal{D}$ is locally given by

$$\mathcal{D}^o = \langle \mu^a = \mu^a_i dq^i ; 1 \leq a \leq m \rangle.$$  

In this manner, the solutions of the nonholonomic Lagrangian system satisfy

$$\nabla_{\dot{c}(t)}\ddot{c}(t) = -\text{grad} \ V(c(t)) + \lambda(\dot{c}(t)), \ \dot{c}(t) \in \mathcal{D}_{c(t)},$$  

(26)

where $\lambda$ is a section of $\mathcal{D}^\perp$ along $c$, and $\mathcal{D}^\perp$ stands for the orthogonal complement of $\mathcal{D}$ with respect to the metric $g$.

Since $g$ is a Riemannian metric, the $m \times m$ matrix $(C^{ab}) = (\mu^a_i g^{ij} \mu^b_j)$ is symmetric and regular. Therefore, we can explicitly determine

$$\lambda(q^i(t), \dot{q}^i(t)) = C_{ab} \left( (-\Gamma^{ij}_{jk} \dot{q}^j \dot{q}^k - g^{ij} \frac{\partial V}{\partial q^j}) \mu^a_i + \dot{q}^i \dot{q}^j \frac{\partial \mu^a_i}{\partial q^j} \right) Z^b$$  

(27)

where $(C_{ab})$ is the inverse matrix of $(C^{ab})$ and the vector field $Z^a$ is defined by

$$g(Z^a, Y) = \mu^a(Y), \text{ for all vector field } Y, \ 1 \leq a \leq m,$$

that is, $Z^a$ is the gradient of the 1-form $\mu^a$. Thus, $\mathcal{D}^\perp = \langle Z^a \rangle$, $1 \leq a \leq m$. In local coordinates, we have

$$Z^a = g^{ij} \mu^a_i \frac{\partial}{\partial q^j}.$$  

By using the metric $g$ and the distribution $\mathcal{D}$ we can obtain two complementary projectors

$$\mathcal{P} : TQ \to \mathcal{D}, \quad \mathcal{Q} : TQ \to \mathcal{D}^\perp,$$

with respect to $g$. The projector $\mathcal{Q}$ is locally described by

$$\mathcal{Q} = C_{ab} Z^a \otimes \mu^b.$$  

Using these projectors we can obtain the equations of motion as follows. A curve $c(t)$ is a motion for the non-holonomic system if it satisfies the constraints, say, $\phi^a(\dot{c}(t)) = 0$, for all $a$, and, in addition, the “projected equation of motion”

$$\mathcal{P}(\nabla_{\dot{c}(t)} \ddot{c}(t)) = -\mathcal{P}(\text{grad} \ V(c(t)))$$  

(28)

is fulfilled. But these conditions are equivalent to

$$\dot{c}(t) \in \mathcal{D}_{c(t)} \quad \nabla_{\dot{c}(t)} \dot{c}(t) = -\mathcal{P}(\text{grad} \ V(c(t))),$$
where $\nabla$ is the modified linear connection defined by

$$\bar{\nabla}_X Y = \nabla_X Y + (\nabla_X \mathcal{Q})(Y)$$

for all vector fields $X$ and $Y$ on $\mathcal{Q}$.

Since the constraints are linear then, from (14)

$$-\mu^a_0(q_0)g^{ij}(q_0) \frac{\partial S^h}{\partial q^0_0}(q_0, q_1) + \mu^a_1(q_0)g^{ij}(q_0) \int_0^h \ddot{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q^0_0} = 0, \quad 1 \leq a \leq m,$$

(29)

or, in terms of projectors,

$$\mathcal{Q}_{|q_0} \left( D_1 S^h(q_0, q_1) \right) = \mathcal{Q}_{|q_0} \left( D_1 \int_0^h \ddot{\Lambda}(q(t), \dot{q}(t)) \right)$$

(30)

Moreover, the dynamics preserves the constraints $\Psi^a$ which implies that

$$\Psi^a(q_1, \frac{\partial S^h}{\partial q^0_1}(q_0, q_1) - \int_0^h \ddot{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q^0_1} = 0,$$

or, in other words,

$$\mathcal{Q}_{|q_1} \left( D_2 S^h(q_0, q_1) \right) = \mathcal{Q}_{|q_1} \left( D_2 \int_0^h \ddot{\Lambda}(q(t), \dot{q}(t)) \right)$$

(31)

Therefore, equations (30) and (31) show that the preservation of the exact constraints is equivalent to give a prescription about the relationship between the “generating function” and the constraint forces.

Thus, equations (31)

$$D_2 S^h(q_{k-1}, q_k) + D_1 S^h(q_k, q_{k+1}) = \int_0^h \ddot{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q^0_1} + \int_h^{2h} \ddot{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q^0_0},$$

can be rewritten using expression (31) as follows

$$\mathcal{P}_{|q_k} \left( D_2 S^h(q_{k-1}, q_k) \right) + D_1 S^h(q_k, q_{k+1}) = \mathcal{P}_{|q_k} \left( \int_0^h \ddot{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q^0_1} \right) + \int_h^{2h} \ddot{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q^0_0},$$

(32)

Now, considering an approximated generating function $\tilde{S}^h$ and an approximate constraint force $\tilde{\alpha}^h = \alpha^h_0(q_0, q_1) dq_0 + \alpha^h_1(q_0, q_1) dq_1$, as in Remark 3.2 from the previous discussion, we now substitute the approximated constraint force by:

$$\tilde{\alpha}^h = \alpha^h_0(q_0, q_1) dq_0$$

$$+ \mathcal{P}_{|q_1} \left( \alpha^h_1(q_0, q_1) dq_1 \right) + \mathcal{Q}_{|q_1} \left( D_2 \tilde{S}^h(q_0, q_1) \right)$$

Therefore for $\tilde{S}^h$ and $\tilde{\alpha}^h$ equations (32) are rewritten as

$$\mathcal{P}_{|q_k} \left( D_2 \tilde{S}^h(q_{k-1}, q_k) \right) + D_1 \tilde{S}^h(q_k, q_{k+1}) = \mathcal{P}_{|q_k} \left( \alpha^h_1(q_{k-1}, q_k) \right) + \alpha^h_0(q_k, q_{k+1}),$$

(33)
for $1 \leq k \leq N - 1$. The importance of equations (33) is that they generate an algorithm which automatically preserves the exact constraint functions $\Phi^a$. In fact, if we apply the projector $Q$ to Equations (33) we obtain:

$$Q_{|q_k} \left( D_1 S^h(q_k, q_{k+1}) \right) = Q_{|q_k} \left( \alpha_0^h(q_k, q_{k+1}) \right)$$

or

$$\tilde{\varphi}^a(q_k, q_{k+1}, h) = \Psi^a(q_k, -\frac{\partial \tilde{S}^h}{\partial q_0}(q_k, q_{k+1}) + \alpha_0^h(q_k, q_{k+1})) = 0$$

that is, the constraints are satisfied.

Therefore the geometric algorithm that we have obtained work as follows:

$$P_{|q_k} \left( D_2 \tilde{S}^h(q_{k-1}, q_k) \right) + D_1 \tilde{S}^h(q_k, q_{k+1}) = P_{|q_k} \left( \alpha_1^h(q_{k-1}, q_k) \right) + \alpha_0^h(q_k, q_{k+1}),$$

with initial condition satisfying:

$$\tilde{\varphi}^a(q_0, q_1, h) = 0$$

Choosing $\alpha_0^h$ and $\alpha_1^h$ in $D^h$, we obtain equations for nonholonomic integrators with more geometric flavour:

**Geometric nonholonomic integrator**

$$P_{|q_k} \left( D_2 \tilde{S}^h(q_{k-1}, q_k) + D_1 \tilde{S}^h(q_k, q_{k+1}) \right) = 0$$

which is interpreted as a discretization of Equations (28)

$$\nabla \dot{c}(t) = -P \left( \text{grad} \left( V(c(t)) \right) \right)$$

In a future work we will study from numerical and geometrical points of view this particular subclass of geometric integrators.

### 5.1 Nonholonomic integrators preserving constraints

For the class of integrators introduced in Section 4 we find the following family of nonholonomic integrators preserving constraints:

$$P_{|q_k} \left( D_2 S^h_{\alpha}(q_{k-1}, q_k) \right) + D_1 S^h_{\alpha}(q_k, q_{k+1}) = \alpha h P_{|q_k} \left( \tilde{\Lambda}((1 - \alpha)q_{k-1} + \alpha q_k, \frac{q_k - q_{k-1}}{h}) \right)$$

$$+ (1 - \alpha) h \tilde{\Lambda}((1 - \alpha)q_k + \alpha q_{k+1}, \frac{q_{k+1} - q_k}{h}), \quad 1 \leq k \leq N - 1 ,$$

with initial condition satisfying

$$-\mu^a_i(q_0) g^{ij}(q_0) \frac{\partial S^h_{\alpha}}{\partial q_0^i}(q_0, q_1) + (1 - \alpha) h \mu^a_i(q_0) g^{ij}(q_0) \tilde{\Lambda}_j((1 - \alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h})) = 0 .$$
Example 5.1 (The nonholonomic particle revisited)

\[
\frac{1}{1 + y_1^2} \left( \frac{x_1 - x_0}{h} - \frac{h}{2} \frac{x_1 + x_0}{2} \right) - \frac{x_2 - x_1}{h} \frac{x_2 + x_1}{2} + \frac{y_1}{1 + y_1^2} \left( \frac{z_1 - z_0}{h} \right)
\]

\[
= -\frac{h}{2} \left[ \frac{1}{1 + y_1^2} \frac{\left( x_1 - x_0 \right) \left( y_1 + y_0 \right)}{2} - \frac{\left( x_1 - x_0 \right) \left( y_1 - y_0 \right)}{h^2} \right] \cdot y_1 + y_0 + \frac{x_2 + x_1}{2} - \frac{\left( x_2 - x_1 \right) \left( y_2 - y_1 \right)}{h^2} \cdot \frac{y_2 + y_1}{2}
\]

\[
\frac{y_1 - y_0}{h} - \frac{h}{2} \frac{y_1 + y_0}{2} - \frac{y_2 - y_1}{h} - \frac{y_2 + y_1}{2} = 0 ,
\]

\[
\frac{y_1^2}{1 + y_1^2} \frac{\left( z_1 - z_0 \right)}{h} - \frac{z_2 - z_1}{h} + \frac{y_1}{1 + y_1^2} \left( \frac{x_1 - x_0}{h} \right) - \frac{x_1 + x_0}{2}
\]

\[
= \frac{h}{2} \left[ \frac{y_1^2}{1 + y_1^2} \frac{\left( x_1 - x_0 \right) \left( y_1 + y_0 \right)}{2} - \frac{\left( x_1 - x_0 \right) \left( y_1 - y_0 \right)}{h^2} \right] + \frac{\left( x_2 + x_1 \right) \left( y_2 + y_1 \right)}{2} - \frac{\left( x_2 - x_1 \right) \left( y_2 - y_1 \right)}{h^2} \cdot \frac{y_1 + y_0}{2}
\]

with initial condition satisfying

\[
\varphi^o (x_0, y_0, z_0, x_1, y_1, z_1, h) = -\frac{z_1 - z_0}{h} - \frac{\left( x_1 + x_0 \right) \left( y_1 + y_0 \right)}{2} - \frac{\left( x_1 - x_0 \right) \left( y_1 - y_0 \right)}{h^2} \cdot \frac{y_1 + y_0}{2}
\]

\[
+ y_0 \left[ \frac{x_1 - x_0}{h} + \frac{h}{2} \frac{x_1 + x_0}{2} - \frac{\left( x_1 + x_0 \right) \left( y_1 + y_0 \right)}{2} - \frac{\left( x_1 - x_0 \right) \left( y_1 - y_0 \right)}{h^2} \cdot \frac{y_1 + y_0}{2} \right]
\]

For the same initial conditions and data, the following graph shows the exact preservation of the constraint function evolution with time of our algorithm.
6 Conclusion

A new numerical algorithm has been proposed for nonholonomic mechanics. This algorithm is based in the underlying geometry of nonholonomic systems. For mechanical systems with linear constraints, a geometric integrator preserving constraints is proposed.

In future work, we will explore reduction schemes for discrete systems using the approach of generating functions. It is also interesting to use generating functions of different kinds; in a recent work [31], we have shown that generating functions of second class generate algorithms which are symplectic (in some sense) for discrete optimal control theory (see also [32]). Moreover, we may easily extend the generating function technique in order to consider variable time stepping and also the time-dependent case and it would be possible to use this formalism for classical field theories.

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