High-order Geometric Nonholonomic Integrators on Vector Spaces and Lie Groups

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Abstract

We have obtained geometrically consistent arbitrarily high-order partitioned Runge-Kutta integrators for nonholonomic systems, both on vector spaces and Lie groups. These methods differ from those of J. Cortés and S. Martínez [1] in that we do not require the discretisation of the constraint, and contrary to L. Jay's SPARK integrators [2] we do not require extraneous combinations of constraint evaluations. Our methods preserve the continuous constraint exactly and can be seen to extend those of M. de León, D. Martín de Diego and A. Santamaría [3].

Introduction to Nonholonomic Mechanics

A mechanical system on a smooth manifold Q is defined by a Lagrangian function $L : TQ \to \mathbb{R}$ and the evolution equations derived from it. For **unconstrained and holonomically constrained** systems these equations can be derived from a **variational** principle called *Hamilton's principle*.

Nonholonomic mechanics is the study of constrained mechanical systems with constraint manifold $N \subset TQ$, which in most cases is a vector subbundle completely described by a non-integral distribution D. In simpler terms these systems have velocity constraints which cannot be reduced to position constraints (such is the case of a rolling disk). It differs from its holonomic counterpart in that its evolution equations are **not variational**. These must be found using the *Lagrange-D'Alembert principle* and so are related to forced systems. Still, the resulting equations are very similar to those of holonomically constrained systems. These take the form:

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} = \left\langle \lambda, \frac{\partial \Phi}{\partial \dot{q}^i} \right\rangle \\ \Phi(q, \dot{q}) = 0 \end{cases}$$

where λ are Lagrange multipliers and $\Phi : TQ \to \mathbb{R}^m$, with $m = \operatorname{codim} N$, are called constraint functions. Locally, when N is a vector subbundle, the constraint takes the form $\Phi_\alpha(q, v) = \mu_{i,\alpha}(q) v^i$, $\alpha = 1, \ldots, m$.

Discrete Mechanics and Variational Integrators

From the Lagrangian of the system we can define another function called energy, $E_L = \Delta L - L$. L is said to be hyperregular if its **fibre derivative** $\mathbb{F}L : TQ \to T^*Q$ $(q, \dot{q}) \mapsto \left(q, \frac{\partial L}{\partial \dot{q}}(q, \dot{q})\right)$ is a global diffeomorphism. In this case we can define the Hamiltonian of the system as $H = E_L \circ \mathbb{F}L^{-1}$. Let $S : Q \times Q \times \mathbb{R} \to \mathbb{R}$ be a complete solution of the *Hamilton-Jacobi PDE*:

$$H\left(q_1, \frac{\partial S}{\partial q_1}(q_0, q_1, t)\right) = \frac{\partial S}{\partial t}(q_0, q_1, t)$$

S defines a pair of diffeomorphisms $\mathbb{F}S^{\pm} : Q \times Q \to T^*Q$ called **discrete fibre derivatives**:

$$\begin{tikzcd}
 & (q_0, q_1) \arrow[dl, "\mathbb{F}S^-"'] \arrow[dr, "\mathbb{F}S^+"] & \\
\left(q_0, p_0 = -\frac{\partial S}{\partial q_0}(q_0, q_1, t)\right) \arrow[rr, mapsto, "F_h"] & & \left(q_1, p_1 = \frac{\partial S}{\partial q_1}(q_0, q_1, t)\right)
\end{tikzcd}$$

and its induced flow $F_h : T^*Q \to T^*Q$ is symplectic, i.e., $F_h^* \omega_Q - \omega_Q = 0$, where ω_Q is the symplectic form in T^*Q. Such an S is *Jacobi's solution*:

$$S(q_0, q_1, t) = \int_0^t L(q(\tau), \dot{q}(\tau)) \mathrm{d}\tau, \text{ with } q \text{ extremal, } q(0) = q_0,\ q(t) = q_1$$

A **discrete Lagrangian** $L_d : Q \times Q \times \mathbb{R}$ is an approximation of the former integral via numerical quadrature:

$$L_d(q_0, q_1, h) \approx h \sum_{i=0}^{s} b_i L(Q^i, V^i), \text{ with appropriately chosen } (Q^i, V^i)$$

The discrete Lagrangian for a certain discrete trajectory $\{q_i\}_{i=0}^{N}$ can be obtained by addition as $L_d(q_0, q_N, Nh) = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}, h)$. Performing the discrete analogue of *Hamilton's principle* we obtain the so-called **discrete Euler-Lagrange equations**:

$$D_2 L_d(q_{k-1}, q_k, h) + D_1 L_d(q_k, q_{k+1}, h) = 0 \Leftrightarrow p_k^-(q_{k-1}, q_k) = p_k^+(q_k, q_{k+1})$$

These equations define numerical integrators for our mechanical system having the property of preserving symplecticity and having excellent long term energy behaviour [5], [4]. The resolution scheme for an IVP becomes:

$$\begin{tikzcd}
Q \times Q : & & (q_0, q_1) \arrow[rr, mapsto, "F_{L_d}"] \arrow[dr, mapsto, "\mathbb{F}L_d^+"] & & (q_1, q_2) \arrow[dl, mapsto, "\mathbb{F}L_d^-"'] \arrow[dr, mapsto, dashed, "\mathbb{F}L_d^+"] & \\
T^*Q : & (q_0, p_0) \arrow[ur, mapsto, "\left(\mathbb{F}L_d^-\right)^{-1}"] \arrow[rr, mapsto, "\tilde{F}_h"] & & (q_1, p_1) \arrow[rr, mapsto, dashed, "\tilde{F}_h"] & & {} \\
TQ : & (q_0, v_0) \arrow[u, mapsto, "\mathbb{F}L"] & & & &
\end{tikzcd}$$

Idea

For simplicity we will focus here on systems subjected to **linear nonholonomic constraints**, even though our method will work in the nonlinear case as well. Systems subjected to linear constraints are energy preserving. The flows of nonholonomic systems are **not symplectic**

$$F_h^* \omega_Q - \omega_Q = \mathrm{d}\left(\int_0^h F_t^* \langle \lambda, \mu \rangle\right) \neq 0$$

yet the use of symplectic algorithms is attractive given their *geometric correctness* and *long term energy behaviour*, which *remains true* in the linear nonholonomic case.

Also for simplicity we will require the Lagrangian of our system to be hyperregular (with a slight modification it is possible to work with regular ones). Thus we may find a constraint subbundle $M \subset T^*Q$ and constraint functions $\Psi : T^*Q \to \mathbb{R}^m$. We begin by discretising the Lagrange-D'Alembert principle:

$$\delta \int_0^{Nh} L(q(\tau), \dot{q}(\tau)) \mathrm{d}\tau + \int_0^{Nh} \langle \lambda, \mu_i \rangle \delta q^i \mathrm{d}t = 0$$

by mimicking the variational results of the holonomic case ([4], [6]):

$$\delta \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}) + h \sum_{k=0}^{N-1} \sum_{i=1}^{s} b_i \left[\left\langle \Lambda_k^i, \mu_i(q_k^i) \frac{\partial q_k^i}{\partial q_k} \right\rangle \cdot \delta q_k + \left\langle \Lambda_k^i, \mu_i(q_k^i) \frac{\partial q_k^i}{\partial q_{k+1}} \right\rangle \cdot \delta q_{k+1} \right]$$

Apart from this, for consistence we must impose the constraints at **every single point** in the trajectory, not only on $\{(q_k, p_k)\}_{k=0}^{N}$ but on every inner step as well $\left\{(q_k^i, p_k^i)\right\}_{k=0,i=1}^{N,s}$, just as in the holonomic case. Instead of artificially generating constraints on $Q \times Q$ from $\Phi(q, \dot{q})$, it is most natural to work with $\Psi(q, p)$:

$$\Psi(q_k, p_k) = 0,\ \Psi(q_k^i, p_k^i) = 0,\ \forall k \in [0, N], \forall i \in [1, s]$$

For the set of resulting equations to be solvable we must restrict to those discretisations where $q_k^1 = q_k$ and $q_k^s = q_{k+1}$, which are collocation methods of the Lobatto type. Partitioned Runge-Kutta methods provide us with a set of inner step values usually noted as (Q_k^i, P_k^i), $\forall i \in [2, s-1]$, where if the Q_k^i come from a continuous collocation method, then the P_k^i come from a discontinuous collocation method. These P_k^i are **not suitable** for our purposes as they diminish the order of our method.

Algorithm

We propose a simple and natural way to generate correct order p_k^i from existing computed values in the integration. The resulting algorithm is as follows:

$$\begin{aligned}
q_{k+1} &= q_k + h \sum_{i=1}^{s} b_i V_k^i, & p_{k+1} &= p_k + h \sum_{i=1}^{s} \tilde{b}_i W_k^i, & q_k^i &= Q_k^i \\
Q_k^i &= q_k + h \sum_{j=1}^{s} a_{ij} V_k^j, & P_k^i &= p_k + h \sum_{j=1}^{s} \tilde{a}_{ij} W_k^j, & p_k^i &= p_k + h \sum_{j=1}^{s} a_{ij} W_k^j \\
W_k^i &= D_1 L(Q_k^i, V_k^i) + \left\langle \Lambda_k^i, D_2 \Phi(Q_k^i, V_k^i) \right\rangle & P_k^i &= D_2 L(Q_k^i, V_k^i) & 0 &= \Psi(q_k^i, p_k^i)
\end{aligned}$$

The work flow of the algorithm is still the same, although we need λ_0 too as an initial condition, which may be obtained from the continuous realm.

$$(q_0, v_0, \lambda_0) \in N \times \mathbb{R}^m \xmapsto{\mathbb{F}L} (q_0, p_0, \lambda_0) \in M \times \mathbb{R}^m \xmapsto{\tilde{F}_h} (q_1, p_1, \lambda_1) \in M \times \mathbb{R}^m \overset{\tilde{F}_h}{\dashrightarrow}$$

Theorem s-stage Lobatto IIIA-IIIB partitioned Runge-Kutta methods of this type preserve the nonholonomic constraint exactly and their order is the same as the order of its corresponding continuous collocation method $p = 2s - 2$.

One can compose methods as usual to easily obtain even higher order methods. This scheme can also be transposed to Runge-Kutta Munthe-Kaas type Lie group methods when $Q = G$, Lie group (cf. [6], [7]):

$$\begin{aligned}
\xi_{k,k+1} &= h \sum_{j=1}^{s} b_j \eta_k^j, \quad \left(\mathrm{d}^L \tau^{-1}_{-\xi_{k,k+1}}\right)^* \mu_{k+1} = \left(\mathrm{d}^L \tau^{-1}_{\xi_{k-1,k}}\right)^* \mu_k + h \sum_{j=1}^{s} b_j \left(\mathrm{d}^L \tau^{-1}_{-\xi_k^j}\right)^* \mathrm{N}_k^j, \\
\xi_k^i &= h \sum_{j=1}^{s} a_{ij} \eta_k^j, \quad \left(\mathrm{d}^L \tau^{-1}_{-\xi_{k,k+1}}\right)^* \mathrm{M}_k^i = \left(\mathrm{d}^L \tau^{-1}_{\xi_{k-1,k}}\right)^* \mu_k + h \sum_{j=1}^{s} b_j \left(\mathrm{d}^L \tau^{-1}_{-\xi_k^j} - \frac{a_{ji}}{b_i} \mathrm{d}^L \tau^{-1}_{-\xi_{k,k+1}}\right)^* \mathrm{N}_k^j,
\end{aligned}$$

$$\left(\mathrm{d}^L \tau^{-1}_{-\xi_k^i}\right)^* \mu_k^i = \left(\mathrm{d}^L \tau^{-1}_{\xi_{k-1,k}}\right)^* \mu_k + h \sum_{j=1}^{s} a_{ij} \left(\mathrm{d}^L \tau^{-1}_{-\xi_k^j}\right)^* \mathrm{N}_k^j$$

$$\mathrm{N}_k^i = \left(\mathrm{d}^L \tau_{\xi_k^i}\right)^* \left[L^*_{g_k \tau(\xi_k^i)} D_1 \ell\left(g_k \tau(\xi_k^i), \mathrm{d}^L \tau_{\xi_k^i} \eta_k^i\right) + \left\langle D_2 \phi\left(g_k \tau(\xi_k^i), \mathrm{d}^L \tau_{\xi_k^i} \eta_k^i\right), \Lambda_k^i \right\rangle \right]$$

$$\mathrm{M}_k^i = \left(\mathrm{d}^L \tau_{\xi_k^i}\right)^* D_2 \ell\left(g_k \tau(\xi_k^i), \mathrm{d}^L \tau_{\xi_k^i} \eta_k^i\right) + h \sum_{j=1}^{s} \frac{b_j a_{ji}}{b_i} \left(\mathrm{dd}^L \tau_{\xi_k^j}\right)^* \left(\eta_k^j, \left(\mathrm{d}^L \tau_{\xi_k^i}\right)^* D_2 \ell\left(g_k \tau(\xi_k^i), \mathrm{d}^L \tau_{\xi_k^i} \eta_k^i\right)\right)$$

$$\psi\left(g_k^i, \left(\mathrm{d}^L \tau^{-1}_{\xi_k^i}\right)^* \mu_k^i\right) = 0, \qquad g_{k+1} = g_k \tau\left(\xi_{k,k+1}\right), \qquad g_k^i = g_k \tau\left(\xi_k^i\right).$$

where $\ell, \phi, \psi : G \times \mathfrak{g} \to \mathbb{R}$ are the corresponding reduced L, Φ, Ψ. $(\xi, \eta) \in T\mathfrak{g}$, $\mu \in \mathfrak{g}^*$. $\tau : \mathfrak{g} \to G$ local diffeomorphism, $\mathrm{d}^L \tau : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, such that $T_\xi \tau \eta = L_{\tau(\xi)_*} \mathrm{d}^L \tau_\xi \eta$, and $\mathrm{dd}^L \tau : \mathfrak{g} \times \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, such that $\partial_\xi \left(\mathrm{d}^L \tau_\xi \eta\right) \zeta = \mathrm{d}^L \tau_\xi \mathrm{dd}^L \tau_\xi (\eta, \zeta)$.

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