Geometric Integration of Degenerate Lagrangian Systems

Michael Kraus

The Geometric Numerical Integration literature describes numerous structure-preserving algorithms for canonical Hamiltonian and regular Lagrangian systems. Noncanonical Hamiltonian and degenerate Lagrangian systems, on the other hand, are rarely discussed. Such systems play an important role in reduced charged particle dynamics like the guiding centre model, magnetic field line flow, population dynamics like the Lotka–Volterra model, or nonlinear oscillators. The following is a short overview of the issues that arise when discretising such systems and a discussion of possible strategies for their structure-preserving integration.

The most general form of the dynamical equations of a Hamiltonian system, also referred to as Poisson system, with state vector $q \in \mathbb{R}^m$ is

$$\dot{q} = \mathcal{P}(q) \, \nabla H(q). \tag{1}$$

Here, $\mathcal{P}(q)$ is an anti-symmetric matrix, possibly degenerate, satisfying

$$\sum_{l=1}^{m} \left[\frac{\partial \mathcal{P}^{ij}(q)}{\partial q^l} \, \mathcal{P}^{lk}(q) + \frac{\partial \mathcal{P}^{jk}(q)}{\partial q^l} \, \mathcal{P}^{li}(q) + \frac{\partial \mathcal{P}^{ki}(q)}{\partial q^l} \, \mathcal{P}^{lj}(q) \right] = 0 \ \text{ for } 1 \leq i, j, k \leq m.$$

In the following, we are concerned with a special case of such systems, namely noncanonical symplectic systems. In that case $\mathcal{P}(q)$ is even-dimensional ($m = 2d$), non-degenerate and thus invertible, so that we can write

$$\mathcal{P}(q) = \Omega^{-1}(q), \tag{2}$$

with Ω a noncanonical symplectic form whose components are in general nonlinear functions of the state variables q. If Ω is constant and takes the values

$$\Omega_c = \begin{pmatrix} \mathbb{0} & -\mathbb{1} \\ \mathbb{1} & \mathbb{0} \end{pmatrix},$$

the system is said to be of canonical symplectic form and with $q = (q, p)$ and $q, p \in \mathbb{R}^d$ Equation (1) recovers Hamilton's equations,

$$\dot{q} = \frac{\partial H}{\partial p}, \qquad \dot{p} = - \frac{\partial H}{\partial q}. \tag{3}$$

Noncanonical symplectic systems are tightly linked to a special class of degenerate Lagrangian systems whose Lagrangian is linear in velocities and given by

$$L(q, \dot{q}) = \vartheta(q) \cdot \dot{q} - H(q). \tag{4}$$

The corresponding Euler–Lagrange equations,

$$\frac{\partial L}{\partial q}(q, \dot{q}) - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}}(q, \dot{q}) \right) = 0, \tag{5}$$

are equivalent to (1) in the case of (2). Here, the symplectic potential ϑ is a general, possibly nonlinear function $\mathbb{R}^{2d} \to \mathbb{R}^{2d}$, such that $\Omega = \mathsf{d}\vartheta$, with d denoting the exterior derivative. Note that by mild abuse of notation we do not distinguish between differential forms ϑ and Ω and their components in some local basis.

This connection suggests that variational integrators [2] should provide suitable means for the construction of structure-preserving integrators for noncanonical symplectic systems. Let us denote the discrete trajectory by $q_d = \{q_n\}_{n=0}^N$. A discrete Lagrangian is constructed as a function of two consecutive points (q_n, q_{n+1}) along that trajectory, by approximating the continuous Lagrangian L via finite difference, Runge–Kutta or other suitable methods. For example, a simple midpoint approximation is given by

$$L_d(q_n, q_{n+1}) = h\, L\left(\frac{q_n + q_{n+1}}{2}, \frac{q_{n+1} - q_n}{h}\right). \tag{6}$$

In a similar fashion as in the continuous case, Hamilton's principle of stationary action leads to the discrete Euler–Lagrange equations,

$$D_2 L_d(q_{n-1}, q_n) + D_1 L_d(q_n, q_{n+1}) = 0 \quad \text{for all} \quad n, \tag{7}$$

where D_i denotes thederivative w.r.t. the i-th argument. In the specific case of degenerate Lagrangians, for which the continuous Euler–Lagrange equations are first-order differential equations, the discrete Euler–Lagrange equations constitute a multi-step method. This implies that these integrators are susceptible to parasitic modes and require two sets of initial data even though the continuous Euler–Lagrange equations are of first order.

A remedy for the initialisation issue can be found by using the discrete fibre derivative to rewrite the discrete Euler–Lagrange equations (7) in the so-called position-momentum (PM) form

$$\begin{aligned} p_n \quad &= -D_1 L_d(q_n, q_{n+1}), \\ p_{n+1} &= \quad D_2 L_d(q_n, q_{n+1}). \end{aligned} \tag{8}$$

Given (q_n, p_n), this system can be solved for (q_{n+1}, p_{n+1}) if the discrete Lagrangian L_d is non-degenerate, i.e.,

$$\det \left| \frac{\partial^2 L_d}{\partial q_n^i \, \partial q_{n+1}^j} \right| \neq 0.$$

Interestingly, most discrete Lagrangians like (6) are non-degenerate even if the corresponding continuous Lagrangian L is degenerate. With the PM-form (8), the continuous fibre derivative can be used to obtain a second initial condition p_0 as function of q_0,

$$p_0 = \frac{\partial L}{\partial \dot{q}}(q_0) = \vartheta(q_0).$$

While this solves the initialisation problem, it does not solve the problem of parasitic modes. Nonetheless, the PM-formulation provides an interesting geometric picture of the parasitic modes developing in solutions of the variational integrator. Introducing the PM-form implicitly amounted to rewriting the equations of motion as an index-two differential-algebraic system,

$$\dot{z} = \Omega_c^{-1}\big(\nabla H(z) + \nabla \phi^T(z)\, v\big), \quad 0 = \phi(z) = p - \vartheta(q), \quad z = (q, p). \tag{9}$$

The problem that arises, is that the variational integrator does not preserve the constraint $\phi(z) = 0$, so that the numerical solution drifts away from the constraint submanifold, i.e., $p_n \neq \vartheta(q_n)$ for $n \geq 1$, even though $p_0 = \vartheta(q_0)$.

This can be remedied by combining the PM-form (8) with projection methods [3]. In particular, symmetric projection methods [1] show very good long-time stability and energy conservation properties, although the resulting projected variational integrators are usually not symplectic. In a similar but more general fashion, applying the SPARK methodology [6] to (9) leads to a large variety of integrators, many of which exhibit good properties although not being symplectic.

For certain degenerate Lagrangians, it is also possible to construct symplectic Runge–Kutta methods as well as one-step variational integrators. This applies to Lagrangians (4) with $q \in \mathbb{R}^{2d}$ and ϑ such that d of its components vanish,

$$\vartheta_\mu = 0 \qquad \text{for} \qquad \mu = d+1, \dots, 2d.$$

In this case, the following family of Runge–Kutta methods can be shown to be symplectic [7],

$$
\begin{aligned}
Q_{n,i} &= q_n + h \sum_{j=1}^{s} a_{ij}\, V_{n,j}, & P_{n,i} &= \frac{\partial L}{\partial \dot{q}}(Q_{n,i}, V_{n,i}), \\
P_{n,i} &= p_n + h \sum_{j=1}^{s} a_{ij}\, F_{n,j}, & F_{n,i} &= \frac{\partial L}{\partial q}(Q_{n,i}, V_{n,i}), \\
q_{n+1}^{\mu} &= q_n^{\mu} + h \sum_{i=1}^{s} b_i\, V_{n,i}^{\mu}, & \mu &= 1, \dots, d, \\
p_{n+1}^{\mu} &= p_n^{\mu} + h \sum_{i=1}^{s} b_i\, F_{n,i}^{\mu}, & \mu &= 1, \dots, d, \\
p_{n+1}^{\mu} &= \vartheta^{\mu}(q_{n+1}), & \mu &= 1, \dots, 2d,
\end{aligned}
$$

if the usual condition holds, namely

$$b_i b_j = b_i a_{ij} + b_j a_{ji}.$$

Note that the same tableau a_{ij} is used for the internal stages of both q and p.

For this specific type of degenerate Lagrangians, it is also possible to construct single-step variational integrators, referred to as Degenerate Variational Integrators (DVIs). It was already pointed out that, although the continuous Lagrangian is degenerate, the corresponding discrete Lagrangians typically are not. Thus a decisive structural property of the continuous system is lost in discretisation: it's degeneracy. When the degeneracy is retained in the discrete Lagrangian, the discrete Euler–Lagrange equations (7) constitute one-step methods referred to as Degenerate Variational Integrators (DVIs) [4, 5]. For simplicity, consider the Lagrangian

$$L(q^1, q^2, \dot{q}^1, \dot{q}^2) = \vartheta_1(q^1, q^2) \cdot \dot{q}^1 - H(q^1, q^2),$$

which is discretised as

$$L_d(q_n^1, q_n^2, q_{n+1}^1, q_{n+1}^2) = h\left[\vartheta_1(q_n^1, q_n^2) \cdot \frac{q_{n+1}^1 - q_n^1}{h} - H(q_n^1, q_n^2)\right].$$

The discrete Euler–Lagrange equations (7) can be written as

$$\begin{aligned}
\vartheta_1(q_n^1, q_n^2) &= \vartheta_1(q_{n-1}^1, q_{n-1}^2) + h\nabla_1\vartheta_1(q_n^1, q_n^2) \cdot v_n^1 \\
&\qquad\qquad - h\nabla_1 H(q_n^1, q_n^2), && \text{for } n = 1, ..., N-1, \\
v_n^1 &= \big(\nabla_2\vartheta_1(q_n^1, q_n^2)\big)^{-1}\nabla_2 H(q_n^1, q_n^2), && \text{for } n = 0, ..., N-1, \\
q_{n+1}^1 &= q_n^1 + hv_n^1, && \text{for } n = 0, ..., N-1.
\end{aligned}$$

Note that this system is underdetermined, as it lacks equations that determine x_N^2. Motivated by the discrete symplecticity condition following from the boundary values in the action principle [2],

$$\begin{aligned}
\delta\mathcal{A}_d[q_{DEL}] = -\delta q_0^1 \cdot \big[\vartheta_1(q_0^1, q_0^2) - h\nabla_1\vartheta_1(q_0^1, q_0^2) \cdot v_0^1 + h\nabla_1 H(q_0^1, q_0^2)\big] \\
+ \delta q_N^1 \cdot \vartheta_1(q_{N-1}^1, q_{N-1}^2),
\end{aligned}$$

the system is closed by adding the equations

$$\begin{aligned}
\vartheta_1(q_N^1, q_N^2) &= \vartheta_1(q_{N-1}^1, q_{N-1}^2) + h\nabla_1\vartheta_1(q_N^1, q_N^2) \cdot v_N^1 - h\nabla_1 H(q_N^1, q_N^2), \\
v_N^1 &= \big(\nabla_2\vartheta_1(q_N^1, q_N^2)\big)^{-1}\nabla_2 H(q_N^1, q_N^2).
\end{aligned}$$

With this closure, the full set of discrete Euler–Lagrange equations preserves the discrete symplectic form $\Omega_d = \mathsf{d}\vartheta_d$ with potential

$$\vartheta_d(q^1, q^2) = \big[\vartheta_1(q^1, q^2) - h\nabla_1\vartheta_1(q^1, q^2) \cdot v^1 + h\nabla_1 H(q^1, q^2)\big]\, \mathsf{d}q^1.$$

The DVI thus obtained is of first-order [4]. While second-order generalisations also exist [5], higher-order DVIs are currently not known. Moreover this approach is limited to the aforementioned special form of the degenerate Lagrangian and thus not always applicable. This and the previous discussion raise several questions:

(1) Can DVIs be generalised to arbitrary order, using e.g. Galerkin or Runge–Kutta discretisations of the Lagrangian?
(2) Can DVIs [4, 5] and symplectic Runge–Kutta methods [7] be obtained for general degenerate Lagrangians of the form (4), without assuming that any of the components of the symplectic potential ϑ vanish?
(3) Do symplectic Runge–Kutta methods [7] follow from a discrete variational principle?

Addressing these questions is of great practical relevance as geometric integrators for degenerate Lagrangian systems and in particular for the guiding centre model are much-needed in application fields such as astro and fusion plasma physics.

References

[1] E. Hairer, *Symmetric projection methods for differential equations on manifolds*, BIT Numerical Mathematics **40** (2000), 726–734.

[2] J. E. Marsden, M. West, *Discrete mechanics and variational integrators*, Acta numerica **10** (2001), 357–514.

[3] M. Kraus, *Projected Variational Integrators for Degenerate Lagrangian Systems*, Preprint (2017), arXiv:1708.07356.

[4] C. L. Ellison, J. M. Finn, J. W. Burby, M. Kraus, H. Qin, W. M. Tang, *Degenerate variational integrators for magnetic field line flow and guiding center trajectories*, Physics of Plasmas **25** (2018), 052502.

[5] J. W. Burby, J. M. Finn, C. L. Ellison, *Improved accuracy in degenerate variational integrators for guiding center and magnetic field line flow*, Preprint (2021), arXiv:2103.05566.

[6] M. Kraus, *SPARK Methods for Degenerate Lagrangian Systems*, in preparation.

[7] M. Kraus, *Symplectic Runge–Kutta Methods for Degenerate Lagrangian Systems*, in preparation.