

GEOMETRIC NUMERICAL INTEGRATION OF NONHOLONOMIC SYSTEMS AND OPTIMAL CONTROL PROBLEMS

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Abstract: A geometric derivation of numerical integrators for nonholonomic systems and optimal control problems is obtained. It is based in the classical technique of generating functions adapted to the special features of nonholonomic systems and optimal control problems.

Keywords: Geometric integrators, nonholonomic systems, optimal control

1. INTRODUCTION

Standard methods for simulating the motion of a dynamical system usually ignore many of the geometric features of this system (simplecticity, conservation laws, symmetries...). 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 system (see [HaLuWa:02]).

In the first part of the paper, we propose a class of geometric integrators for nonholonomic systems [Leomar:96D,NeiFuf:72] based on a discretization of the Lagrangian function (in a more precise sense, we discretize the action function) and a coherent discretization of the constraint forces (see [LeMaSa:02]). These equations will be conceptually equivalent to the proposed for systems with external forces (see [MarWes:01]). Finally, second part concerns with the construction of symplectic integrators for optimal control theory by using generating functions of the second kind.

2. NONHOLONOMIC SYSTEMS

2.1 Geometrical formulation of nonholonomic systems

Let Q be a n -dimensional differentiable manifold, with local coordinates (q^i) and tangent bundle TQ , with induced coordinates (q^i, \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 ϕ^a (the “constraint functions”), satisfying the rank condition $\text{rank} \left(\frac{\partial \phi^a}{\partial \dot{q}^i} \right) = m$.

In the sequel, we will follow a Hamiltonian point of view. The canonical coordinates on T^*Q (the cotangent bundle of Q) are denoted by (q^i, p_i) . Assume, for simplicity, that the Lagrangian L is hyperregular, that is, 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. $\Psi^a(q^i, p_i) = \phi^a(q^i, \frac{\partial H}{\partial p_i})$, where the Hamiltonian $H : T^*Q \rightarrow \mathbb{R}$ is defined by $H = E_L \circ \text{Leg}^{-1}$. Here, E_L denotes the energy of the system, locally defined by $E_L = \dot{q}^i \frac{\partial L}{\partial \dot{q}^i} - L$. Since

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locally $Leg^{-1}(q^i, p_i) = (q^i, \frac{\partial H}{\partial p_i})$, 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 by using Leg^{-1} .

The equations of motion for the nonholonomic system on T^*Q can now be written as follows (see [CaLeMa:99,Marl:95] and references therein)

$$\begin{cases} \dot{q}^i = \frac{\partial H}{\partial p_i} \\ \dot{p}_i = -\frac{\partial H}{\partial q^i} - \lambda_a \frac{\partial \Psi^a}{\partial p_j} \mathcal{H}_{ji}, \end{cases} \quad (1)$$

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

$$\left(\frac{\partial \Psi^a}{\partial p_j} \mathcal{H}_{ji} \right)(q, p) = \left(\frac{\partial \phi^a}{\partial \dot{q}^i} \circ Leg^{-1} \right)(q, p).$$

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 $F^\circ = Leg_*(\tilde{F}^\circ)$. Here, \tilde{F}° represents the constraint forces subbundle, locally defined by

$$\tilde{F}^\circ = \text{span}\{\mu^\alpha = \frac{\partial \phi^\alpha}{\partial \dot{q}^i} dq^i\}$$

The Hamiltonian equations of motion of the nonholonomic system can be then rewritten in intrinsic form as

$$\begin{aligned} (i_X \omega_Q - dH)|_M &\in F^\circ \\ X|_M &\in TM, \end{aligned} \quad (2)$$

where $\omega_Q = -d\theta_Q = dq^i \wedge dp_i$ (with $\theta_Q = p_i dq^i$) is the canonical symplectic form on T^*Q . Suppose in addition that the following *compatibility condition* $F^\perp \cap TM = \{0\}$ holds, where “ \perp ” denotes the symplectic orthogonal with respect to ω_Q . Observe that, locally, this condition means that the matrix $(C^{ab}) = \left(\frac{\partial \Psi^a}{\partial p_i} \mathcal{H}_{ij} \frac{\partial \Psi^b}{\partial p_j} \right)$ is regular. The compatibility condition is not too restrictive, since 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 \mathcal{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 (2) which, henceforth, will be denoted by $X_{H,M}$ on the Hamiltonian side and $Leg_*^{-1}(X_{H,M}) = \xi_{L,D}$ on the Lagrangian side.

Moreover, if we denote by X_H the Hamiltonian function of H , i.e., $i_{X_H} \omega_Q = dH$ then, using the constraint functions, we may explicitly determine the Lagrange multipliers λ_a as $\lambda_a = -\mathcal{C}_{ab} X_H(\Psi^b)$. Next, writing the 1-form $\Lambda = -\mathcal{C}_{ab} X_H(\Psi^b) \frac{\partial \Psi^a}{\partial p_j} \mathcal{H}_{ji} dq^i$ then, the nonholonomic equations are equivalently rewritten as

$$\begin{cases} \dot{q}^i = \frac{\partial H}{\partial p_i}, \\ \dot{p}_i = -\frac{\partial H}{\partial q^i} - \Lambda_i, \end{cases} \quad (3)$$

for initial conditions $(q_0, p_0) \in M$ and $\Lambda = \Lambda_i dq^i$. We also denote by $\tilde{\Lambda} = Leg^*(\Lambda)$ the 1-form on TQ which represents the constraint force once the Lagrange multipliers have been determined.

Now, consider the flow $F_t : M \rightarrow M$, $t \in I \subseteq \mathbb{R}$ of the vector field $X_{H,M}$, solution of the nonholonomic problem. Since (3) is geometrically rewritten as

$$i_{X_{H,M}} \omega_Q = dH + \Lambda,$$

then

$$L_{X_{H,M}} \theta_Q = d(i_{X_{H,M}} \theta_Q - H) - \Lambda,$$

or, equivalently, $L_{X_{H,M}} \theta_Q = d(L \circ Leg^{-1}) - \Lambda$. Therefore, integrating

$$F_h^* \theta_Q - \theta_Q = d \left(\int_0^h L \circ \tilde{F}_t dt \right) - \int_0^h F_t^* \Lambda, \quad (4)$$

where \tilde{F}_t is the flow of the vector field $\xi_{L,D}$.

2.2 “Generating functions” and nonholonomic mechanics

In what follows, we will follow similar arguments for the construction of generating functions for symplectic or canonical maps [Arn:78]. However, because of equation (4), we have that the nonholonomic flow is not a canonical transformation; i.e.,

$$F_h^* \omega_Q - \omega_Q = d \left(\int_0^h F_t^* \Lambda \right). \quad (5)$$

This description will allow us to construct a new family of nonholonomic integrators for equations (19). Denote by $\pi_i : T^*Q \times T^*Q \rightarrow T^*Q$, $i = 1, 2$, the canonical projections. Consider the following forms

$$\begin{aligned} \Theta &= \pi_2^* \theta_Q - \pi_1^* \theta_Q, \\ \Omega &= \pi_2^* \omega_Q - \pi_1^* \omega_Q = -d\Theta. \end{aligned}$$

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 (4) $i_{F_h}^* \Theta$ is equal to

$$(\pi_1|_{\text{Graph}(F_h)})^* \left[d \left(\int_0^h L \circ \tilde{F}_t dt \right) - \int_0^h F_t^* \Lambda \right].$$

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 $\text{Graph}(F_h)$, $q_1 = q_1(q_0, p_0)$, $p_1 = p_1(q_0, p_0)$ and

$$p_1 dq_1 - p_0 dq_0 = d \left(\int_0^h L(q(t), \dot{q}(t)) dt \right) - \int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)), \quad (6)$$

where $(q(t), \dot{q}(t)) = \tilde{F}_t(q_0, \dot{q}_0)$ with $Leg(q_0, \dot{q}_0) = (q_0, p_0)$. Here, \tilde{F}_t denotes the flow of $\xi_{L,D}$. Equation (6) 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 $q(h) = q_1$ and an adequate extension of S^h . It is easy to show that this solution always exists for adequate values of q_0 and q_1 .

Thus, we deduce that

$$\begin{cases} p_0 = -\frac{\partial S^h}{\partial q_0} + \int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_0}, \\ p_1 = \frac{\partial S^h}{\partial q_1} - \int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_1}, \end{cases} \quad (7)$$

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

$$\varphi^a(q_0, q_1, h) = \Psi^a(q_0, -\frac{\partial S^h}{\partial q_0}(q_0, q_1) + \int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_0}), \quad (8)$$

where $q(t)$ is a solution of the nonholonomic problem with $q(0) = q_0$ and $q(h) = q_1$.

Next, we will show how the group composite law of the flow F_h , $F_{Nh} = \underbrace{F_h \circ \dots \circ F_h}_N$, 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.

Theorem 2.1. 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

$$D_2 S^h(q_{k-1}, q_k) + D_1 S^h(q_k, q_{k+1}) = \int_0^h \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_1} + \int_h^{2h} \tilde{\Lambda}(q(t), \dot{q}(t)) \frac{\partial q}{\partial q_0}, \quad (9)$$

and $q(t)$ is a solution curve of the nonholonomic problem with $q(0) = q_{k-1}$ and $q(h) = q_k$ (respec-

tively, $q(h) = q_k$ and $q(2h) = q_{k+1}$) for the first integral (resp., second integral) of the right-hand side.

Proof: It 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 (9).

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

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

Since the variables q_1 do not appear on the left-hand side term, we obtain expression (9). Moreover, for this choice of q_1 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} . ■

Equations (9) determine an implicit system of difference equations which permit us to obtain q_2 from the initial data q_0 and q_1 .

2.3 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 $q(h) = q_1$, 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

$$S_\alpha^h(q_0, q_1) = hL((1-\alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h}), \quad (10)$$

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

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, we obtain the following numerical method for nonholonomic systems

$$D_2 S_\alpha^h(q_{k-1}, q_k) + D_1 S_\alpha^h(q_k, q_{k+1}) = \alpha h \tilde{\Lambda}((1-\alpha)q_{k-1} + \alpha q_k, \frac{q_k - q_{k-1}}{h}) + (1-\alpha)h \tilde{\Lambda}((1-\alpha)q_k + \alpha q_{k+1}, \frac{q_{k+1} - q_k}{h}),$$

with $1 \leq k \leq N-1$ and initial condition satisfying

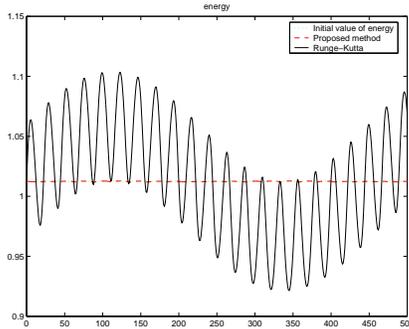
$$\tilde{\varphi}^a(q_0, q_1, h) = \Psi^a(q_0, -\frac{\partial S_\alpha^h}{\partial q_0}(q_0, q_1) + (1-\alpha)h \tilde{\Lambda}((1-\alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h})) = 0.$$

Example 2.2. Nonholonomic particle.

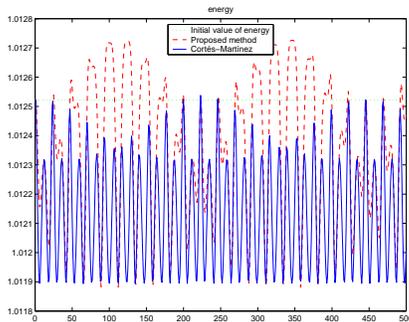
Consider the Lagrangian $L : T\mathbb{R}^3 \rightarrow \mathbb{R}$

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

subject to the constraint $\phi = \dot{z} - y\dot{x} = 0$. Taking $\alpha = 1/2$ in (10) we obtain a geometric integrator for the continuous nonholonomic problem. 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.



The second figure is a comparison between our method and the one proposed in [CorMar:01]. 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.



3. OPTIMAL CONTROL THEORY

3.1 Geometric formulation of optimal control problems

A general optimal control problem consists of a set of differential equations

$$\dot{q}^i = \Gamma^i(q(t), u(t)), \quad 1 \leq i \leq n, \quad (11)$$

where q^i denote the states and u the control variables, and a cost function $L(q, u)$. Given some boundary conditions (usually $q_0 = q(t_0)$ and $q_F = q(t_f)$) the aim is to find a C^2 -piecewise smooth curve $c(t) = (q(t), u(t))$, satisfying the control equations (11) and minimizing the functional

$$\mathcal{J}(c) = \int_{t_0}^{t_f} L(q(t), u(t)) dt. \quad (12)$$

In a global description, one assumes a fiber bundle structure $\pi : U \rightarrow Q$, where Q is the configuration manifold with local coordinates q^i and U is the bundle of controls, with local coordinates (q^i, u^a) , $1 \leq i \leq n$, $1 \leq a \leq m$.

The ordinary differential equations (11) on Q depending on the parameters u can be seen as a vector field Γ along the projection map π , that is, Γ is a smooth map $\Gamma : U \rightarrow TB$ such that the diagram

$$\begin{array}{ccc} U & \xrightarrow{\Gamma} & TQ \\ & \searrow \pi & \swarrow \tau_Q \\ & & Q \end{array}$$

is commutative. This vector field is locally written as $\Gamma = \Gamma^i(q, u) \frac{\partial}{\partial q^i}$.

The solutions of such problem are provided by Pontryaguin's maximum principle. If we construct the Hamiltonian function

$$H(q, p, u) = L(q, u) + p_i \Gamma^i(q, u) \quad (13)$$

where p_i , $1 \leq i \leq n$, are now considered as Lagrange's multipliers, then a curve $\gamma : \mathbb{R} \rightarrow U$, $\gamma(t) = (q(t), u(t))$ is an optimal trajectory if there exists functions $p_i(t)$, $1 \leq i \leq n$ such that they are solutions of the Hamilton equations:

$$\begin{cases} \dot{q}^i(t) = \frac{\partial H}{\partial p_i}(q(t), p(t), u(t)) \\ \dot{p}_i(t) = -\frac{\partial H}{\partial q^i}(q(t), p(t), u(t)) \end{cases} \quad (14)$$

and

$$H(q(t), p(t), u(t)) = \min_v H(q(t), p(t), v), \quad (15)$$

with $t \in [t_0, t_f]$. This last condition is usually replaced by

$$\frac{\partial H}{\partial u^a} = 0, \quad 1 \leq a \leq m \quad (16)$$

when we are looking for extremal trajectories.

It is well known that the Pontryaguin's necessary conditions for extremality have a geometric interpretation in terms of presymplectic hamiltonian system. The total space of the system will be $T^*Q \times_Q U$. Let ω_Q be the canonical symplectic form on T^*Q and consider the canonical projection $\text{pr}_1 : T^*Q \times_Q U \rightarrow T^*Q$. Denote by $\omega = \text{pr}_1^* \omega_Q$ the induced closed 2-form on $T^*Q \times_Q U$. The 2-form ω is degenerate and its characteristic distribution is locally spanned by $\partial/\partial u^a$, $1 \leq a \leq m$. Define the Pontryaguin's hamiltonian function $H : T^*Q \times_Q U \rightarrow \mathbb{R}$ as follows $H(\alpha_q, u_q) = L(u_q) + \alpha_q(\Gamma(u_q))$ where $\alpha_q \in T_q^*Q$ and $u_q \in \text{pr}^{-1}(q)$. Obviously, the coordinate expression of H is (13).

Equations (14) (15) and (16) are intrinsically written as

$$i_X \omega = dH \quad (17)$$

Applying the Dirac-Bergmann-Gotay-Nester algorithm to the presymplectic system $(T^*Q \times_Q U, \Omega, H)$ we obtain that equations (16) correspond to the primary constraints for the presymplectic system: $\phi^a = \frac{\partial H}{\partial u^a} = 0$. The equations have solution along the first constraint submanifold P_0 determined by the vanishing of the primary constraints. On the points of P_0 there is at least a pointwise solution of Equation (17) but such solutions are not, in general, tangent to P_0 . These points must be removed leaving a subset $P_1 \subset P_0$ (it is assumed $\tan P_1$ is also a submanifold). Then, we have to restrict P_1 to a submanifold where the solutions of (17) are tangent to P_1 . Proceeding further, we obtain a sequence of submanifolds

$$\dots \hookrightarrow P_k \hookrightarrow \dots \hookrightarrow P_2 \hookrightarrow P_1 \hookrightarrow P_0 \hookrightarrow T^*Q \times_Q U$$

If this algorithm stabilizes, i.e. there exists a positive integer $k \in \mathbb{N}$ such that $P_k = P_{k+1}$ and $\dim P_k \neq 0$, then we will obtain a stable submanifold $P_f = P_k$, on which a vector field exists such that

$$(i_X \omega = dH)|_{P_f} \quad (18)$$

The constraints determining P_f are known in the control literature as higher order conditions for optimality. Therefore, a necessary condition for optimality of the curve $\gamma : \mathbb{R} \rightarrow U$, $\gamma(t) = (q(t), u(t))$ will be the existence of a lift $\tilde{\gamma}$ of γ to P_f such that $\tilde{\gamma}$ will be an integral curve of a solution of Equations (18).

In the regular case, the final constraint algorithm is P_0 (that is, $P_0 = P_f$) and all the constraints are second class following the classical classification of Dirac. In such case (P_0, ω_0) is a symplectic manifold, where Ω_0 denotes the restriction of the presymplectic 2-form to the constraint submanifold P_0 . Locally, the symplecticity of (P_0, ω_0) is equivalent to the regularity of the

matrix $\left(\frac{\partial^2 H}{\partial u^a \partial u^b} \right)_{1 \leq a, b \leq m}$. The dynamical equations for the optimal control problem will be

$$i_{X_{P_0}} \omega_0 = dH|_{P_0} \quad (19)$$

Taking coordinates (q^i, p_i) on P_0 , then the dynamical equations are:

$$\begin{cases} \dot{q}^i(t) = \frac{\partial H|_{P_0}}{\partial p_i}(q(t), p(t)) \\ \dot{p}_i(t) = \frac{\partial H|_{P_0}}{\partial q^i}(q(t), p(t)) \end{cases} \quad (20)$$

where we have substituted in (14) the control variables u^a by its value $\bar{u}^a = f^a(q, p)$ applying the implicit function theorem to the primary constraints $\phi^a = 0$. In such case, there exists a unique solution X_{P_0} of Equation (19) and its flow preserves the symplectic 2-form ω_0 , i.e. it is a canonical transformation.

3.2 Generating functions of the second kind

Let (\mathcal{M}, Ω) be an exact symplectic manifold (Ω is symplectic and exact, $\Omega = -d\Theta$) and suppose that $F : \mathcal{M} \rightarrow \mathcal{M}$ is a transformation from \mathcal{M} to itself and $\text{Graph}(F)$ the graph of F , $\text{Graph}(F) \subset \mathcal{M} \times \mathcal{M}$. Denote by $\pi_i : \mathcal{M} \times \mathcal{M} \rightarrow \mathcal{M}$, $i = 1, 2$ the canonical projections and the forms:

$$\begin{aligned} \bar{\Theta} &= \pi_2^* \Theta - \pi_1^* \Theta \\ \bar{\Omega} &= \pi_2^* \Omega - \pi_1^* \Omega = -d\bar{\Theta} \end{aligned}$$

Denote by $i_F : \text{Graph}(F) \hookrightarrow \mathcal{M} \times \mathcal{M}$ the inclusion map. Then, F is a canonical transformation if and only if $i_F^* \bar{\Omega} = 0$, that is, if $\text{Graph}(F)$ is a lagrangian submanifold of $(\mathcal{M} \times \mathcal{M}, \bar{\Omega})$. In such a case, $i_F^* \bar{\Omega} = -di_F^* \bar{\Theta} = 0$ and, at least locally, there exists a function $S : \text{Graph } F \rightarrow \mathbb{R}$ such that

$$i_F^* \bar{\Theta} = dS \quad (21)$$

Taking (q^i, p_i) as natural coordinates in $\text{Graph}(F)$ and $(q^i, p_i, \mathbf{q}^i, \mathbf{p}_i)$ the coordinates in $\mathcal{M} \times \mathcal{M}$, then, along $\text{Graph}(F)$, $\mathbf{q}^i = q^i(q, p)$ and $\mathbf{p}_i = p_i(q, p)$ and $\mathbf{p}_i dq^i - p_i dq^i = dS(q, p)$. Suppose that (q^i, \mathbf{p}_i) are independent local coordinates on $\text{Graph}(F)$ (see [Arn:78]); i.e. $S = S(q, \mathbf{p})$ Since

$\mathbf{p}_i dq^i - p_i dq^i = -\mathbf{q}^i dp_i + d(\mathbf{q}^i \mathbf{p}_i) - p_i dq^i = dS$, if we define $S_2(q, \mathbf{p}) = \mathbf{q}^i \mathbf{p}_i - S(q, \mathbf{p})$, where \mathbf{p} is expressed in terms of p and \mathbf{q} , then $\mathbf{q}^i dp_i + p_i dq^i = dS_2(q, \mathbf{p})$

Definition 3.1. The function $S_2(q, \mathbf{p})$ will be called a **generating function of the second kind** of the canonical transformation F .

Now, suppose that (\mathcal{M}, Ω, H) is a hamiltonian system and X_H its hamiltonian vector field, say $i_{X_H} \Omega = dH$. Denote by $F_h : \mathcal{M} \rightarrow \mathcal{M}$ its flow.

Theorem 3.2. Let a function S_2^{Nh} be defined by

$$S_2^{Nh}(q_0, p_{Nh}) = \sum_{k=0}^{N-1} (S_2^h(q_k, p_{k+1}) - q_{k+1}p_{k+1})$$

where q_k , $1 \leq k \leq N$, and p_k , $0 \leq k \leq N-1$, are stationary points of the right-hand side, that is

$$\begin{aligned} q_{k+1} &= \frac{\partial S_2^h}{\partial p}(q_k, p_{k+1}), \quad 0 \leq k \leq N-1 \\ p_k &= \frac{\partial S_2^h}{\partial q}(q_k, p_{k+1}), \quad 0 \leq k \leq N-1 \end{aligned}$$

then S_2^{Nh} is a generating function of the second kind for $F_{Nh} : \mathcal{M} \rightarrow \mathcal{M}$.

Proof: It is similar to that of Theorem 2.1. ■

Finally, we have the following

Proposition 3.3. A generating function of the second kind for F_h is given by

$$S_2^h(q_0, p_h) = p_h q_h - \int_0^h (p dq - H dt)$$

where $t \rightarrow (q(t), p(t))$ is an integral curve of the Hamilton equations such that $q(0) = q_0$ and $p(h) = p_h$.

3.3 Generating functions of the second kind and discrete optimal control problems

From Proposition 3.3 a generating function of the second kind for the Hamiltonian system $(P_0, \Omega_0, H|_{P_0})$ which determines the dynamics of the optimal control problem given by (11) and (12) is

$$\begin{aligned} S_2^h(q_0, p_h) &= p_h q_h \\ &- \int_0^h (p(t)\dot{q}(t) - H|_{P_0}(q(t), p(t))) dt \quad (22) \end{aligned}$$

where $t \rightarrow (q(t), p(t))$ is an integral curve of the vector field X_{P_0} with $(q(0), p(0)) = (q_0, p_0)$ and $(q(h), p(h)) = (q_h, p_h)$.

We now turn to the construction of a numerical integrator for the Hamiltonian system $(P_0, \omega_0, H|_{P_0})$ by using an approximation of the generating function. The proposed methods also realize the integration steps by canonical transformations; therefore, they are symplectic integrators.

Example 3.4. Consider, for instance, the following approximation to S_2^h :

$$\begin{aligned} \tilde{S}_2^h(q_k, p_{k+1}) &= p_{k+1}q_{k+1} - hp_{k+1} \left(\frac{q_{k+1} - q_k}{h} \right) \\ &+ h\tilde{L}_d(q_k, p_{k+1}) + hp_{k+1}\tilde{\Gamma}_d(q_k, p_{k+1}) \end{aligned}$$

where \tilde{L}_d and $\tilde{\Gamma}_d$ are adequate approximations to $L|_{P_0}$ and $\Gamma|_{P_0}$, respectively.

Denote by $\tilde{f}(q_k, p_{k+1})$ the function $\tilde{f}(q_k, p_{k+1}) = h\Gamma_d(q_k, p_{k+1}) + q_k$. Since $\frac{q_{k+1} - q_k}{h} = \tilde{\Gamma}_d(q_k, p_{k+1})$ then,

$$\tilde{S}_2^h(q_k, p_{k+1}) = \tilde{L}_d(q_k, p_{k+1}) + p_{k+1}\tilde{f}(q_k, p_{k+1})$$

and hence the equations

$$\begin{cases} p_k = \frac{\partial \tilde{S}_d^h}{\partial q}(q_k, p_{k+1}) \\ q_{k+1} = \frac{\partial \tilde{S}_d^h}{\partial p}(q_k, p_{k+1}) \end{cases} \quad (23)$$

are exactly the discrete equations corresponding to the classical discrete optimal control problem (see [Lew:86]), determined by the control equations: $q_{k+1}^i = \tilde{f}^i(q_k, u_k)$, $((q_0)$ given) and with associate performance index: $J = \sum_{k=0}^{N-1} \tilde{L}_d(q_k, u_k)$ Observe that this discrete optimal control problem is symplectic in the sense explained in the subsection above.

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