The Poincare-Cartan form and conservative numerical methods

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Abstract

The variational route to the Poincare-Cartan form for general variational problems is proposed in the lines of [8], [14]. Some conservative numerical schemes for Euler-Lagrange equations are derived.

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1 The Poincare-Cartan form

In the paper [8] the authors ask if the Poincare-Cartan form can be defined from the lagrangeian as a boundary term. They solved the problem for lagrangeians on J^1Y and in the paper [14] the problem is solved for J^2Y.Here is a general solution to this problem.

Let $\pi_{X,Y}: Y \to X$ a differential fibration and J^kY the fibration of k jets of its sections. Let dim X=n+1, the dimension of the fiber equals N and let $(x^i, y^A)_{i=0..n,\ A=1..N}$ a system of local coordinates on Y, where $(x_i)_{i=0..n}$ are the coordinates on the base X and $(y^A)_{A=1..N}$ the coordinates on the fiber. Let (x_i, y^A, y^A_J) the derived system of local coordinates on J^kY, $J=(j_1, j_2..)$ with $j_1+j_2+..\leq k$.As notation, π_{X,J^kY} is the canonical projection from J^kY on X, π_{J^s,J^kY} is the canonical projection from J^kY to J^sY for s$<k$,etc. We shall use the notation $D_i = \frac{\partial}{\partial x^i} + \sum_{A,J} y^A_{J,i} \frac{\partial}{\partial y^A_J}$ for the total derivative on direction x^i and $D_J = D_{j_1} D_{j_2} ... D_{j_k}$ if $J=(j_1, j_2..j_k)$.Let $\Lambda_X J^kY$ the set of π_{X,J^kY} horizontal forms on J^kY. A lagrange form is a differential form $\mathcal{L} \in \Lambda^{n+1}_X J^kY$. Locally

$$\mathcal{L} = L\left(x^i, y^A, y^A_J\right) \cdot dx^0 \wedge dx^1 \wedge .. \wedge dx^n$$

For any section $s: X \to Y$, $j^k(s)^* \mathcal{L} = \mathcal{L}\left(x^i, s^A(x), \frac{\partial^{|J|} s^A}{\partial x^J}\right) \cdot dx^0 \wedge dx^1 \wedge .. \wedge dx^n$ and may be integrated over X to get the action $S(s) = \int_X j^k(s)^* \mathcal{L}$. Sometimes we have

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to integrate over a submanifold of X. Let U a differentiable manifold of C^{∞} class, with smooth boundary and let

$$(1.1) \quad C_U^{\infty} = \{\varphi \,|\} \, \varphi : U \to Y, \varphi \text{ of } C^{\infty} \text{ class}, \, \pi_{X,Y} \circ \varphi : U \to X \text{ is embeeding}$$

Let $\varphi_X : U \to X$, $\varphi_X = \pi_{X,Y} \circ \varphi$ and $U_X = \varphi_X(U) = \pi_{X,Y}(\varphi(U))$. Let C_U the closure ofi C_U^{∞} in a Banach manifold topology. The topology is not very important here and it is omitted. The tangent space to $\varphi \in C_U^{\infty}$ is

$$(1.2) \quad T_{\varphi} C_U^{\infty} = \{\mathcal{V} \in C^{\infty}(U, TY), \, \pi_{Y,TY} \circ \mathcal{V} = \varphi\}$$

If V is a vector field on Y then for any $\varphi \in C_U^{\infty}$ the map $\mathcal{V} =.V \circ \varphi$ belongs to $T_{\varphi} C_U^{\infty}$. V so it generates a field of tangent vectors on C_U^{∞} denoted by $\tilde{V}$.

Let G the group of projectable diffeomorphisms of Y so we have the commutative diagramm

$$(1.3) \quad \begin{array}{ccc} Y & \xrightarrow{\eta_Y} & Y \\ \downarrow \pi_{X,Y} & & \downarrow \pi_{X,Y} \\ X & \xrightarrow{\eta_X} & X \end{array}$$

The action of G on C_U^{∞} is defined by $\phi : G \times C_U^{\infty} \to C_U^{\infty}$, $\phi(\eta_Y, \varphi) = \eta_Y \circ \varphi$. It follows $(\eta_Y \circ \varphi)_X = \eta_X \circ \varphi_X$. For any $\varphi \in C_U^{\infty}$ it follows $s = \varphi \circ \varphi_X^{-1}$ is a section of Y restricted to U_X so the action $\mathcal{S} : C_U^{\infty} \to R$ may defined by

$$(1.4) \quad \mathcal{S}(\varphi) = \int_{U_X} j^k \left(\varphi \circ \varphi_X^{-1}\right)^* \mathcal{L}$$

A stationary point of $\mathcal{S}$ is $\varphi \in C_U^{\infty}$ such that for any smooth path on G, $\lambda \to \eta^{\lambda}$ with $\eta^0 = id$ the following condition is fulfilled

$$\frac{\partial}{\partial \lambda}|_{\lambda=0} \mathcal{S}\left(\phi\left(\eta_Y^{\lambda}, \varphi\right)\right) = \frac{\partial}{\partial \lambda}|_{\lambda=0} \int_{U_{\lambda,X}} j^k \left(\varphi\lambda \circ \varphi_{\lambda,X}^{-1}\right)^* \mathcal{L} = 0$$

where $\varphi_{\lambda} = \eta_Y^{\lambda} \circ \varphi$, $\varphi_{\lambda,X} = \pi_{X,Y} \circ \varphi_{\lambda}$, $U_{\lambda,X} = \varphi_{\lambda,X}(U)$. Let V the infinitesimal generator of η_Y^{λ} and $j^p(V)$ the extension of V to J^pY. Let $\theta_J^A = dy_J^A - y_{J,i}^A dx^i$, $\omega = dx^0 \wedge dx^1 \wedge ... \wedge dx^n$ and $\omega_i = \frac{\partial}{\partial x^i} \lrcorner \, \omega = (-1)^i dx^0 \wedge ..\widehat{dx^i} \wedge ..dx^n$. Let $\theta_{\mathcal{L}}$ the form defined on a coordinate syatem of $J^{2k-1}Y$ by

$$(1.5) \quad \theta_{\mathcal{L}} = \sum_{A=1}^{N} \sum_{1 \le |J| \le k} \sum_{J=(J',j^i,J'')} (-1)^{|J''|} D_{J''} \frac{\partial L}{\partial y_J^A} \cdot \theta_{J'}^A \wedge \omega_{j^i} + L\omega$$

In the sum (1.5) the multiindexes J, J', J'' are increasingly ordered and if $J = (j^1 j^2 ... j^l)$, then $J' = (j^1 .. j^{i-1})$, $J'' = (j^{i+1} ... j^l)$, for $i = 1, 2, ...l$.Then we have the following theorem

Theorem 1.1. *Under the above conditions:*
a) the variation of $\mathcal{S}$ is (if U_X is included in a system of coordinates)

$$\begin{aligned} &\frac{\partial}{\partial\lambda}\Big|_{\lambda=0}\mathcal{S}\left(\varphi^{\lambda}\right) \\ (1.6)\qquad &= \int_{U_X} j^{2k-1}\left(\varphi\circ\varphi_X^{-1}\right)^{*}\left(j^{2k-1}V\lrcorner\, d\theta_{\mathcal{L}}\right) \\ &+\int_{\partial U_X} j^{2k-1}\left(\varphi\circ\varphi_X^{-1}\right)^{*}\left(j^{2k-1}\left(V\right)\lrcorner\, \theta_{\mathcal{L}}\right)\end{aligned}$$

b) There is the identity

$$\mathcal{L}\left(j^{k}\left(\varphi\circ\varphi_X^{-1}\right)\right)=\left(j^{2k-1}\left(\varphi\circ\varphi_X^{-1}\right)\right)^{*}\theta_{\mathcal{L}}$$

c) If R and S are $\pi_{X,J^{2k-1}Y}$ vertical fields, then $R\lrcorner\, S\lrcorner\, \theta_{\mathcal{L}}=0$ and $\theta_{\mathcal{L}}$ depends on each point $j^{2k-1}(s)(x)$ only on dx^i, i=0..n and dy^A_J, with $|J|\le k-1$.
d) If W is a vector field on $J^{2k-1}Y$, tangent lto the fibers of $\pi_{Y,J^{2k-1}Y}$, then $j^{2k}\left(\varphi\circ\varphi_X^{-1}\right)^{*}\left(W\lrcorner\, d\theta_{\mathcal{L}}\right)=0$.
e) Any form $\theta\in\Lambda^{n+1}J^{2k-1}Y$, which in a coordinate system has the proprieties a), b), c), d) above, is identical to $\theta_{\mathcal{L}}$.
f) There is an unique differential form $\Theta_{\mathcal{L}}\in\Lambda^{n+1}J^{2k-1}Y$ depending on the Lagrange form $\mathcal{L}$, with the properties a), b), c), d) above and such that the formula (1.6) *is true for any U_X . In local coordinates $\Theta_{\mathcal{L}}$ is expressed by* (1.5)
g) $\varphi\in C_U^{\infty}$ is a stationary iff

$$(1.7)\qquad j^{2k-1}\left(\varphi\circ\varphi_X^{-1}\right)^{*}\left(W\lrcorner\, d\Theta_{\mathcal{L}}\right)=0$$

for any vector field W on $J^{2k-1}Y$, that is the Euler-Lagrange equations

$$(1.8)\qquad \sum_{0\le|J|\le k}(-1)^{|J|}\left(\frac{\partial^{|J|}}{\partial x^J}\left(\frac{\partial L}{\partial y^A_J}\left(\varphi\circ\varphi_X^{-1}\right)\right)\right)=0,\ A=1,2,..N$$

are equivalent to (1.7).

The proof cosists in a lengthy computation with differntial forms.

Example 1. *n=0,N=1, $k>1$, $\mathcal{L}=L\left(t,q,\dot q,q^{(2)},..q^{(k)}\right)dt$, then* (1.5) *becomes*

$$\begin{aligned}\Theta_{\mathcal{L}} &= \sum_{s=1}^{k}\sum_{a=0}^{s-1}(-1)^a\frac{d^a}{dt^a}\left(\frac{\partial L}{\partial q^{(s)}}\right)\theta_{s-a-1}+Ldt \\ &= \sum_{b=0}^{k-1}\sum_{a=0}^{k-b-1}(-1)^a\frac{d^a}{dt^a}\left(\frac{\partial L}{\partial q^{(a+b+1)}}\right)\theta_b+Ldt\end{aligned}$$

where $\theta_b=dq^{(b)}-q^{(b+1)}dt$.

2 Conservative numerical schemes

Consider a variational problem with the lagrange form $\mathcal{L} = L\left(q, \dot{q}, q^{(2)}, ..q^{(k)}\right) dt$ on $J^k Y$ where $Y = R \times Q$ and assume the matrix $\left(\frac{\partial^2 L}{\partial q^{i(k)} \partial q^{j(k)}}\right)_{i,j=1..\dim(Q)}$ is nondegenerate. A point $\gamma \in J^{2k-1}Y$ is represented by $\left(t, q(t), q'(t), ...q^{(2k-1)}(t)\right)$ where q is a curve from R to Q. Two fibers of $J^k Y$ over t_0 and over t_1 are identified by translation $j^k(s)(t_0) \to j^k(s')(t_1)$ where $s'(t) = s(t - t_1 + t_0)$. Any such fiber is called the k tangent space $T^k Q$. The solution of the Euler-Lagrange equations with initial conditions $\left(t_0, q(t_0), q'(0), ...q^{(2k-1)}(t_0)\right)$ gives at time t_1 the point $\left(t_1, q(t_1), q'(t_1), ...q^{(2k-1)}(t_1)\right)$ and this correspondence defines a diffeomorphism $F_{t_0,t_1} : \pi^{-1}_{R,J^{2k-1}Y}(t_0) \to \pi^{-1}_{R,J^{2k-1}Y}(t_1)$ or equivalently $F_t : T^{2k-1}Q \to T^{2k-1}Q$ with $t = t_1 - t_0$, because L is independent of t. Let

$$S_t\left(q(t_0), q'(0), ...q^{(2k-1)}(t_0)\right) = \int_{[t_0,t_1]} L\left(q(t), q'(t), ...q^{(k)}(t)\right) dt$$

In this way S_t is defined on $T^{2k-1}Q$. We have

Proposition 2.1. *If* $\Theta_{\mathcal{L}} = \sum_{b=0}^{k-1} \sum_{a=0}^{k-b-1} (-1)^a \frac{d^a}{dt^a}\left(\frac{\partial L}{\partial q^{(a+b+1)}}\right) \theta_b$ *then*

$$F_t^*(\Theta_{\mathcal{L}}) - \Theta_{\mathcal{L}} = dS_t$$

and

$$F_t^*(d\Theta_{\mathcal{L}}) = d\Theta_{\mathcal{L}}$$

Proof. In the formula (1.6) U_X is $[t_0, t_1]$, $\varphi \circ \varphi_X^{-1}(t) = q(t)$ and $V = j^{2k-1}(V_0)$ where V_0 is the projection of V on Q and V is the field generated by a variation of initial conditions $\left(q(t_0), q'(0), ...q^{(2k-1)}(t_0)\right)$. One remarks that $V = 0\frac{\partial}{\partial t} + ..$ The first integral is zero thanks to point g) of the above theorem. The second is

$$\begin{aligned} &\Theta_{\mathcal{L}}\left(V\left(t_1, q(t_1), q'(t_1), ...q^{(2k-1)}(t_1)\right)\right) \\ &-\Theta_{\mathcal{L}}\left(V\left(t_0, q(t_0), q'(0), ...q^{(2k-1)}(t_0)\right)\right) \\ = \;& \left(F_t^*(\Theta_{\mathcal{L}}) - \Theta_{\mathcal{L}}\right)\left(V\left(t_0, q(t_0), q'(0), ...q^{(2k-1)}(t_0)\right)\right) \end{aligned}$$

which is $dS_t\left(V\left(t_0, q(t_0), q'(0), ...q^{(2k-1)}(t_0)\right)\right)$ by (1.6).

QED.

The numerical method tries to emulate the invariance of $d\Theta$ of this proposition. In the lines of [10] , in a way which differs in some points from [11] here is proposed a scheme for k order variational problems for unidimensional integrals. The lagrange form is $L\left(q, q', ...q^{(k)}\right) dt$. For small positive h, the solution is uniquely defined by 2k points of Q, $(q_0, q_1..q_{k-1}q_k, q_{k+1}, ..q_{2k-1})$ such that $q(0) = q_0$, $q(h) = q_1$, ... $q((2k-1)h) = q_{2k-1}$. We take the discrete analogue of $T^{2k-1}Q$ as $Q^{2k} = Q^k \times Q^k$ where $Q^k = Q \times Q \times ... \times Q$ (k times). A point $(q_0, q_1..q_{k-1}q_k, q_{k+1}, ..q_{2k-1}) \in Q^{2k}$ is split into two groups $(q_0, q_1..q_{k-1}) \in Q^k$ and $(q_k, q_{k+1}, ..q_{2k-1}) \in Q^k$ denoted by

$q_{(0,k-1)}$ and $q_{(2k,2k-1)}$. In what follows, h is a constant time stamp, $L\left(q(t), q'(t), ..q^{(k)}(t)\right)$ is approximated on $[0,h]$ by

$$L_d(q_0, q_1, ..q_k) = L\left(q_0, \frac{q_1 - q_0}{h}, \frac{q_2 - 2q_1 + q_0}{h^2}, ..\right)$$

and analogously on $[h, 2h]$ etc.

The integral $\int_0^h L\left(q(t), q'(t), ..q^{(k)}(t)\right) dt$ is approximated by $hL_d(q_0, q_1, ..q_k)$ whence $\int_0^{kh} L\left(q(t), q'(t), ..q^{(k)}(t)\right) dt$ is approximated by the dicrete action

$$S_d\left(q_{(0,k-1)}, q_{(k,2k-1)}, h\right) = h\sum_{i=0}^{k-1} L_d(q_i, q_{i+1}, ..q_{i+k-1})$$

The discrete dynamics consists in passing from $\left(q_{(0,k-1)}, q_{(k,2k-1)}\right) \in Q^{2k}$ to $\left(q_{(k,2k-1)}, q_{(2k,3k-1)}\right) \in$ Q^{2k} in such a way that the discrete action $S_d\left(q_{(0,k-1)}, q_{(k,2k-1)}, h\right) + S_d\left(q_{(k,2k-1)}, q_{(2k,3k-1)}, h\right)$ is minimum for variations with fixed endpoints. If D_1 is the derivative by respect of the first group of variables and D_2 is the derivative by respect of the second group of variables then minimum condition reads

$$D_2S_d\left(q_{(0,k-1)}, q_{(k,2k-1)}, h\right) + D_1S_d\left(q_{(k,2k-1)}, q_{(2k,3k-1)}, h\right) = 0 \tag{2.9}$$

This is the discrete analogue of Euler-Lagrange equations. The (2.9) is an implicit equation which gives $q_{(2k,3k-1)}$ as function of $\left(q_{(0,k-1)}, q_{(k,2k-1)}\right)$ and h and defines $F_d : Q^{2k} \to Q^{2k}$ by $\left(q_{(0,k-1)}, q_{(k,2k-1)}\right) \to \left(q_{(k,2k-1)}, q_{(2k,3k-1)}\right)$. One defines as in [10] the differential forms on Q^{2k} by

$$\Theta^+_{L_d}\left(q_{(0,k-1)}, q_{(k,2k-1)}\right) = D_2S_d\left(q_{(0,k-1)}, q_{(k,2k-1)}, h\right) \cdot dq_{(k,2k-1)}$$

and

$$\Theta^-_{L_d}\left(q_{(0,k-1)}, q_{(k,2k-1)}\right) = -D_1S_d\left(q_{(0,k-1)}, q_{(k,2k-1)}, h\right) \cdot dq_{(0,k-1)}$$

It follows

$$dS_d = \Theta^+_{L_d} - \Theta^-_{L_d}$$

whence $d\Theta^+_d = d\Theta^-_d$ and we define $\Omega_{L_d} = d\Theta^+_d = d\Theta^-_d$. Using local coordinates we get

$$\Omega_{L_d} = \frac{\partial^2 S_d\left(q_{(0,k-1)}, q_{(k,2k-1)}, h\right)}{\partial q_{(0,k-1)}\partial q_{(k,2k-1)}} dq_{(0,k-1)} \wedge q_{(k,2k-1)} \tag{2.10}$$

The following proposition is the discrete analogue of proposition (2.1)

Proposition 2.2. *With the above notations a)* $F^*_d\Theta^+_{L_d} - \Theta^-_{L_d} = dS_d + dF^*_dS_d$ *and b)* $F^*_d\left(\Omega_{L_d}\right) = \Omega_{L_d}$..

Proof. Using the discrete Euler-Lagrange equations we get (d=exterior derivative)

$$\begin{aligned}
&\left(dS_d + dF_d^* S_d\right)\left(q_{(0,k-1)}, q_{(k,2k-1)}, h\right) \\
= \; & dS_d\left(q_{(0,k-1)}, q_{(k,2k-1)}, h\right) + dS_d\left(q_{(k,2k-1)}, q_{(2k,3k-1)}, h\right) \\
= \; & D_1 S_d\left(q_{(0,k-1)}, q_{(k,2k-1)}, h\right) dq_{(0,k-1)} \\
& + D_2 S_d\left(q_{(k,2k-1)}, q_{(2k,3k-1)}, h\right) dq_{(k,2k-1)} \\
= \; & \left(-\Theta_{L_d}^- + F_d^* \Theta_{L_d}^+\right)\left(q_{(0,k-1)}, q_{(k,2k-1)}\right).
\end{aligned}$$

The exterior derivative of a) gives b).
QED.
This numerical scheme conseves the form (2.10).

Example 2. *Let $L(q,q',q'') = \frac{1}{2}q''^t A q'' + \frac{1}{2}q'^t B q' - V(q)$ where A and B are $N \times N$ symmetric matrices, A nosingular and V is a function defined on $Q = R^N$. Then*

$$\begin{aligned}
& S_d\left(q_{(0,1)}, q_{(2,3)}\right) \\
= \; & h \begin{bmatrix} \left(\frac{q_2-2q_1+q_0}{h^2}\right)^t A \left(\frac{q_2-2q_1+q_0}{h^2}\right) + \left(\frac{q_1-q_0}{h}\right)^t B \left(\frac{q_1-q_0}{h}\right) - V(q_0) \\ \left(\frac{q_3-2q_2+q_1}{h^2}\right)^t A \left(\frac{q_3-2q_2+q_1}{h^2}\right) + \left(\frac{q_2-q_1}{h}\right)^t B \left(\frac{q_2-q_1}{h}\right) - V(q_1) \end{bmatrix}
\end{aligned}$$

The equations (2.9) *are* $D_2 S_d\left(q_{(0,1)}, q_{(2,3)}\right) + D_1 S_d\left(q_{(2,3)}, q_{(4,5)}\right) = 0$ *which finally give*

$$\text{(2.11)} \quad q_4 = 4q_3 - 6q_2 + 4q_1 - q_0 + h^2 A^{-1} B\left(q_3 - 2q_2 + q_1\right) + \frac{h^4}{2} A^{-1} V'\left(q_2\right)$$

$$\text{(2.12)} \quad q_5 = 4q_4 - 6q_3 + 4q_2 - q_1 + h^2 A^{-1} B\left(q_4 - 2q_3 + q_2\right) + \frac{h^4}{2} A^{-1} V'\left(q_3\right)$$

that is $F_d : Q^4 \to Q^4$ is given by $F_d\left(q_0, q_1, q_2, q_3\right) = \left(q_2, q_3, q_4, q_5\right)$ with q_4, q_5 given by previous formula. By iteration q_{2k+4} and q_{2k+5} are given by translation of $(2.11 - 2.12)$ *as functions of $q_{2k+3}, q_{2k+2}, q_{2k+1}$ and q_{2k}. The form Ω_{L_d} invariated by F_d is* (2.10)

$$\begin{aligned}
\Omega_{L_d} = \; & \frac{1}{h^3} A_{i,j}\left(2dq_0^i \wedge dq_2^j - 8dq_1^i \wedge dq_2^j + 2dq_1^i \wedge dq_3^j\right) \\
& - \frac{2}{h} B_{i,j} dq_1^i \wedge dq_2^j \cdot
\end{aligned}$$

To control the quality of approximation let

(2.13)

$$S_d^E\left(q_{(0,k-1)}, q_{(k,2k-1)}, h\right) = \int_0^{kh} L\left(\tilde{q}_{(0,2k-1)}(t), \tilde{q}'_{(0,2k-1)}(t), ..\tilde{q}^{(k)}_{(0,2k-1)}(t)\right) dt$$

where $\tilde{q}_{(0,2k-1)}(t)$ is the unique solution of Euler-Lagrange equations such that $\tilde{q}_{(0,2k-1)}(0) = q_0$, $\tilde{q}_{(0,2k-1)}(h) = q_1, \ldots$ $\tilde{q}_{(0,2k-1)}((2k-1)h) = q_{2k-1}$. This discrete action generates a discrete dynamics F_d^E by discrete Euler-Lagrange equations (2.9). Let F^E : $Q^k \times Q^k \to Q^k \times Q^k$ the diffeomorphism

$$\begin{aligned}
& F^E\left(q_0; q_1, ..q_{k-1}, q_k, ..q_{2k-1}\right) \\
= \; & \left(q_k, ..q_{2k-1}, \tilde{q}_{(0,2k-1)}(2kh), \tilde{q}_{(0,2k-1)}((2k+1)h), ..\tilde{q}_{(0,2k-1)}((3k-1)h)\right)
\end{aligned}$$

In other words the points obtained from $(q_0, q_1, ..q_{k-1}, ..q_{2k-1})$ by iteration of F^E are situated on the exact solution $\bar{q}_{(0,2k-1)}(t)$ of the Euler-Lagrange equations. Then is not true that $F_d^E = F^E$ as in [10] for k=1. This has severe impact on the convergence of the approximate solution to the exact solution as $h \to 0$. Numerical experiments show that the formulas $(2.11 - 2.12)$ keep the shape of the exact solution but is severe translated from it. A new numerical method which uses at each point $q \in Q$ the derivatives up to k-1 gives a better result. The details will be published later.

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