Integrator for Lagrangian Dynamics

C. Udrişte, M. Postolache and I. Ţevy

Abstract

In §1 we bring the reader gently along from the theory of discrete single-time Lagrangian dynamics (for details see [3]). §2 develops the theory of discrete multi-time Lagrangian dynamics, emphasizing the possibility of computer modelling via Newton method (for details see [8], [9]).

Mathematics Subject Classification: 49KXX, 65P10
Key words: Lagrangian energy, extremals, discrete Euler-Lagrange equations

1 Single-time Lagrangian dynamics

Let $x \in R^n$ and let $\gamma = \{(t,x) | x = x(t), t_0 \leq t \leq t_1\}$ be a curve in the space $R \times R^n$. Let Γ be the set of all curves γ which join the point (t_0, x_0), (t_1, x_1). A differentiable function

$$L: R \times R^n \times R^n \to R$$

is called *Lagrangian density energy.*

Theorem 1.1 *A C^2 curve γ is an extremal of the functional*

$$E(\gamma) = \int_{t_0}^{t_1} L\left(t, x, \frac{dx}{dt}\right) dt, \quad \gamma \in \Gamma$$

iff it is a solution of Euler-Lagrange equations

$$\frac{\partial L}{\partial x^k} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \left(\dfrac{dx^k}{dt}\right)} = 0, \quad k = 1, \dots, n.$$

This is a differential system of n equations of second order and therefore the solutions depend on $2n$ arbitrary constants. For fixing one solution there are used $2n$ boundary conditions

$$x(t_0) = x_0, \ x(t_1) = x_1.$$

Balkan Journal of Geometry and Its Applications, Vol.6, No.2, 2001, pp. 109-115

Since the property for γ to be an extremal of the functional E does not depend on the choice of the system of coordinates, the previous explanations extend easily to (Riemannian) manifolds.

The Lagrangian L produces the Hamiltonian

$$H(t,x,\dot{x}) = \dot{x}^i \frac{\partial L}{\partial \dot{x}^i}(t,x,\dot{x}) - L(t,x,\dot{x}),$$

which is conserved along the extremals only if it does not depend on the parameter t.

The discretization of L can be made by using the midpoint rule which consists in the substitution of t by h, of the point x with $\frac{x_{k+1}+x_k}{2}$, and of the velocity $\dot{x}$ by $\frac{x_{k+1}-x_k}{h}$, where h is the time step. One obtains the discrete Lagrangian

$$L_d\colon R \times R^n \times R^n \to R, \quad L_d(h,u,v) = L\left(h, \frac{u+v}{2}, \frac{v-u}{h}\right).$$

This determines the action

$$S\colon R \times (R^n)^{N+1} \to R, \quad S(h; x_0, x_1, \ldots, x_N) = \sum_{k=0}^{N-1} L(h, x_k, x_{k+1}),\ x_k \in R^n.$$

The discrete variational principle characterizes the sequence $(x_0, x_1, \ldots, x_N) \in (R^n)^{N+1}$ for which the action S is stationary, for any family $x_k(\varepsilon) \in R^n$, $\varepsilon \in I \subset R$, $0 \in I$, with $x_k(0) = x_k$, and x_0, x_N fixed points. Using the variation of the first order we find

Theorem 1.2 *The sequence (x_k), $k = 0, 1, \ldots, N$ is stationary for the action S iff it is generated by the discrete Euler-Lagrange equations (variational integrator)*

$$\frac{\partial L_d}{\partial x_k^i}(h, x_{k-1}, x_k) + \frac{\partial L_d}{\partial x_k^i}(h, x_k, x_{k+1}) = 0, \quad i = 1, \ldots, n;\ k = 1, \ldots, N-1.$$

Denoting

$$A_i(k) = \frac{\partial L_d}{\partial x_k^i}(h, x_{k-1}, x_k), \quad f_i(u) = \frac{\partial L_d}{\partial x_k^i}(h, x_k, u) + A_i(k),$$
$$i = 1, \ldots, n;\ u = (u^1, \ldots, u^n);\ F = (f_1, \ldots, f_n),$$

the preceding equations tansfer into a nonlinear equation system

$$F(u) = 0, \tag{1}$$

at each step k. The solution of the system (1) can be approximated by using $u(e) = x_k$ in the Newton method

$$J_F(u(e)) \begin{pmatrix} u^1(e+1) \\ \cdots \\ u^n(e+1) \end{pmatrix} = J_F(u(e)) \begin{pmatrix} u^1(e) \\ \cdots \\ u^n(e) \end{pmatrix} - \begin{pmatrix} f_1(u(e)) \\ \cdots \\ f_n(u(e)) \end{pmatrix},$$

$e = 1, 2, \ldots, \bar{e}$. The matrix J_F is the Jacobi matrix of the function F, and the integer number $\bar{e}$ is determined by the condition

$$\frac{\left| \sum_{i=1}^{n} f_i^2(u(e)) - \sum_{i=1}^{n} f_i^2(u(e+1)) \right|}{1 + \sum_{i=1}^{n} f_i^2(u(e+1))} < \varepsilon.$$

Next, we put $x_{k+1} = u(\bar{e})$.

The discrete Lagrangian L_d produces the discrete Hamiltonian

$$H_d(k) = \frac{x_k^i - x_{k-1}^i}{h} \frac{\partial L_d}{\partial \dot{x}^i}(h, x_{k-1}, x_k) - L_d(h, x_{k-1}, x_k).$$

2 Multi-time Lagrangian dynamics

In the preceding section the space coordinate and time played quite distinct roles: the space coordinate was merely an index numbering freedom degrees, and the time coordinate was the usual physical time in which the system evolves. According Dickey [1], such a theory is satisfactory unless we turn our attention to relativistic invariant equations, e.g. chiral fields, sine-Gordon, and others. Also considering the KP-hierarchy for arbitrary m and n, the variables x_m and x_n are quite equal in rights and there is no reason to prefer one to the other by choosing it as time. In such cases a new field theory is useful which involves many time variables. The multi-time formalism is of interest even for all examples where the variables are involved in a distinctly asymmetric way.

The multi-time calculus of variations is of course not new. Let $T_0 \subset R^p$ be a relatively compact domain. Let $\varphi = \{(t, x) | x = x(t), t \in T_0, x \in R^n\}$ be a parametrized sheet in the space $R^p \times R^n$. Let Φ be the set of all parametrized sheets φ satisfying the boundary condition $\varphi|_{\partial T_0} = f$, where f is a given continuous function. A differentiable function

$$L: R^p \times R^n \times R^{np} \to R$$

is called *Lagrangian density energy.*

Theorem 2.1 *A C^2 parametrized sheet is an extremal of the functional*

$$E(\varphi) = \int_{T_0} L\left(t^\alpha, x^i, \frac{\partial x^i}{\partial t^\alpha}\right) dt^1 \wedge \cdots \wedge dt^p$$

iff it is a solution of Euler-Lagrange equations

$$\frac{\partial L}{\partial x^k} - \frac{\partial}{\partial t^\alpha} \frac{\partial L}{\partial x_\alpha^k} = 0, \quad x_\alpha^k = \frac{\partial x^k}{\partial t^\alpha}, \quad k = 1, \ldots, n.$$

This is a PDEs system with n equations of second order. Therefore the solutions depend on $2n$ arbitrary functions. For fixing one solution we use the boundary condition.

Since the property of φ to be an extremal of the functional E does not depend on the choice of the system of coordinates, the previous explanations extend easily to Riemannian manifolds.

The Lagrangian L produces the Hamiltonian

$$H(t^\alpha, x^i, x^i_\alpha) = x^j_\beta \frac{\partial L}{\partial x^j_\beta}(t^\alpha, x^i, x^i_\alpha) - L(t^\alpha, x^i, x^i_\alpha),$$

but this function is not conserved along the extremals.

Suppose $p = 2$. The discretization of L can be made by using the *centroid rule* which consists in the substitution of the point t with the step (h_1, h_2), of the point x with $\frac{x_{k\ell} + x_{k+1\ell} + x_{k\ell+1}}{3}$, and of partial velocities x_α, $\alpha = 1, 2$, by $\frac{x_{k+1\ell} - x_{k\ell}}{h_1}$, $\frac{x_{k\ell+1} - x_{k\ell}}{h_2}$. One obtains the discrete Lagrangian

$$L_d\colon R^2 \times R^n \times R^n \times R^n \to R, \quad L_d(u, v, w) = L\left(h_1, h_2, \frac{u+v+w}{3}, \frac{v-u}{h_1}, \frac{w-u}{h_2}\right).$$

This determines the 2-dimensional discrete action

$$S\colon R^2 \times (R^n)^{(M+1)(N+1)} \to R,$$

$$S(h_1, h_2; A) = \sum_{k=0}^{M-1} \sum_{\ell=0}^{N-1} L(h_1, h_2; x_{k\ell}, x_{k+1\ell}, x_{k\ell+1}), \quad x_{k\ell} \in (R^n)^{(M+1)(N+1)},$$

$$A = \begin{pmatrix} x_{00} & x_{01} & \cdots & x_{0N} \\ x_{10} & x_{11} & \cdots & x_{1N} \\ \cdots & & & \\ x_{M0} & x_{M2} & \cdots & x_{MN} \end{pmatrix}.$$

We fix the 2-step (h_1, h_2). The discrete variational principle consists in the characterization of the matrix A for which the action S is stationary, for any family $x_{k\ell}(\varepsilon) \in R^n$, $k \in \{0, 1, \ldots, M-1\}$, $\ell \in \{0, 1, \ldots, N-1\}$, $\varepsilon \in I \subset R$, $0 \in I$ with $x_{k\ell}(0) = x_{k\ell}$, and fixed lines $(x_{00}, x_{01}, \ldots, x_{0N})$, $(x_{M0}, x_{M2}, \ldots, x_{MN})$, fixed columns ${}^t(x_{00}, x_{10}, \ldots, x_{M0})$, ${}^t(x_{0N}, x_{1N}, \ldots, x_{MN})$. The discrete variational principle is obtained using the variation of S of the first order.

Theorem 2.2 *The first variation of the discrete action S is*

$$\begin{aligned} \delta S(A)(\eta) \;=\; & \frac{\partial L}{\partial x^i_{00}}(x_{00}, x_{10}, x_{01})\eta^i_{00} + \frac{\partial L}{\partial x^i_{10}}(x_{10}, x_{20}, x_{11})\eta^i_{10} + \frac{\partial L}{\partial x^i_{01}}(x_{01}, x_{11}, x_{02})\eta^i_{01} \\ & + \sum_{k=1}^{M_1} \sum_{\ell=1}^{N-1} \left[\frac{\partial L}{\partial x^i_{k\ell}}(x_{k\ell}, x_{k+1\ell}, x_{k\ell+1}) + \frac{\partial L}{\partial x^i_{k\ell}}(x_{k-1\ell}, x_{k\ell}, x_{k-1\ell+1})\right. \\ & \left. + \frac{\partial L}{\partial x_{k\ell^i}}(x_{k\ell-1}, x_{k+1\ell-1}, x_{k\ell})\right]\eta^i_{k\ell} + \sum_{k=1}^{M-1} \frac{\partial L}{\partial x^i_{k0}}(x_{k-10}, x_{k0}, x_{k-11})\eta^i_{k0} \\ & + \sum_{\ell=0}^{N-1} \frac{\partial L}{\partial x^i_{M\ell}}(x_{M-1\ell}, x_{M\ell}, x_{M-1\ell+1})\eta^i_{M\ell} + \sum_{\ell=1}^{N-1} \frac{\partial L}{\partial x^i_{0\ell}}(x_{0\ell-1}, x_{1\ell-1}, x_{0\ell})\eta^i_{0\ell} \\ & + \sum_{k=0}^{M-1} \frac{\partial L}{\partial x^i_{kN}}(x_{kN-1}, x_{k+1N-1}, x_{kN})\eta^i_{kN}, \end{aligned}$$

where

$$\eta = \begin{pmatrix} \eta_{00} & \eta_{01} & \cdots & \eta_{0N} \\ \eta_{10} & \eta_{11} & \cdots & \eta_{1N} \\ \cdots & & & \\ \eta_{M0} & \eta_{M1} & \cdots & \eta_{MN} \end{pmatrix}, \quad \eta_{k\ell} = \left.\frac{\partial x_{k\ell}}{\partial \varepsilon}\right|_{\varepsilon=0},$$

$x_{k\ell}(\varepsilon) \in Q$, $\varepsilon \in I$, $0 \in I$, $x_{k\ell}(0) = x_{k\ell}$.

Proof. We use the family of curves $x_{k\ell}(\varepsilon) \in R^n$, $\varepsilon \in I$. Then

$$S(A(\varepsilon)) = \sum_{k=0}^{M-1}\sum_{\ell=0}^{N-1} L(x_{k\ell}(\varepsilon), x_{k+1\ell}(\varepsilon), x_{k\ell+1}(\varepsilon)).$$

We find

$$\begin{aligned} \delta S(A)(\eta) \;=\; & \left.\frac{\partial}{\partial \varepsilon} S(A(\varepsilon))\right|_{\varepsilon=0} = \sum_{k=0}^{M-1}\sum_{\ell=0}^{N-1} \frac{\partial L}{\partial x^i_{k\ell}}(x_{k\ell}, x_{k+1\ell}, x_{k\ell+1})\eta^i_{k\ell} \\ & + \sum_{k=0}^{M-1}\sum_{\ell=0}^{N-1} \frac{\partial L}{\partial x^i_{k+1\ell}}(x_{k\ell}, x_{k+1\ell}, x_{k\ell+1})\eta^i_{k+1\ell} \\ & + \sum_{k=0}^{M-1}\sum_{\ell=0}^{N-1} \frac{\partial L}{\partial x^i_{k\ell}}(x_{k\ell}, x_{k+1\ell}, x_{k\ell+1})\eta^i_{k\ell+1}. \end{aligned}$$

Corollary 2.1 *(discrete Euler-Lagrange equations). The matrix $A = (x_{k\ell})$ is stationary for the action S iff*

$$\frac{\partial L}{\partial x^i_{k\ell}}(x_{k\ell}, x_{k+1\ell}, x_{k\ell+1}) + \frac{\partial L}{x^i_{k\ell}}(x_{k-1\ell}, x_{k\ell}, x_{k-1\ell+1}) + \frac{\partial L}{\partial x^i_{k\ell}}(x_{k\ell-1}, x_{k+1\ell-1}, x_{k\ell}) = 0,$$

$$i = 1, \ldots, n; \quad k \in \{1, \ldots, M-1\}, \quad \ell \in \{1, \ldots, N-1\}.$$

Proof. Since the boundary of the grid is fixed, the lines

$$(\eta_{00}, \eta_{01}, \ldots, \eta_{0N}), \quad (\eta_{M0}, \eta_{M1}, \ldots, \eta_{MN}),$$

and the columns

$$^t(\eta_{00}, \eta_{10}, \ldots, \eta_{M0}), \quad ^t(\eta_{0N}, \eta_{1N}, \ldots, \eta_{MN})$$

must be zero, and $\eta_{k\ell}$, $k \in \{1, \ldots, M-1\}$, $\ell \in \{1, \ldots, N-1\}$ are arbitrary.

The variational integrator described by the discrete Euler-Lagrange equations works as follows:

- we give the lines $(x_{00}, x_{01}, \ldots, x_{0N})$, $(x_{10}, x_{11}, \ldots, x_{1N})$;
- we denote

$$u = x_{k\ell+1},$$

$$A_i(k\ell) = \frac{\partial L}{\partial x^i_{k\ell}}(x_{k-1\ell}, x_{k\ell}, x_{k-1\ell+1}), \quad B_i(k\ell) = \frac{\partial L}{\partial x^i_{k\ell}}(x_{k\ell-1}, x_{k+1\ell-1}, x_{k\ell}),$$

$$f_i(u) = \frac{\partial L}{\partial x^i_{k\ell}}(x_{k\ell}, x_{k+1\ell}, u) + A_i(k\ell) + B_i(k\ell), \quad F = (f_1, \ldots, f_n);$$

- we solve the nonlinear system (4) $F(u)=0$, at each step (k,ℓ) using six points of starting as shown a part of the grid,

$$\begin{array}{lll} \bullet & \bullet x_{k-1\ell} & \bullet x_{k-1\ell+1} \\ \bullet x_{k\ell-1} & \bullet x_{k\ell} & * u = x_{k\ell+1} \\ \bullet x_{k+1\ell-1} & \bullet x_{k+1\ell} & \circ \end{array}$$

Newton Method

The solution of the nonlinear system (4) can be approximated by using $u(\ell) = x_{k\ell+1}$ in the Newton method

$$J_F(u(e))\begin{pmatrix} u^1(e+1) \\ \vdots \\ u^n(e+1)\end{pmatrix} = J_F(u(e))\begin{pmatrix} u^1(e) \\ \vdots \\ u^n(e)\end{pmatrix} - \begin{pmatrix} f_1(u(e)) \\ \vdots \\ f_n(u(e))\end{pmatrix},$$

$e = 1,2,\ldots,\bar{e}$. The matrix J_F is the Jacobi matrix of the function F, and the integer $\bar{e}$ is determined by the condition

$$\frac{\left|\sum\limits_{i=1}^{n} f_i^2(u(e)) - \sum\limits_{i=1}^{2} f_i^2(u(e+1))\right|}{1+\sum\limits_{i=1}^{n} f_i^2(u(e+1))} < \varepsilon.$$

Next, we put $x_{k\ell+2} = u(\bar{e})$.

The discrete Lagrangian L_d produces the discrete Hamiltonian

$$\begin{aligned} H_d(k,\ell) = {} & \frac{x^i_{k+1\ell} - x^i_{k\ell}}{h_1}\frac{\partial L}{\partial x^i_1}\left(h_1,h_2,x_{k\ell},x_{k+1\ell},x_{k\ell+1}\right) \\ & + \frac{x^i_{k\ell+1} - x^i_{k\ell}}{h_2}\frac{\partial L}{\partial x^i_2}\left(h_1,h_2,x_{k\ell},x_{k+1\ell},x_{k\ell+1}\right) - L_d\left(h_1,h_2,x_{k\ell},x_{k+1\ell},x_{k\ell+1}\right). \end{aligned}$$

Acknowledgements. A version of this paper was presented by the first two authors at the third Conference of Balkan Society of Geometers, Workshop on Electromagnetic Flows and Dynamics, July 31-August 3, 2000, University POLITEHNICA of Bucharest, Romania.

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Politehnica University of Bucharest
Department of Mathematics I
Splaiul Independenţei 313, 77206 Bucharest, Romania
E-mail:udriste@mathem.pub.ro