

MA189 Course Project

# **Conserving Integrators by Generating Function**

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## 1. Introduction

This project explores the use of a special type of generating function for deriving conserving integrators. The basic idea follows Zhong and Marsden[1], that is, find an approximate solution to Hamilton-Jacobi equation and generate a symplectic transformation,

$$\begin{aligned} p_{n+1} &= \frac{\partial S(q_{n+1}, q_n, t_{n+1}, t_n)}{\partial q_{n+1}} \\ p_n &= -\frac{\partial S(q_{n+1}, q_n, t_{n+1}, t_n)}{\partial q_n} \end{aligned} \quad (1)$$

This produces a one-step integration algorithm. First note that the ensuing integrator, by design, is symplectic, hence it preserves the symplectic two-form in phase space, see Marsden[2]. In addition, as is pointed out in [1], if the generating function is invariant under certain group action, then the integrator also preserves corresponding momentum map.

Attention here will be concentrated on a special type of generating function, namely the "action integral". Recall the action integral integrated along the extremal path exactly satisfies the Hamilton-Jacobi equation, thus by (1) recovers the exact Hamiltonian flow. The question then is how to judiciously construct appropriate approximation, and also to satisfy invariant requirement that may apply. In what follows a way to construct the approximation will be described, and the process will first be applied to Hamiltonian system in linear (flat) configuration space, and later, application to rigid body dynamics, in which the configuration space is the rotation group, will be outlined. It will be shown that in linear configuration case this approach leads to the symplectic momentum conserving integrators derived by Simo[4] in a different setting.

Before closing, it may be remarked that, this procedure may bring into connection with the so-called "temporal finite element" (or "space-time finite element" in some literature), in which the time-stepping relations are derived from a weak form formulation, e.g., see Zienkiewicz[8]. The viewpoint here is different, however, the procedure is analogous and

the results indicate that one can expect more out of these approaches than the traditional time integration, namely, the conserving properties.

## 2. Hamiltonian System in Linear Space

### 2.1 Time Stepping Integrator

As stated before, attention is focused on a special type of generating function,

$$S = \int_{\gamma} L(\dot{q}, q, t) dt \quad (2)$$

Seek the following *discretized* version of  $\dot{q}$ ,  $q$ , and  $L$ . In a time step  $[t_n, t_{n+1}]$ ,

$$\begin{aligned} \dot{q} &= \frac{q_{n+1} - q_n}{\Delta t} \\ q_{n+\alpha} &= (1 - \alpha)q_n + \alpha q_{n+1}, \quad 0 \leq \alpha \leq 1 \end{aligned} \quad (3)$$

and construct *discretized* action integral

$$S(q_{n+1}, q_n, \Delta t) = \int_{\Delta t} L\left(\frac{q_{n+1} - q_n}{\Delta t}, q_{n+\alpha}\right) dt \quad (4)$$

A Taylor series expansion shows that,  $S$  given above is a first order approximation to (2). This ensures the consistency of approximation. In what follows it is assumed that the Lagrangian is of the form,

$$L(\dot{q}, q) = K(\dot{q}) - U(q) \quad (5)$$

where  $K: TQ \rightarrow R$  is the kinetic energy, and  $U: Q \rightarrow R$  is the potential energy. Assume further that  $K$  is positive definite quadratic form in canonical momentum,

$$K(p) = \frac{1}{2} p \cdot M^{-1} p, \quad M = M^T \quad (6)$$

Then the discretized action integral may be worked out as,

$$S(q_{n+1}, q_n, \Delta t) = \frac{1}{2\Delta t} (q_{n+1} - q_n) \cdot M(q_{n+1} - q_n) - \Delta t U(q_{n+\alpha}) \quad (7)$$

In view of (1), the time stepping integrator is derived as,

$$\begin{aligned} p_{n+1} &= \frac{M}{\Delta t} (q_{n+1} - q_n) - \alpha \Delta t U'((1-\alpha)q_n + \alpha q_{n+1}) \\ -p_n &= \frac{M}{\Delta t} (q_n - q_{n+1}) - (1-\alpha) \Delta t U'((1-\alpha)q_n + \alpha q_{n+1}) \end{aligned} \quad (8)$$

Where  $U' = \frac{dU(\xi)}{d\xi}$ .

## 2.2 Invariance Under Group Action, Conserving Properties

As an example, assume the generating function is invariant under the left action of rotation group, in sense that  $S(q_{n+1}, q_n, t) = S(gq_{n+1}, gq_n, t)$  for  $g \in SO(3)$ . A simple case could be that both kinetic and potential energy are invariant. Following the argument of Marsden[1], algorithm (8) should conserve the *angular* momentum map  $J: P \rightarrow R^3$ . This can be verified by the following calculation. From (8),

$$J_{n+1} - J_n := \sum_A q_{n+1}^A \times p_{n+1}^A - \sum_A q_n^A \times p_n^A = -\Delta t \sum_A q_{q_{n+\alpha}}^A \times U'(q_{q_{n+\alpha}}^A) \quad (9)$$

Recall the algorithmic invariance condition given by Simo[4, Equation (2.18<sub>2</sub>)], namely

$$\sum_A q_{n+\alpha}^A \times U'(q_{n+\alpha}^A) = 0$$

It is clear that  $J_{n+1} - J_n = 0$ . Another way to see is to recast (7) into the following form,

$$\begin{aligned} p_{n+1} - p_n &= -\Delta t U'((1-\alpha)q_n + \alpha q_{n+1}) \\ q_{n+1} - q_n &= \Delta t M^{-1}((1-\alpha)p_{n+1} + \alpha p_n) \end{aligned} \quad (10)$$

Which can be readily identified as the momentum conserving algorithm by Simo[4, Equation(2.19)] with  $\kappa_1 = \kappa_2 = 1$ . (Parameter  $\kappa$ 's are introduced to enforce conservation

of energy, which may be regarded as algorithmic representation of "reparameterization in time". This will be addressed briefly in next sub-section). Noted also if the Lagrangian does depend on  $q$ , then, by (10<sub>a</sub>),  $p_{n+1} = p_n$ , the conservation of *linear* momentum map is trivially satisfied.

A few remarks may be included here. First, equation(10) actually furnishes a first order discretization to Hamilton equation, and is second order as  $\alpha = 0.5$ . Second, generation functions in term of pairs  $(q_{n+1}, p_n)$ ,  $(q_n, p_{n+1})$  may also be used, with a proper approximation analogous to (3) (4) and the following rules

$$\begin{aligned} p_{n+1} &= \frac{\partial S(q_{n+1}, p_n, t_{n+1}, t_n)}{\partial q_{n+1}} \\ q_n &= \frac{\partial S(q_{n+1}, p_n, t_{n+1}, t_n)}{\partial p_n} \end{aligned} \quad (11)$$

or,

$$\begin{aligned} q_{n+1} &= -\frac{\partial S(q_n, p_{n+1}, t_{n+1}, t_n)}{\partial p_{n+1}} \\ p_n &= -\frac{\partial S(q_n, p_{n+1}, t_{n+1}, t_n)}{\partial q_n} \end{aligned} \quad (12)$$

### 2.3 Conservation of Energy

It seems that the difficulty associated with the conservation of energy may be attributed to the fact that the potential energy function lacks a unified mathematical structure. (The kinetic energy, on the other hand, always induces a Riemannian metric in configuration space). Hence there may not exist a general way for constructing energy conserving algorithm. Conservation of energy may only be enforced, say, numerically, and on a case-to-case basis. The general issue will not be discussed herein, rather, a special example will be examined, with emphasis on "reparameterization of time".

Recall that middle point rule conserves the total energy in linear Hamiltonian system, we then set  $\alpha = 0.5$ , and apply it to linear oscillation of a one degree of freedom system, the mass of which is unite. (Or, one may regard this as modal coordinates of general linear Hamiltonian system). First check that the energy is indeed conserved. Recall

$$E_m = \frac{1}{2}p_m^2 + \frac{\omega^2}{2}q_m^2, \quad m = n, n+1 \quad (13)$$

The difference in energy between time steps is worked out to be

$$E_{n+1} - E_n = (\alpha - 0.5)\omega^2(q_{n+1}p_n - q_n p_{n+1}) \quad (14)$$

Then the conservation of energy is obvious. Recall we have the integrator i) symplectic, ii) conserve angular momentum, iii) conserve energy. For this particular problem, which has two integral invariance and thus is completely integrable, the integrator should integrate the exact trajectory to within a reparameterization of time. Recall Hamilton's equation,

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\omega^2 & 0 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} \quad (15)$$

the solution of which gives a time-stepping relation,

$$\begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = e^{\begin{pmatrix} 0 & 1 \\ -\omega^2 & 0 \end{pmatrix} \Delta t} \begin{pmatrix} q_n \\ p_n \end{pmatrix} = \begin{pmatrix} \cos(\omega\Delta t) & \sin(\omega\Delta t)/\omega \\ -\omega \sin(\omega\Delta t) & \cos(\omega\Delta t) \end{pmatrix} \begin{pmatrix} q_n \\ p_n \end{pmatrix} \quad (16)$$

And the integrator yields the following,

$$\begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = \frac{1}{1 + (\omega\Delta\tau)^2/4} \begin{pmatrix} 1 - (\omega\Delta\tau)^2/4 & 1 \\ -\omega^2\Delta\tau & 1 - (\omega\Delta\tau)^2/4 \end{pmatrix} \begin{pmatrix} q_n \\ p_n \end{pmatrix} \quad (17)$$

Comparing (16), (17), it's clear that if one relates  $\Delta t$  and  $\Delta\tau$  by

$$\Delta t = \cos^{-1} \frac{1 - (\omega\Delta\tau)^2/4}{1 + (\omega\Delta\tau)^2/4} \quad (18)$$

then integrator essentially integrate the exact solution.

The above discussion leads to the following observation, that one may introduce other parameters, put them as function of time in (4), to represent the reparameterization. First

order accuracy could be ensured by imposing consistency condition on these parameters. This may provided an explanation for the parameter  $\kappa$ 's in Simo [4][5].

### 3. Rigid Body Dynamics

There seems to be a number of ways to apply the method to rigid body dynamics. The first is to use coordinate at the onset, for example, the Euler angles. By a proper choice of coordinates, the coordinates may be globally canonical, so the procedure above can be applied directly. However, these coordinate may have singularities as in the case of Euler angles, hence caution should be exercised. Another drawback is the loss of "intrinsic" feature that the theory originally possesses.

Another way is to use the reduction (symmetry) theory[1, 2]. This theory provides a systematic way to transform the dynamics from symplectic cotangent space to the reduced symplectic space and vice versa, as well as transformation form the configuration to its Lie algebra. With these transformation in hand, one may write the dynamic in the induced space and/or Lie algebra, formulate the updating there and transform back[1,5]. This is an elegant approach. The author needs time to digest this theory and understand the details.

Without going to reduction theory, the above procedure may be also be applied to rigid bodies, as outlined below. Recall the configuration space is the rotation group  $SO(3)$ , one may use the following discretization,

$$\hat{\Omega} = \frac{\ln(Q_{n+1}) - \ln(Q_n)}{\Delta t} \quad (19)$$

$$Q_{n+\alpha} = Q_n^{1-\alpha} Q_{n+1}^\alpha$$

which is the counterpart of (3) in nonlinear case.  $\hat{\Omega} \in \mathfrak{so}(3)$  is the (body) angular velocity and  $Q_n, Q_{n+1}$  the configurations. Equation (19<sub>b</sub>) may be used when potential is involved. Make the connection between skew symmetric matrix and vector by the usual way, one may define vectorial form of angular velocity and momentum. Follow the notation in Zhong & Marsden [1], one may write the Lagrangian for a free rigid body as,

$$L = \frac{1}{4} \text{trace} \left( \hat{\Omega} \hat{I} \cdot \hat{\Omega} \right) \quad (20)$$

And the generating function, from the integration of the Lagrangian over time step, is,

$$S = \frac{1}{4\Delta t} \text{trace} \left( (\ln(Q_{n+1}) - \ln(Q_n)) \hat{I} \cdot (\ln(Q_{n+1}) - \ln(Q_n)) \right) \quad (21)$$

The "momentum", i.e., the matrix form of body angular momentum, may be derived as,

$$\begin{aligned} \hat{p}_{n+1} &= Q_{n+1}^{-1} \frac{\partial S}{\partial Q_{n+1}} \\ \hat{p}_n &= -Q_n^{-1} \frac{\partial S}{\partial Q_n} \end{aligned} \quad (22)$$

Equation (22) may provide a time integration scheme. Conservation properties will not be discussed.

#### 4. Conclusion

A process of constructing symplectic conserving integrators is briefly discussed. The method falls into the category of using generating function. Use is made of a discretized action integral as a generating function. Conservation properties in linear configuration space is discussed, and is shown lead to algorithms by Simo. Possible application to rigid body dynamics is suggested.

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