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Noether's theorem and one-step corrections method for holonomic system*

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In this paper, a new computational method for improving the accuracy of numerically computed solutions is introduced. The computational method is based on the one-step method and conserved quantities of holonomic systems are considered as kinematical constraints in this method.

Keywords: conserved quantities, one-step method, holonomic system
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1. Introduction

Dynamical systems are usually represented as a set of first-order equations. Various computational methods, such as Euler's method, the Runge–Kutta method and many other integration algorithms,[1] can be used to accomplish the numerical integration of ordinary differential equations. In assessing the accuracy of numerically computed solutions to the equations of motion of a dynamical system, it is helpful to have relatively simple check solutions available. A common approach is to use integrals of the motion or conserved quantities, that is, functions whose values remain constant during the course of the solution, as checks on accuracy. For example, the energy integral may be used for conservative systems. Other systems may have one or more conserved quantities. Integrals of the motion are particularly effective in detecting programming errors. In this paper, a method for representing constraints that are integrals of motion or conservative quantities of dynamical systems is presented and one example is analysed to illustrate the method.

2. Equation of motion of holonomic system

Let us consider first a dynamical system which is subjected to m holonomic constraints of the form

$$\varphi_j(q,t)=0, \quad (j=1,\ldots,m). \tag{1}$$

Suppose there are n second-order dynamical equations written in the fundamental Lagrangian form

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{\partial T}{\partial \dot{q}_s}\Big)-\frac{\partial T}{\partial q_s}=\sum_{j=1}^{m}\lambda_j\frac{\partial \varphi_j}{\partial q_s}+Q_s(q,\dot{q},t),$$

$$(s=1,\ldots,n), \tag{2}$$

where λs are Lagrange multipliers, Q_s are generalized applied forces.

Solve these n equations for the $n\ddot{q}_s$ $(s=1,\ldots,n)$:

$$\ddot{q}_s=\ddot{q}_s(q,\dot{q},\lambda,t), \quad ,(s=1,\ldots,n)\,. \tag{3}$$

The m holonomic constraint functions are differentiated twice with respect to time, with the result

$$\ddot{\varphi}_j(q,\dot{q},\ddot{q},t)=0,(j=1,\ldots,m)\,. \tag{4}$$

Then the $n\ddot{q}$ expressions obtained from the dynamical equations are substituted into Eq.(4). These m equations are solved for the m Lagrange multipliers $\lambda_j(q,\dot{q},t)$ which are then substituted back into the $\ddot{q}$ expressions. At this point, we have n dynamical equations without λs, namely,

$$\ddot{q}_s=\ddot{q}_s(q,\dot{q},t), \quad (s=1,\ldots,n)\,. \tag{5}$$

These n second-order equations are integrated numerically, usually by converting them into $2n$ first-order equations. A one-step error correction takes place at each time step.

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3. Conserved quantities of dynamical systems

The theory of symmetries and conserved quantities is an important research field in mathematics and physics. A conservative quantity or constant of motion $C(\boldsymbol{q},\dot{\boldsymbol{q}})$ is any function that satisfies $\mathrm{d}C/\mathrm{d}t=0$, where $\boldsymbol{q}(t)$ is a solution of the equation of motion. For example, in a 'conservative' system, energy is conserved, so $E(\boldsymbol{q},\dot{\boldsymbol{q}})$ is a constant of motion.

A theorem proved by Emmy Noether provides a powerful way of extracting constants of motion from Lagrangians. Noether's theorem[2] involves the process of identifying a flow in configuration space that leaves L invariant. A 'flow' is an infinitesimal transformation

$$\boldsymbol{q}\ \rightarrow\ \boldsymbol{q}'=\boldsymbol{q}+\frac{\mathrm{d}\boldsymbol{q}(\boldsymbol{q})}{\mathrm{d}\lambda}\delta\lambda\,. \tag{6}$$

A flow changes the path $\boldsymbol{q}(t)$ into the path $\boldsymbol{q}'(t)$ and thus changes the value of the Lagrangian at time t by

$$\delta L=\frac{\partial L}{\partial\boldsymbol{q}}\cdot\delta\boldsymbol{q}+\frac{\partial L}{\partial\dot{\boldsymbol{q}}}\cdot\delta\dot{\boldsymbol{q}}\,. \tag{7}$$

Notice that $\delta\dot{\boldsymbol{q}}$ is well defined: $\delta\dot{\boldsymbol{q}}=\partial\delta\boldsymbol{q}/\partial\boldsymbol{q}\cdot\dot{\boldsymbol{q}}$.

Invariance of L just means that L takes the same value at all points that are joined by the flow. Noether's theorem states that if δL vanishes along the dynamically determined path, then $\mathrm{d}\boldsymbol{q}/\mathrm{d}\lambda\cdot\partial L/\partial\dot{\boldsymbol{q}}$ is a constant of motion. The proof of Noether's theorem is simple. Equating to zero Eq.(7) for δL, we have

$$\begin{aligned}0=&\delta L=\frac{\partial L}{\partial\boldsymbol{q}}\cdot\delta\boldsymbol{q}+\frac{\partial L}{\partial\dot{\boldsymbol{q}}}\cdot\delta\dot{\boldsymbol{q}}\\ =&\frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{\partial L}{\partial\dot{\boldsymbol{q}}}\Big)\cdot\delta\boldsymbol{q}+\frac{\partial L}{\partial\dot{\boldsymbol{q}}}\cdot\delta\dot{\boldsymbol{q}}\\ =&\frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{\partial L}{\partial\dot{\boldsymbol{q}}}\cdot\delta\boldsymbol{q}\Big)=\frac{\mathrm{d}}{\mathrm{d}t}\big(\frac{\partial L}{\partial\dot{\boldsymbol{q}}}\cdot\frac{\mathrm{d}\boldsymbol{q}}{\mathrm{d}\lambda}\delta\lambda\big)\,.\end{aligned}$$

Thus from the invariance of L under translation $\boldsymbol{x}\rightarrow\boldsymbol{x}+\boldsymbol{i}\delta\lambda$ along the x-axis, Noether's theorem deduces the constancy of

$$\boldsymbol{i}\cdot\frac{\partial L}{\partial\dot{q}}=\frac{\partial L}{\partial\dot{x}}\,.$$

For a particle moving in a velocity-independent potential this is just the x-momentum $m\dot{x}$.

After Noether's work, many Chinese[3−10] and foreign[11−14] researchers have done a lot of work. Hence more general and more important results have been obtained.

Define an infinitesimal transformation of time and generalized coordinates

$$t^*=t+\Delta t,\quad q_s^*(t^*)=q_s(t)+\Delta q_s\,, \tag{8}$$

or their linear expansions

$$\begin{aligned}&t^*=t+\varepsilon\xi_0(t,\boldsymbol{q},\dot{\boldsymbol{q}}),\\ &q_s^*(t^*)=q_s(t)+\varepsilon\xi_s(t,\boldsymbol{q},\dot{\boldsymbol{q}})\,,\end{aligned} \tag{9}$$

where ε is an infinitesimal real parameter, ξ_0 and ξ_s are infinitesimal generators.

Noether's symmetry means that the action of Hamilton's variational principle is invariant under an infinitesimal transformation. Noether's theorem says that if we can find r functions $G^\alpha=G^\alpha(t,\boldsymbol{q},\dot{\boldsymbol{q}})$ such that

$$\begin{aligned}&\frac{\partial L}{\partial t}\xi_0^\alpha+\frac{\partial L}{\partial q_s}\xi_s^\alpha+\frac{\partial L}{\partial\dot{q}_s}\dot{\xi}_s^\alpha\\ &+\Big(L-\frac{\partial L}{\partial\dot{q}_s}\dot{q}_s\Big)\dot{\xi}_0^\alpha=-\dot{G}^\alpha\,,\\ &(\alpha=1,\ldots,r)\,,\end{aligned} \tag{10}$$

then it will yield r conserved quantities or constants of the motion

$$\begin{aligned}J_\alpha=&L\xi_0^\alpha+\frac{\partial L}{\partial\dot{q}_s}(\xi_s^\alpha-\dot{q}_0^\alpha)+G^\alpha\\ &=\text{const.}\quad(\alpha=1,\ldots,r)\,.\end{aligned} \tag{11}$$

Conserved quantities or integrals of the motion can be used to check the accuracy of numerically computed solutions. Integrals of the motion are also particularly effective in detecting programming errors.

4. One-step method for holonomic system

The accuracy of numerical results for a dynamical system can be improved by using a one-step method.[15] The correction is very significant when a system is subjected to more than one constraint. The goal of the one-step method is to completely eliminate the constraint errors at the end of each time step. Integrals of the motion or conserved quantities are often used as checks on accuracy.

For any given configuration, velocity errors result in a separation of the solution point from the constraint surface in velocity space. These errors can be detected and corrections can be made for the $\dot{q}s$.

Suppose $J_j(q,\dot{q},t)=C_j=$ const. be conserved quantities of the system. Let $I_j(q,\dot{q},t)=J_j(q,\dot{q},t)-C_j=0$, then we have $I_j(q,\dot{q},t)=0\,,\quad(j=1,\ldots,m)$.

We can use one-step procedure to correct the velocities in such a manner that all the $I_j s$ go to zero. The gradient in the velocity space of I_j is

$$\nabla I_j = \Big[\frac{\partial I_j}{\partial \dot{q}_1}, \ldots, \frac{\partial I_j}{\partial \dot{q}_n}\Big]^{\mathrm{T}}. \tag{12}$$

Choose the velocity vector correction $\Delta\dot{\boldsymbol{q}}$ of the form

$$\Delta\dot{\boldsymbol{q}} = \sum_{j=1}^{r} K_j \nabla I_j \,, \tag{13}$$

where the values of Ks are such that

$$\nabla I_j \cdot \Delta\dot{\boldsymbol{q}} = -I_j \,, \quad (j = 1, \ldots, r) \,. \tag{14}$$

We can write Eqs.(13) and (14) more explicitly as

$$\Delta\dot{q}_s = \sum_{j=1}^{r} K_j \frac{\partial I_j}{\partial \dot{q}_s} \,, \quad (s = 1, \ldots, n) \,, \tag{15}$$

where the Ks are obtained by solving

$$\sum_{s=1}^{n}\sum_{l=1}^{r} K_l \frac{\partial I_j}{\partial \dot{q}_s}\frac{\partial I_l}{\partial \dot{q}_s} = -f_j \,, \quad (j = 1, \ldots, r) \,. \tag{16}$$

Knowing the values of the Ks, one can obtain the velocity corrections from Eq.(15).

5. Example

Example 1[3] Consider the Emden equation

$$\ddot{q} + \frac{2}{t}\dot{q} + q^5 = 0 \,. \tag{17}$$

This second-order equation is usually converted into two first-order equations and integrated numerically.

The corresponding Lagrangian of the system is

$$L = t^2\Big(\frac{1}{2}\dot{q}^2 - \frac{1}{6}q^6\Big) \,. \tag{18}$$

According to Eq.(10), we can find its generator function is

$$\xi_0 = t, \quad \xi = -\frac{1}{2}q \,. \tag{19}$$

Noether's theorem implies

$$J = -\frac{1}{2}t^3\dot{q}^2 - \frac{1}{2}t^2 q\dot{q} - \frac{1}{6}t^3 q^6 = \text{const.} \tag{20}$$

First, we require the velocity correction in the velocity space,

$$\Delta\,\dot{q} = K\frac{\partial I}{\partial \dot{q}} \,, \tag{21}$$

where $I = J - C = 0$. Next, the correction must exactly cancel the constraint error, that is

$$\frac{\partial I}{\partial \dot{q}} \cdot \Delta\,\dot{q} = -I \,. \tag{22}$$

Or

$$K\frac{\partial I}{\partial \dot{q}} \cdot \frac{\partial I}{\partial \dot{q}} = -I. \tag{23}$$

This equation is solved for K and then the velocity correction is made using Eq.(21):

$$K = \frac{-I}{\big(t^3\dot{q} + \frac{1}{2}t^2 q\big)^2} \,. \tag{24}$$

Hence the one-step velocity correction is

$$\Delta\,\dot{q} = \frac{I}{t^3\dot{q} + \frac{1}{2}t^2 q} \,. \tag{25}$$

Thus, at end of each time step in the numerical integration, the value of the conserved quantity is approximately zero.

Example2 A pendulum of particle mass m and length l is forced to rotate about a vertical axis with a constant angular velocity Ω. The pendulum angle θ is measured downward from the horizontal axis η, as shown in Fig.1.

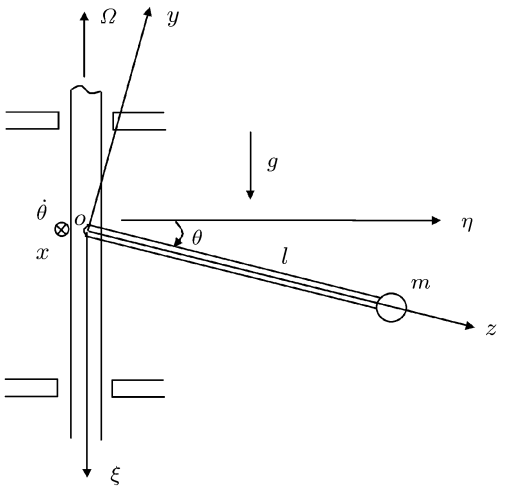


Figure 1

The system is described by Lagrange's equation of the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{\partial L}{\partial \dot{\theta}}\Big) - \frac{\partial L}{\partial \theta} = 0 \,.$$

The Lagrangian function is

$$L = T - V = \frac{1}{2}ml^2\dot{\theta}^2 + \frac{1}{2}ml^2\Omega^2\cos^2\theta + mgl\sin\theta \,.$$

The corresponding motion equation of the system is

$$ml^2\ddot{\theta} - m(gl - l^2\Omega^2\sin\theta)\cos\theta = 0 \,.$$

After simplifying it, we have

$$\ddot{\theta} - (g/l - \Omega^2\sin\theta)\cos\theta = 0 \,.$$

Assume that $g/l = 4$ m/s^2 and $\Omega = \sqrt{10}$ rad/s, then substitute these values into Eq.(27), we obtain

$$\ddot{\theta} + (10\sin\theta - 4)\cos\theta = 0\,. \tag{28}$$

This second-order equation can be converted into two first-order equations and integrated numerically under the initial conditions $\theta(0) = 0$ and $\omega(0) = 0$.

$$\dot{\theta} = \omega\,, \quad \dot{\omega} = (4 - 10\sin\theta)\cos\theta\,. \tag{29}$$

Let us consider the corrections of one-step method. Noether's theorem implies

$$\begin{aligned} E &= T_2 - T_0 + V \\ &= \frac{1}{2}ml^2\dot{\theta}^2 - \frac{1}{2}ml^2\Omega^2\cos^2\theta - mgl\sin\theta = E_0\,, \end{aligned} \tag{30}$$

where E_0 is evaluated under the initial conditions.

The individual angular velocity correction is

$$\Delta\dot{\theta} = K\frac{\partial T}{\partial\dot{\theta}}\,, \tag{31}$$

where

$$K = -\Delta E\Big[\Big(\frac{\partial T}{\partial\dot{\theta}}\Big)^2\Big]^{-1}$$

and $\Delta E = E - E_0$.

In the case of $\dot{\theta}$ remaining small, it is preferable to make the correction in configuration space

$$\Delta\theta = -\Delta E\Big[\Big(\frac{\partial V'}{\partial\theta}\Big)^2\Big]^{-1}\frac{\partial V'}{\partial\theta}\,, \tag{32}$$

where $V' = V - T_0 = -ml^2\Omega^2\cos^2\theta/2 - mgl\sin\theta$.

The numerical results of Eqs.(29) are presented in table 1 with time step h=0.001s. Tabulated values of θ and ω over the time interval $0 \le t \le 1.5$s are shown in Table 1.

Table 1. Numerical results of Eqs.(29).

Step N	t/s	θ/rad	ω/(rad/s)
1	0.001	2e-006	0.00399999
100	0.1	0.0198336	0.393352
200	0.2	0.0773546	0.74733
300	0.3	0.166776	1.02589
400	0.4	0.279102	1.20207
500	0.5	0.403383	1.26469
600	0.6	0.528487	1.22121
700	0.7	0.644813	1.09352
800	0.8	0.745298	0.908899
900	0.9	0.825516	0.691691
1000	1	0.88313	0.459049
1100	1.1	0.91714	0.220673
1200	1.2	0.927219	–0.0191867
1300	1.3	0.913306	–0.25895
1400	1.4	0.875489	–0.496805
1500	1.5	0.814167	–0.727807

6. Conclusions

We have discussed the integrals of motion or the conserved quantities of holonomic systems that can be used for error correction at the end of each time step in the numerical integration. The method presented in this paper generalizes the work of Ref.[15] in which the kinematical constraints and classical integrals of motion are taken as constraints to improve and correct the numerical results at each time step. The concepts of integrals of motion in this paper have more comprehensive meaning and are thus applicable to all kinds of conserved quantities such as Noether's conserved quantities.

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