Indicator of chaos based on the Riemannian geometric approach

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Using the Riemannian geometric approach to Hamiltonian systems, we show that the empirical indicator of chaos proposed by Kosloff and Rice [J. Chem. Phys. **74**, 1947 (1981)], an improved version of the well-known Toda-Brumer criterion, is equivalent to sectional curvature of the Jacobi equation when the Eisenhart metric is chosen for the Riemannian manifold. Further, we present a relation among the sectional curvature, the Lyapunov exponents, and the Kolmogorov-Sinai entropy. By using this relation, the empirical indicator by Kosloff and Rice, which is local, can be used as a global indicator of chaos.

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A study on the stability of dynamical systems has been extensively done to find the methods and the criteria for determining the onset of chaotic motion in the Hamiltonian system since the pioneer work by Toda [1] and Brumer [2]. The Toda-Brumer (TB) criterion for the onset of chaos is based on local instability due to separation of neighboring trajectories in phase space. The instability of these trajectories relates closely to the sign of the Gaussian curvature of the potential function of the system [1]. Owing to its simplicity, this criterion has been widely used to predict the critical value for intramolecular energy transfer [2] and several chemical systems [3] in chemical dynamics as well as the threshold energy for the onset of chaos in dynamical systems [4,5]. However it is also known that the TB criterion sometimes fails to correctly predict these values.

In order to remove this defect in the TB criterion, it is necessary to impose stronger conditions to specify the trajectories responsible for chaotic motion. Based on the observation that chaotic motion occurs by the trajectory which diverges in the direction perpendicular to the flow in phase space, which is found by the analysis of the Hénon-Heiles system, Kosloff and Rice have proposed an empirical indicator of chaos, i.e., an improved version of the Toda-Brumer criterion [6]. This improved TB (ITB) criterion seems to be very effective for two-dimensional Hamiltonian systems to obtain the precise information about the onset of chaos. The degree of chaos is characterized by the quantity related to the curvature of the potential energy surface perpendicular to the trajectory. The ITB criterion is, however, introduced in an empirical way so that its base is not clear from the viewpoint of both physics and mathematics.

Recently there has been much attention to investigation about Hamiltonian chaos from the Riemannian geometric approach [7]. In this approach, the trajectory of a dynamical system can be viewed as a geodesic on the Riemannian manifold endowed with a suitable metric. The stability of the trajectory is connected to the curvature of the manifold on which the trajectory is defined. Especially the sectional curvature plays a central role to determine the local instability of trajectories. The usefulness of this approach has been confirmed for the two-dimensional Hamiltonian systems such as the Hénon-Heiles system [5], the homogeneous Yang-Mills-Higgs system [8] and the Abelian-Higgs system [9].

The purpose of this paper is to show that the ITB criterion can be understood from the framework of the Riemannian geometric approach. Indeed, it is shown that the indicator of chaos used in the ITB criterion is equivalent to the sectional curvature of the Jacobi equation in the Riemannian geometric approach when the Eisenhart metric is chosen. From this equivalence we can explain the reason why the original TB criterion does not necessarily work well. Furthermore, we point out an interesting relation among the sectional curvature, the Lyapunov exponents and the Kolmogorov-Sinai (KS) entropy that connects the ITB criterion to a global indicator of chaos.

Let us start by briefly reviewing the TB criterion [1,2], which is derived by the analysis of the linear stability of trajectories. For the Newtonian system with two degrees of freedom as

$$\frac{d^2q^i}{dt^2} = -\frac{\partial V(\boldsymbol{q})}{\partial q^i} \quad (i=1,2), \tag{1}$$

the perturbation ξ^i to the trajectory q^i evolves under the tangent dynamics equation as

$$\frac{d^2\xi^i}{dt^2} + m_{ij}\xi^j = 0, \quad m_{ij} = \frac{\partial^2 V}{\partial q^i \partial q^j}, \tag{2}$$

where V is the potential energy function of the system. The stability of the motion is determined by the eigenvalues of the stability matrix with elements m_{ij}. The eigenvalues are

$$\lambda_\pm = h \pm \sqrt{h^2 - G}, \tag{3}$$

where h and G are defined as

$$h = m_{11} + m_{22}, \quad G = m_{11}m_{22} - m_{12}m_{21}. \tag{4}$$

If we have a region where G is negative in Eq. (3), λ_- becomes negative. For this negative eigenvalue the perturbation ξ^i grows exponentially with time because of $\xi \propto \exp(\sqrt{-\lambda}t) = \exp(\sqrt{|\lambda_-|}t)$. In this case the system exhibits an exponential instability. The TB criterion claims that the onset of chaos starts at the threshold energy determined by $G=0$ in Eq. (4). Since the expression of G is the same as the numera-

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tor of the Gaussian curvature of the potential function V, the quantity G has the same sign as the Gaussian curvature. Hereafter we call G the Gaussian curvature tersely.

The ITB criterion comes from the empirical fact that chaotic motion can be triggered by the trajectory diverging in the direction perpendicular to the flow in phase space [6]. In other words, if the motion for some time sweeps across the region where the curvature of the potential surface is negative, we ultimately observe that the motion becomes chaotic at longer periods.

To formulate the curvature appropriate for describing such a motion, it is convenient to introduce a set of coordinates $(z_\parallel, z_\perp)$ which moves with the trajectory, where $z_\parallel$ and $z_\perp$ are parallel and transverse to an arbitrary direction of flow, respectively. The coordinate $z_\perp$ is related to the coordinates (q_1, q_2) by

$$z_\perp = -q_1 \sin\theta + q_2 \cos\theta, \tag{5}$$

where θ is the angle between q_1 and $z_\parallel$. Thus the curvature perpendicular to the direction of the flow can be described by the quantity $d^2V/dz_\perp^2$. This quantity is calculated as

$$V^{(2)} \equiv \frac{d^2V(q_1,q_2)}{dz_\perp^2} = m_{11}\sin^2\theta + m_{22}\cos^2\theta - m_{12}\sin 2\theta, \tag{6}$$

where m_{ij} is the element of the stability matrix in Eq. (2).

Since the curvature $V^{(2)}$ is defined in the direction perpendicular to the motion, the empirical fact mentioned above is characterized by the condition $V^{(2)}<0$. Indeed it has been numerically shown that the chaotic degree of the Hénon-Heiles system increases with the amount of such negative region. Based on these observations it is proposed that $V^{(2)}$ is a more precise indicator of chaos than G used in the TB criterion. In other words, the ITB criterion claims that the onset of chaos depends on the measure of the region with negative $V^{(2)}$.

From now, let us try to show that the quantity $V^{(2)}$ is closely related to the sectional curvature of a Riemannian manifold whose sign is relevant for the stability of a geodesic. In the Riemannian geometric approach [7,10], the stability of a geodesic flow is studied by means of the Jacobi equation as

$$\frac{D^2\boldsymbol{J}}{Ds^2} + R(\boldsymbol{J},\boldsymbol{v})\boldsymbol{v} = 0, \tag{7}$$

where s is the proper time, $R(\cdot,\cdot)$ is the Riemannian curvature tensor, D/Ds is the covariant derivative along the geodesic and $\boldsymbol{v}=d\boldsymbol{q}/ds$ is the velocity of the geodesic. This equation comes from the second-order variation of the geodesic equation with respect to a perturbed geodesic. Thus Eq. (7) describes the evolution of a vector field $\boldsymbol{J}$ called the Jacobi field or the geodesic variation field, which measures the spread between nearby geodesics.

In order to clarify the meaning of $V^{(2)}$ in Eq. (6), by multiplying Eq. (7) by $\boldsymbol{J}$ we consider its scalar version, i.e., the norm equation, as follows:

$$\left\langle \frac{D^2\boldsymbol{J}}{Ds^2}, \boldsymbol{J} \right\rangle + \langle R(\boldsymbol{J},\boldsymbol{v})\boldsymbol{v}, \boldsymbol{J}\rangle = 0, \tag{8}$$

where $\langle X, Y\rangle = g_{ij}X^iY^j$ stands for a scalar product. It is well known that once the sectional curvature is introduced this norm equation can be transformed to a generalized Hill equation of the form (11) or (13) as will be shown below. For these derivations we follow the procedure presented in Ref. [5] although we can find similar manipulation in many standard books of the Riemannian geometry [10]. The second term of Eq. (8) is written by the sectional curvature K as

$$\langle R(\boldsymbol{J},\boldsymbol{v})\boldsymbol{v},\boldsymbol{J}\rangle = K(\boldsymbol{J},\boldsymbol{v})(\langle \boldsymbol{J},\boldsymbol{J}\rangle\langle \boldsymbol{v},\boldsymbol{v}\rangle - \langle \boldsymbol{J},\boldsymbol{v}\rangle^2). \tag{9}$$

By noting that $\boldsymbol{J}$ is orthogonal to $\boldsymbol{v}$, i.e., $\langle \boldsymbol{J},\boldsymbol{v}\rangle=0$, and the condition of $\langle \boldsymbol{v},\boldsymbol{v}\rangle=1$, we can derive from Eq. (8) the following equation as

$$\frac{1}{2}\frac{d^2\|\boldsymbol{J}\|^2}{ds^2} + K(\boldsymbol{J},\boldsymbol{v})\|\boldsymbol{J}\|^2 - \left(\frac{d\|\boldsymbol{J}\|}{ds}\right)^2 = 0, \tag{10}$$

where $\|\boldsymbol{J}\| = \sqrt{\langle \boldsymbol{J},\boldsymbol{J}\rangle}$.

From Eq. (10) we arrive at the norm equation describing the evolution of the norm $\|\boldsymbol{J}\|$ as

$$\frac{d^2\|\boldsymbol{J}\|}{ds^2} + K(\boldsymbol{J},\boldsymbol{v})\|\boldsymbol{J}\| = 0, \tag{11}$$

where the sectional curvature $K(\boldsymbol{J},\boldsymbol{v})$ is given by

$$K(\boldsymbol{J},\boldsymbol{v}) = R_{\mu\nu\lambda\eta}\frac{J^\mu}{\|\boldsymbol{J}\|}\frac{dq^\nu}{ds}\frac{J^\eta}{\|\boldsymbol{J}\|}\frac{dq^\lambda}{ds}. \tag{12}$$

Up to this point the results are independent of choice of the metric.

Here we use the Eisenhart metric. This metric allows that the arc length ds is parametrized by $ds^2=C^2dt^2$ with C a constant and the physical time t is by $q^0=t$. Under this metric the nonvanishing component of $R_{\mu\nu\lambda\eta}$ in Eq. (12) is R_{i0j0} alone, which equals m_{ij} in Eq. (2), and then $R_{i0j0}(dq^0/ds)\times(dq^0/ds)=m_{ij}/C^2$. Since the first term of the Jacobi equation (11) becomes $d^2\|\boldsymbol{J}\|/C^2dt^2$, Eq. (11) can be finally rewritten as follows

$$\frac{d^2\|\boldsymbol{J}\|}{dt^2} + K^{(2)}\|\boldsymbol{J}\| = 0, \tag{13}$$

where the sectional curvature $K^{(2)}$ is defined as

$$K^{(2)} = m_{ij}\frac{J^i}{\|\boldsymbol{J}\|}\frac{J^j}{\|\boldsymbol{J}\|}. \tag{14}$$

It should be noticed here that the sectional curvature (12) becomes a simple expression (14) owing to the Eisenhart metric. For the two-dimensional Hamiltonian systems [5,9] we can assign $J^1=p_2$ and $J^2=-p_1$ to the components of $\boldsymbol{J}$ of Eq. (14). Thus the sectional curvature $K^{(2)}$ of Eq. (14) can be written as

$$K^{(2)}(\boldsymbol{p},\boldsymbol{q}) = \frac{1}{p^2}(m_{11}p_2^2 + m_{22}p_1^2 - 2m_{12}p_1p_2), \tag{15}$$

where $p^2=p_1^2+p_2^2$ and the relation of $m_{12}=m_{21}$ is used. By using the relation as $p_1=p\cos\theta$ and $p_2=p\sin\theta$, we can finally show that $K^{(2)}$ of Eq. (15) is the same expression as $V^{(2)}$ of Eq. (6). In other words, the quantity $V^{(2)}$ proposed empirically in Ref. [6] is nothing but the sectional curvature $K^{(2)}$ of the Jacobi equation (7) when the Eisenhart metric is used. If $K^{(2)}<0$ the nearby geodesics starting out parallel tend to diverge, while if $K^{(2)}>0$ they tend to converge. Thus the sign of the curvature $K^{(2)}$ is relevant for the stability of a geodesic. This fact is reflected in the instability condition $V^{(2)}<0$ in the ITB criterion. In conclusion, we have shown that the ITB criterion is understood from the viewpoint of the Riemannian geometry and its empirical indicator of chaos, $V^{(2)}$, is exactly the same as the sectional curvature $K^{(2)}$ in the Jacobi equation with the Eisenhart metric.

Let us briefly comment on our results. First, we would like to show that the sectional curvature $K^{(2)}$ of Eq. (15) explains the reason why the TB criterion sometimes fails to predict the threshold energy for the onset of chaos. For this purpose, it should be noticed that the expression of Eq. (15) or Eq. (6) can be rewritten as

$$K^{(2)} = V^{(2)} = h + \sqrt{h^2 - G}\,\sin(2\theta + \phi), \tag{16}$$

where h and G are defined by Eq. (4) and $\phi=\arctan[(m_{11}-m_{22})/2m_{12}]$. The TB criterion is based on the sign of G. We can understand the reason of the defect in the TB criterion by considering the inclusive relation between G and $K^{(2)}$ in Eq. (16). For the criterion of chaos, the ITB imposes the condition $K^{(2)}<0$ while the TB imposes the condition $G<0$. It is obvious from Eq. (16) that $K^{(2)}>0$ holds for $G>0$ because the condition $h>0$ is satisfied for the usual Hamiltonian systems. This means that the stable condition of the TB criterion, $G>0$, is a sufficient condition for $K^{(2)}>0$, i.e., $G>0 \Rightarrow K^{(2)}>0$. Its contraposition is that $K^{(2)}<0 \Rightarrow G<0$. In other words, $G<0$ does not necessarily imply $K^{(2)}<0$. This fact allows the TB criterion of chaos, $G<0$, to have two cases: (i) $G<0$ and $K^{(2)}<0$, and (ii) $G<0$ and $K^{(2)}>0$. Thus the defect in the TB criterion appears when the case (ii) occurs dominantly.

Second, owing to the equivalence of $V^{(2)}$ and $K^{(2)}$, we would like to point out that the global indicator of chaos in the Riemannian geometric approach can be used for the ITB criterion. In this geometric approach to the Hamiltonian system $H(\boldsymbol{p},\boldsymbol{q})$, the global indicator is assumed to be the microcanonical average of the local sectional curvature $K^{(2)}$ as follows

$$\langle K^{(2)}_{(-)}\rangle = \frac{\int d\boldsymbol{p}d\boldsymbol{q}\,\Theta(-K^{(2)})K^{(2)}(\boldsymbol{p},\boldsymbol{q})\,\delta(H(\boldsymbol{p},\boldsymbol{q})-E)}{\int d\boldsymbol{p}d\boldsymbol{q}\,\delta(H(\boldsymbol{p},\boldsymbol{q})-E)}, \tag{17}$$

where Θ is the step function, i.e., $\Theta(x)=0$ for $x<0$ while $\Theta(x)=1$ for $x\geqslant 0$. The quantity $\langle K^{(2)}_{(-)}\rangle$ is motivated by the fact that the norm $\|J\|$ in Eq. (13) grows with time when $K^{(2)}<0$ and then the region of the phase space with $K^{(2)}<0$ becomes inevitably unstable. Since concrete formula of the indicator in the ITB criterion was not explicitly presented in Ref. [6], it will be worth pointing out that the indicator (17) is available for the ITB criterion also.

Finally, we would like to discuss the reason why the quantity (17) in the Riemannian geometric approach plays a role of the global indicator, whose base has not been seriously addressed so far. For this end, we use the formula connecting the KS entropy h_{KS} to the Lyapunov exponents λ_L as follows [11]

$$h_{KS} = \overline{\lambda_L}(E)r(E), \tag{18}$$

where $\overline{\lambda_L}$ is the average value of λ_L. Here r is the relative weight of the chaotic part of the energy shell defined as

$$r(E) = \frac{\int d\boldsymbol{p}d\boldsymbol{q}X(\boldsymbol{p},\boldsymbol{q})\,\delta(H(\boldsymbol{p},\boldsymbol{q})-E)}{\int d\boldsymbol{p}d\boldsymbol{q}\,\delta(H(\boldsymbol{p},\boldsymbol{q})-E)}, \tag{19}$$

where X is the characteristic function depending on the value of λ_L at a point $(\boldsymbol{p},\boldsymbol{q})$ in the phase space as follows: $X=1$ for $\lambda_L>0$ while $X=0$ for $\lambda_L=0$. From the definition of r in Eq. (19) we can expect that the behavior of r will closely resemble that of $\langle K^{(2)}_{(-)}\rangle$ in Eq. (17). Indeed, it has been numerically shown that both quantities r and $\langle K^{(2)}_{(-)}\rangle$ exhibit almost the same behavior [9], i.e., $r\approx|\langle K^{(2)}_{(-)}\rangle|$. Thus we obtain the relation from Eq. (18) as follows

$$h_{KS} \approx \overline{\lambda}(E)|\langle K^{(2)}_{(-)}\rangle|. \tag{20}$$

Since the KS entropy h_{KS} characterizes the global property of dynamical systems, the relation (20) strongly suggests that $\langle K^{(2)}_{(-)}\rangle$ is qualified to be a global indicator of chaos. Although it is difficult to verify rigorously whether the relation (20) holds in general for the two-dimensional Hamiltonian systems, the numerical results for several dynamical systems [5,8,9] seem to support the relation (20).

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