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Emergence of local ergodicity from the space-time properties of Lyapunov vectors

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Abstract Tangent space basis vector fields, Lyapunov vectors, are fundamental objects of chaotic dynamical systems. Two bases used in numerical calculations, the Gram-Schmidt vectors and the covariant Lyapunov vectors, are propagated with numerical trajectories of a Hamiltonian dynamical system, the Lennard-Jones trimer. Space-time properties measuring stability and localization characterize each vector set and probe the tangent space directions important to the system's evolution. The tangent vector directions and their properties further elucidate the emergence of local ergodicity in this model of an atomic system and an improved estimation of the separate time scales involved.

Keywords Hamiltonian system · Chaos · Lyapunov vector · Lyapunov exponent · Ergodicity

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Introduction

Finite-time Lyapunov exponents are statistical observables of chaos in dynamical systems [4]. They are properties of yet more fundamental objects: tangent space basis vector fields, often called Lyapunov vectors [7]. The nature and utility of various basis fields and their numerical calculation has only recently been studied in few degree of freedom systems [5] and extended systems [9]. Relatively little is known about their role in the chaotic dynamics of finite size Hamiltonian systems.

Space-time properties of Lyapunov vectors are of particular use in probing the emergence of local ergodicity in Hamiltonian systems, such as the Lennard-Jones trimer [2,1]. Local ergodicity emerges in the time history of a chaotic trajectory of the trimer when distinct regions of phase space are filled on different time scales [8]. The statistics of Lyapunov vector properties collected in different phase space locales and time spans along a trajectory reflect this phenomenon. The Lyapunov vectors themselves give additional physical insight into the relevant tangent space directions [6].

In addition to finite-time Lyapunov exponents, another property of Lyapunov vectors is the inverse participation ratio, a localization measure of each Lyapunov vector in the tangent fiber bundle. They give a rough estimate of the inverse number of degrees of freedom contributing to each vector on average, in a time span. For a range of time span lengths they give insight into the space and time localization of tangent vectors and further aid analysis of the emergence of local ergodicity [6]. Numerically, the tangent space basis vector field quantitatively and qualitatively affects the finite-time Lyapunov exponents and consequently the examination of local ergodicity as it emerges.

Computational methodology

Trajectories of a model, three-atom Lennard-Jones cluster were propagated with the "velocity Verlet" algorithm. Both Lyapunov vector sets were propagated using a linearized form of the "velocity Verlet" [6]. Gram-Schmidt vectors (GSVs) were calculated with the method of Benettin et al. [3] and the covariant Lyapunov vectors (CLVs) with the method of Ginelli et al. [5].

Initiated from various initial conditions, trajectories were partitioned into uniform time segments of varying length. Distributions of finite-time Lyapunov exponents and inverse participation ratios from the time segments characterize the trajectory, partition, and basis field. These distributions were analyzed for a range of total energies, time scales, and initial conditions, relating GSV and CLV directions and their properties to features of the potential energy landscape. For brevity, we discuss the distribution $f(\lambda, l)$ for finite-time Lyapunov exponents λ from CLVs for a time segment length $l = 200$.

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Results and discussion

Once converged, the GS basis vectors define mutually orthogonal, maximally expanding or contracting directions at which initially nearby trajectories diverge or converge exponentially [7]. Converged CLVs are a coordinate (independent) basis, time-reversal invariant under the linearized dynamics, and coincide with the local stable and unstable manifolds at each point of the trajectory [5].

Our results have shown that CLVs are time-reversal invariant, but similarly localized to GSVs in trajectory tangent fiber bundles. Lyapunov exponents and inverse participation ratios of both basis vector sets are in good quantitative agreement in the long time limit. Differences in the distributions of finite-time Lyapunov exponents for the two basis vector fields are dramatic. Qualitatively, in the range of timescales and total energy examined, exponent distributions from CLVs are narrower than those from GSVs; in this sense, they are more localized.

In both λ_1 and λ_2 GSV exponent distributions, multi-modality is present at total energies above the potential energy of the linear saddle. This result suggests that ergodicity emerges locally on different time scales for these trajectories [6]. The bimodality of the covariant exponent distributions $f(\lambda_2, 200)$ confirms that ergodicity emerges on different time scales, when the trajectory spans different phase space regions (Figure 1).

Peaks in $f(\lambda_2, 200)$ reflects the separation of motion into a region of highly chaotic behavior, characterizing motion in the potential well, and a region with much more regular dynamics, characterizing motion across the saddles. The CLV exponent distribution $f(\lambda_1, 200)$ is only bimodal at the highest total energy (Figure 1), reflecting bound motion and motion near the dissociation threshold. Multi-modality of both GS exponent distributions over a wide energy range and time segment length, is thus, in part, due to the coordinate dependence of GSVs.

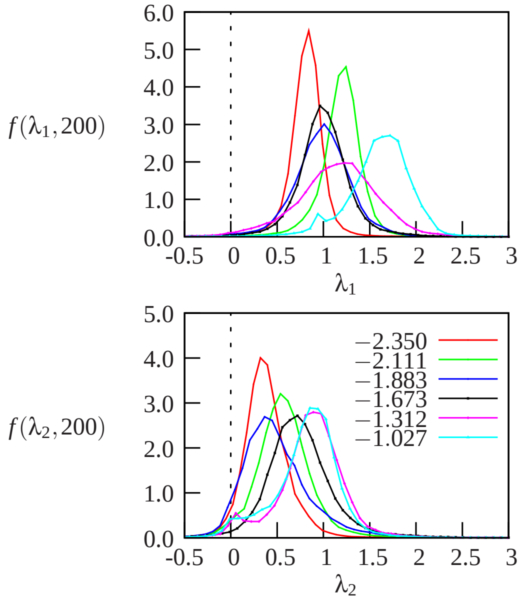

Fig. 1 Covariant Lyapunov exponent λ_1 and λ_2 distributions $f(\lambda_1, 200)$ and $f(\lambda_2, 200)$ from trajectories at different total energies. λ_1 and λ_2 were collected from 200 time step segments. The total energy of each trajectory was initially deposited in the symmetric stretch mode of the equilateral triangle configuration.

Conclusions

Our results demonstrate that CLVs are more appropriate than GSVs for finite-time estimation of Lyapunov exponents. The lack of coordinate dependence of the CLVs clearly revealed the emergence of local ergodicity phase space allowing more accurate estimation of the separate time scales involved.

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