Detecting chaos and determining the dimensions of tori in Fermi-Pasta-Ulam lattices by the GALI method

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Abstract
The recently introduced Generalized Alignment Index (GALI) method of chaos detection [1] is applied to distinguish differently regular and chaotic orbits of multi-dimensional Hamiltonian systems. The GALI of order k (GALK) is proportional to volume elements formed by k initially linearly independent unit vector quantities whose magnitude is normalized to unity from time to time. For chaotic orbits, GALI lies exponentially to zero with eigenvalues that involve the values of several Lyapunov exponents, while in the case of regular orbits, GALI fluctuates around nonzero values or goes to zero following particular power laws that depend on the dimension of the torus and on the order k. We apply these indices to rapidly detect chaotic motion and identify low-dimensional tori of Fermi-Pasta-Ulam (FPU) lattices [2]. We also present an efficient computation scheme of the GALI's, based on the Singular Value Decomposition (SVD) algorithm.

1 The GALI method

1.1 Definition
Following [1] we consider a Hamiltonian system of N degrees of freedom having a Hamiltonian H(q₁,...,qₙ, p₁,...,pₙ) where qᵢ and pᵢ are 1,...,N the generalized coordinates and momenta respectively. An orbit of this system is defined by a vector \( \mathbf{r}(t) = (q_1(t),... ,q_N(t)) \), with \( q_i = x_i, \quad \dot{x}_i = p_i, \quad i = 1,...,N \). This orbit is a solution of Hamilton's equations \( \dot{q} = \nabla E/S(\mathbf{r}(t)), \quad \dot{p} = -\nabla H(\mathbf{r}(t)) \), where the evolution of a deviation vector \( \delta \mathbf{r} \) from \( \mathbf{r}(t) \) obeys the variational equations \( \delta \dot{\mathbf{r}} = H/M(\mathbf{r}(t)) \), where \( M = \partial^2 H / \partial \mathbf{r} \partial \mathbf{r} \) is the Jacobian matrix of \( H \).

We follow k normalized deviation vectors \( \mathbf{v}_{\mathbf{r}}, \ldots, \mathbf{v}_k \) (2 ≤ k ≤ 2N) in time, and determine when they become linearly dependent, by checking if the volume of the corresponding \( k \)-parallelogram goes to zero. This volume is equal to the norm of the wedge or exterior product of these vectors. Hence we are led to define the following ‘volume’ element:

\[
GALI(k,t) = \left| \mathbf{v}_{\mathbf{r}} \wedge \cdots \wedge \mathbf{v}_k(t) \right| \quad (N = k \text{ or } k = 2N - s),
\]

which we call the Generalized Alignment Index (GALI) of order k. We note that the hat (•) over a vector denotes that it is of unit magnitude. Clearly, if at least two of these two vectors become linearly dependent, the wedge product in (1) becomes zero and the volume element vanishes.

1.2 Behavior
In the case of a chaotic orbit, all deviation vectors tend to become linearly dependent, aligning in the direction which corresponds to the maximal Lyapunov exponent and GALI tends to zero exponentially following the law [1]:

\[
GALI(t) \sim e^{-\lambda t}, \quad \lambda = \ln(v_{\mathbf{r}}), \quad \lambda = \ln(v_{\mathbf{r}}) \quad \text{constant}, \quad \text{if } 2 \leq k \leq N,
\]

\[
GALI(t) \sim \frac{1}{e^{2\pi^{2}}}, \quad \text{constant}, \quad \text{if } k = 2N - s
\]

while for regular orbits lying on an s-dimensional torus, with \( s \leq N \), GALI behaves as [2]:

\[
GALI(t) \sim \frac{1}{e^{2\pi^{2}}}, \quad \text{constant}, \quad \text{if } 2 \leq k \leq s
\]

\[
GALI(t) \sim e^{2\pi^{2}}, \quad \text{constant}, \quad \text{if } k = 2N - s
\]

Note that from (4) we deduce that for \( s = N \), GALI remains constant for \( 2 \leq k \leq N \) and decreases to zero as \( t \to \infty \) for \( s = N \) in accordance with (3).

1.3 Numerical computation
In order to numerically compute GALI, we perform the Singular Value Decomposition (SVD) of the 2N × 2N matrix \( \mathbf{A} \) as having the columns the coordinates of the k normalized deviation vectors \( \mathbf{v}_{\mathbf{r}}, \ldots, \mathbf{v}_k \). Then GALI is equal to the product of the singular values \( z_{\mathbf{r}}, k = 1,...,k \) of matrix \( \mathbf{A} \) [2], so that

\[
\log(GALI) = \sum_{i=1}^{k} \log(z_{\mathbf{r}}),
\]

2 Numerical application to the FPU system
We apply the GALI method to study chaotic and quasiperiodic motion in a multi-dimensional Hamiltonian system. In particular, we consider the FPU 3-lattice of N particles with Hamiltonian

\[
H = \sum_{i=1}^{N} \left[ \frac{p_{i+1}^2}{2} + \frac{g_{i+1}}{2} + \beta \frac{\left( q_{i+1} - q_i \right)^2}{4} \right], \quad \text{with } q_1 = q_{N+1}, \quad p_1 = p_{N+1}, \quad i = 1,...,N
\]

where \( g_{i+1} \) and \( p_{i+1} \) are the displacements of the particles with respect to their equilibrium positions, and \( g_{i+1} p_{i+1} \) the corresponding momenta. It is well known that if we define normal mode variables by

\[
\begin{align*}
Q_k &= \sqrt{\sum_{i=1}^{N} \sum_{j=1}^{N} \frac{q_i}{\sin \left( \frac{k i}{N} \right)}}, \quad P_k = \sqrt{\sum_{i=1}^{N} \sum_{j=1}^{N} \frac{p_i}{\sin \left( \frac{k i}{N} \right)}},
\end{align*}
\]

the unperturbed Hamiltonian (Eq. (6) for \( \beta = 0 \)) is written as the sum of the so-called harmonic energies \( E_k \) having the form

\[
E_k = \frac{1}{2} (Q_k^2 + P_k^2), \quad \omega_k = 2 \sin \left( \frac{i \pi}{N+1} \right), \quad i = 1,...,N,
\]

with \( \omega_k \) being the corresponding harmonic frequencies. In our study we imposed fixed boundary conditions \( q_1 = q_{N+1}, p_1 = p_{N+1} \), and fix the number of particles to \( N = 8 \) and the system's parameter to \( \beta = 1.5 \).

Figure 1. (a) The time evolution of quantities \( E_i, i = 1,...,7 \), having as limits for \( t \to \infty \) the seven positive Lyapunov exponents \( \alpha_i, i = 1,...,7 \), for a chaotic orbit with initial conditions \( Q_1 = Q_2 = 0.5, Q_3 = Q_4 = 0.7, J_2 = J_3 = 0, J_1 = J_4 = 0 \), \( i = 1,...,8 \) of the N = 8 particle FPU lattice (6). The time evolution of the corresponding GALI is plotted in (b) for \( k = 2,...,8 \) and in (c) for \( k = 7, 7.9, 10, 12, 14, 16 \). The plotted lines in (b) and (c) correspond to exponentials that follow the asymptotic lines (2) for \( \alpha_1 = 0.179, \alpha_2 = 0.141, \alpha_3 = 0.114, \alpha_4 = 0.090, \alpha_5 = 0.064, \alpha_6 = 0.042, \alpha_7 = 0.020 \). Note that \( \alpha = 0 \) is linear and that the slope of each line is written explicitly in (b) and (c).

Figure 2. (a) The time evolution of harmonic energies \( E_k, i = 1,...,8 \), for a regular orbit with initial conditions \( q_1 = q_2 = q_3 = q_4 = 0.05, q_5 = q_6 = q_7 = q_8 = 0.1, p_1 = p_2 = p_3 = p_4 = p_5 = p_6 = p_7 = p_8 = 0 \), for the N = 8 particle FPU lattice (6). The time evolution of the corresponding GALI is plotted in (b) for \( k = 2,...,8 \) and in (c) for \( k = 10, 12, 14, 16 \). The plotted lines in (b) and (c) correspond to precisely the power laws predicted in (4) for \( s = 2 \).

Figure 3. (a) The time evolution of harmonic energies for a regular orbit lying on a 2-dimensional torus of the N = 8 particle FPU lattice (6). Recurrences occur between \( E_1, E_2, E_3, E_4 \), while all other harmonic energies remain practically zero. The time evolution of the corresponding GALI is plotted in (b) for \( k = 2,...,8 \) and in (c) for \( k = 9, 11, 13, 14, 16 \). The plotted lines in (b) and (c) correspond to precisely the power laws predicted in (4) for \( s = 2 \).

Figure 4. (a) The time evolution of harmonic energies for a regular orbit lying on a 4-dimensional torus of the N = 8 particle FPU lattice (6). Recurrences occur between \( E_1, E_2, E_3, E_4 \), while all other harmonic energies remain practically zero. The time evolution of the corresponding GALI is plotted in (b) for \( k = 3,...,8 \) and in (c) for \( k = 9, 11, 13, 14, 16 \). The plotted lines in (b) and (c) correspond to precisely the power laws predicted in (4) for \( s = 4 \).

References