Learning the Intrinsic Dimensionality of Fermi-Pasta-Ulam-Tsingou Trajectories using a Deep Autoencoder Model

Gionni Marchetti [1]

[1]Postillón XAI, Barcelona, Spain

Introduction

Recently, using a data-driven approach based on principal component analysis (PCA), Ref. [3] demonstrated a key relationship between the nonlinearity strength and the intrinsic dimension m^* of trajectories in the Fermi–Pasta–Ulam–Tsingou (FPUT) β model [1], consisting of a one-dimensional chain of $N = 32$ weakly coupled harmonic oscillators.

In particular, PCA applied to trajectories comprising 4,000,000 data points estimates $m^* = 2$–3 for $\beta \in [0, 1.1]$, where characteristic energy recurrences are observed and the dynamics is therefore **non-ergodic**. This remarkable finding is further confirmed for $\beta = 0.1$ by a Riemannian learning approach based on the multi-chart flows method, recently proposed by Yu et al. [5]. The latter suggests that the trajectories lie on a low-dimensional Riemannian manifold. Consequently, due to the inherent limitations of PCA, these results make it necessary to validate them using another nonlinear manifold learning method.

We propose an approach based on a deep-learning autoencoder (DEA) [2], which effectively learns the data representation and generalizes successfully, yielding reconstruction errors negligible compared to those from PCA.

Fermi-Pasta-Ulam-Tsingou β Model

The FPUT Hamiltonian $H(q,p)$ where $q = (q_0, q_1, \cdots, q_N)$ and $p = (p_0, p_1, \cdots, p_N)$, reads [1]

$$H(q,p) = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \frac{1}{2}\sum_{i=0}^{N}(q_{i+1}-q_i)^2 + \frac{\beta}{4}\sum_{i=0}^{N}(q_{i+1}-q_i)^4 \,. \tag{1}$$

The trajectories, embedded in a 64-dimensional phase space, are obtained by a symplectic integration algorithm, assuming the following initial condition (first mode excitation), setting $k = 1$, $A = 10$:

$$q_i(0) = A\sqrt{\frac{2}{N+1}}\sin\left(\frac{ik\pi}{N+1}\right) . \tag{2}$$

Furthermore, we assume fixed ends for this one-dimensional chain of harmonic oscillators.

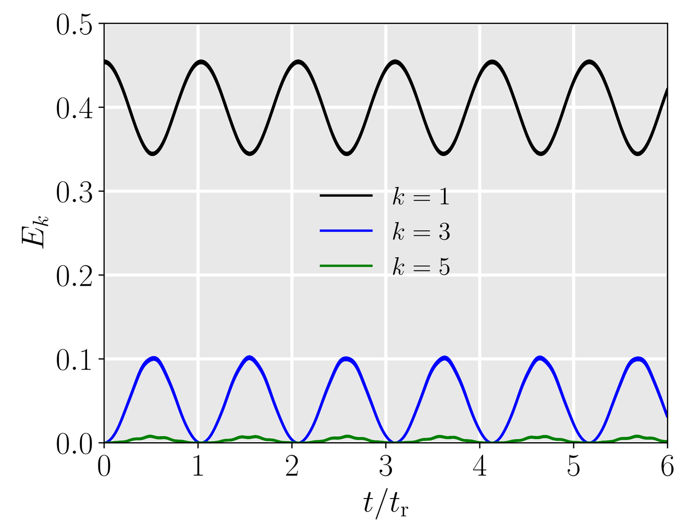

Figure 1. The energy E_k of modes for $k = 1, 3, 5$ as a function of time t in units of recurrence time t_r ($t_r = 2 \times 10^5$) for β model with $\beta = 0.3$, assuming $N = 32$.

A Deep Autoencoder Model

DEA is a deep neural network that aims to find a low-dimensional data representation, minimizing the reconstruction loss, which is given by the mean square error (MSE). Roughly, it can be considered a nonlinear PCA.

We chose the DEA architecture sketched in Fig. 2 below, due to its excellent performance [4]

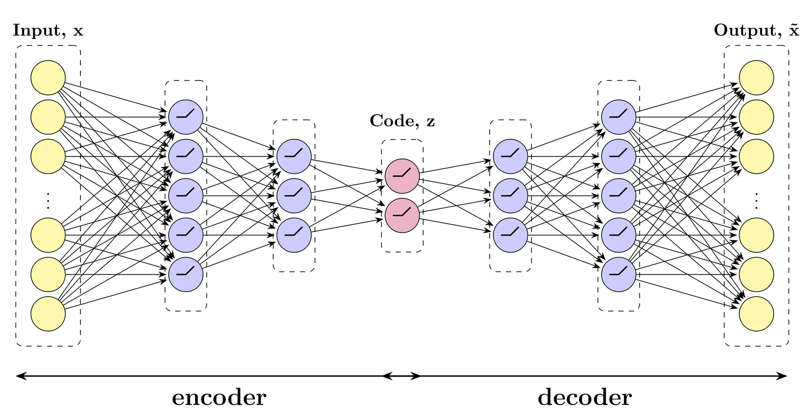

Figure 2. The symbol on the hidden units (or nodes) represents ReLu activation function, see Table 1 for details.

Layer Type	Nodes	Activation Function
input layer	64	-
encoder layer 1	32	ReLu
encoder layer 2	16	ReLu
hidden layer	m	ReLu
decoder layer 1	16	ReLu
decoder layer 2	32	ReLu
output layer	64	Linear

Table 1. The deep autoencoder architecture used in the present work.

Results

We compare the estimated intrinsic dimension m^* from PCA and DEA applied to entire trajectories (4, 000, 000 datapoints) in Fig. 3. For the case of DEA, m^* is inferred from the reconstruction error curves, by looking at their elbows. This task is achieved using Kneedle algorithm (KA). In contrast, participation ratio D_{PR} is used in PCA, that is, the following formula:

$$D_{\mathrm{PR}} = \frac{\left(\sum_{i=1}^{n}\lambda_i\right)^2}{\sum_{i=1}^{n}\lambda_i^2} , \tag{3}$$

where λ_i denote the PCA eigenvalues. The two approaches yield the very same results.

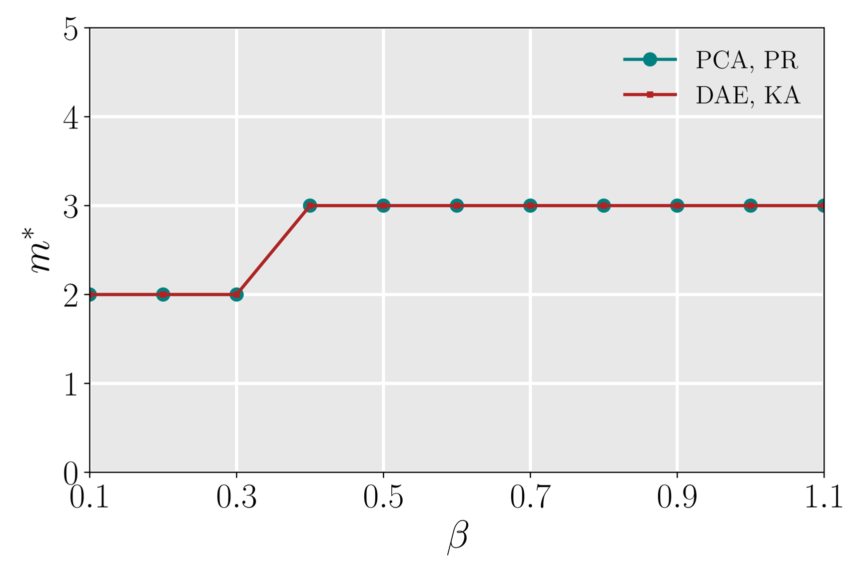

Figure 3. Estimated intrinsic dimension m^* as function of parameter β. Square and Circle symbols refer to DAE + KA and PCA + PR, respectively.

Using DAE, the 2-dimensional embeddings of the original high-dimensional trajectory data ($\beta = 0.1$) are shown in Fig. 4. ReLu and Linear functions on the bottleneck layer are shown on panels (a) and (b), respectively, assuming $\beta = 0.1$. These embeddings confirm that FPUT orbits are due to a regular, possibly quasi-periodic, motion, for weak nonlinearities.

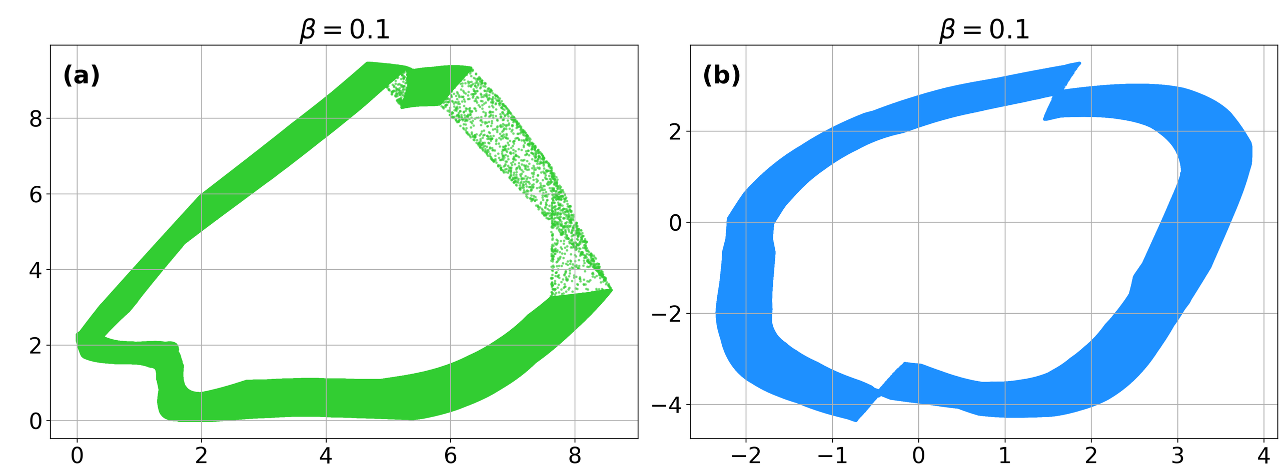

Figure 4. ReLu and Linear functions on the bottleneck layer in (a) and (b), respectively. In both cases MSE $\approx 6 \times 10^{-4}$.

Conclusions

The deep learning approach agrees with the linear PCA results, confirming that the trajectories lie on a 2- or 3-dimensional Riemannian manifold at weak nonlinearities. However, determining the elbows from the DAE reconstruction curves may introduce some uncertainty due to the heuristic nature of the method. Therefore, further investigation is required to ensure the robustness and accuracy of our findings.

Possible directions for future research include:

1. Inferring the intrinsic dimensionality using alternative methods, such as the multi-chart flows approach [5].
2. Characterizing the geometry and topology of the manifold on which the trajectories lie [3].

Acknowledgments

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