LDDS: Python package for computing and visualizing Lagrangian Descriptors for Dynamical Systems

19 May 2021

Statement of Need

Nonlinear dynamical systems are ubiquitous in natural and engineering sciences, such as fluid mechanics, theoretical chemistry, ship dynamics, rigid body dynamics, atomic physics, solid mechanics, condensed matter physics, mathematical biology, oceanography, meteorology and celestial mechanics (Wiggins 1994 and references therein). There have been many advances in understanding phenomena across these disciplines using the geometric viewpoint of the solutions and the underlying structures in the phase space; for example MacKay, Meiss, and Percival (1984), V Rom-Kedar, Leonard, and Wiggins (1990), Ozorio de Almeida et al. (1990), V. Rom-Kedar and Wiggins (1990), Meiss (1992), Koon et al. (2000), Waalkens, Burbanks, and Wiggins (2005), Meiss (2015), Wiggins (2016), Zhong, Virgin, and Ross (2018), Zhong and Ross (2020). Chief among these phase space structures are the invariant manifolds that form a barrier between dynamically distinct solutions. In most nonlinear systems, the invariant manifolds are computed using numerical techniques that rely on some form of linearization around equilibrium points followed by continuation and globalization. However, these methods become computationally expensive and challenging when applied to the high-dimensional phase space of vector fields defined analytically, from numerical simulations or experimental data. This points to the need for techniques that can be paired with trajectory calculations, without the excessive computational overhead and at the same time can allow visualization along with trajectory data. The Python package, `LDDS`, serves this need for analyzing deterministic and stochastic, continuous and discrete high-dimensional nonlinear dynamical systems described either by an analytical vector field or from data obtained from numerical simulations or experiments.

To the best of our knowledge, no other open-source software exists for computing Lagrangian descriptors. However, a variety of computational tools are available for obtaining phase space structures in fluid mechanics, such as the identification of Lagrangian coherent structures via finite-time Lyapunov exponents (Briol and d'Ovidio (2011), Nelson and Jacobs (2016), Onu, Huhn, and Haller (2015), Finn and Apte (2013), Dabiri Lab (2009), Haller et al. (2020)) and finite-size Lyapunov exponents (Briol and d'Ovidio (2011)), Eulerian coherent structures (Katsanoulis and Haller (2018)). Our goal with this software is to make Lagrangian descriptors available to the wider scientific community and enable the use of this method for reproducible and replicable computational dynamical systems.

Summary and Functionalities

The `LDDS` software is a Python-based module that provides the user with the capability of analyzing the phase space structures of both continuous and discrete nonlinear dynamical systems in the deterministic and stochastic settings using Lagrangian descriptors (LDs). The main idea of this method is to define a scalar valued functional called Lagrangian descriptor as the integral of a non-negative function $g(\mathbf{x}(t); \mathbf{x}_0)$ which encodes a dynamical property of a trajectory at the initial condition, $\mathbf{x}_0$. Different formulations of the Lagrangian descriptor exist in the literature where the non-negative function $g(\mathbf{x}(t); \mathbf{x}_0)$ is given by: the arclength of a trajectory in phase space (Jiménez Madrid and Mancho (2009), Mancho et al. (2013)), the arclength of a trajectory projected on the configuration space (Craven and Hernandez (2015)), the p-norm or p-quasinorm (Lopesino et al. (2017)), and the Maupertuis' action of Hamiltonian mechanics (Gonzalez Montoya and Wiggins (2020)). The approach provided by Lagrangian descriptors for revealing phase space structure has also been adapted to address discrete-time systems (maps) and stochastic systems.

Briefly, for a continuous-time dynamical system:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}\left(\mathbf{x}(t), t\right) \tag{1}$$

where $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{f}$ is the vector field, starting from an initial condition $\mathbf{x}_0 = \mathbf{x}(t_0)$ at time $t = t_0$, $g(\mathbf{x}(t); \mathbf{x}_0)$ is integrated along with the trajectory in forward and backward time over the interval $[t_0 - \tau, t_0 + \tau]$, respectively, to obtain the Lagrangian descriptor,

$$\mathcal{L}\left(\mathbf{x}_0, t_0, \tau\right) = \int_{t_0-\tau}^{t_0+\tau} g(\mathbf{x}(t); \mathbf{x}_0)\, dt. \tag{2}$$

at the initial condition. When this computation is performed for a 2D grid of initial conditions over long enough integration time interval and the corresponding contour map is visualized, one can detect phase space structures at the points with extremum LD values that also have a singularity (non-differentiability) (Lopesino et al. (2017), Naik, García-Garrido, and Wiggins (2019)).

This open-source software incorporates the following features:

- Computation of LDs for two dimensional maps.
- Computation of LDs for two dimensional continuous-time dynamical systems.
- Computation of LDs for two dimensional stochastic differential equations with additive noise.
- Computation of LDs on two-dimensional sections of Hamiltonian systems with 2 or more degrees of freedom (DoF).
- Computation of LDs for 2 DoF Hamiltonian systems where the potential energy surface is known on a grid of points in the configuration space of a chemcial reaction.
- Computation of LDs from a spatio-temporal discretization of a two-dimensional time-dependent vector field.
- Numerical gradient based identification of the invariant stable and unstable manifolds from the LD contour map.
- Addition of time-dependent external forcings in two-dimensional continuous dynamical systems.
- Different formulations of the Lagrangian descriptor available in the literature.

All the features of the package and their usage across different settings are illustrated using Jupyter notebooks as hands-on tutorials. These tutorials are meant to be worked through to understand how to set up a model dynamical system to which LDs is applied and use different options for visualizing the computational results. We believe that these notebooks are effective in integrating this method into classroom courses, independent study, and research projects. Moreover, the tutorials will encourage future contributions from the scientific community to expand the features and application of the Lagrangian descriptor method in other areas of computational science and engineering.

Example systems

To illustrate the use of this software, we have applied the method to some of the benchmark dynamical systems. These are included as examples:

Maps:

- Standard map

The standard map is a two-dimensional map used in dynamical systems to study a number of physical systems such as the cyclotron particle accelerator or a kicked rotor (Chirikov (1971), Meiss (1992), Meiss (2008)). The equations of the discrete system are given by the expressions:

$$\begin{cases} x_{n+1} = x_n + y_n - \dfrac{K}{2\pi}\sin(2\pi x_n) \\ y_{n+1} = y_n - \dfrac{K}{2\pi}\sin(2\pi x_n) \end{cases} \tag{3}$$

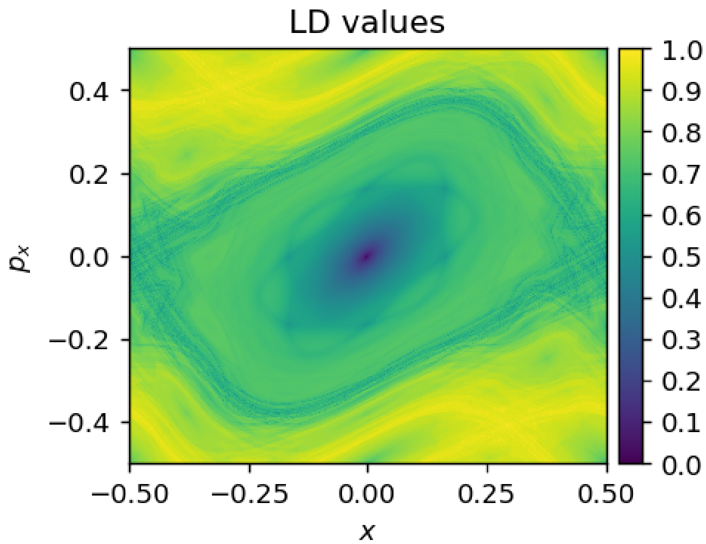

Figure 1: Lagrangian descriptor contour plot for the standard map, using $p = 0.5$-quasinorm and integration time $\tau = 15$.

where K is the parameter that controls the forcing strength of the perturbation. The inverse map is described by:

$$\begin{cases} x_n = x_{n+1} - y_{n+1} \\ y_n = y_{n+1} + \dfrac{K}{2\pi}\sin(2\pi(x_{n+1} - y_{n+1})) \end{cases} \tag{4}$$

In the following figure, we show the output produced by the LDDS software package for the standard map using the model parameter value $K = 1.2$.

Flows:

- Forced undamped Duffing oscillator

The Duffing oscillator is an example of a periodically driven oscillator with nonlinear elasticity (Duffing (1918), Kovacic and Brennan (2011)). This can model the oscillations of a pendulum whose stiffness does not obey Hooke's law or the motion of a particle in a double-well potential. It is also known as a simple system that can exhibit chaos.

As a special case, the forced undamped Duffing oscillator is described by a time-dependent Hamiltonian given by:

$$H(x, p_x, t) = \frac{1}{2}p_x^2 - \frac{\alpha}{2}x^2 + \frac{\beta}{4}x^4 - f(t)x \tag{5}$$

where α and β are the model parameters and $f(t)$ is the time-dependent focing added to the system. The non-autonomous vector field that defines the dynamical system is given by:

$$\begin{cases} \dot{x} = \dfrac{\partial H}{\partial p_x} = f_1(x, p_x) = p_x \\ \dot{p}_x = -\dfrac{\partial H}{\partial x} = f_2(x, p_x, t) = \alpha x - \beta x^3 + f(t) \end{cases} \tag{6}$$

In the following figure we show the output produced by the LDDS software package for the forced Duffing oscillator using the model parameter value $\alpha = \beta = 1$. The initial time is $t_0 = 0$ and the perturbation used is of the form $f(t) = A\sin(\omega t)$ where $A = 0.25$ and $\omega = \pi$.

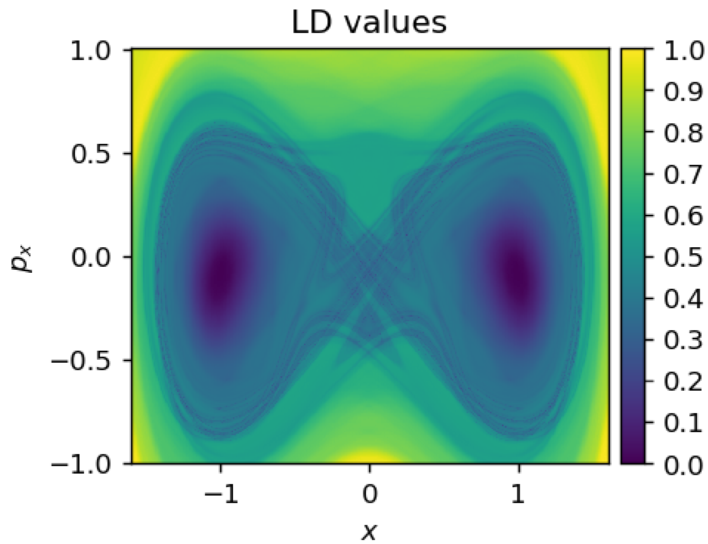

Figure 2: Lagrangian descriptor contour plot for the Duffing oscillator, using $p = 0.5$-quasinorm and integration time $\tau = 15$.

- A double gyre flow with stochastic forcing

The double gyre is a recurrent pattern occurring in geophysical flows (Coulliette and Wiggins (2001)). The stochastic dynamical system for a simplified model of this flow (Shadden, Lekien, and Marsden (2005)) with additive noise is described by the following stochastic differential equations (Balibrea-Iniesta et al. (2016)):

$$\begin{cases} dX_t = \left(-\pi A \sin\left(\dfrac{\pi f(X_t,t)}{s}\right) \cos\left(\dfrac{\pi Y_t}{s}\right) - \mu X_t \right) dt + \sigma_1 \, dW_t^1 \\ dY_t = \left(\pi A \cos\left(\dfrac{\pi f(X_t,t)}{s}\right) \sin\left(\dfrac{\pi Y_t}{s}\right) \dfrac{\partial f}{\partial x}(X_t,t) - \mu Y_t \right) dt + \sigma_2 \, dW_t^2 \end{cases} \tag{7}$$

where W^1 and W^2 are Wiener processes and we have that:

$$f(X_t,t) = \varepsilon \sin(\omega t + \psi) X_t^2 + (1 - 2\varepsilon \sin(\omega t + \psi)) \; X_t \tag{8}$$

In the following figure we show the output produced by the LDDS software package for the stochastically forced double gyre using a noise amplitude of $\sigma_1 = \sigma_2 = 0.1$. The double gyre model parameters are $A = 0.25$, $\omega = 2\pi$, $\psi = \mu = 0$, $s = 1$, $\varepsilon = 0.25$, and the initial time is $t_0 = 0$.

Four-dimensional phase space:

- Hénon-Heiles Hamiltonian.

The Hénon-Heiles system is a simplified model describing the restricted motion of a star around the center of a galaxy (Henon and Heiles (1964)). This system is a paradigmatic example of a time-independent Hamiltonian with two degrees of freedom, given by the function:

$$H(x,y,p_x,p_y) = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + x^2 y - \frac{1}{3} y^3 \tag{9}$$

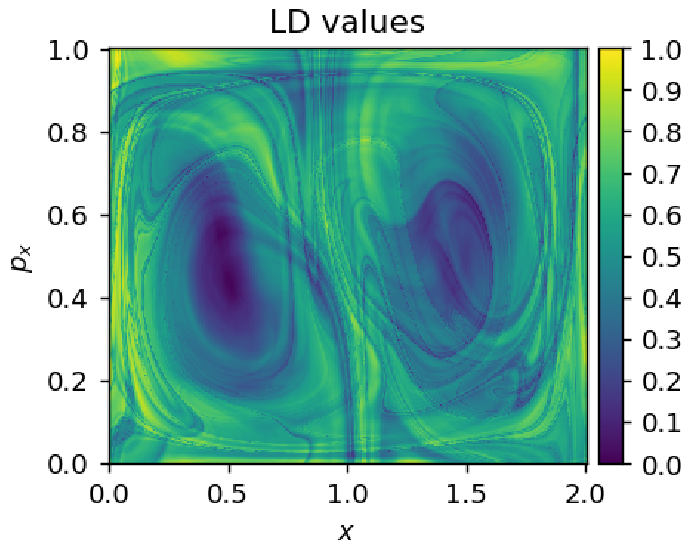

Figure 3: Lagrangian descriptor contour plot for the Double-gyre with stochastic forcing, using $p = 0.5$-quasinorm and integration time $\tau = 15$.

where the vector field is:

$$\begin{aligned}\dot{x} =& \frac{\partial H}{\partial p_x} = p_x \\ \dot{y} =& \frac{\partial H}{\partial p_y} = p_y \\ \dot{p}_x =& -\frac{\partial H}{\partial x} = -x - 2xy \\ \dot{p}_y =& -\frac{\partial H}{\partial y} = -x^2 - y + y^2\end{aligned} \tag{10}$$

In the next figure, we show the computation of Lagrangian descriptors with the LDDS software package on the phase space slice described by the condition $x = 0$, $p_x > 0$ for the energy of the system $H_0 = 1/5$.

Relation to ongoing research projects

Lagrangian descriptors form the basis of several past and ongoing research projects (Cámara et al. (2012), Cámara et al. (2013), Lopesino et al. (2015), Craven and Hernandez (2015), Craven and Hernandez (2016), García-Garrido et al. (2016), Balibrea-Iniesta et al. (2016), Demian and Wiggins (2017), Craven, Junginger, and Hernandez (2017), Feldmaier et al. (2017), Junginger et al. (2017), García-Garrido et al. (2018), Ramos et al. (2018), Patra and Keshavamurthy (2018), Naik, García-Garrido, and Wiggins (2019), Naik and Wiggins (2019), Curbelo et al. (2019b), Curbelo et al. (2019a), Revuelta, Benito, and Borondo (2019), García-Garrido, Naik, and Wiggins (2020), García-Garrido, Agaoglou, and Wiggins (2020), Krajňák, Ezra, and Wiggins (2020), Naik and Wiggins (2020), Gonzalez Montoya and Wiggins (2020), Katsanikas, García-Garrido, and Wiggins (2020)). The common theme of all these projects is the investigation of phase space structures that govern phase space transport in nonlinear dynamical systems. We have also published an open-source book using Jupyter Book Executable Books Community (2020) on the theory and applications of Lagrangian descriptors Agaoglou et al. (2020). This open-source package is the computational companion to the book.

Acknowledgements

We acknowledge the support of EPSRC Grant No. EP/P021123/1 (CHAMPS project) and Office of Naval Research (Grant No. N00014-01-1-0769).

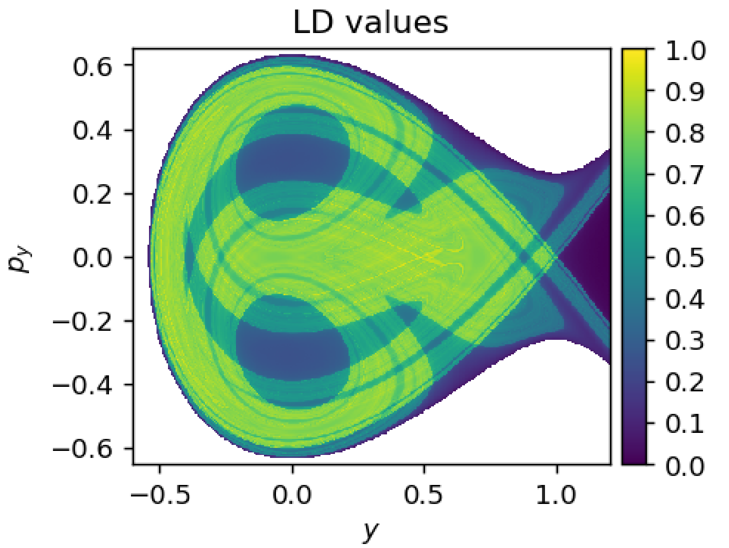

Figure 4: Lagrangian descriptor contour plot for the Hénon-Heiles Hamiltonian, using $p = 0.5$-quasinorm and integration time $\tau = 15$.

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