

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

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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 et al., 1984](#)), ([V. Rom-Kedar et al., 1990](#)), ([Ozorio de Almeida et al., 1990](#)), ([V. Rom-Kedar & Wiggins, 1990](#)), ([J. D. Meiss, 1992](#)), ([Koon et al., 2000](#)), ([Waalkens et al., 2005](#)), ([J. D. Meiss, 2015](#)), ([Wiggins, 2016](#)), ([Zhong et al., 2018](#)), ([Zhong & 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 software for calculating Lagrangian descriptors exists. A variety of computational tools is available for competing approaches popular in fluid mechanics, such as the identification of Lagrangian coherent structures via finite-time Lyapunov exponents ([Briot & d'Ovidio, 2011](#)), ([Nelson & Jacobs, 2016](#)), ([Onu et al., 2015](#)), ([Finn & Apte, 2013](#)), ([Dabiri Lab, 2009](#)), ([Haller et al., 2020](#)) and finite-size Lyapunov exponents ([Briot & d'Ovidio, 2011](#)) or Eulerian coherent structures ([Katsanoulis & Haller, 2018](#)).

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 through the method of Lagrangian descriptors (LDs). The main idea behind this methodology is to define a Lagrangian descriptor as the integral of a non-negative function g that captures a dynamical property of the evolution of a trajectory. Different formulations of the Lagrangian descriptor exist in the literature where the non-negative function g is: the arclength of a trajectory in phase space ([Jiménez](#)

43 [Madrid & Mancho, 2009](#)), ([Mancho et al., 2013](#)), the arclength of a trajectory projected on
44 the configuration space ([Craven & Hernandez, 2015](#)), the p -norm or p -quasinorm ([Lopesino
45 et al., 2017](#)), and the Maupertuis' action of Hamiltonian mechanics ([Montoya & Wiggins,
46 2020](#)). The approach provided by Lagrangian descriptors for revealing phase space structure
47 has also been adapted to address discrete-time systems (maps) and stochastic systems.

48 Consider a continuous-time dynamical system:

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

49 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
50 $t = t_0$, $g(\mathbf{x}(t); \mathbf{x}_0)$ is integrated together with the trajectory forward and backward time over
51 the interval $[t_0 - \tau, t_0 + \tau]$ to give the Lagrangian descriptor,

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

52 Large differences in values obtained for initial conditions on a predefined grid indicate the
53 presence of the phase space structures in the system and provide insight into their geometry.
54 One of the main goals we pursue with this software is to make Lagrangian descriptors available
55 to a large scientific audience and enable them to use this tool for reproducible research.

56 This open-source package incorporates the following features:

- 57 ■ Computation of LDs for two-dimensional maps.
- 58 ■ Study of the phase space structure of two-dimensional continuous dynamical systems
59 with LDs.
- 60 ■ Computation of LDs for a system of two stochastic differential equations with additive
61 noise.
- 62 ■ Computation of LDs on two-dimensional phase space planes for Hamiltonian systems
63 with 2 or more degrees of freedom (DoF).
- 64 ■ Application of LDs to Hamiltonian systems with 2 DoF where the potential energy
65 surface is known on a discrete spatial grid.
- 66 ■ Computation of LDs from a spatio-temporal discretization of a two-dimensional time-
67 dependent vector field.
- 68 ■ Visual extraction of the invariant stable and unstable manifolds from the LD scalar field
69 values.
- 70 ■ Addition to time-dependent external forcings for two-dimensional continuous dynamical
71 systems.
- 72 ■ Different definitions for the Lagrangian descriptor function found in the literature.

73 All the different features of the module, and their usage across different settings, are illustrated
74 through Jupyter-notebook tutorials. These tutorials would help users better understand how
75 to set up a model dynamical system to which LDs is applied, and present them with different
76 options for visualizing the results obtained from the analysis. We believe that these resources
77 provide useful material for the development of an effective learning process that could motivate
78 the integration of this tool into users' research/academic projects. Moreover, this will surely
79 encourage future contributions from the scientific community to extend the features and
80 applicability of this software package to other areas.

81 Example systems

82 The following dynamical systems are included in this software package as examples to illustrate
83 the application of Lagrangian descriptors:

84 Maps:

85 ▪ Standard map

86 The standard map is a two-dimensional map used in dynamical systems to study a number
87 of physical systems such as the cyclotron particle accelerator or a kicked rotor (Chirikov,
88 1971),(J. D. Meiss, 1992),(J. D. Meiss, 2008). The equations of the discrete system are given
89 by the expressions:

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

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

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

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

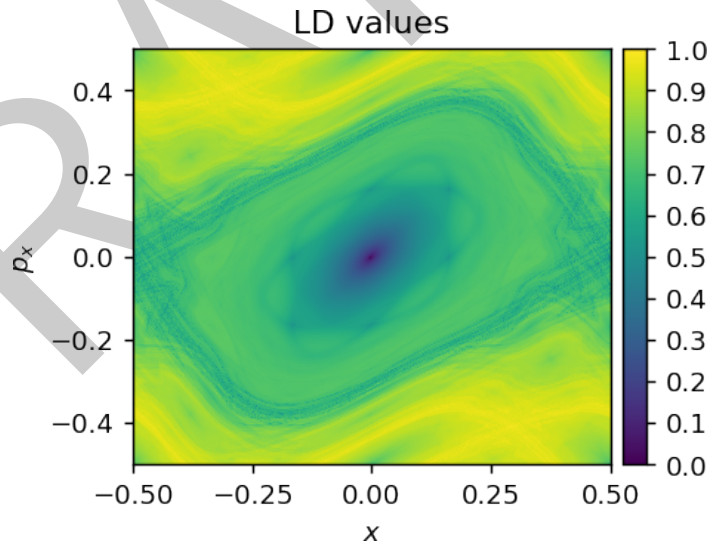


Figure 1: Lagrangian descriptor contour plot for the standard map, using $p = 0.5$ -quasinorm and integration time $\tau = 15$.

94 Flows:

95 ▪ Forced undamped Duffing oscillator

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

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

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

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

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

104 In the following figure we show the output produced by the LDDS software package for the
105 forced Duffing oscillator using the model parameter value $\alpha = \beta = 1$. The initial time is
106 $t_0 = 0$ and the perturbation used is of the form $f(t) = A \sin(\omega t)$ where $A = 0.25$ and $\omega = \pi$.

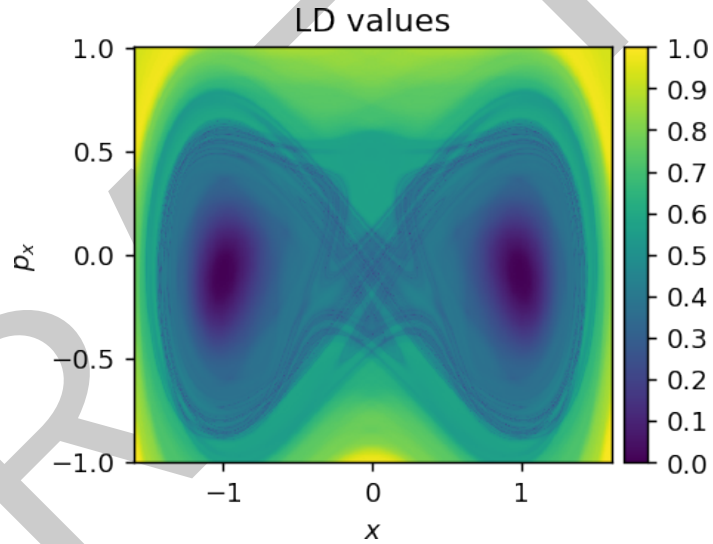


Figure 2: Lagrangian descriptor contour plot for the Duffing oscillator, using $p = 0.5$ -quasinorm and integration time $\tau = 15$.

107 ■ A double gyre flow with stochastic forcing

108 The double gyre is a recurrent pattern occurring in geophysical flows (Coulliette & Wiggins,
109 2001). The stochastic dynamical system for a simplified model of this flow (Shadden et
110 al., 2005) with additive noise is described by the following stochastic differential equations
111 (Balibrea-Iniesta et al., 2016):

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

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

$$f(X_t, t) = \varepsilon \sin(\omega t + \psi) X_t^2 + (1 - 2\varepsilon \sin(\omega t + \psi)) X_t \quad (8)$$

113 In the following figure we show the output produced by the LDDS software package for the
114 stochastically forced double gyre using a noise amplitude of $\sigma_1 = \sigma_2 = 0.1$. The double gyre
115 model parameters are $A = 0.25$, $\omega = 2\pi$, $\psi = \mu = 0$, $s = 1$, $\varepsilon = 0.25$, and the initial time is
116 $t_0 = 0$.

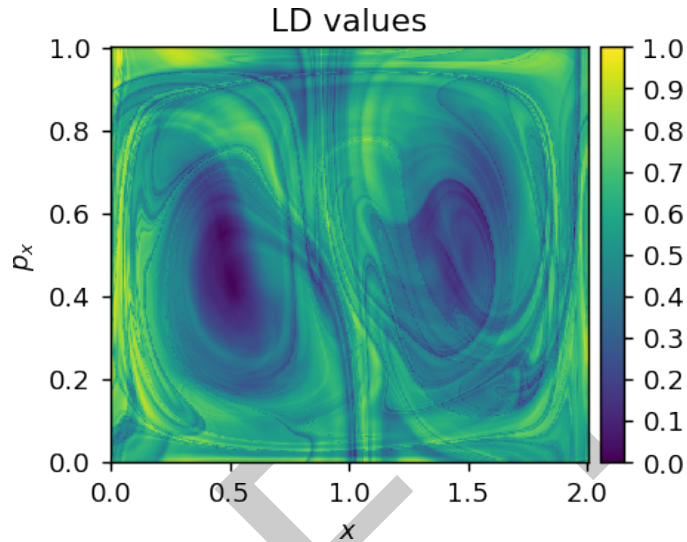


Figure 3: Lagrangian descriptor contour plot for the Double-gyre with stochastic forcing, using $p = 0.5$ -quasinorm and integration time $\tau = 15$.

117 Four-dimensional phase space:

- 118 ■ Hénon-Heiles Hamiltonian.

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

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

122 where the vector field is:

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

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

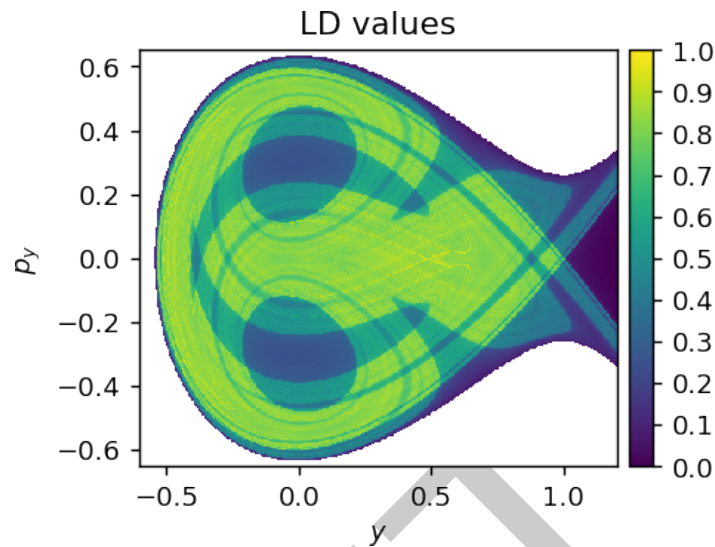


Figure 4: Lagrangian descriptor contour plot for the Hénon-Heiles Hamiltonian, using $p = 0.5$ -quasinorm and integration time $\tau = 15$.

Relation to ongoing research projects

Lagrangian descriptors form the basis of several past and present research projects (Cámara et al., 2012), (Cámara et al., 2013), (Lopesino et al., 2015), (Craven & Hernandez, 2015), (Craven & Hernandez, 2016), (García-Garrido et al., 2016), (Balibrea-Iniesta et al., 2016), (Demian & Wiggins, 2017), (Craven et al., 2017), (Feldmaier et al., 2017), (Junginger et al., 2017), (García-Garrido et al., 2018), (Ramos et al., 2018), (Patra & Keshavamurthy, 2018), (Naik et al., 2019), (Naik & Wiggins, 2019), (Curbelo et al., 2019a), (Curbelo et al., 2019b), (Revuelta et al., 2019), (García-Garrido, Naik, et al., 2020), (García-Garrido, Agaoglou, et al., 2020), (Krajňák et al., 2020), (Naik & Wiggins, 2020), (Montoya & Wiggins, 2020), (Katsanikas et al., 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 co-authored an open-source book project 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 that book.

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