Path-based measures of transport and expansion rates in stochastic flows

Michał Branicki and Kenneth Uda

Department of Mathematics, University of Edinburgh, Scotland, UK

Summary. We present a new information-theoretic framework for trajectory-based characterisation of transport and mixing in stochastic dynamical systems which are non-autonomous and known over a finite time interval. This work is motivated by the desire to study time-dependent transport and provide Lagrangian (i.e., trajectory-based) predictions in multi-scale systems based on simplified, data-driven models with errors affecting path-based predictions in a non-local fashion. In deterministic dynamical systems techniques exploiting stable and unstable manifolds of finite-time hyperbolic trajectories or finite-time Lyapunov exponents (FTLE) are frequently used as a means to estimate transport barriers. Alternatively, a formulation relying on spectral properties of (probability) transfer operator leads to identifying almost-invariant sets which remain 'quasi-coherent' under the dynamics. While these techniques often give compatible numerical results in the deterministic setting, a rigorous connection between the two approaches has remained elusive. Here, we provide a mathematical link between the two approaches in the case of deterministic dynamics, and we extend the framework to deal with transport and evolution of path-based uncertainty in stochastic flows. In this new framework the average finite-time expansion along trajectories in stochastic dynamical systems is based on a finite-time rate of certain probabilistic divergencies which provide a notion of 'distance' on manifolds of probability measures and capture nonlinear stretching from the growth of cross-entropy under the stochastic flow. Finally, we develop a numerical method to illustrate the relationship of the new probabilistic approach to FTLE fields in the deterministic setting, and to illustrate the uncertainty bounds on path-based functionals in the general stochastic setting.

Extended Abstract

Organised or 'coherent' structures in fluid flows have been a subject of intense study for some time, especially since the seminal paper of Brown and Roshko [2]. The dynamical systems approach to describe and quantify general transport concepts based on the structure and topology of trajectories, $x(t) = \varphi_{t_0}^t(x_0)$, determined by the flow, $\varphi_{t_0}^t : \mathcal{M} \to \mathcal{M}$, on the phase manifold $\mathcal{M}$ became widespread in the 1980's and 90's. These efforts have led to various notions of 'organised structures' in the underlying flows, as well as a variety of techniques for determining the existence of such objects. Historically, the developed approaches fall roughly into two classes:

(i) Geometric/topological methods which make use of flow-invariant manifolds of certain hyperbolic sets and the so-called Lagrangian coherent structures,

(ii) Probabilistic techniques which exploit spectral properties of an operator evolving probability densities, leading to notions of almost-invariant and finite-time coherent sets.

Hyperbolic trajectories and their associated stable and unstable manifolds have provided the first mathematical approach to this problem - in both the periodic and aperiodic time-dependent deterministic settings - with applications dating back to the beginning of studies of 'chaotic advection' in fluid flows (e.g., [11]). Apart from the purely theoretical aspects a major motivation for these efforts arose from the desire to study time-dependent transport and provide Lagrangian (i.e., trajectory-based) predictions in geophysical flows; more recent applications include trajectory-based predictions in molecular dynamics or systems biology based on simplified models with errors affecting the dynamics in a complicated and non-local fashion. Important obstacles for deriving a general theory of Lagrangian transport arise from the need to account for the effects of transient phenomena (e.g., time-localised mixing) which cannot be captured by the infinite-time notions (e.g., hyperbolicity, ergodicity, etc.), and to account for errors and uncertainty in trajectory-based functionals inferred from reduced-order models. In deterministic non-autonomous dynamical systems $(\mathcal{M}, \mathcal{I}, \varphi_{t_0}^t)$ on a finite time interval $\mathcal{I}$ with the flow map $\varphi_s^t \circ \varphi_{t_0}^s = \varphi_{t_0}^t$ on $\mathcal{M}$ such that $t_0 \leq s \leq t$, for $t_0, t \in \mathcal{I}$, generalised techniques exploiting notions of stable and unstable manifolds of finite-time hyperbolic trajectories, or finite-time Lyapunov exponents (FTLE) and related stretching indicators are frequently used as a means to estimate transport barriers. These geometric structures in non-autonomous flows, be it invariant manifolds of hyperbolic sets or their approximately invariant generalisations, are known to play a key role in dynamical transport and mixing (e.g., lobe dynamics [12, 13]). In particular, the approximately invariant 'Lagrangian coherent structures' are often studied computationally (e.g. [9, 10, 1]) based on FTLE maps whose ridges may indicate transport barriers. Alternatively, probabilistic approaches - originating from [3, 4] and so far largely confined to deterministic systems - focus on the evolution of probability densities on trajectories with the aim to detect regions in the phase manifold $\mathcal{M}$ that are, on average, little affected under the flow of the dynamical system. These regions are known as almost-invariant, finite-time coherent sets, or time-asymptotic coherent sets (e.g., [7]) depending on whether eigenvectors, singular vectors, or Oseledets vectors of the associated transfer operator acting on probability densities are considered. Both approaches (i.e., geometric and probabilistic) have advantages and disadvantages, but usually give compatible answers in deterministic case studies [7, 1]. However, rigorous or even formal results on the connection between the two frameworks remain elusive (e.g., [8]). The results presented in this paper are threefold:

(I) We propose a new information-theoretic methodology for estimating both the average finite-time expansion along trajectories, as well as the evolution and bounds on uncertainty in non-autonomous stochastic dynamical systems.

(II) We provide a further insight into the mathematical link between the approaches (i) and (ii) in the case of deterministic dynamics by deriving bounds on the FTLE fields in terms of certain information measures and vice versa.

(III) We systematically extend the theoretical framework to deal with transport and evolution of path-based uncertainty in general stochastic flows. Bounds on uncertainty of path-based functoinals (e.g., Lyapunov exponents) are derived in terms of the generators of the stochastic dynamics which provides a connection between the Eulerian (field-based) and Lagrangian (trajectory-based) viewpoints, and allows for further analytical treatment.

The approach is based on utilising certain class of divergencies, $D_\alpha(\mu\|\nu) > 0$, which provide a notion of a pseudo-distance between measures μ and ν on manifolds of probability measures on a measurable space $(\Omega, \mathcal{F}, \mathbb{P})$ and the stochastic flow $\mathcal{P}^t_{t_0}(\cdot,\omega)$ on $\mathcal{M}$ s.t. $\mathcal{P}^t_s \circ \mathcal{P}^s_{t_0} = \mathcal{P}^t_{t_0}$ a.s. for each $t_0 \leq s \leq t$. We subsequently introduce the notion of a finite-time divergence rate (FTDR) field, $D^t_\alpha(\mu\|\nu) > 0, t > 0$, which captures nonlinear stretching directly from the growth of cross-entropy under the stochastic flow. The FTDR framework elucidates the connection between the evolution of probability measures and the average local stretching; in particular, this allows for a rigorous definition of finite-time nonlinear expansion rates based on the Lyapunov exponents for probability measures, owing to the multiplicative ergodic theorem. We then show that under fairly general conditions the FTDR field exists and provides a well-defined notion of stretching which is a continuous on the phase manifold $\mathcal{M}$. Moreover, under some weak conditions on the differentiability of the flow, we prove the existence of FTDR in the limit when the measure of the support of the initial density tends to zero. In the deterministic setting these results allow for derivation of rigorous bounds on the FTLE in terms of the probabilistic finite-time divergence rates in the general form

$$\big|\mathbb{E}^{\mu_t}[\Lambda^t_{t_0}]\big| \leq \mathscr{A}_t\big(D^t_\alpha\,(\mu_t\|\mu_0)\big), \qquad \mathscr{A}_t \geq 0, \quad \mu_t \ll \mu_0,$$

where $\Lambda^t_{t_0}(x_0)$ is the largest finite-time Lyapunov exponent and μ_0 is the measure on the initial conditions $x_0 \in \mathcal{M}$, and $\mu_t = (\mathcal{P}^t_{t_0})^*\mu_0$ with the family of Markov evolutions $\{(\mathcal{P}^t_{t_0})^*\}_{t_0,t\in\mathcal{I}}$ given by the dual of $\mathcal{P}^t_{t_0}$. Conversely, the finite-time divergence rates are shown to be bounded by certain minimal FTLE fields.

Reduced order modelling of complex systems characterised by a wide range of spatio-temporal scales is unavoidably affected by incomplete information about the true state which enters the problem as a dynamical model error or a parametric uncertainty. The evolution of both types of uncertainty relative to the initial measure μ_0 can be captured in terms of the evolution of the appropriate divergence. For path-based functionals the uncertainty bounds can be derived either in terms of a measure-valued process on the phase manifold $\mathcal{M}$ or based on the measure on the (infinite-dimensional) path space associated with the stochastic flow. We derive such uncertainty bounds in the two aforementioned cases for Markov processes (specifically, Îto diffusions) in terms of information-theoretic measures on a finite time interval. Consequently, this framework avoids the use of asymptotic notions (e.g., flow-invariant measures) and the bounds are not restricted to long-time regimes. However, extra care is needed in the infinite-dimensional setting when dealing with path-space measures; the problem simplifies and regularises in finite-dimensional approximations of the dynamics on a finite subset of times in the evolution. Similar to the Pinsker inequality, the bounds are of the general form (details to be published)

$$d\big(\mathbb{E}^\mu[f], \mathbb{E}^\nu[f]\big) \leq \mathscr{B}\big(f, \mathbb{E}^\mu[f], \mathbb{E}^\nu[f]\big)\,\mathscr{C}\big(D_\alpha\,(\mu\|\nu)\big), \qquad \mathscr{B}, \mathscr{C} > 0, \quad \mu \ll \nu,$$

where d is some metric, the measure μ is absolutely continuous w.r.t the measure ν, and the bound factorises into a product of a term that depends on the dynamics and a term involving the expectation of the functional under the measure associated with the dynamics. Such bounds connect sensitivity analysis based on stochastic gradient-descent with information-theoretic methods, and they are derived from appropriate variational formulations of information measures in a similar spirit to those in [5] or more recently in [6]. However, in the present work more general information measures are employed and the explicit connection to the generator of the underlying stochastic process is utilised (cf. (III) above), making the results amenable to further analysis. Moreover, this approach provides computational advantages when dealing with high-dimensional stochastic systems or models with a high-dimensional parameter space when the gradient-type methods for computing sensitivity to perturbations become formidably costly. Finally, in order to illustrate the relationship between the FTLE and FTDR fields, and the uncertainty bounds, we develop a simple numerical method for estimating the FTDR field; more sophisticated, adaptive methods focusing on high-value FTDR regions are under development for practical applications. A follow-up work based on this abstract framework involves uncertainty quantification and optimal path-space tuning of reduced-order Lagrangian predictions of multi-scale stochastic dynamical systems.

References

[1] Branicki M., Wiggins S. (2010) Finite-time Lagrangian transport analysis: stable and unstable manifolds of hyperbolic trajectories and finite-time Lyapunov exponents, *Nonlin. Processes Geophys.* **17**, 1–36.

[2] Brown G.L., Roshko A. (1974) Density effect and large structure in turbulent mixing layers, *J. Fluid Mech.*, **64**, 775–816.

[3] Dellnitz M., Junge O. (1999) On the approximation of complicated dynamical behaviour, *SIAM J. Numer. Anal.* **36**(2), 491–515.

[4] Deuflhard P., Huisinga W., Fischer A., Schütte C. (2000) Identification of almost invariant aggregates in nearly uncoupled Markov chains, *Linear Algebra Appl.* **315**, 39–59.

[5] Donsker M.D., Varadhan S.R.S (1975) Asymptotic evaluation of certain Markov process expectation for large time, *Comm. Pure Appl. Math*, 1-47.

[6] Dupuis P., Katsoulakis M. A., Pantazis Y., Plechác P. (2016) Path-Space Information Bounds for Uncertainty Quantification and Sensitivity Analysis of Stochastic Dynamics, *SIAM J. Uncertainty Quant.* **4**, 80-111.

[7] Froyland G., Padberg K. (2009) Almost-invariant sets and invariant manifolds – connecting probabilistic and geometric descriptions of coherent structures in flows, *Physica D* **238**, 1507–1523.

[8] Froyland G., Padberg-Gehle K. (2012) Finite-time entropy: A probabilistic approach for measuring nonlinear stretching, *Physica D* **241**, 1612–1628.

[9] Haller G. (2000) Finding finite-time invariant manifolds in two-dimensional velocity fields, *Chaos* **10**, 99–108.

[10] Haller G. (2001) Distinguished material surfaces and coherent structures in three-dimensional fluid flows, *Physica D* **149** 248–277.

[11] Ottino J. (1989) *The Kinematics of Mixing: Stretching, Chaos, and Transport*, Cambridge University Press, Cambridge.

[12] Rom-Kedar V., Wiggins S., (1990) Transport in two-dimensional maps, *Arch. Ration. Mech. Anal.* **109**, 239–298.

[13] Wiggins S., (1992) *Chaotic Transport in Dynamical Systems*, Springer.