

New methods for analysing metastable structures in closed, open or non-autonomous dynamical systems

11frg168

Chris Bose (University of Victoria),
Gary Froyland (University of New South Wales),
Cecilia González–Tokman (University of Victoria),
Rua Murray (University of Canterbury)

October 23–October 30, 2011

1 Overview of the Field

Dynamical systems $\hat{T} : I \rightarrow I$ typically model complicated deterministic processes on a phase space I . The map \hat{T} induces a natural action on probability measures η on I via $\eta \mapsto \eta \circ \hat{T}^{-1}$. Of particular interest in ergodic theory are those probability measures that are \hat{T} -invariant; that is, η satisfying $\eta = \eta \circ \hat{T}^{-1}$. By Birkhoff’s Ergodic Theorem, if η is ergodic and invariant, then it describes the time-asymptotic distribution of orbits of η -almost-all initial points $x \in I$. This picture is part of a well established classical mathematical understanding of dynamical systems.

From an applications point of view, it is desirable to find the invariant measures η , and analyse the way that typical orbits are “mixed” to the consequent equilibrium distribution. When the space I is equipped with a natural “smooth” measure m (such as the Lebesgue measure on subsets of \mathbb{R}^d), the action of \hat{T} on $\eta \ll m$ can be studied via the so-called *Frobenius–Perron* (transfer) operator:

$$\mathcal{L} \frac{d\eta}{dm} = \frac{d(\eta \circ \hat{T}^{-1})}{dm}$$

(see [32] for an introductory account). Numerical representation of \mathcal{L} can be accomplished via *Ulam’s method* [39]—a Galerkin type projection onto the space of piecewise constant functions on partitions of I . As the underlying partitions are refined, the fixed points of Ulam’s method are known to converge to densities of interesting \hat{T} -invariant measures in a variety of settings [34, 15, 16, 18, 20, 17, 3, 37]. The quality of approximation is determined in part by the speed at which orbits are “mixed” by \hat{T} , and the speed of mixing is often controlled by the gap between the leading eigenvalue, and the rest of the spectrum of \mathcal{L} (on a suitable Banach space of test functions). Although the behaviour of this *spectral gap* can be well-behaved under Ulam-type approximations [29, 11], the gap is often small, frustrating efforts to control approximation errors. It has recently become clear [21, 19, 27, 25, 26, 22] that small spectral gaps are actually associated with *metastable structures*—subsets of phase space I which exchange mass very slowly. Moreover, these structures crop

up in a variety of real applications (*eg*, molecular conformation dynamics [14], spacecraft orbits [12], large-scale ocean circulation [13]).

Consequently, the development of computational tools for identifying metastable states is interesting and important. A particularly fruitful idea is to regard a (closed) dynamical system as a union of interacting open subsystems. Essentially arbitrary *open systems* can be obtained from (\hat{T}, I) by excising a “hole” H_0 from I . Orbits are computed as normal on $X_0 := I \setminus H_0$, but are lost to the system when they fall into H_0 . Because trajectories are being lost to the hole, in many cases, there is no T -invariant probability measure. One can, however, consider *conditionally invariant* probability measures, which satisfy $\eta \circ T^{-1} = \rho \eta$ for some $\rho \in (0, 1)$. This idea has a long history [38, 9, 8, 10], and has seen an explosion of interest in recent years [35, 36, 30, 23, 7], with many of the aforementioned references being focussed on the existence (or analytical approximation) of conditionally invariant probability measures. Very recently, attention has focussed on practical means of calculating these measures numerically [1, 2] and connecting them with metastable behaviour in dynamical systems [28, 22].

2 Scientific progress made and open problems

Our activities at BIRS were in two main directions:

1. Rigorous analysis of the application of Ulam’s method [39] to the calculation of conditionally invariant probability measures for Lasota-Yorke type maps [33] into which “large” holes have been put. Using an analytical setup similar to that of Liverani and Maume-Deschamps [35], we proved that Ulam’s method produces a sequence of density functions which converge (in L^1) to the density of the (unique) absolutely continuous conditionally invariant probability measure for the open system, as well as a sequence of measures which converge weak* to the conformal measure of the open system (concentrated on the surviving repelling Cantor set). Unlike previous work [1, 2] these results are not based in spectral perturbation theory [29, 30], so are not limited to “small” holes. A manuscript containing these results will shortly be submitted for publication [5]. Open problems include: generalising the setup to higher dimensions; controlling rigorously the rate of convergence; and using the method to study the interaction between multiple metastable states within a closed system (as in [28, 22]).
2. Investigating alternatives to Ulam’s method for computation of invariant measures, conditionally invariant measures and metastable states [6, 4, 31, 24]. This work threw up many questions, which will form the basis of future projects by the group participants.

3 Acknowledgements

All four of us thank BIRS for the splendid working and living conditions provided. The work in [5] would not have happened without this meeting. CB is supported by an NSERC grant. GF was partially supported by the UNSW School of Mathematics and an ARC Discovery Project (DP110100068). CGT thanks the Pacific Institute for the Mathematical Sciences (PIMS) and the University of Victoria for financial support. RM thanks the College of Engineering (University of Canterbury) for funding to attend the workshop, and the Department of Mathematics and Statistics (University of Victoria) for hospitality during an adjacent visit.

References

- [1] Wael Bahsoun. Rigorous numerical approximation of escape rates. *Nonlinearity*, 19(11):2529–2542, 2006.
- [2] Wael Bahsoun and Christopher Bose. Quasi-invariant measures, escape rates and the effect of the hole. *Discrete Contin. Dyn. Syst.*, 27(3):1107–1121, 2010.
- [3] C. Bose and R. Murray. The exact rate of approximation in Ulam’s method. *Discrete Contin. Dyn. Syst, Series A*, 7(1):219–235, 2001.
- [4] C Bose and R Murray. Duality and the computation of approximate invariant densities for nonsingular transformations. *SIAM Journal on Optimization*, 18(2):691–709, 2007.
- [5] Christopher Bose, Gary Froyland, Cecilia González Tokman, and Rua Murray. Ulam’s method for Lasota–Yorke maps with holes. In preparation, 2011.
- [6] Christopher J. Bose and Rua Murray. Minimum ‘energy’ approximations of invariant measures for nonsingular transformations. *Discrete Contin. Dyn. Syst.*, 14(3):597–615, 2006.
- [7] H Bruin, M Demers, and I Melbourne. Existence and convergence properties of physical measures for certain dynamical systems with holes. *Ergod. Th. & Dynam. Sys.*, 30:687–728, 2010.
- [8] Pierre Collet, Servet Martínez, and Bernard Schmitt. Quasi-stationary distribution and Gibbs measure of expanding systems. In *Instabilities and nonequilibrium structures, V (Santiago, 1993)*, volume 1 of *Nonlinear Phenom. Complex Systems*, pages 205–219. Kluwer Acad. Publ., Dordrecht, 1996.
- [9] P Collet, S Martínez, and B Schmitt. The Yorke–Pianigiani measure and the asymptotic law on the limit cantor set of expanding systems. *Nonlinearity*, 7:1437–1443, 1994.
- [10] P Collet, S Martínez, and B Schmitt. The Pianigiani–Yorke measure for topological markov chains. *Israel J. Math.*, 97:61–70, 1997.
- [11] M. Dellnitz, G. Froyland, and S. Sertl. On the isolated spectrum of the Perron-Frobenius operator. *Nonlinearity*, 13(4):1171–1188, 2000.
- [12] M. Dellnitz, O. Junge, M.W. Lo, J.E. Marsden, K. Padberg, R. Preis, S.D. Ross, and B. Thiere. Transport of Mars-crossing asteroids from the quasi-Hilda region. *Physical Review Letters*, 94(23):231102, 2005.
- [13] Michael Dellnitz, Gary Froyland, Christian Horenkamp, Kathrin Padberg-Gehle, and Alex Sen Gupta. Seasonal variability of the subpolar gyres in the southern ocean: a numerical investigation based on transfer operators. *Nonlinear Processes in Geophysics*, 16:655–664, 2009.
- [14] P. Deuffhard and C. Schütte. Molecular conformation dynamics and computational drug design. In *Applied Mathematics Entering the 21st Century, Invited Talks from the ICIAM 2003 Congress*, pages 91–119, 2004.
- [15] J. Ding and A. Zhou. Finite approximations of Frobenius-Perron operators. a solution of Ulam’s conjecture to multi-dimensional transformations. *Physica D*, 92(1-2):61–68, 1996.
- [16] G. Froyland. Finite approximation of Sinai-Bowen-Ruelle measures for Anosov systems in two dimensions. *Random and Computational Dynamics*, 3(4):251–264, 1995.

- [17] G. Froyland. Ulam’s method for random interval maps. *Nonlinearity*, 12:1029, 1999.
- [18] G. Froyland. Using Ulam’s method to calculate entropy and other dynamical invariants. *Nonlinearity*, 12:79–101, 1999.
- [19] G. Froyland. Statistically optimal almost-invariant sets. *Physica D*, 200(3-4):205–219, 2005.
- [20] G. Froyland and K. Aihara. Rigorous numerical estimation of lyapunov exponents and invariant measures of iterated function systems and random matrix products. *International Journal of Bifurcation and Chaos*, 10(1):103–122, 2000.
- [21] G Froyland and M Dellnitz. Detecting and locating near-optimal almost-invariant sets and cycles. *SIAM J. Sci. Comput.*, 24(6):1839–1863, 2003.
- [22] G. Froyland, R. Murray, and O. Stancevic. Spectral degeneracy and escape dynamics for intermittent maps with a hole. *Nonlinearity*, 24:2435–2463, 2011.
- [23] G Froyland and O Stancevic. Escape rates and perron-frobenius operators: open and closed dynamical systems. *Discrete Contin. Dyn. Syst. Ser. B*, 14(2):457–472, 2010.
- [24] Gary Froyland, Oliver Junge, and Peter Koltai. Estimating long term behaviour of flows without trajectory integration: the infinitesimal generator approach. Submitted, 2011.
- [25] Gary Froyland, Simon Lloyd, and Anthony Quas. Coherent structures and isolated spectrum for perron-frobenius cocycles. *Ergodic Theory and Dynamical Systems*, 30:729–756, 2010.
- [26] Gary Froyland, Simon Lloyd, and Naratip Santitissadeekorn. Coherent sets for nonautonomous dynamical systems. *Physica D*, 239:1527–1541, 2010.
- [27] Gary Froyland and Kathrin Padberg. Almost-invariant sets and invariant manifolds—connecting probabilistic and geometric descriptions of coherent structures in flows. *Phys. D*, 238(16):1507–1523, 2009.
- [28] Cecilia González Tokman, Brian Hunt, and Paul Wright. Approximating invariant densities for metastable systems. *Ergodic Theory and Dynamical Systems*, 31:1345–1361, 2011.
- [29] G. Keller and C. Liverani. Stability of the spectrum for transfer operators. *Ann. Scuola Norm. Sup. Pisa Cl. Sci.(4)*, 28(1):141–152, 1999.
- [30] G Keller and C Liverani. Rare events, escape rates and quasistationarity: some exact formulae. *J. Stat. Phys.*, 135(3):519–534, 2009.
- [31] Péter Koltai. *Efficient approximation methods for the global long-term behavior of dynamical systems – Theory, algorithms and examples*. PhD thesis, Technische Universität München, 2010.
- [32] A Lasota and M C Mackey. *Chaos, Fractals and Noise: stochastic aspects of deterministic dynamics*. Springer, 2 edition, 1994.
- [33] A Lasota and J A Yorke. On the existence of invariant measures for piecewise monotonic transformations. *Trans. Amer. Math. Soc.*, 186:481–488, 1973.
- [34] Tien Yien Li. Finite approximation for the Frobenius-Perron operator. A solution to Ulam’s conjecture. *J. Approximation Theory*, 17(2):177–186, 1976.

- [35] Carlangelo Liverani and Véronique Maume-Deschamps. Lasota-Yorke maps with holes: conditionally invariant probability measures and invariant probability measures on the survivor set. *Ann. Inst. H. Poincaré Probab. Statist.*, 39(3):385–412, 2003.
- [36] M Mark F Demers and L-S Young. Escape rates and conditionally invariant measures. *Nonlinearity*, 19:377–397, 2006.
- [37] R. Murray. Ulam’s method for some non-uniformly expanding maps. *Discrete Contin. Dyn. Syst, Series A*, 26(3):1007–1018, 2010.
- [38] G Pianigiani and J Yorke. Expanding maps on sets which are almost invariant: decay and chaos. *Trans. Amer. Math. Soc.*, 252:351–366, 1979.
- [39] S. M. Ulam. *A collection of mathematical problems*. Interscience Tracts in Pure and Applied Mathematics, no. 8. Interscience Publishers, New York-London, 1960.