

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

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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.

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