A tutorial on transfer operator methods for numerical analysis of dynamical systems

Gary Froyland

School of Mathematics and Statistics
University of New South Wales, Sydney

BIRS Workshop on Uncovering transport barriers in geophysical flows
BIRS, 22–27 September 2013

Transfer Operators

- A transfer operator $\mathcal{P} : L^1(X) \circlearrowleft$ is a natural push-forward on densities under the action of a map $T : X \circlearrowleft$.
- Think of a density $f : X \to \mathbb{R}$ as represented by a pile of sand grains.
- At the base of each pile of sand grains is a point x. Take the vertical column of sand grains at x and reposition that column at $T(x)$.
- Do this for each $x \in X$. The result is $\mathcal{P}f(x)$.
- If T is volume-preserving, $\mathcal{P}f(x) = f \circ T^{-1}(x)$.

Transition matrices

- Now let's work with a finite set of columns of sand grains.
- Lay down a finite grid on X, call the sets $\{B_1, \ldots, B_n\}$, and populate each grid set with sand grains (or a tower of sand grains if you like).
- Take a grid set B_i and apply T to each sand grain x in B_i. The image sand grains cover $T(B_i)$.
- Count #grains in $B_i \cap T^{-1}B_j$; this looks odd, but it is the number of grains in B_i that are mapped into B_j by T.
- Form the transition matrix

$$P_{ij} = \frac{\#\text{grains in } B_i \cap T^{-1}B_j}{\#\text{grains in } B_i}.$$

- The matrix P gives us the action of T at a coarse-grained level given by the grid.

P generates a Markov chain

- The matrix P captures the short-time evolution of *all* points in X up to the resolution of the grid.
- We can now very efficiently push distributions forward by matrix multiplication.
- Let p_i^0 denote the initial mass contained in grid set B_i.
- If we want to push p^0 forward k steps with our discretised system, we just calculate $p^0 P^k$; the matrix P is sparse so this is an $O(n)$ operation.
  - See eg. "**Origin and evolution of the ocean garbage patches derived from surface drifter data**", van Sebille/England/F, *Environmental Research Letters*, 2012.
- If P is irreducible (eg. if T is ergodic), then there is a unique p^∞ that satisfies $p^\infty = p^\infty P$ (one can easily approximate by choosing k large).

What happens as $n \to \infty$? (Grid becomes finer)

- I'm going to be using the Markov chain P to compute all sorts of objects related to T. Are there convergence results as $n \to \infty$?
- For example, does p^∞ converge to an invariant measure of T? Yes. (not too hard to show). But which invariant measure? (more difficult, but positive results).
- **Beyond the scope of this tutorial!** At a broad level, the question boils down to stability of the property of T to small perturbations.
  - See F, "**Extracting dynamical behaviour via Markov modelling**", chapter in *Nonlinear Dynamics and Statistics*, Birkhauser, 2001, and references therein.
- It is instructive to think of P as "T plus noise", where the noise is localised with magnitude of the order of the grid set diameters.

GAIO

- GAIO (Global analysis of invariant objects) is software created by Michael Dellnitz and Oliver Junge to facilitate "set-oriented" investigations of dynamical systems.
- One main focus of GAIO is topological; efficiently and rigorously computing invariant manifolds, invariant sets, attractors, chain-recurrent sets, etc...and I'm not discussing these today.
- For the purposes of today, GAIO has two very useful built-in functions. One creates a box collection, and the other creates the transition matrix P on that box collection.
- Oliver has kindly given me a beta-version of GAIO for windows and that's what I'm using today. A linux version has existed since the late 90s.
- Documentation for GAIO is: Dellnitz/F/Junge "**The algorithms behind GAIO – Set oriented numerical methods for dynamical systems**", chapter in "Ergodic Theory, Analys, and Efficient Simulation of Dynamical Systems, Springer 2001.

Numerics

- The important output from GAIO for today is a box collection, an $N \times 2d$ array containing N box centres and radii in $\mathbb{R}^d$, and an $N \times N$ transition matrix P describing the coarse-grained dynamics between boxes.
- With these two objects, one is back in MATLAB, and uses simple matlab functions (which I've prepared for today).
- **Note:** This presentation is highly me-centric, and the list of references is intended to support the demonstrations and code, as I'm presenting them today. I've made no attempt to create a full survey of the areas discussed.

Eigenvectors of P, time-asymptotic almost-invariant sets

- All eigenvalues λ of P satisfy $|\lambda| \leq 1$. If T is ergodic, $\lambda = 1$ is the only eigenvalue on the unit circle.
- Let $0 < \lambda_2 < 1$ denote the second largest eigenvalue of P. If T is volume-preserving, the corresponding left eigenvector v_2 of P represents a signed density (a fluctuation from equilibrium if you like) that *decays at the slowest time-asymptotic rate*.
- Level-set thresholding yields time-asymptotic almost-invariant sets.

References:

Dellnitz/Junge "**Almost invariant sets in Chua's Circuit**", *Int. J. Bifur. Chaos*, 1997.

Dellnitz/Junge "**On the approximation of complicated behaviour**", *SIAM J. Num. Anal.*, 1999.

Eigenvectors of $R = (P + \hat{P})/2$, finite-time AI sets

- If we are interested in sets that are almost-invariant over a finite-time duration, then right eigenvectors of $R = (P + \hat{P})/2$ solve the right optimisation problem.
- For volume-preserving systems, $\hat{P}$ is the transpose of P with row sums renormalised to 1 (a matrix operation). $\hat{P}$ is the transition matrix describing backward-time dynamics.
- Level-set thresholding yields finite-time almost-invariant sets.

References:

See F, "**Statistically optimal almost-invariant sets**", Physica D, 2005, for development.

F/Padberg, "**Almost-invariant sets and invariant manifolds – connecting probabilistic and geometric descriptions of coherent structures in flows**", *Physica D*, 2009, for relationship to invariant manifolds.

Geophysical applications: F/Padberg/England/Treguier, "**Detecting coherent oceanic structures via transfer operators**". *PRL*, 2007.

and Dellnitz/F/Horenkamp/Padberg-Gehle/Sen Gupta, "**Seasonal variability of the subpolar gyres in the Southern Ocean: a numerical investigation based on transfer operators**", *Nonlin. Proc. in Geophys.*, 2009.

Singular vectors of P, finite-time coherent sets

- Suppose we now allow sets to move, rather than stay fixed.
- We'd like to find sets that are not long, thin, and filament-like, don't become stretched into long, thin, filament-like sets, but rather remain "blob-like" over a specified finite-time duration.
- If u_2, (resp. v_2) are the left, (resp. right) singular vectors corresponding to the second largest singular value σ_2, then $u_2 L = \sigma_2 v_2$, so that u_2 is mapped onto v_2 with a small scaling down factor.
- Level-set thresholding yields finite-time coherent sets.

References:

See F/Santitissadeekorn/Monahan, "**Transport in time-dependent dynamical systems: Finite-time coherent sets**", *Chaos*, 2010, for matrix version and atmospheric dynamics example,

F, "**An analytic framework for identifying finite-time coherent sets in time-dependent dynamical systems**", *Physica D*, 2013, for the operator version.

F/Padberg-Gehle, "**Almost-invariant and finite-time coherent sets: directionality, duration, and diffusion**", (Available on my website).

Geophysical appl.: F/Horenkamp/Rossi/Santi./SenGupta, "**Three-dimensional characterization and tracking of an Agulhas Ring**", *Ocean Mod.*, 2012.

Nonlinear stretching from P, finite-time entropy

- A uniform density on a single box will be stretched out under the action of P, however the image density will never be thinner than a box-width.
- The log of the stretching that a box B_i undergoes after k iterates of T can be estimated as $\frac{1}{|k|}\sum_{j=1}^{n} P_{ij}^{(k)} \log P_{ij}^{(k)}$.
- In two lines of matlab code, one can create an "FTE-field" directly from P.
- It is immaterial to the method whether P models purely advective dynamics or a combination of advective and diffusive dynamics.

Reference:

See F/Padberg-Gehle, "**Finite-time entropy: a probabilistic approach for measuring nonlinear stretching**", *Physica D*, 2012.

Absorption/hitting times

- Choose a target set of boxes $\mathcal{I} \subset \{1, \dots, n\} =: \mathcal{N}$.
- We wish to find the mean time it takes points in box $j \in \mathcal{N} \setminus \mathcal{I}$ to hit $\mathcal{I}$.
- This can be computed using classical Markov chain theory; solve

$$(Id - P|_{\mathcal{N}\setminus\mathcal{I}}) = [1, 1, \dots, 1],$$

using eg. "backslash" in MATLAB

References:

See most classical Markov chain books, eg. Norris, **Markov Chains**, Cambridge, 1997.

See Hsu, **Cell-to-Cell Mapping**, Springer, 1987, for early calculations in a dynamical context.

See F "**Extracting dynamical behaviour via Markov modelling**", chapter in *Nonlinear Dynamics and Statistics*, Birkhauser, 2001, also in a dynamical context.

Geophysical application: Dellnitz/F/Horenkamp/Padberg-Gehle/Sen Gupta, "**Seasonal variability of the subpolar gyres in the Southern Ocean: a numerical investigation based on transfer operators**", *Nonlin. Proc. in Geophys.*, 2009.

Topological entropy from P

- Choose a coarse partition of X, and assign an alphabet of size H to this coarse partition.
- Topological entropy with respect to this partition is exponential growth rate of new "words" with the length N of the words: $\lim_{N\to\infty} \frac{1}{N} \log |\#\text{words of length } N|$.
- Tight upper bounds for this rate can be obtained directly from P, and as the box diameters go to zero, the estimate rate converges to the true rate from above.
- As with all transfer operator algorithms, the dimension is unimportant, so the theory and algorithms work in $\mathbb{R}^d$, $d \geq 1$ (even on fractal sets, eg. Hénon attractor, Lorenz attractor).

Reference:

F/Junge/Ochs. "**Rigorous computation of topological entropy with respect to a finite partition**", *Physica D*, 2001.