Global Numerics II:
Isolating Neighborhoods and Statistics

Combinatorial Objects

- $X \subset \mathbb{R}^d$ cubical, $F : X \rightrightarrows \mathbb{R}^d$, $\mathcal{B}$ partition of X into elementary cubes (cubical grid).
- For $\mathcal{S} \subset \mathcal{B}$, $|\mathcal{S}|$ is the union of the elements in $\mathcal{S}$.
- Smallest representable neighborhood of $\mathcal{S}$

$$o(\mathcal{S}) = \{B \in \mathcal{B} \mid B \cap |\mathcal{S}| \neq \emptyset\}$$

- Combinatorial multivalued map $\mathcal{F} : \mathcal{B} \rightrightarrows \mathcal{B}$

$$\mathcal{F}(B) = \{B' \in \mathcal{B} \mid F(B) \cap B' \neq \emptyset\}\,;$$

(storage: sparse matrix, graph).

- Full combinatorial trajectory of $\mathcal{F}$ through $B \in \mathcal{B}$: $\gamma_B : \mathbb{Z} \to \mathcal{B}$, $\gamma_B(0) = B$ and $\gamma_B(n+1) \in \mathcal{F}(\gamma_B(n))$ for all $n \in \mathbb{Z}$.
- $\mathcal{S} \subset \mathcal{B}$ is a combinatorial invariant set if for every $B \in \mathcal{S}$ there exists a full solution $\gamma_B : \mathbb{Z} \to \mathcal{S}$.
- The maximal combinatorial invariant set in $\mathcal{I} \subset \mathcal{B}$ is

$$\mathrm{Inv}(\mathcal{I}, \mathcal{F}) := \{B \in \mathcal{I} \mid \text{there exists a full trajectory } \gamma_B : \mathbb{Z} \to \mathcal{I}\}.$$

- A combinatorial isolating neighborhood for $\mathcal{F}$ is a set $\mathcal{I} \subset \mathcal{B}$ such that

$$o(\mathrm{Inv}(\mathcal{I}, \mathcal{F})) \subset \mathcal{I}.$$

- **Proposition 1** *If $\mathcal{I}$ is an isolating neighborhood for $\mathcal{F}$, then $|\mathcal{I}|$ is an isolating neighborhood for F.*

Index pairs

A continuous selector of $\mathcal{F}$ is a continuous map $f : X \to \mathbb{R}^d$ such that

$$f(B) \subset \text{int } |\mathcal{F}(B)|$$

for all $B \in \mathcal{B}$.

Theorem 1 (Szymczak, 97) *Let $\mathcal{S}$ be an isolated invariant set for $\mathcal{F}$ and let*

$$\mathcal{N}_1 = \mathcal{S} \cup \mathcal{F}(\mathcal{S}), \quad \mathcal{N}_0 = \mathcal{N}_1 \backslash \mathcal{S}.$$

Then $\mathcal{N} = (|\mathcal{N}_1|, |\mathcal{N}_0|)$ is an index pair for every continuous selector of $\mathcal{F}$.

Computing Isolating Neighborhoods

- Consider the transition matrix

$$P = (p_{ij}), \quad p_{ij} = \begin{cases} 1, & \text{if } B_i \in \mathcal{F}(B_j), \\ 0, & \text{else.} \end{cases}$$

  k-periodic points of $\mathcal{F} \leftrightarrow$ nonzero diagonal entries of P^k;

- Consider the graph $G = (\mathcal{B}, V)$,

$$V = \{(B, B') : B' \in \mathcal{F}(B)\}.$$

  - recurrent sets of $\mathcal{F} \leftrightarrow$ strongly connected components of G;
  - connecting orbits of $\mathcal{F} \leftrightarrow$ shortest paths (Dijkstra's algorithm);

Turning the guess into a true isolating nbhd

Input: guess $\tilde{\mathcal{I}}$ for an isolating neighborhood.

$\mathcal{I}$ `= make_isolated(`$\tilde{\mathcal{I}}$`)`

$\mathcal{I}$ `:=` $\mathrm{Inv}(\tilde{\mathcal{I}}, \mathcal{F})$

`while` $o(\mathcal{I}) \not\subset \tilde{\mathcal{I}}$

$\tilde{\mathcal{I}}$ `:=` $\tilde{\mathcal{I}} \cup o(\mathcal{I})$

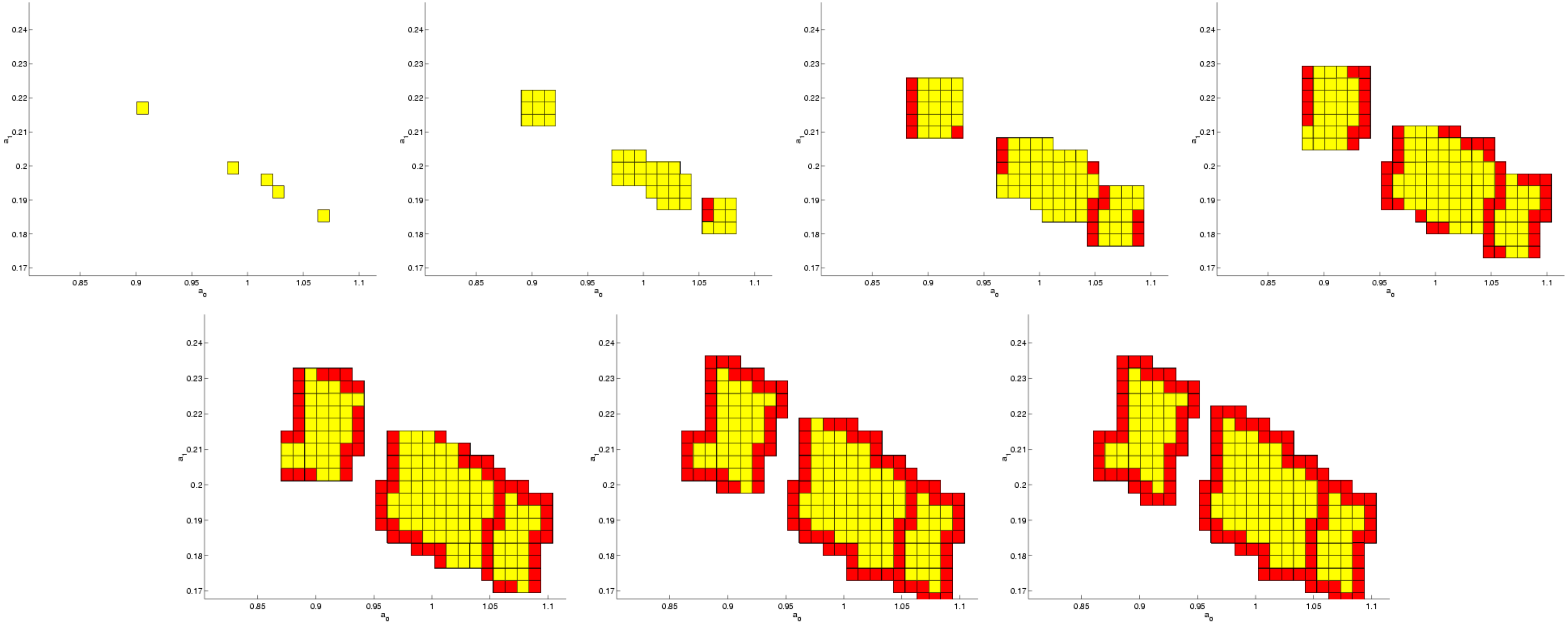
$\mathcal{I}$ `:=` $\mathrm{Inv}(\tilde{\mathcal{I}}, \mathcal{F})$

`if` $|\mathcal{I}| \subset \operatorname{int} |o(\mathcal{I})|$ `return` $\mathcal{I}$

`else return` $\emptyset$

Output: combinatorial isolating neighborhood $\mathcal{I}$ for $\mathcal{F}$ or $\emptyset$ (=failure).

Illustration: isolating neighborhood for a connecting orbit



Constructing Minimal Index Pairs

Input: combinatorial isolating neighborhood $\mathcal{I}$.

$[\mathcal{N}_1, \mathcal{N}_0]$ `= build_ip(`$\mathcal{I}$`)`

    $\mathcal{N}_0$ `:=` $\emptyset$

    $\mathcal{E}$ `:=` $(\mathcal{F}(\mathcal{I}) \cap o(\mathcal{I})) \setminus \mathcal{I}$

    `while` $\mathcal{E} \neq \emptyset$

        $\mathcal{N}_0$ `:=` $\mathcal{N}_0 \cup \mathcal{E}$

        $\mathcal{E}$ `:=` $(\mathcal{F}(\mathcal{N}_0) \cap o(\mathcal{I})) \setminus \mathcal{N}_0$

    $\mathcal{N}_1$ `:=` $\mathcal{I} \cup \mathcal{N}_0$

    `return` $[\mathcal{N}_1, \mathcal{N}_0]$

Output: combinatorial index pair $(\mathcal{N}_1, \mathcal{N}_0)$.

Measures

$\mathcal{A}$: set of measurable sets (i.e. Borel-σ-Algebra on X)

Measure: function $\mu : \mathcal{A} \to [0, \infty)$, such that

$$\text{(1)} \qquad \mu(\emptyset) = 0,$$

$$\text{(2)} \qquad \mu\left(\bigcup_{i\in\mathbb{N}} A_i\right) = \sum_{i\in\mathbb{N}} \mu(A_i) \quad \text{if } A_i \cap A_j = \emptyset \text{ for } i \neq j.$$

Probability measure: $\mu(X) = 1$.

$\mathcal{M}$: space of probability measures on X.

m: Lebesgue-measure (“volume” measure in $\mathbb{R}^n$).

Measures (2)

Example: Dirac-measure

$$\delta_x(A) = \begin{cases} 1, & \text{if } x \in A, \\ 0, & \text{if } x \notin A \end{cases}$$

Integration with respect to δ_x:

$$\int g \, d\delta_x = g(x).$$

Lebesgue-measure m: unique "volume" measure, i.e. if Q is a box (rectangle) then $m(Q)$ is the volume of Q.

Invariant measures

Invariant measure: probability measure μ, such that

$$\mu(A) = \mu(f^{-1}(A))$$

for all measurable A.

Example: $f : [0,1] \to [0,1]$, $f(x) = 2x \bmod 1$, $\mu = m$.

Ergodic measure: invariant measure μ, such that

$$A \ f\text{-invariant} \ \Rightarrow \mu(A) \in \{0,1\}.$$

Example: Dirac-measure δ_p supported on a fixed point $p = f(p)$.

The Birkhoff Ergodic Theorem

Theorem 2 (Birkhoff) *Let μ be an ergodic measure. Then for μ-almost all $x \in X$*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{k=0}^{N-1} \phi(f^k(x)) = \int \phi \, d\mu$$

for all $\phi \in L^1(\mu)$.

Example: Choose $\phi = \chi_A$ for some set A, then

$$\begin{aligned} \lim_{N\to\infty} \frac{1}{N} \sum_{k=0}^{N-1} \phi(f^k(x)) &= \text{“relative no of points of } \{f^k(x)\}_{k\in\mathbb{N}} \text{ in } A\text{“} \\ &= \int \chi_A \, d\mu = \mu(A). \end{aligned}$$

Example: a stable fixed point

p: (globally) asymptotically stable fixed point, i.e.

$$f^k(x) \to p \text{ as } k \to \infty \text{ for all } x \in X.$$

δ_p: ergodic measure.

Birkhoff's Ergodic Theorem: statement for $x = p$ only.

Of interest: statement for (m-almost) all $x \in X$.

Natural invariant measures (SRB measures)

Definition 1 *An ergodic measure μ is called an SRB measure (Sinai-Ruelle-Bowen measure), if there is a set U of positive Lebesgue-measure such that*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{k=0}^{N-1} \phi(f^k(x)) = \int \phi \, d\mu$$

for all $x \in U$ and all continuous ϕ.

Interpretation: An SRB-measure describes the asymptotic distribution of the orbits of a "large" set of initial points.

Example: $f : [0,1] \to [0,1]$, $f(x) = 2x \bmod 1$, $\mu = m$.

The Perron-Frobenius operator

The Perron-Frobenius operator

$$P : \mathcal{M} \to \mathcal{M}, \quad (P\mu)(A) = \mu(f^{-1}(A)).$$

Observation: μ invariant $\Leftrightarrow \mu = P\mu. \qquad (*)$

Goal: Discretize the fixed point problem (*) and compute a (discrete) fixed point as an approximation to an invariant measure.

Discretization

$\mathcal{B} = \{B_1, \ldots, B_d\}$ a grid, $f(|\mathcal{B}|) \subset |\mathcal{B}|$.

Transition matrix

$$P_d = (p_{ij}) = \frac{m(B_j \cap f^{-1}(B_i))}{m(B_j)}, \quad i, j = 1, \ldots, d.$$

p_{ij} is the probability for a point in B_j to get mapped into B_i (transition probability with respect to m).

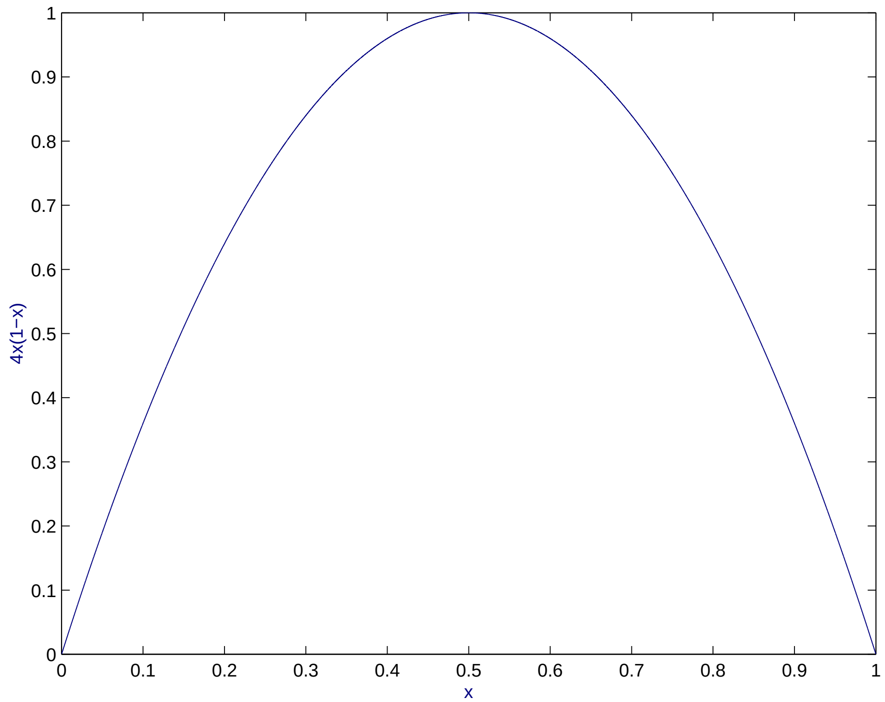
P_d is (column) stochastic: $\sum_{i=1}^{d} p_{ij} = 1$. Thus its maximal eigenvalue is 1.

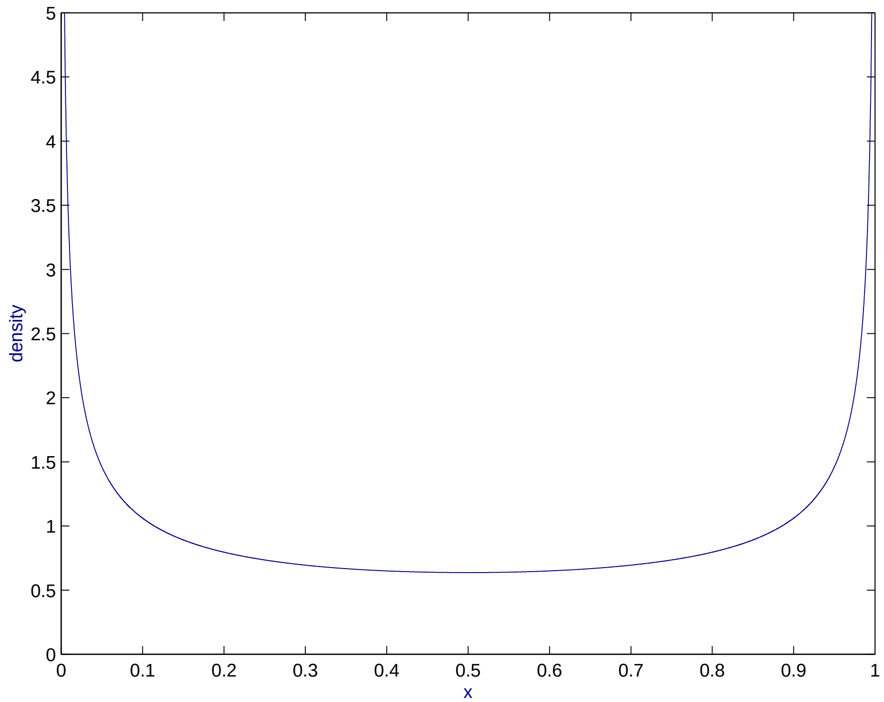
A corresponding eigenvector approximates an invariant measure.

Example: The logistic map

Consider

$$f : [0,1] \to [0,1], \quad f(x) = 4x(1-x).$$





Convergence: the expanding case

$(u_d)_d$ sequence of fixed points of P_d,

$$h_d \in L^1([0,1],\mathbb{R}), \quad h_d|_{B_i} = u_d(B_i)/m(B_i)$$

the corresponding density.

Theorem 3 (Li, 76) *Let $f : [0,1] \to [0,1]$ be a piecewise C^2-map, such that*

$$\inf_x |f'(x)| > 2.$$

If f has a unique absolutely continuous invariant measure μ with density h, then

$$\|h_d - h\|_1 \to 0 \quad \textit{as } d \to \infty.$$

Weak convergence of measures

Let X be compact and $C^0(X)$ be the vector space of continuous functions $f : X \to \mathbb{R}$ endowed with the norm

$$\|f\|_0 = \sup_{x \in X} |f(x)|.$$

Definition 2 *A sequence $(\mu_n)_{n\in\mathbb{N}}$ of probability measures converges weakly to some measure $\mu \in \mathcal{M}$, if*

$$\lim_{n\to\infty} \int g \, d\mu_n = \int g \, d\mu$$

for all $g \in C^0(X)$.

Random perturbations

Replace the deterministic evolution

$$x_{k+1} = f(x_k), \quad k = 0, 1, \ldots$$

by the randomly perturbed evolution

$$x_{k+1} = f(x_k) + \xi_k, \quad k = 0, 1, \ldots$$

where ξ_k is chosen randomly from some ball $B_\varepsilon(0)$ according to (e.g) a uniform distribution.

Stochastic transition functions

Stochastic transition function

$$p : X \times \mathcal{A} \to [0,1],$$

where for every x the probability measure $p(x,\cdot)$ determines the distribution of the perturbation ξ_k (for all k).

Example:

$$p(x,A) = p_\varepsilon(x,A) = \frac{m(A \cap B_\varepsilon(f(x)))}{m(B_\varepsilon(0))}.$$

Small random perturbations

Definition 3 *A family p_ε of stochastic transition functions is a small random perturbation of (the deterministic system) f, if*

$$\lim_{\varepsilon \to 0} \sup_{x \in X} \left| \int g(y)\, p_\varepsilon(x, dy) - g(f(x)) \right| = 0.$$

Theorem 4 (Kifer, 86) *Let p_ε be a small random perturbation of f. For every ε let μ_ε be the unique invariant measure of p_ε, supported on a neighbourhood of some attractive hyperbolic invariant set of f. Let μ be the corresponding SRB-measure of f. Then (under additional assumptions)*

$$\mu_\varepsilon \to \mu \quad \text{weakly as } \varepsilon \to 0.$$

Convergence: the hyperbolic case

Fix ε, consider p_ε, respectively the corresponding Perron-Frobenius operator P^ε.

Discretize P^ε as usual by computing the associated transition matrix P_d^ε.

Let u_d^ε be a fixed point of P_d^ε.

Theorem 5 (Dellnitz, J., 99) *Let μ be the unique SRB-measure supported on a topologically transitive hyperbolic attractor. Then*

$$\lim_{\varepsilon \to 0} \lim_{d \to \infty} u_d^\varepsilon \to \mu.$$

GAIO code

Recall: matrix of transition probabilities

$$P_d = (p_{ij}) = \frac{m(B_j \cap f^{-1}(B_i))}{B_j}, \quad i, j = 1, \dots, d,$$

between the boxes of some collection $\mathcal{B} = \{B_1, \dots, B_d\}$.

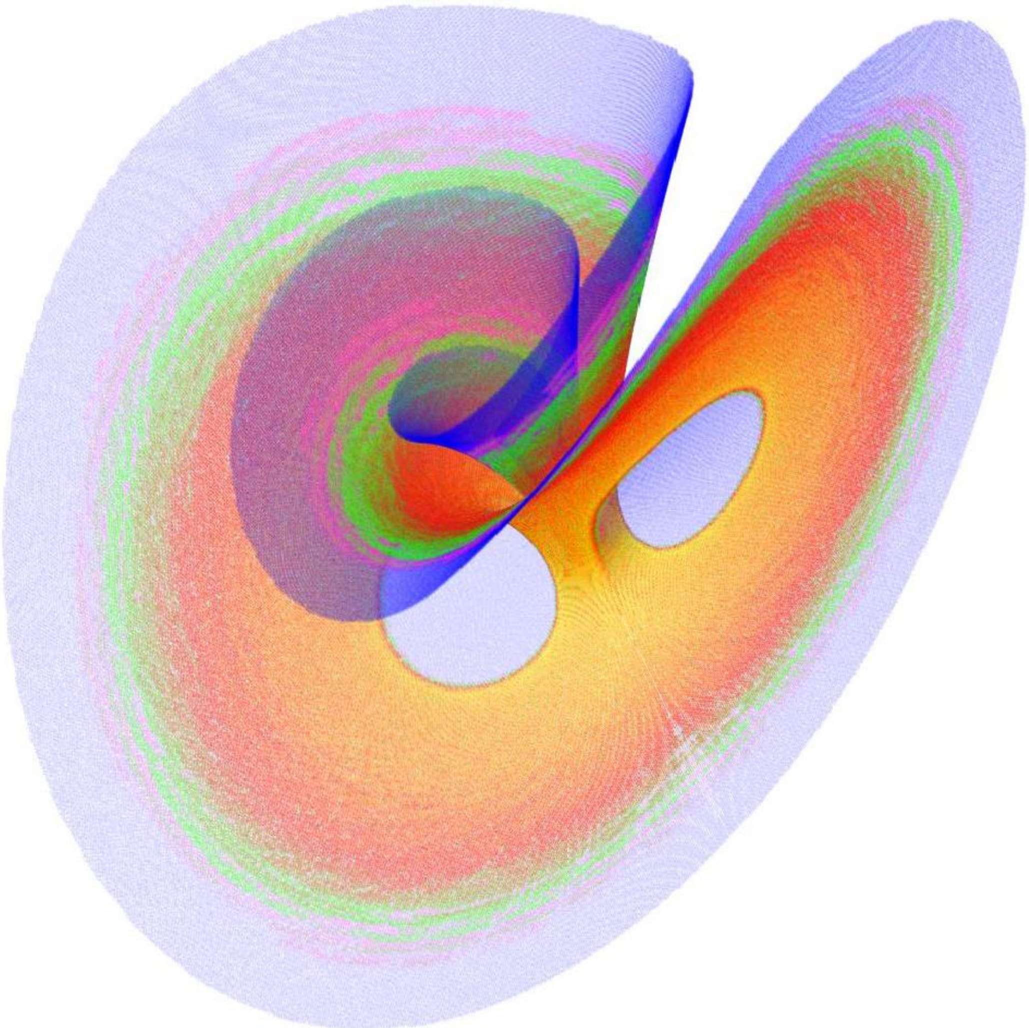
Question: How to compute p_{ij}?

Monte-Carlo method: choose a finite set $T \subset B_j$ and set

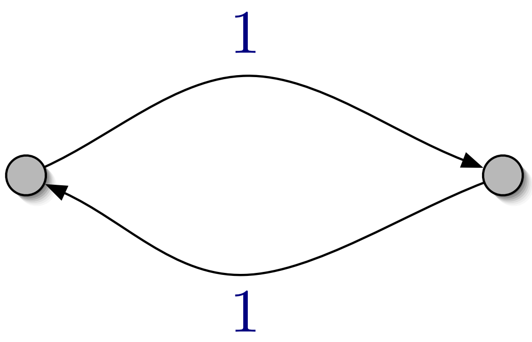
$$p_{ij} \approx \frac{|\{x \in T : f(x) \in B_i\}|}{|T|}$$

```
>> T = Points('MonteCarlo', 2, 20)
>> P = tree.matrix(T)
>> [l,v]=eigs(P)
>> l(1,1)
ans =
0.99999244
```

Invariant measure in the Lorenz system



Cyclic behaviour

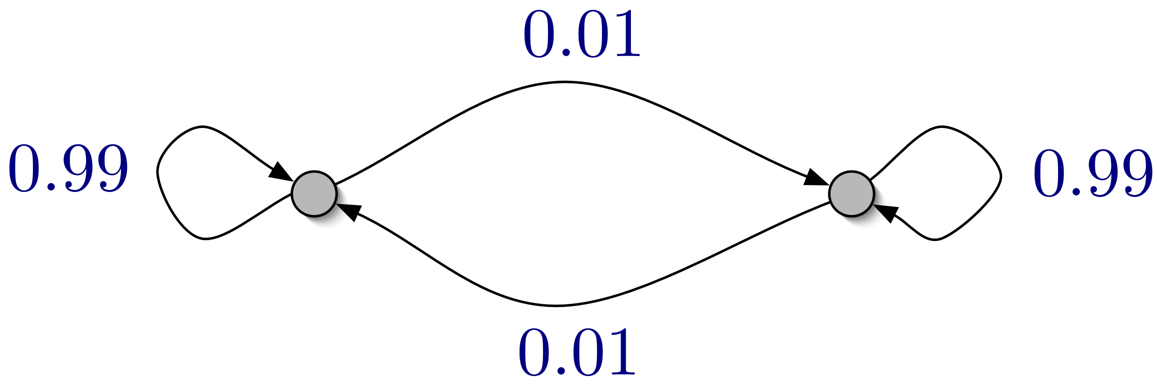


Transition matrix

$$P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Eigenvalues: $1, -1,$
Eigenvectors: $(1,1)^T, (-1,1)^T.$

Almost Invariant Sets



Transition matrix

$$P = \begin{bmatrix} 0.99 & 0.1 \\ 0.1 & 0.99 \end{bmatrix}$$

Eigenvalues: $1, 0.98$,

Eigenvectors: $(1,1)^T, (-1,1)^T$.

Almost Invariant Sets

Definition 4 *The set* $A \subset X$ *is* *δ-almost invariant* *with respect to the probability measure* ν, *if* $\nu(A) \neq 0$ *and*

$$\nu(f^{-1}(A) \cap A) = \delta\nu(A).$$

Now let

$$P\nu = \lambda\nu,$$

$\lambda \neq 1$, ν real valued (signed) measure ($\Rightarrow \nu(X) = 0$).

Relation to Spectrum

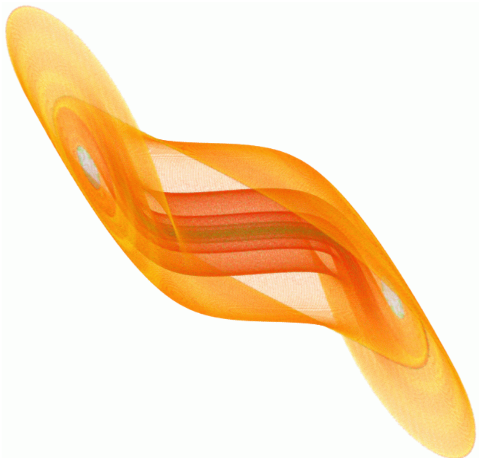
Lemma 1 (Dellnitz-J., 99) *Let $A \subset X$ be a set with $\nu(A) = \frac{1}{2}|\nu(X)|$ which is δ-almost invariant. If $X - A$ is σ-almost invariant, then*

$$\delta + \sigma = \lambda + 1.$$

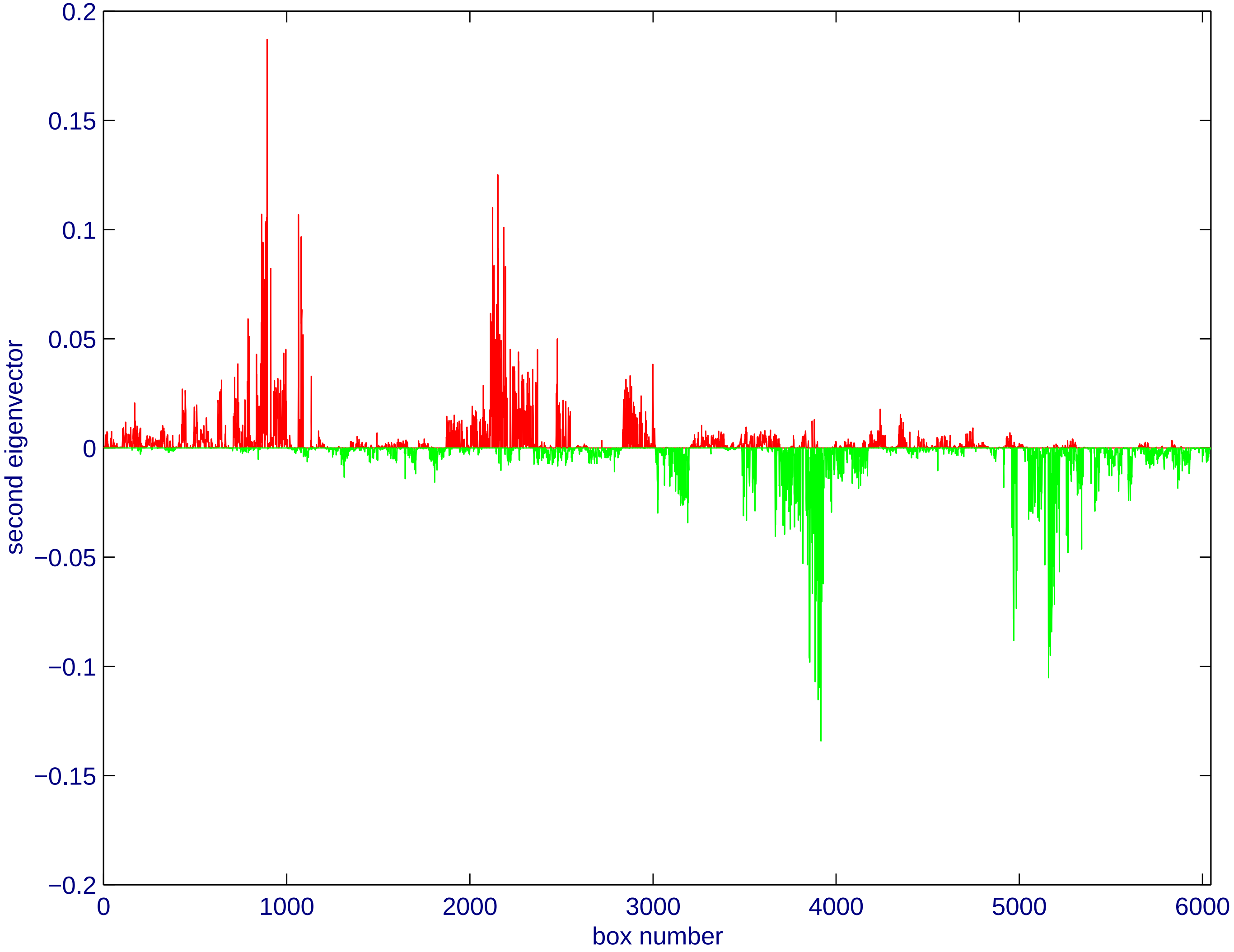
Idea: use the sign structure of the eigenmeasures at eigenvalues $\neq 1$ in order to identify cyclic and almost invariant sets.

Chua's circuit

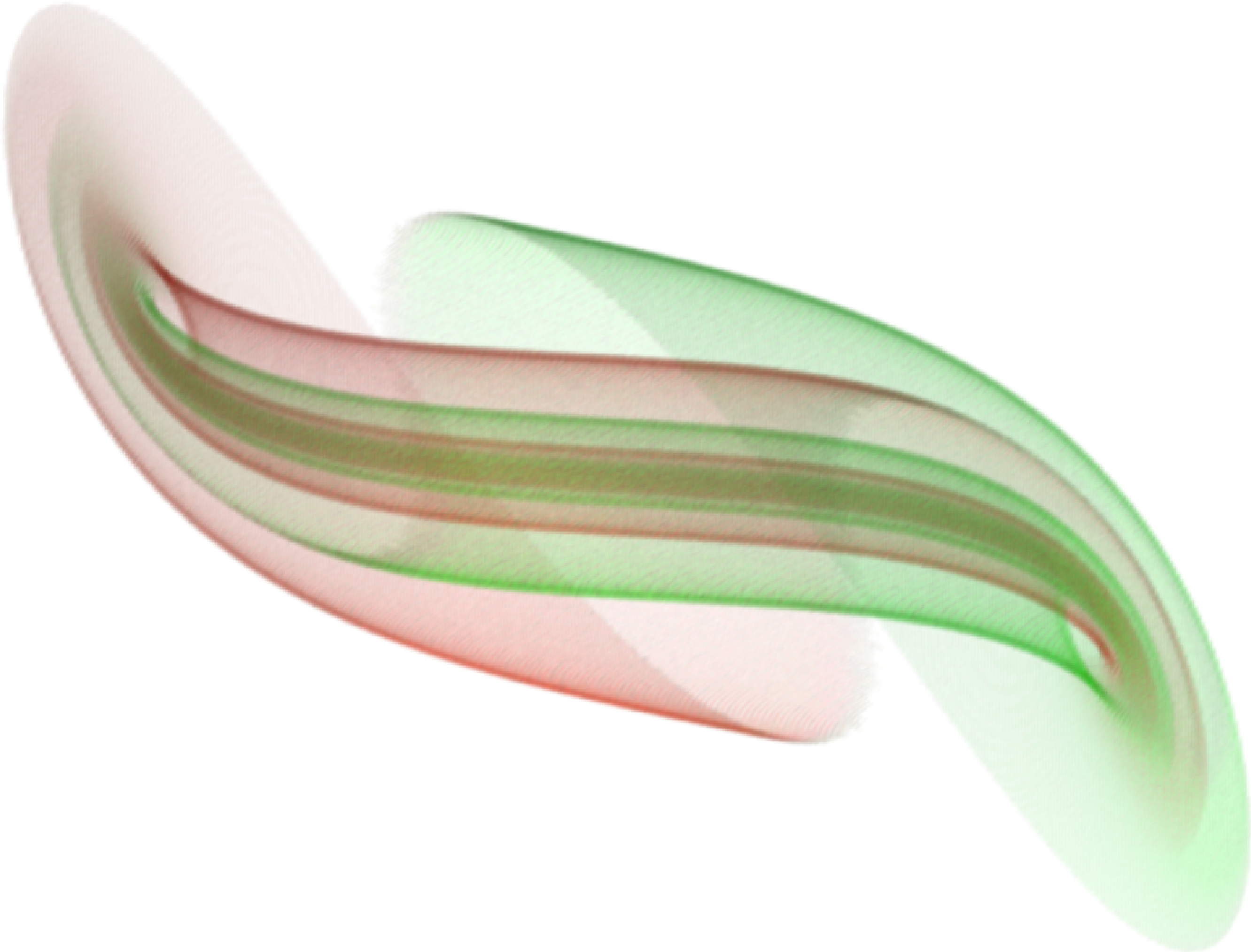
$$\begin{aligned}\dot{x} &= \alpha(y - m_0 x - \frac{1}{3} m_1 x^3)\\ \dot{y} &= x - y + z\\ \dot{z} &= -\beta y.\end{aligned}$$



Chua' circuit: eigenvector at $\lambda = 0.93$



Chua's circuit: two almost invariant sets



Application: Molecular Dynamics

- Almost invariant sets in configuration space correspond to certain conformations;
- Transition probability between conformations can be estimated by the size of the corresponding eigenvalues;
- Different approach: use graph partitioning algorithms.